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ORIGINAL ARTICLE

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From approximation of dissipative systems to representative space-time volume elements for metamaterials

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Abstract In this paper we present some relatively unexpected mathematical questions emerging from the idea to approximate dissipative mechanical systems using Lagrangian formalism. We also explain potential consequences of these constructions for definition of representative space-time volume elements in modelling of metamaterials.

Keywords Dissipative Lagrangians · Approximation · Space-time formalism · Representative volume elements · Metamaterials

1 Introduction/motivation

This short paper starts a series of works devoted to developping a rigorous mathematical understanding of the problem of dissipative mechanical systems and eventually constructing an appropriate geometric formalism for them. In this latter sense the paper is also a part of a big project of "geometrizing" mechanics, which is one of the key interests of the authors with various other collaborators. It includes several stages: starting from spelling out geometric structures appropriate for various classes of mechanical systems (those often come from advanced differential geometry), all the way through to numerical methods respecting those structures and thus providing robust, reliable and scalable simulation tools. For a brief review of the subject see Ref. [1] and references therein.

For conservative mechanics, the approaches are several decades if not centuries old. The Lagrangian formalism actually dates back to the epoch of Lagrange and is now part of textbooks, together with its Hamiltonian counterpart and the relation to symplectic / Poisson geometry, which is obviously more recent, but still well established. Then, unfortunately (or fortunately), most mechanical systems are not conservative, either due to kinetic energy being transformed to heat by some dissipative process, or when the system is subject to external forces or control, like it is often the case for architectured materials or metamaterials.

Taking into account dissipation or interaction can be done relatively easily at the level of equations of motion of the system, by adding ad-hoc empiric terms to the right hand sides, for example as in mechanical

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thermostats (see Ref. [2] and references therein). But the question of finding a global structure of such resulting equations, i.e. a way to derive them by some general procedure, is a long-standing problem with no sufficiently generic solution. One approach may be so-called port-Hamiltonian systems [3], which in the end of the day turns out to be a game of notations, although useful for distributed parallel computations. Together with systems with constraints, it eventually fits to (almost) Dirac structures [4,5], for some class of those the variational formulation has been obtained in Ref. [6]. Another approach, which we are revisiting in this paper, is *dissipative Lagrangians*. Without context, the term 'dissipative Lagrangian' obviously sounds paradoxical, which can be resolved if one asks appropriate questions. One of the meaningful discussions in the context may be whether a dissipative system can be approximated, in some sense to be defined, by a (possibly large) number of interacting conservative systems. The question is studied for example in the papers [7,8], a communication with the authors of those has been the starting point for the study in this paper.

The goal of this paper is thus twofold. First, we address the idea of approximating dissipative systems by a number of conservative ones, that we mentioned above. In particular we explain why the technique of harmonic oscillators works as it was presented in the simple academic case, and discuss how it can be transferred to more general cases. Second, we sketch what mathematical "tools" we consider appropriate for more complicated problems. And more importantly, we discuss the conceptual constructions that emerge from them, in particular the one that we call 'representative space-time volume element'.

The paper is organized as follows. The next Sect. 2 is a fleeting overview of the state of the art of some approaches to fomalization of dissipative systems, including dissipative Lagrangians. Then Sect. 3 is devoted to two mathematical constructions appearing in the context: one directly – Fourier analysis, and one in generalizations – the problem of small divisors. We sketch in Sect. 4 how these constructions can be useful to attack real-life applications, in particular metamaterials. We conclude by formulating some near-at-hand future directions and open problems in the context.

Disclaimer. This paper is intended for a rather broad audience of specialists in mechanics and applications, we thus avoid technical and theoretical details as much as possible. While we do recall some minimal mathematical working knowledge, a more detailed "definition–lemma–theorem style" paper will follow elsewhere.

2 A glimpse of state of the art

As mentioned above, the problem of formalizing the description of dissipative systems is complex and has multiple facets. There is not much use in repeating the overview of all what could be related to it. A nice survey about Lagrangian description can be found for example in Ref. [7], we only mention here several ideas that are important for future discussions, and also some more applied aspects that have motivated this study on the long run.

As we have already pointed out, claiming that a dissipative system is Lagrangian in the classical sense of the term, is somehow contradictory. More precisely, it means that if one is able to derive the equations of motion of such a system by some analogue of variational principal, the Lagrangian used in the construction will no longer have any interpretation in terms of energy of the system. However the resulting system then has to possess some conserved quantities or equivalently symmetries [9], that is has to satisfy some compatibility conditions. Those conditions are typically rather strong and restrictive, but the question is still meaningful. Examples of dissipative systems derived by using a variational formulation may be found in Ref. [10]. Considering some conservation laws for non-dissipative systems one can obtain some bounds even for dissipative ones such as for plastic behaviour (see Ref. [11]). Various modifications of the usual formalism have been studied, for example the Rayleigh functional is an important tool for the so-called hemivariational approach for continuum systems [12]. It can also be defined for viscous thermoelasticity [13].

A more straightforward question in the absence of energy conservation may be phrased as: given a dissipative system, reconstruct the conservation laws or equivalently at each moment of time the power balance – this means find a bigger closed (conservative) system which contains the initial one, and study the Lagrangian formalism for it. While conceptually it sounds much more treatable, there are still a lot of subtleties to handle. For instance the problem is ill-posed, in a sense that the solution is far from being unique – this results in natural optimization problems. While we are not addressing it in this paper, let us still mention two important observations. First, the problem may have a Hamiltonian counterpart and be related to port-Hamiltonian systems, the link is rather clear, we explored some 'academic' parts of it in Ref. [14,15] and intend to elaborate the real-life applications in a separate paper. Second, there is a more surprising link to theoretical physics, namely field theory and quantization techniques [16,17]. A very concrete example may be related to nuclear

decay: the whole system is conservative at all levels, but disregarding electrons (which is done in practice) one can view it as a dissipative subsystem. In this setting the question of equivalence makes a lot of sense, and that one is related to model reduction in mechanics and gauge theories in physics. This message also deserves a separate text and is a part of our roadmap.

The idea of describing a dissipative system as a part of a conservative one is not only a mathematical abstraction, it could be confirmed by examples of resonating metasurfaces which absorb some of acoustic energy that looks as a loss of energy in the bulk (see e.g. [18–20]). Remembering physics but on a more down-to-earth level, the theory of electrodynamics from the point of continuum mechanics is discussed in Ref. [21].

And on top of the elegant theoretical formalism, there are some "engineering" applications, for example the hemivariational approach has been succesfully used for discrete models for masonry systems [22–24] and for fracture propagation in continuum macroscopic systems [25], as well as for continuum granular micromechanics based systems [26–31].

The third natural question, also present in Ref. [7], which is probably the most pragmatic in the context, is approximation of dissipative systems with conservative ones. That is given a (small) dissipative system we want to find a conservative / Lagrangian / Hamiltonian one which is close enough to the initial one in some sense. One of the natural criteria is simply to approximate the trajectory of the initial system by some quantities deduced from the constructed systems – one may call these quantities *observables*, again in the direct analogy with gauge theories [32,33]. One may say that in some sense this setting is similar to the previous paragraph: the system is being extended to make sure that the qualitative behaviour related to failure of conservation of energy is captured. The key difference is that we do not have to perform the extension exactly, and thus do not run into danger of an obstruction result.

Let us recall here the results of [8], where the above question is answered positively for a simple yet instructive example of a damped harmonic oscillator. The authors consider the following equation

$$\ddot{x} + 2\gamma\dot{x} + \omega^2 x = 0 \tag{1}$$

as a test case for a numerical study of the possibility to approximate the solution of the Cauchy problem by an undamped harmonic oscillator coupled to N other ones with different frequencies, described by the equations of the form:

$$\ddot{\xi}_k = \omega_k^2(\xi_{k+1} - \xi_k) - \omega_{k-1}^2(\xi_k - \xi_{k-1}). \tag{2}$$

These latter equations come from the Lagrangian

$$L = \frac{1}{2}\sum \left(\dot{\xi}_k^2 + \omega_k^2(\xi_{k+1} - \xi_k)^2\right). \tag{3}$$

The solution of (1) is well studied and everything is known about fine-tuning of it, which makes it a convenient tool to check the approximation results. The authors present numerical benchmarking of the frequencies optimization problem for the approximating system. The conclusion is rather natural: the proof of concept is established, i.e. some approximation is produced; and as soon as this is done, the optimization problem admits a better solution when there are more degrees of freedom. In the next section we will explain the origin of both of these facts.

3 Mathematical interpretations and observations

A mathematically rigorous way to justify that the observables from the system (2) approximate the solution of (1) is to study the space of those solutions and convince oneself that its subspaces provide a filtration of the space of solutions of (1). This statement will become clear in the next subsection, and the following one will explain some details of the process.

3.1 Trigonometric polynomials and Fourier expansion

Recall that $\zeta(t, \omega) = e^{i\omega t}$ is the fundamental solution of the equation describing an independent harmonic oscillator

$$\ddot{\zeta} + \omega^2 \zeta = 0.$$

The space of such functions is often called *trigonometric polynomials* and from the point of view of functional analysis, possesses some remarkable properties. We use here the complex notation for them for conciseness, but can always rewrite them as sums of a sine and a cosine with coefficients.

On the space of trigonometric polynomials, given some segment I, one considers the usual L^2 scalar product:

$$< f, g >:= \frac{1}{|I|} \int_I f(t)\bar{g}(t)dt.$$

With respect to this scalar product two ζ's with ω's being different multiples of some frequency are orthogonal and functionally independent.

This means that by an appropriate selection of a set of frequencies ω_k in (2) one can generate a family of functions $\{f_k(t) = e^{i\omega_k t}\}$ and start filtering the space of functions. More precisely, for a given function $x(t)$ one defines the quantity:

$$c_k(x) := \frac{1}{|I|} \int_I x(t)e^{i\omega_k} dt,$$

called its k-th Fourier coefficient. Then according to the Fourier theorem [34] any periodic sufficiently smooth function can be represented in the form of a series:

$$x(t) = \sum_k c_k(x)e^{i\omega_k t}. \tag{4}$$

It is now straightforward to say that any finite truncation of this convergent series (i.e. fixing the set of frequencies of (2)) precisely provides an approximation of the solution of (1). This also explains the phenomenon that increasing the size of the approximating system permits to achieve smaller discrepancy.

3.2 Characteristic frequencies and small divisors

The above subsection explains why the proof of concept from Ref. [8] actually works. However there are some details and subtleties worth being mentioned.

First of all, we have mentioned periodicity in the formulation of the Fourier theorem, but have left this without comments. This is actually very important, since generic functions characterizing dissipative systems are not periodic. On the contrary, they typically have some definite gradient "direction" in the phase space – think of the energy for example. At the first glance this again seems to be a contradiction, but in fact it is not, it only means that the choice of the base frequencies in ω_k cannot be arbitrary. More precisely it is enough to consider the whole motion of the system as observed during the half of the largest period of the approximating oscillators and complete this motion by some other half period, not necessarily governed by (1), but bringing the system to its initial state. It would mean that physically we are approximating a dissipative process by one phase of a conservative one up to fine-tuning the minor corrections, and then just stop observing the system.

Second, we manipulate the approximating oscillators rather freely, saying that we can fix the frequencies at our convenience. This is true up to a technical detail, where we actually need to justify the strategy of selecting the frequencies in (2). The approximating system is not a sum of independent oscillators, it is rather a system of the form

$$\ddot{X} + AX = 0$$

for some matrix A read-off from the quadratic form in the Lagrangian (3). This means that to recover the needed frequencies we need to study the orthogonalization procedure for A. This is exactly where one may run into the difficulty of a very vast range of its spectrum. While theoretically for Lagrangian formulation this is not an issue, in numerical computations this can result in technical difficulties. The problem is however relatively well studied, it may be related to so-called small divisors and resonances (see Ref. [35] or a more

general audience oriented [36]). Those, in turn, are eventually responsible for the distinction between chaotic and quasi-periodic motions.

Both of these statements can not only shed light on why the suggested procedure works, but also provide insights on how to optimize the procedure not going through heavy brute force computations.

3.3 Consequences and generalizations

Note that the approach above permits not only to prove the theoretical statement of the approximation result, it is also constructive. Given a solution, the coefficients of the Fourier expansion are explicitly computable, with optimized codes using discrete Fourier transform. While for one particular solution this has no practical sense, it can be useful in the philosophy of model reduction. Phrased like this, the idea is rather straightforward. The strategy is to compute the expansions in terms of (2) for several solutions of (1), varying the parameters and initial conditions – these expansion are afterwards used to interpolate solutions for other initial data and values of parameters. Viewing the whole problem through the lens of Fourier formalism permits to claim uniform convergence and thus justify the approach. Note also that the formalism is suitable for any version of the dissipative system (1), i.e. if the solution is sufficiently regular the same approximation logic works verbatim.

One important remark is in place here, it concerns non-linearity. While the filtration generated by the Fourier modes is linear in the essence, i.e. the finer approximation is constructed from a coarser one by adding new terms with coefficients, this is true for one solution (observable) given a finite time interval. For families of solutions depending on parameters, severe non-linearities may and systematically will enter the play: this is related to the structure of equations and subspaces of solutions, the proper language for which can be Grassmannian manifolds. Then, the first step to uniformly approximate the solutions would be Fourier filtrations, followed by the interpolations on manifolds (see Ref. [37] and references therein).

Moreover, nothing prevents us from considering dissipative systems in higher dimension and even infinite dimensional (continuous media). As promised, leaving the technical mathematical details for a separate text, we just say that the same Fourier inspired formalism is appropriate.

4 Instead of conclusion

4.1 Discussion about applications to metamaterials

It has been clear from the very beginning that we are not presenting these constructions for mathematical elegance of them. A little bit, yes, but primarily to formulate constructive conclusions. Clearly, the results of Ref. [8] could have been used as empiric observations with the status “they work when they work”; now however we understand the reason why the suggested method is not an exceptional coincidence, but is valid for generic situations. This permits us to dare to apply it to interesting and complex real-life problems – one we are having in mind would be dynamics of metamaterials.

We are not even trying to tell the whole story of metamaterials [38], which are now extremely important for industrial applications and have thus raised a lot of interest in modelling communities (our favourite example would be pantographic architectured materials [39]). Let us just note a couple of features relevant in the context of this paper.

The spacial structure of metamaterials is simultaneosly complex and simple. On the one hand they are designed to realize non-trivial, sometimes counterintuitive, phenomena. But on the other, by construction, they have a very specific internal structure, which is now more or less mastered at the production stage, i.e. their modelling should be technically easier than generic heterogenious media, but conceptually new tools and approaches are needed. To name a few: introduction of higher displacement gradients, to explain exotic mechanical interactions [40,41], principal of virtual work [42], “mathematically-driven” design [43].

Another important thing to note is that these complicated phenomena are often not long-term behaviour, but rather switch-like short transitions, which means that in the dynamical “active” regime metamaterials have a relatively short time scale. In the pantographic material this is clearly observed [44–48], and present even for complex 3-dimensional structures [49]. And once again, the observation is not purely theoretical, it has been validated through imaging techniques [50]. Similar behaviour is exhibited for “origami” structures [51] and extreme buckling [52–57].

In view of the results of Sect. 3, these two observation lead to a rather natural idea to include this time-dimension to the modelling approaches. An example of such approaches can be the analogue of FFT-based

homogenisation techniques [58]. A couple of decades ago the passage from modelling of 2-dimensional composite materials to 3-dimensional ones used to be a computational challenge, nowadays one has enough resources to perform reasonable computations in honest 4-dimensional space-time [59].

In the pure spacial dimension, homogenization leads to higher order models by using continuum [60] or discrete technniques [61], the latter approach is inspired by a similar logic as in Ref. [8]. This higher order model is needed to properly handle the length scale [62]. In the context, damage mechanics with higher order theories and their computational implementation can be studied using phase field approches [63]. Homogenization by using asymptotic analysis in mechanics [64,65] delivers parameters for systems with a prescribed microstructure [66,67]. The approach is generalizable to thermomechanics [68].

For the time dimension, there are experimental evidence on higher order terms in inertia [69]. Some relatively fast motion is observed studying the macro and microscopic scales for strongly non-homogeneous materials [70], as well as, shearable, extensible alternatives to Timoshenko beams [71]. It is also important to take into account surface waves and wave transmission across surfaces [72,73]. We refer to [74] for a comparison of some of those techniques and [75] for a benchmark case to verify computational methods. And finally, from the mathematical point view, eigen-modes of a perfect system, for example, elastic ones, which could be treated as an extension of the harmonic oscillator, could be rather useful for approximation of more complex systems [76–78].

The only conceptual step that was missing in this increasing dimension is the way to consider the time-dimension on equal footing with the spacial ones. With the observation about Fourier expansion and intuition from theoretical physics, the way out is realistic: the notion of Representative Volume Element becomes *'Representative space-time Volume Element* (RstVE). By this we mean that in the 3 spacial dimensions there is a clear characteristic size governed by the architecture of metamaterials, and in the time-dimension the non-linear process defines the characteristic period. Put together, they form a 4-dimensional RstVE. Zooming out from the 4-dimensional microstructure, the result of the computation or simulation will then be the macroscopic "homogenized" data about the behavior of a dynamical system approximating the initial material with controlled precision. And this in turn, may be used as a building block in more complex reduced or digital-twin like models.

4.2 Towards a roadmap

As we have stated in the beginning, the aim of this paper is to start some longer discussion. We thus "conclude" by mentioning some near-at-hand steps to be made following the map.

First, as we promised in the introduction, a separate text about exact mathematical formulations and proofs from Sect. 3 is in preparation. It will include in particular a more detailed study of the uniform convergence of the parametric families of Fourier series, and more importantly a study of strategies of choices and optimization of the approximating frequencies—more deterministic than the brute force one.

Second, we have observed that the space of trigonometric polynomials provides a proof of concept for the approximation problems. This is the first very natural educated guess, but other spaces may also be considered and prove to be more efficient.

Third, quantitatively more demanding would be the benchmarking of the same techniques for bigger systems and as the next step and the ultimate goal for continuous media and metamaterials—phrased in 3 lines it actually opens a totally new direction.

And on top of that, all these steps, once again, fit naturally to the "big picture" of revisiting theoretical mechanics and geometrization of mechanical problems.

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Declarations

Author contributions V.S. and O.C. wrote the main manuscript; F.D'A reviewed it and provided important comments.

Data availability No datasets were generated or analysed during the current study.

Conflict of interest The authors declare no conflict of interest.

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