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Computational models for multi-scale coupled dynamic problems

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Abstract

In this paper we describe a systematic methodology for the construction of computational models for coupled multi-scale dynamic problems with a major focus given to a case study example related to the design of shape memory alloy actuators controlled by thermoelectric effect. From a mathematical point of view, the problem in hand is a coupled dynamic system of partial differential equations which is not amenable to analytical treatments and requires an efficient computational tool for its solution. The developed methodology is based on a combination of the analysis of such invariant sets that keep the essentials of the system dynamics and on the reduction procedures of the original model on such sets. A presented numerical example demonstrates the efficiency of the developed tool in describing phase transformations in actuators based on materials with shape memory effects.

Keywords: Coupled problems; Dynamics of phase transitions; Invariant sets; Multi-scale analysis

1. Introduction

There is a growing recognition in scientific and engineering communities that many, if not all, real world problems are intrinsically coupled. The coupling may have different sources, e.g. different physical fields coupled together. Electroelasticity, thermoelasticity, viscoelasticity, magnetoelasticity are examples of such problems. Different states of matter should often be also treated together, giving other examples of coupled problems such as fluid–structure interactions, aeroelasticity, various phase transitions. Sometimes such problems are termed as multi-physics problems. This term, however, does not include explicitly many other important coupled problems where, for example, chemical, biological fields, or a combination of those could be a major source of coupling. In climate modelling, for instance, we need to account for physical, chemical, biochemical, geological, and many other features of the planet and its surrounding in their intrinsic interactions [13]. Such seemingly distant fields as biomechanics, climate modelling, geomechanics, and nanotechnological applications all have in common that further advances in these areas are closely connected with our ability to solve efficiently *coupled problems* [12].

The class of coupled problems has been continuously expanded, reflecting the nature of scientific discovery and needs of practical applications. However, it would be proper to say that the coupling most often originates from:

- the phenomenon under consideration which requires accounting for several different fields,
- a multi-scale nature of the problem where different effects and/or structure properties may be more

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pronounced at a specific scale, while being negligible at other scales,
- a combination of the above factors.

Most of such coupled problems are not amenable to analytical treatments, especially when dynamic phenomena are at the focus of interest. At the same time, computational cost of such problem solutions is often prohibitively high to allow their efficient solution on modern computers.

By now, with ready availability of computer power many coupled problems are already possible to attack directly, without restricting our attention to just one phenomenon or field. However, there is a large and expanding class of coupled problems that requires the development of efficient computational algorithms for the solution of these problems. In fact, many problems in this class involve strongly coupled *nonlinear* dynamics. Practically important, mathematically fruitful, and computationally challenging examples of such coupled problems are provided by advances in smart materials and structure technology. Indeed, a better understanding of magnetostrictive and piezoelectric materials, magneto- and electro-rheological fluids, and materials with memory such as shape memory alloys (SMA) can only be achieved with efficient computational models describing these materials. For this reason, our discussion is centred around a case study example dealing with one of the most important problems in this field requiring an adequate description of the dynamics of materials with shape memory as part of multi-layered structures.

The paper is organised as follows:

- In Section 2 we provide details of our approach, highlight its main features, generic to a large class of coupled problems, and discuss the differences and similarities of our approach with other existing approaches.
- Section 3 gives a necessary background in and examples of coupled dynamic problems arising in smart materials and structures applications. Major attention is given to thermoelectric SMA-based actuators which are currently in the focus of experimental studies aiming at developing new devices for microtechnology and microsystem engineering.
- In Section 4 we give details of the governing equations describing both thermoelectric and thermomechanical processes in the system chosen as a case study example. In this section we also give details of the reduced computational model, derived with the developed technique, and demonstrate the effectiveness of the proposed approach in the analysis of coupled thermomechanical dynamics of the SMA layer in the actuator.
- Concluding remarks are given in Section 5.

2. Multi-scale analysis and low-dimensional modelling

It is well known that standard approaches in developing numerical discretisations neither explicitly take into account subgrid scales, nor allow to rescale the system in terms of a set of parameters responsible for the contribution of small effects [2]. In the analysis of singular perturbed systems, such as

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \epsilon\mathcal{L}\mathbf{u} + \mathbf{f}(\mathbf{u}), \tag{2.1}$$

it is a common practice to rescale the system in terms of a single parameter which leads to rescaling the time as $t = \tau/\epsilon$

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}\tau} = \mathcal{L}\mathbf{u} + \frac{1}{\epsilon}\mathbf{f}(\mathbf{u}), \tag{2.2}$$

where ϵ is a small parameter, $\mathcal{L}$ and $\mathbf{f}$ are linear and nonlinear (at least quadratic) parts of the system, respectively. Difficulties with this approach are well known and lie in the fact that lowering ϵ leads to a decreasing influence of the contribution of the dissipative term $\epsilon\mathcal{L}\mathbf{u}$ and that a lower value of ϵ may produce a manifold (e.g., an inertial manifold $\mathcal{M}$) of higher dimension. More precisely, if, for example, $A = -\mathcal{L}$ is self-adjoint and $\mathbf{f} : D(A^\alpha) \to D(A^\beta)$ is bounded and satisfies the following conditions:

$$\begin{aligned} &|A^\beta \mathbf{f}(\mathbf{u})| \le K_1, \\ &|A^\beta[\mathbf{f}(\mathbf{u}) - \mathbf{f}(\mathbf{v})]| \le K_1 |A^\alpha[\mathbf{u} - \mathbf{v}]|, \\ &\mathrm{supp}(\mathbf{f}) \subset \{\mathbf{u} : |A^\alpha \mathbf{u}| \le \rho\}, \end{aligned} \tag{2.3}$$

then the standard arguments of the inertial manifold would require the spectral gap condition

$$\lambda_{k+1} - \lambda_k > 2K_1[\lambda_k^{\alpha-\beta} + \lambda_{k+1}^{\alpha-\beta}] \tag{2.4}$$

for such a manifold $\mathcal{M}$ to exist. In (2.3) and (2.4) we assume that $0 \le \alpha - \beta < \gamma$ with $\gamma = 1$ (the standard

arguments apply for $\gamma = 1/2$, inclusive) and that

$$A\omega_k = \lambda_k, \quad \lambda_{k+1} \geq \lambda_k. \tag{2.5}$$

The condition (2.4) leads to severe *computational* restrictions on the applicability of the described methodology to a number of practically important problems. The standard methodologies of multiple scales and singular perturbation are efficient tools for the analysis of *weakly nonlinear* problems. In some cases these methodologies can be applied directly to some PDE-based models and even can result in obtaining normal forms. However, since the systems we are interested in this paper are infinite dimensional, it is quite natural to apply a centre manifold reduction first, and in doing so to balance the order of small effects at the stage of the model construction, rather than at a later stage. In what follows we explain how a combination of the centre manifold technique and the computer-algebra approach would allow us to construct efficient computational models even in the situations where the standard approaches highlighted above would lead to serious difficulties.

Firstly, we recall that centre manifold is a technique of reducing the model dimensionality and restricting attention to an invariant subspace, known as the centre manifold, which contains all of the essential dynamics of the system described by the original model. The technique has been used widely in the context of ODE, including bifurcation analysis and general nonlinear delay-differential equation (e.g., [17] and references therein). From a theoretical point of view the technique is well established (see, e.g., [4,16,18,20] and references therein). Although the technique was conceived for ordinary differential equations, at present time application areas of the centre manifold technique to PDE-based models are growing rapidly. Moreover, the normal form methodology and centre manifold technique often considered in conjunction (e.g., [11]), and historically the key publications on both of these tools appeared around the same time.

Secondly, it is important to note that the centre manifold methodology can deal with problems where invariant sets might become non-hyperbolic, which is an important element in phase transition problems and in a number other coupled models based on systems of PDEs consisting of different type equations (e.g., hyperbolic and parabolic, hyperbolic and elliptic, etc.). It is known that non-hyperbolic sets cannot persist in general, so the task is to construct a normally hyperbolic (invariant) manifold which contains the invariant set of the smallest possible dimension. A key to the current success stories of applying the centre manifold technique to complicated applied problems, as diverse as nonlinear aeroelasticity, nonlinear optics, delay PDEs, thin film fluid dynamics, combustion systems of reaction–diffusion types, turbulent flows and climate models, magneto-hydrodynamic plasma, and many other applications (e.g., [5,11,19] and references therein), is the *link between the centre manifold and computer-algebra methodologies*. This link allows one to derive low-dimensional models *systematically*.

We recall the main idea of centre manifold by highlighting major steps of associated numerical procedures. If we have already approximated the spatial part of our PDE-based model, we come to a fairly generic system in the form (e.g., [5] and references therein)

$$\begin{aligned} \frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} &= \mathcal{L}\mathbf{x} + f(\mathbf{x}, \mathbf{y}), \qquad \mathbf{x} \in \mathbb{R}^n, \\ \frac{\mathrm{d}\mathbf{y}}{\mathrm{d}t} &= \mathcal{K}\mathbf{y} + g(\mathbf{x}, \mathbf{y}), \quad \mathbf{y} \in \mathbb{R}^m. \end{aligned} \tag{2.6}$$

Bringing an analogy with the classical Tichonov singular perturbation system, we can say that if $\mathbf{x}$ is a "slow" variable (the real parts of the eigenvalues of $\mathcal{L}$ are zero), and $\mathbf{y}$ is a "fast" variable, relaxing exponentially quickly to the instantaneous equilibrium value (the real parts of the eigenvalues of $\mathcal{K}$ are negative), we can then construct systematically an approximation to (2.6) by considering $\mathbf{y}$ as a function of $\mathbf{x}$, $\mathbf{y} = h(\mathbf{x})$ (where $h(\mathbf{x})$ is called a centre manifold), in the form

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathcal{L}\mathbf{u} + f[\mathbf{u}, h(\mathbf{u})], \quad \mathbf{u} \in \mathbb{R}^n. \tag{2.7}$$

If the origin is an equilibrium point of (2.6), then the solutions of (2.7) relax exponentially quickly to the solutions of (2.6). It is rarely possible to find centre manifold $h(\mathbf{x})$ analytically, and hence to write down Eq. (2.7) explicitly. Even in this, relatively simple case, the equation for evolution of $h(\mathbf{x})$ has a complexity comparable with the second equation of system (2.6) (see, e.g., [5]). Since $h(\mathbf{x})$ and (2.7) can rarely be constructed analytically, the construction of model (2.7) and the derivation of the equation for the centre manifold $\mathbf{y} = h(\mathbf{x})$ are conducted simultaneously with a *computer-algebra-based numerical procedure*. Since h is found in an iterative manner, model (2.7) can be

thought as a set of models, each of which can be represented in the following form:

$$\frac{\mathrm{d}\mathbf{u}}{\mathrm{d}t} = \mathcal{L}\mathbf{u} + f[\mathbf{u}, \boldsymbol{\epsilon}], \tag{2.8}$$

where $\boldsymbol{\epsilon}$ is a vector of parameters. This idea allows us to generalise the classical singular perturbation approach. Rather than to rescale all variables with respect to a single parameter, as shown by (2.1) and (2.2), we aim at balancing as many small effects as needed in a particular problem.

From a theoretical point of view, the idea of centre manifold is ultimately connected with that of inertial manifolds introduced by Foias, Sell, and Temam in the mid-1980s, in particular in the context of approximate inertial manifolds (AIM) (e.g., [22]). Similar to the centre manifold technique the (approximate) inertial manifold methodology allows us to reduce infinite-dimensional PDEs to a finite set of ODEs, but the tools of such a reduction are somewhat different in these two cases. While in the inertial manifold methodology we use asymptotic "slaving rules" (or exponential tracking properties that follow from (2.4)) in an attempt to achieve the asymptotic completeness of the model, in the centre manifold technique the main emphasis is placed on a *constructive procedure* of obtaining a model, solutions of which are attracted exponentially quickly to the solutions of the original system (see also [16]).

In general, *approximations* obtained with any of these two approaches are distinct from the standard Galerkin approximation. A more general nonlinear Galerkin method becomes one of the most popular approaches in constructing AIMs. However, at the computational level this approach is quite demanding computationally, and, as it has been pointed out in [8], it is not clear at the moment whether better accuracy of this methodology (say, compared to the standard Galerkin technique) is worth its computational cost. Recent attempts have been made to remedy this deficiency via multi-level multi-grid procedures and post-processing Galerkin methodologies (see, e.g., [3,8,23] and references therein).

We note also that in its essence our approach has similar features to that of multiple scale methodologies where two-scale models achieve certain degree of maturity (e.g., macro–micro, or macro–meso [24,25]). Among multi-scale approaches widely used in the literature we mention the wavelet method for the numerical approximation of PDEs, Harten's multi-scale framework, level-set-based method of multiple scales, incremental unknowns and other techniques of the non-linear Galerkin type. A quite promising method based on variational multi-scale techniques has recently been described in [2]. Its main steps are:

- at the initial stage, the presence of the unresolved scales is included ab initio;
- then, the problem is decomposed into two coupled sub-problems, so that we can carry out computations of: (a) the fine scales as driven by the residuals of the visible modes, and (b) the coarse scales, accounting for the effects of the invisible modes.

No computational results have been reported so far to test this methodology. It is well known, however, that the method of two-scale asymptotic expansions may fail to give the appropriate multi-scale governing equation for general nonlinear problems [24]. At the same time, iterative schemes, developed within the multi-scale methodology framework, that allow us to alternate between macroscopic and microscopic solutions (e.g., [24]) could lead to unjustifiably high computational cost. In our approach we balance contributions of small effects at the stage of the model construction, and the centre manifold technique allows us to treat effectively as many small effects as we wish by choosing as many different parameters (and orders in the amplitudes) as needed for a specific problem.

In the next sections, our goal is to apply our approach to the description of the dynamics of phase transitions in the SMA layer of thermoelectric actuators. The problem has recently been analysed by experimentalists [1], and an efficient computational methodology would lead to a further insight into the physical processes that are crucial for the design of these devices. Firstly, note that the problem in hand is a strongly nonlinear problem. Moreover, since we need to deal with different (possibly co-existent) phases of the material, the problem is a multi-equilibrium problem. These features of the problem under consideration would require a quite efficient computational methodology in order to simulate phase transformations in the material. Before moving to technicalities of this problem, we summarise the most important

features of our approach:

- computational implementations of the centre manifold technique do not require a restrictive spectral gap condition typical for a number of other numerical algorithms, including AIM constructions;
- the methodology can be applied to multi-equilibrium problems, which is an essential factor for phase transition models;
- the centre manifold technique can be effectively applied to multi-scale problems; it allows treatment of multiple small effects by choosing as many different small parameters as needed;
- last, but not least, the centre manifold can be constructed to any desired degree of accuracy with respect to the chosen small parameters.

In what follows, we demonstrate our approach on the example of modelling a thermoelectric SMA actuator. The approach, which is a combination of the centre manifold technique and computer algebra, is *systematic* in a sense that it allows us to derive computational models with arbitrary order of accuracy with respect to a pre-defined set of small parameters.

3. Multi-scale coupled dynamic problems in smart material and structure technologies

A wide range of computationally challenging problems is provided by recent advances in smart material and structure technologies. Not only do new materials require an efficient treatment of *spatio-temporal multiple scale effects*, they lead to mathematical models which are essentially *coupled*. In many applications of smart material and structure technologies, coupled phenomena are in the very essence of the successful design of systems and devices. Classical examples include electromechanical and magnetomechanical systems. As a part of modelling such systems, in some cases we have to adequately describe the dynamic behaviour of complex materials these systems made of, subject to different loadings. This is known to be *one of the most difficult tasks in computational sciences*, which is complicated even further as soon as an intrinsic nonlinear interplay between different physical fields, such as mechanical, electric, and/or thermal, is at the heart of the process of interest. Typical examples of the materials that are usually classified as "smart" (due to their ability to respond to environmental changes or external loading conditions) include electro-rheological fluids, magnetostrictive materials, piezoelectrics to name just a few. In what follows, we consider a specific example which has recently attracted a considerable interest of experimentalists. It has been known for a long time that under external stimuli (e.g., a mechanical force, a temperature impulse, or a magnetic field) some materials can restore their original configurations after being permanently deformed. The materials that have attracted a lot of attention in the context of microtechnology and microsystems engineering are SMAs. However, these promising materials have a disadvantage which only recently has been overcome by experimentalists. Indeed, it is known that the control of the SMA phase transformations can be made by temperature or mechanical field or a combination of both, but what is problematic is the low dynamic response of these materials. For example, we can use SMA elements to actuate microrobots, but their low dynamic response may not allow us to do so efficiently, in particular in the situations where it is difficult to control the external temperature or where such actuators operate in confined environments. This is especially true due to cooling mechanisms [1]. Hence, it is our next goal to develop a model which would work for such SMA-based systems. In particular, we want to describe adequately phase transformations occurring in the SMA layer of thermoelectric actuators such as those that have recently been studied experimentally in [1]. The design of new devices and systems requires a better understanding of the dynamics of these materials, including phase transition and hysteresis phenomena [15]. The modelling of SMA dynamics is a challenging field of computational science where interdisciplinary efforts are required. The adequate modelling of SMA-based multi-layered structures represents even a greater challenge. It is a novel, interesting, and important task, and it is this class of problems that is in a focus of our analysis in the next two sections.

We consider a SMA actuator whose operation is based on the so-called solid–solid phase transitions, a process which can be understood only by considering the dynamics of thermal and mechanical fields as coupled. From a practical point of view, such actuators, which could be quite small in size, can outperform classical piezoelectric-based actuators in terms of their

ability to generate larger stresses and strains. SMA can be used for actuating purposes in shape and vibration control problems, as well as in applications ranging from various mechatronics products (e.g., flexible grippers for the assembly of tiny workpieces in the semiconductor industry and the sample collection for microscopic observations in the biochemical labs) to SMA actuators in the area of underwater vehicle design, artificial valves in bioengineering applications, etc. However, as we have already mentioned, SMA actuators have a fairly low frequency response and slow cooling rates [1,6,7,10]. Hence, substantial research efforts have been recently directed to overcome this disadvantage of SMA-based devices by controlling their operation with thermoelectric, magnetic, or other externally generated fields. It has been confirmed by experimentalists that the Peltier effect can be used effectively for these purposes [1]. This effect is intrinsic to thermoelectric materials. The fundamentals of modelling thermoelectric (thermodynamically reversible) processes were laid by A.F. Ioffe, and based on those early results, semiconductors have been used for localised cooling in various applications. Several factors contribute to a renewed and rapidly growing interest in thermoelectric materials. As the size of semiconductor devices continues to decrease, this leads to an increasing power dissipation per unit area. Thermal effects become even more critical for photonic devices where the heat generation density could be very high. In the context of our further discussion, thermoelectric effects are used for thermal cycling of the SMA, so that the desired phase change for actuation purposes can be induced, subject to appropriate mechanical conditions. In order to model such thermoelectrically controlled SMA actuators based on an SMA layer surrounded by layers of thermoelectrics (typically semiconductors), we have to deal with two levels of coupling. Firstly, we have the coupling between thermal and electric fields in the semiconductor layers, and secondly, we have the coupling between mechanical and thermal fields in the SMA layer. In its generality, a complete dynamic description of such multi-layered structures is difficult to obtain, and efficient computational models should be developed to attack the problem. In order to demonstrate the methodology described in Section 2 in modelling such devices, we use a simple model for thermoelectric "surroundings" of the SMA layer.

4. Case study example: thermoelectrically controlled SMA actuators

We consider a single SMA module (a realistic structure consists of a set of such modules) depicted in Fig. 1. The idea here is essentially the same as in more classical applications of thermoelectrics in power conversion and refrigeration industries, where the cooling efficiency can be achieved with semiconductor thermoelements (in fact, much progress in the field has been connected with the development in solid-state electronics). For SMA-based actuators cooling is important as soon as the control of SMA phase transformations (and a subsequent mechanical power generation) is made by the temperature. If the dynamic response of such actuators is low in low cooling rates, it deteriorates their usefulness. Note that the efficiency of traditional "cooling" technologies such as thermal convection and conduction, usually applied to SMA samples at larger scales, decreases with scaling down SMA devices. A novel engineering idea, developed here further from a computational

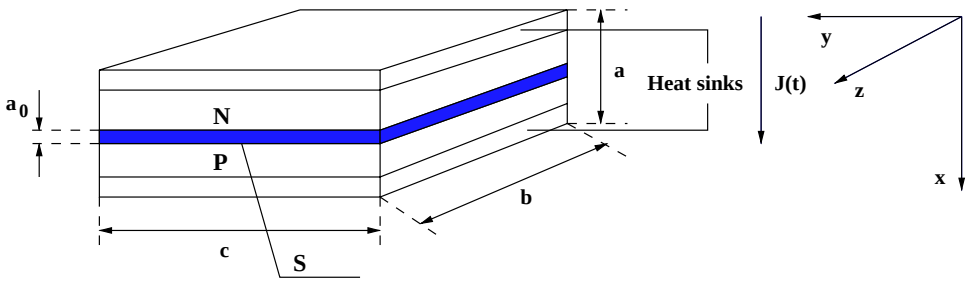

Fig. 1. Schematic representation of a single multi-layered SMA actuator module.

point of view, originates from the fact that the Peltier effect is known to be quite effective for cooling electronic chips in electronic industry. The use of this effect is based on the fact that whenever we apply an electric current to a system composed of two dissimilar conductors, heat is evolved at one junction and absorbed at the other leading to a situation where one junction becomes cold and the other becomes hot. From a computational point of view, this fact brings difficulties in modelling these devices due to a jump in the heat flux at the interface caused by the Peltier effect.

In Fig. 1, P and N stand for oppositely doped semiconductors (e.g., bismuth telluride TeBi), and S stands for the SMA layer of this multi-layered structure. We assume that the density of applied current is $J(t)$, and the current direction for this specific case is indicated schematically in Fig. 1.

The modelling of thermoelectrically cooled/heated SMA actuators is typically limited in the literature to thermal analyses only (e.g., [1,7] and references therein) where the SMA module is described on the basis of the heat equations with different approximations for the internal heat productions. Such models cannot describe the dynamics of phase transitions that would require considering displacements coupled to temperature changes. In addition, until recently such models were based on the assumption of a small ratio between the SMA layer thickness and the thickness of semiconductors (see discussion in [7]). This assumption might be violated in practice. Nevertheless, such models allow us to obtain a first approximation to the temperature at the interface between the SMA and semiconductor layers. This fact will be used in the models discussed below.

4.1. Accounting for thermoelectric effects in the thermomechanical analysis of the system

We denote the temperature by θ, the thermal conductivity coefficient by k, the perimeter and area of the cross-section by P and A, respectively, the heat convection coefficient by H, the electrical resistivity by ρ (so that ρJ^2 is the Joule heat), the heat capacity per unit volume by C_v, and the Seebeck coefficient by α. The structure is symmetric, the thickness of the SMA layer is a_0, and the thickness of each semiconductor layer is a (see Fig. 1). Two other dimensions of the structure, denoted by b and c, are used in the definition of A and P, so that $A = bc$ and $P = 2(b+c)$. Following [6], we consider a thermal model for the multi-layered SMA actuator based on a system of three heat equations written for each layer i (either N-semiconductor layer, P-semiconductor layer, or SMA layer, that is, for instance, θ_s denotes the temperature in the SMA layer)

$$k_i \frac{\partial^2 \theta_i}{\partial x^2} + \rho_i J^2(t) - H\frac{P}{A}(\theta_i - \theta_0) = C_v^i \frac{\partial \theta_i}{\partial t}, \qquad (4.1)$$

and coupled together by the flux interface conditions, e.g.,

$$-k_s \frac{\partial \theta_s}{\partial x} = -k_p \frac{\partial \theta_p}{\partial x} + \alpha_p \theta_p J(t). \qquad (4.2)$$

Model (4.1) and (4.2) provides a good approximation especially in the case where the temperature in each layer does not vary significantly in the plane perpendicular to the x-axis. This simple analysis allows us to set a background for the analysis of the SMA layer.

Note that by considering a special case where the thermal conductivity of SMA, k_s, is much larger compared to thermal conductivity of semiconductors, k_n, and k_p (e.g., by assuming a small ratio between the layer thickness of SMA and semiconductor $a_0/a \ll 1$), the strong thermomechanical coupling, intrinsic to the SMA layer, has often been neglected (e.g., [6]). Although the assumption $a_0/a \ll 1$ (dubious in many applications) has been recently removed in [7], most approaches developed in this field so far can account only partly for the thermomechanical coupling in the SMA layer [6,7,10]. However, it is this *coupling that is responsible for phase transformations*, and due to this coupling, the often made assumption that $\theta_s(x,t)$ is independent of x (e.g., [6]) cannot be justified in any realistic situations involving phase transformations. A partial phase transformation (and hence the effect of coupling) has been considered in [10], where the assumption of an almost uniform temperature distribution in the SMA layer has been removed. The authors of [10] used a phenomenological model based on gradual transformations of SMA polycrystals and evolution equations for field variables which were then solved with a Runge–Kutta method. Similar to their previous works, the procedure was limited to

stress-free boundaries, and therefore could be applied to a specific form of thermomechanical coupling only.

Despite limitations mentioned above, models proposed in [6,7,10] are an important step forward, indicating clearly a way of reducing the problem (4.1) and (4.2) to a relatively simple heat transfer problem with coupling effects implemented at the boundaries, as a result of the dependency of the temperature in semiconductor layers on the heat capacity of the SMA material. Indeed, as shown in [6], this problem can be effectively reduced to an integro-differential equation, which in its turn is reduced further to the solution of a Volterra equation. By considering θ as a function of J in the SMA layer, it can be shown that certain conditions, such as bounds on J, should be satisfied in order to achieve a monotonic decay of the SMA temperature. This is an important observation since a major disadvantage in utilising SMA actuators is the low rate of cooling. However, no possible austenite-to-martensite transformations as a result of this cooling has been discussed. It is one of our purposes here to demonstrate that our computational model can reproduced very well such transformations under appropriate cooling conditions. Before proceeding with this task, thermal boundary conditions for the SMA layer should be specified.

In describing coupled thermomechanical fields in the SMA layer, we follow a two-step procedure. Our first step is equivalent to that described in [7]. This leads us to an approximation of the temperature on the boundary of semiconductor layers, and by using its continuity a fully coupled model for the SMA layer can be formulated at the second step. If $J(t)$ is assumed to be constant, the exact solution to the problem at step 1, considered as a "purely" thermal analysis of the multi-layered structure, can be found. In this analysis, the heat transfer behaviour along the SMA layer is dominated by the temperature at the interface between the SMA layer and the semiconductor layer. The analysis can be reduced to an integro-differential equation with respect to an auxiliary function, as discussed in [7]. More precisely, we consider Eq. (4.1) for $i = s$, that is for the SMA layer, where, due to symmetry, it is sufficient to consider the interval $0 < x < a_0/2$ only. This equation is supplemented by the initial condition $\theta(x, 0) = \theta_0$, "symmetry" boundary condition $(\partial\theta/\partial x)(0, t) = 0$, and the "interface" boundary condition at $x = a_0/2$:

$$\frac{\partial\theta}{\partial x} = -\frac{2k}{ak_s}\int_0^t G_1(t-\tau)\left[\frac{\mathrm{d}\theta}{\mathrm{d}t} + \frac{HP}{C_v A}(\theta-\theta_0)\right]\Big|_{t=\tau}\mathrm{d}\tau + \left(1-\frac{k}{\alpha a}\right)\theta + F(t), \quad t > 0, \tag{4.3}$$

obtained by using the solution for the semiconductor layer, as explained in [7]. In (4.3) $G_1(t) = \sum_{n=1}^{\infty}\exp(-\beta_n t)$ and function F has the following form:

$$F(t) = \frac{4\rho k}{C_v k_s a}\int_0^t \sum_{n=1}^{\infty}\exp(-\beta_{2n-1}(t-\tau)J^2(\tau))\,\mathrm{d}\tau + \frac{k}{ak_s}\theta_0. \tag{4.4}$$

Indices of the coefficients of the semiconductor adjacent to the SMA layer are omitted in (4.3) and (4.4), and $\beta_n = n^2\pi^2 + H$. It is this problem that is reduced to an integro-differential equation. Existence and uniqueness of its solution is established in a standard manner by equivalence with a Volterra equation, and its solution is found numerically by employing a finite difference scheme. Temperature profiles at the interface between the SMA and semiconductor layers can be quite different for different values of the current density J, but once such a profile is found we can proceed to the next step of our procedure.

4.2. Thermomechanical interactions in the actuator SMA layer

The methodology discussed in Section 2 can be applied to the description of solid–solid phase transitions in the SMA layer of the thermoelectrically controlled actuator. The behaviour of one-dimensional SMA samples is reasonably well understood, and austenitic–martensitic transformations, as well as the associated hysteresis phenomena, can be reproduced computationally (see [15,16] and references therein). However, the extension of such computational models allowing to describe multidimensional responses is more difficult. We consider the fully coupled thermomechanical dynamic system of the SMA layer by employing a general procedure, similar to that discussed in [15] for a single layer structure. In particular, starting from the 3D coupled model consisting of the

equation of motion and the energy balance equation

$$\rho\frac{\partial^2\mathbf{u}}{\partial t^2} = \nabla\cdot\mathbf{s} + \mathbf{F},$$
$$\rho\frac{\partial e}{\partial t} + \rho\tau_0\frac{\partial^2 e}{\partial t^2} - \mathbf{s}^{\mathrm{T}} : (\nabla\mathbf{v}) - \tau_0\frac{\partial}{\partial t}[\mathbf{s}^{\mathrm{T}} : (\nabla\mathbf{v})] - \nabla\cdot(k\nabla\theta) = G, \tag{4.5}$$

we aim at developing efficient computational models allowing to reproduce austenite-to-martensite phase transformations observed under thermoelectric cooling of SMA actuators. In (4.5) $\mathbf{u}$ denotes displacements, $\mathbf{s}$ is the stress tensor, $\mathbf{v} = \partial\mathbf{u}/\partial t$ the velocity vector, e the internal energy, τ_0 the relaxation time, ρ the density of the material, $\mathbf{F}$ and G are forcing terms (further details can be found in [14]).

Solving problem (4.5) is a quite challenging computational task. Note, for example, that the invariant directions in the definition of strain are associated with a representation of the 48th order symmetry group, and the complexity of the problem can be appreciated better if one writes explicitly the resulting strain invariants (e.g., [14]). Even in a relatively simple (due to a straightforward relationship between microscopic strain and displacements $\epsilon = \partial u/\partial x$) one-dimensional case the system (4.5) reads as follows:

$$C_v\left[\frac{\partial\theta}{\partial t}\right] - k_1\left[\theta\frac{\partial u}{\partial x}\frac{\partial^2 u}{\partial t\partial x}\right] - \frac{\partial}{\partial x}\left(k\frac{\partial\theta}{\partial x}\right) = G,$$
$$\rho\frac{\partial^2 u}{\partial t^2} - \frac{\partial}{\partial x}\left[k_1\frac{\partial u}{\partial x}(\theta-\theta_1) - k_2\left(\frac{\partial u}{\partial x}\right)^3 + k_3\left(\frac{\partial u}{\partial x}\right)^5\right] = F, \tag{4.6}$$

where θ is the temperature field, k the thermal conductivity of the material, C_v the specific heat constant of the material, θ_1 is a positive constant that characterises a critical temperature of the material, and k_i, $i = 1, 2, 3$ are material-specific constants that characterise the material free energy which was chosen in the Landau–Devonshire form. Note that in (4.6) we neglect relaxation time effects and the dependency of the stress on the rate of the deformation gradient and temperature. The stress is defined via the free energy function as $s = \rho(\partial\psi/\partial\epsilon)$.

In moving to the three-dimensional case note that each specific type of phase transformation brings some restrictions to the definition of the free energy function. Even if the free energy function is chosen, it is not always easy to proceed with such a function to the computational level. A classical example is the Ericksen–James functional, for which it is difficult to construct computationally a minimising sequence due to increasing oscillations with grid refinement. Different remedies have been proposed in the literature to overcome this deficiency. For example, a number of procedures have been proposed to approximate the free energy function, e.g. by considering its quasi-convex counter-part (see [9] and references therein). However, hysteresis effects have not been included into such simplified models.

Constitutive models used in this paper are based on the general representation of the free energy function in the form

$$\Psi(\boldsymbol{\epsilon}) = \psi^0(\theta) + \sum_{i=1}^{\infty}\sum_{j=1}^{j^i}\psi_j^i\mathcal{I}_j^i \tag{4.7}$$

with $\mathcal{I}_i^j$ being the strain invariants, ψ_i^j the temperature dependent functional coefficients, and $\boldsymbol{\epsilon}$ the strain tensor. Function (4.7) is made invariant with respect to the symmetry group of austenite, and the upper limits j^i are chosen appropriately to satisfy this condition [14].

Further, we determine the stress component due to mechanical dissipations as $\mathbf{s}^q = \rho(\partial\Psi/\partial\boldsymbol{\epsilon})$. As with the one-dimensional system (4.6), thermal dissipations, plasticity, and other effects can be incorporated into the model, but in what follows we describe our methodology for the Landau–Devonshire type constitutive models as an example, where we take $\mathbf{s} = \mathbf{s}^q$. In particular, for the general 3D model we use the Falk–Konopka representation of the free energy function (4.7) with 10 strain invariant directions, valid for the copper-based SMA materials [14].

Model (4.5), supplemented by appropriate constitutive laws for the SMA materials, boundary and initial conditions, represents a tremendous computational challenge in the general 3D case. Any computational treatment of this model aiming at the description of the dynamics of SMA-based system responses will necessarily require essential simplifications of this model in order to be tractable. Such simplifications should be developed in a systematic way, and below we apply our methodology for improving computational models for the description of SMA dynamics.

4.3. Centre manifold analysis of the phase transformations in SMA-based actuators

As described in Section 2, our idea is based a combination of the centre manifold technique and computer algebra, and we apply this idea to developing reduction procedures for the original model (4.5) on centre manifolds, while retaining essential properties of the system. Our approach allows considering different patterns of thermomechanical coupling implemented via appropriate choices of the free energy function, constitutive models, initial and boundary conditions. In the dimensions higher than one computational results are virtually absent in this field, and little is known on how to simplify such models as (4.5) and (4.7) systematically. In the spirit of our previous works [14,15] we consider an SMA slab, and associate the qualitative change in system behaviour with the subset of eigenvalues having zero real parts. In the case analysed here, if dissipations are omitted, there is a zero eigenvalue of multiplicity 5 and the rest are purely imaginary. Then, critical variables are chosen as those that are responsible for the essential behaviour of the system. This leads to the following steps in our computational procedure:

- Analysis of eigenvalues of the cross-slab modes, as required by centre manifold theory.
- Construction of a sub-centre manifold based upon the relevant eigenmodes as they evolve slowly.

Therefore, the sub-centre manifold is constructed based on these five eigenmodes. Note that for simplicity we consider here the critical eigenvalues that are zeros (see comments on pure imaginary eigenvalues in [20,21]). The initial conditions for the detailed (original) dynamics also have to be projected onto the low-dimensional manifold, as well as the boundary conditions (see further details on this in [14,15]). The low-dimensional invariant manifold should be parameterised by the amplitudes of the critical modes, which constitute a subset of all modes, and determine the essential dynamic behaviour of the system [20]. A computational model is constructed with respect to these amplitudes, and since the leading order structure of the critical eigenmodes are constant across the slab (the longitudinal variations were neglected in the first approximation), we associate these amplitudes with the y-averages of displacements, velocities, and temperature, denoted here as $\mathbf{U} = (U_1, U_2)$, $\mathbf{V} = (V_1, V_2)$, and $\theta' = \theta - \theta_0$ (θ_0 is taken as 300 K). The connection between these variables, and the variables of the original model is established in an approximate form by employing the low-dimensional invariant manifold and asymptotic sum representations (explicit formal power series representations maybe prohibitive even for the modern computer). The small parameters used in this paper are ∂_x, $\mathcal{E} = \|U_x\| + \|V_x\|$ and $\vartheta = \|\Theta'\|$, and our computer-algebra program balances their small effects in such a way that in the model construction the strains are treated as small, as measured by $\mathcal{E}$, while asymptotically large displacements and velocities are permitted. After the decision on how to parameterise the centre manifold model is taken, and the critical modes are identified in order to project the dynamics onto the "slow" modes of interest, we complete our computational procedure by:

- Substituting the asymptotic sums into the governing equations.
- Evaluating residuals by using computer-algebra tools to get the result with the required accuracy.

These steps are performed in a computationally very efficient manner by using an iterative algorithm analogous to that discussed in [20]. By applying the above procedure, we have derived the reduced model

$$
\begin{aligned}
&\rho\frac{\partial V_1}{\partial t} = \frac{\partial s}{\partial x} + F, \qquad \frac{\partial U_1}{\partial t} = V_1,\\
&C_v\frac{\partial \Theta'}{\partial t} = k\frac{\partial^2 \Theta'}{\partial x^2} + (c_{11} + c_{12}\Theta' - c_{13}(\Theta')^2)\frac{\partial U_1}{\partial x}\frac{\partial V_1}{\partial x}\\
&\qquad + (c_{14} + c_{15}\theta')\frac{\partial V_1}{\partial x}\left(\frac{\partial U_1}{\partial x}\right)^3\\
&\qquad + c_{18}\frac{\partial V_1}{\partial x}\left(\frac{\partial U_1}{\partial x}\right)^5 + g,\\
&s = (c_1 + c_2\theta' - c_3(\theta')^2)\frac{\partial U_1}{\partial x} - (c_4 - c_5\theta')\left(\frac{\partial U_1}{\partial x}\right)^3\\
&\qquad + c_6\left(\frac{\partial U_1}{\partial x}\right)^5,
\end{aligned}
\tag{4.8}
$$

where coefficients c_k are positive material constants (taken here as in [14]). This model, derived from the general 3D model (4.5), is exact up to the fourth order with respect to the small parameters, and preserves all essential features of the dynamics of the original

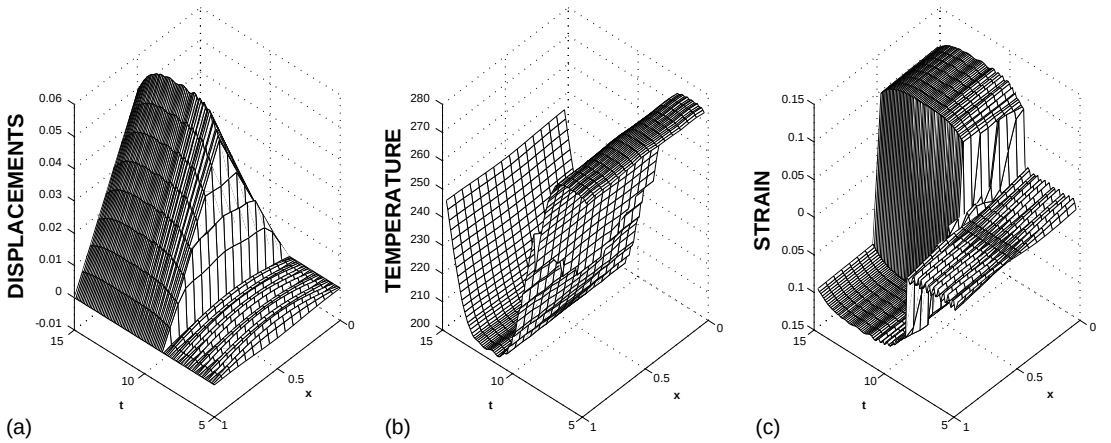

Fig. 2. Austenite-to-martensite phase transformation in the SMA layer of the thermoelectric actuator (from left to right): (a) displacements; (b) temperature; (c) strain.

system. The resulting model (4.8) is solved by its reduction to a system of differential-algebraic equations, and the displacements and temperature of the slab are recovered by using critical eigenmodes.

The developed computational procedure provides an efficient tool for analysing multi-layered SMA actuators. In Fig. 2 we present a typical result of computation based on this procedure. Profiles for thermal cycling used in these experiments are analogous to those used in thermal analyses of these devices [6,7]. Starting with high temperature phase (austenite) (represented in Fig. 2(a) and (c) by zero displacements and zero strain, respectively) it is shown how the cooling of the SMA layer (Fig. 2(b)) leads to the martensitic phase.

5. Concluding remarks

By using a realistic case study example based on thermoelectrically controlled thermomechanical SMA actuators, we have demonstrated a systematic methodology for improving computational efficiency of models describing the coupled dynamics of nonlinear systems. The approach, based on a combination of the centre manifold and computer-algebra techniques, allows us to derive computational models with arbitrary degree of accuracy with respect to a priori chosen small parameters. The methodology can be applied to other complicated multi-scale problems where as many such small parameters can be chosen as needed in order to allow an effective treatment of contributions from many different small effects.

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