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Efficient Computational Models for Coupled Nonlinear Dynamics of Materials with Memory

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1. INTRODUCTION

Many models of science and engineering are essentially coupled dynamically in a sense that the response of system components should be obtained concurrently. This dynamic coupling is an intrinsic feature of many systems, processes, and phenomena with numerous examples in mechatronics, geophysics, biomechanics, and many other fields (e.g. [6] and references therein). In some cases the interacting components of the system could be structures, fluid, or solid media, as, e.g., in geophysical applications, while in other cases the interacting components could be given in the form of fields such as mechanical and thermal, or electrical and mechanical, invoking a unification of two or more physical theories that have been considered separately before, e.g. thermoelasticity, electroelasticity, hydroelasticity, etc.
A common feature of all these problems is that in most practically interesting cases the resulting mathematical models are not amenable to the analytical treatment, and the development of efficient numerical procedures for their solutions is required. In this paper I am interested in efficient scientific computing tools allowing us to adequately describe the complex nonlinear behaviour of materials with memory, in particular shape memory alloys. My main tool will be the centre manifold technique [2] linked together with effective computational procedures for the model construction.

2. MATHEMATICAL MODELS FOR MATERIAL DYNAMICS WITH HYSTERESIS

It is often argued that in dealing with the description of nonlinear dynamics based on laws of continuum mechanics the main freedom we have nowadays in constructing models lies in the description of material response. However, some materials have fairly complicated responses leading to hysteresis and other strongly nonlinear effects [1]. The major interest in this paper is the developing systematically computational tools for materials with memory, in particular for shape memory alloys. The basic model for describing the dynamics of shape memory alloys is a nonlinear coupled system of partial differential equations consisting of the energy balance equation and the equation of motion

$$\rho\frac{\partial^2\mathbf{u}}{\partial t^2} = \nabla\cdot\mathbf{s} + \mathbf{f}, \quad \rho\frac{\partial e}{\partial t} - \mathbf{s}^T : (\nabla\mathbf{v}) + \nabla\cdot\mathbf{q} = g\,. \tag{1}$$

The system should be solved with respect to the displacement $\mathbf{u} = (u_1, u_2, u_3)$ and temperature θ. In (1) ρ is the density of the material, $\mathbf{s}$ is the stress tensor, e is the internal energy of the system, $\mathbf{v}$ is the velocity vector ($\mathbf{v} = \partial\mathbf{u}/\partial t$), $\mathbf{q}$ is the heat flux, and $\mathbf{f}$, g give the mechanical and thermal loading, respectively.

For the heat flux we use the hyperbolic equation based on the Cattaneo-Vernotte model, accounting for the finite speed of heat propagation (see [10]):

$$\mathbf{q} + \tau_0\frac{\partial\mathbf{q}}{\partial t} = -k(\theta,\boldsymbol{\epsilon})\nabla\theta\,, \tag{2}$$

where τ_0 is the thermal relaxation time, and $k(\theta, \boldsymbol{\epsilon})$ is the thermal conductivity of the material, $\boldsymbol{\epsilon}$ is the strain tensor. A simplified model (1)–(2) has been already studied computationally (e.g., [7] and references therein), but little is known about efficient computational models based on the general 3D systems (1).

The major computational difficulties are coming from two sources. The first is a strong nonlinear coupling between mechanical and thermal fields for this type of problems pronounced in a complex stress-strain constitutive relationship for these materials. In this paper I use a quintic nonlinear dependency, as resulted from the Landau-Devonshire model. The second source of difficulties is the definition of the internal energy function. Both these sources merge at the choice of the free energy function for the system. In a quite general setting we can use the following definition

$$\Psi(\boldsymbol{\epsilon}, \theta) \equiv e - \theta\eta = \psi^0(\theta) + \sum_{n=1}^{\infty} \psi^n(\boldsymbol{\epsilon}, \theta) \quad \psi^n = \sum_{j=1}^{j^n} \psi_j^n \mathcal{I}_j^n, \quad \psi^0(\theta) = \psi_0(\theta)\,, \tag{3}$$

where $\eta = -\dfrac{\partial \Psi}{\partial \theta}$ is the entropy density of the system, and $\mathcal{I}_j^n$ are the strain invariants with j^n being the number of all invariant directions associated with a representation of the 48th order cubic symmetry group of the parent phase phase of the material, as in [3]. It is appropriate to recall here that shape memory alloys have two main phases, the austenite (the parent, high temperature phase) and the martensite (the low temperature phase) obtained from each other by a simple shearing motion of the atoms within the crystal structure of the material (this is the reason why it's often called a diffusionless transformation, not requiring large movements of atoms like atomic plane dislocations, etc).

Having Ψ, we define the internal energy and the stress-strain relationship as follows

$$e = \Psi - \theta \frac{\partial \Psi}{\partial \theta}, \quad \mathbf{s} = \rho \frac{\partial \Psi}{\partial \boldsymbol{\epsilon}}. \tag{4}$$

The initial conditions for this problem are defined in a straightforward way, while thermal and mechanical boundary conditions vary from an application to application, e.g. stress-free, pinned-end, or mixed mechanical boundary conditions, thermal insulation, controlled flux, or fixed temperature ("uncontrolled energy flow") thermal boundary conditions.

3. MODELS BASED ON THE RESIDUAL MINIMISATION AND A DIRECT CODING OF THE GOVERNING EQUATIONS

The development of computational models based on (1)–(4) should be carried out bearing in mind three important points:

- the material we are dealing with has several different equilibrium configurations, so we need a computational method that is not linked to just a single equilibrium;
- since we deal with dynamically interacting fields, it is important to realise that just a single parameter, as it is often used in singular perturbation theory, may not be sufficient to scale all other variables, - a range of such parameters is required to balance carefully the order of small effects in the model construction (rather than in its use [9]);
- the model itself should be flexible enough to incorporate further possible improvements in the physics of the model, e.g. by incorporating new effects such as porosity, plasticity, by using different forms of the free energy functions (see discussion in [4]), by accounting for complex multiaxial conditions, by using improved constitutive models, etc.

Under these circumstances the methodologies requiring the fulfillment of the spectral gap condition might not be the best method of choice. Such a condition is very restrictive in a computational sense since it usually requires some form of the global exponential decay in order to construct an approximate inertial manifold of the dynamics, being guided by an asymptotically complete inertial manifold idea. In this paper the construction of computational models is carried out on the basis of a local exponential decay following the centre manifold technique empowered by computer algebra. In particular, based on the existence, relevance, and approximation theorems (e.g., [9]) we can construct a hierarchy of models for materials with memory depending on their order of accuracy. Consider, for example, the case where the critical eigenvalues of a linear (initial) approximation to the dynamics are zero of arbitrary multiplicity M and amplitudes U_i, $i = 1, ..., M$ (critical eigenvalues with a non-zero imaginary part are included into the analysis when necessary). We chose a vector $\boldsymbol{\varepsilon}$ to measure the contribution of small effects, and then express our model in terms of asymptotic sums in $\boldsymbol{\varepsilon}$, balancing carefully the order of these effects at *the stage of the model construction* by using computer algebra. Note that the direct application of power series for such complex infinite dimensional systems as (1)–(4) is usually computationally prohibitive due to a quick growth of terms that are required to be accounted for. Our aim is to find a low-dimensional model

$$\frac{d\mathbf{U}}{dt} = \mathbf{g}(\mathbf{U}), \quad \mathbf{U} \in \mathbb{R}^M, \quad \mathbf{u} = \boldsymbol{\nu}(\mathbf{U}), \tag{5}$$

for the evolution of M amplitudes $\mathbf{U}$ with the low-dimensional dynamics occurring on the exponentially attractive centre manifold described parametrically in (5) by $\boldsymbol{\nu}$ (a vector function to be found). The important feature of our approach is that this function can be found approximately with arbitrary degree of accuracy by using computer algebra. First, we use a linear approximation to the centre manifold, and then modify the projection onto the slow modes of interest by nonlinear terms, correcting our approximation to the actual nonlinear "shape" of the manifold. This is implemented via the estimation of the residual of the governing equation (1) implemented into the program via a direct coding. The iterative procedure is organised in the spirit of [9] and works in a way similar to the Newton algorithm for systems of nonlinear algebraic equations by improving at each step the previous approximation (denoted by J)

$$\mathbf{u} \approx \boldsymbol{\nu}^J(\mathbf{U}) + \Delta\boldsymbol{\nu}(\mathbf{U}) \quad \text{such that} \quad \frac{d\mathbf{U}}{dt} \approx \mathbf{g}^J(\mathbf{U}) + \Delta\mathbf{g}(\mathbf{U}) \tag{6}$$

leading to a higher order approximation to the original dynamics. This is organised by an iterative sub-procedure which deals with physically meaningful expressions, while the evaluation of the residual itself is carried out with a computer algebra package Reduce. Improving at each iteration the order of error in terms on β_1 and β_2 (we took two parameters as an example for estimating the residual), we improve the accuracy of the model according to the centre manifold approximation theorem [9].

The methodology has been already tested on an example reported in [5], and other examples will be given during the presentation. Below we provide an example of the model of a shape memory alloy slab with thickness 2b for its longitudinal dynamics on the slow manifold determined up to the fifth order in terms of $\|\mathbf{U}_x\| + \|\mathbf{V}_x\|$ and the second order with respect to the spatial derivatives and temperature:

$$\begin{aligned}\rho\frac{\partial V_1}{\partial t} &= 1.91\text{e}6\,\frac{\partial^2 U_1}{\partial x^2} + 5.15\text{e}5\,b^2\frac{\partial^4 U_1}{\partial x^4} \\ &+ \frac{\partial}{\partial x}\left[(592\,\Theta' - 0.00931\Theta'^2)\frac{\partial U_1}{\partial x} - (2.75\text{e}9\ - 8.42\text{e}6\,\Theta')\left(\frac{\partial U_1}{\partial x}\right)^3 + 4.56\text{e}11\,\left(\frac{\partial U_1}{\partial x}\right)^5\right.\end{aligned}$$

$$+ (1811 - 5.64\,\Theta')b^2 \left(\frac{\partial V_1}{\partial x}\right)^2 \frac{\partial U_1}{\partial x} + 0.728\,b^4 \left(\frac{\partial V_1}{\partial x}\right)^4 \frac{\partial U_1}{\partial x} - 2.51\text{e}3\,b^2 \left(\frac{\partial V_1}{\partial x}\right)^2 \left(\frac{\partial U_1}{\partial x}\right)^3 \Bigg],$$

$$\rho \frac{\partial V_2}{\partial t} = -6.36\text{e}5\,b^2 \frac{\partial^4 U_2}{\partial x^4}$$

$$\begin{aligned} C_v \frac{\partial \Theta'}{\partial t} &= \kappa \frac{\partial^2 \Theta'}{\partial x^2}, + (1.78\text{e}5 + 586\,\Theta' - 5.94\,\Theta'^2) \frac{\partial U_1}{\partial x} \frac{\partial V_1}{\partial x} \\ &+ (2.53\text{e}9 + 8.11\text{e}6\ \Theta') \frac{\partial V_1}{\partial x} \left(\frac{\partial U_1}{\partial x}\right)^3 - (36.8 + 0.00761\,\Theta')b^2 \left(\frac{\partial V_1}{\partial x}\right)^3 \frac{\partial U_1}{\partial x} \\ &+ 1.08\text{e}12\, \frac{\partial V_1}{\partial x} \left(\frac{\partial U_1}{\partial x}\right)^5 - 1.016\text{e}6\,b^2 \left(\frac{\partial V_1}{\partial x}\right)^3 \left(\frac{\partial U_1}{\partial x}\right)^3 - 0.0116\,b^4 \left(\frac{\partial V_1}{\partial x}\right)^5 \frac{\partial U_1}{\partial x} \\ &+ 1.05\text{e}4\,b^2 \frac{\partial^2 U_1}{\partial x^2} \frac{\partial^2 V_1}{\partial x^2} + 5.92\text{e}4\,b^2 \frac{\partial^2 U_2}{\partial x^2} \frac{\partial^2 V_2}{\partial x^2} + \frac{\partial^2}{\partial x^2} \left[-5228\,b^2 \frac{\partial U_1}{\partial x} \frac{\partial V_1}{\partial x}\right]. \end{aligned}$$

where C_v is the specific heat constant of the material. In the above model the critical eigenvalues are associated with the y-averages of the amplitudes U_i, V_i and $\theta' = \theta - 300°\text{K}$. The model reflects well the temperature dependent quintic stress-strain relation of the shape memory alloy.

The methodology proposed in this paper allows us to derive systematically new efficient mathematical models and to construct relatively simple, robust and flexible computer codes [9, 5, 7]. It can also be applied to computational analysis of multilayered structures [8].

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