Low dimensional nonlinear thermomechanical models describing phase transformations and their applications

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Low Dimensional Nonlinear Thermomechanical Models Describing Phase Transformations and Their Applications

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Abstract: This paper focuses on the development of low dimensional approximations to coupled nonlinear systems of partial differential equations (PDE) describing phase transformations. The methodology is explained on the example of nonlinear ferroelastic dynamics. We start from the general three-dimensional Falk-Konopka model and with the center manifold reduction obtain a Ginzburg-Landau-Devonshire one-dimensional model. The Chebyshev collocation method is applied for the numerical analysis of this latter model, followed by the application of an extended proper orthogonal decomposition. Finally, we present several numerical results where we demonstrate performance of the developed methodology in reproducing hysteresis effects occurring during phase transformations.

Key–Words: Coupled systems, Nonlinearities, Phase transformations, Proper Orthogonal Decomposition, Dynamics of ferroelastic materials, Galerkin projection.

1 Introduction

Applied materials science provides mathematicians with a number of challenging problems at the forefront of applied mathematics, stimulating the development of new numerical methods and mathematical modelling tools often applicable in other areas of science, engineering, finance and industry. One of the reasons for that lies with the fact that basic physics of complicated materials is still only partially known and in most practically-relevant situations mathematicians should necessarily deal with multiscale multiphysics nature of the corresponding problems [13]. Furthermore, at the optimization and design level these materials become part of complex systems bringing about further difficulties in controlling such systems [15, 21].

In this paper we consider PDE-based mathematical models for the description of materials exhibiting phase transformations. Although our discussion is relevant to a wider group of materials, most of our examples here will be referring to ferroelastic materials which can sense and respond or actuate upon mechanical or thermal loadings. Materials with such properties belong to the group of smart materials. Most of the currently existing mathematical models for dynamic behaviors of smart materials are given by partial differential equations with couplings between various, often nonlinear, physical fields [1, 14, 5]. For ferroelastic materials involving the first order martensite phase transformation, the mathematical models can be formulated by coupling the thermal and elastic fields [7, 6, 18, 19, 20]. Due to the nonlinear nature of phase transformations, the dynamics of the mechanical field is strongly nonlinear amplified by nonlinear coupling with the thermal field. Since the dynamics of ferroelastic materials can be described by a system of nonlinear coupled PDEs, we usually have to deal with an infinite dimensional space. However, for control and design optimization purpose, an infinite dimensional model is difficult to deal with [3, 21], especially when the system is nonlinear. Having this in mind, starting with a general three-dimensional model, we reduce it to a simpler model and develop an efficient numerical methodology to construct the low-dimensional model for the dynamics of such materials.

2 Mathematical Model

The starting point of our consideration in this paper is the nonlocal model developed in [11] based on the equation of motion

$$\rho\frac{\partial^2\mathbf{u}}{\partial t^2}=\nabla_{\mathbf{x}}\cdot\mathbf{s}+\mathbf{F}\quad\text{with}\quad\mathbf{F}=\rho(\mathbf{f}+\hat{\mathbf{f}})-\hat{\rho}\mathbf{v}\,,\quad(1)$$

and the energy balance equation

$$\rho\frac{\partial e}{\partial t}-\mathbf{s}^T:(\nabla\mathbf{v})+\nabla\cdot\mathbf{q}=g\,,\qquad(2)$$

where $\mathbf{u}$ is the displacement vector, ρ is the density of the material, e is the internal energy (per unit mass), $\mathbf{q}$ is the heat flux, $\mathbf{f}$ is a given body force per unit mass, $\hat{\rho}$ and $\hat{\mathbf{f}}$ are nonlocal mass and force residuals respectively (similarly, g accounts for both local and non-local contributions), $\mathbf{v}=\partial\mathbf{u}/\partial t$ is the velocity vector, $\mathbf{s}$ is the stress tensor, $\mathbf{a}^T:\mathbf{b}=\sum_{i,j=1}^{3}a_{ij}b_{ij}$ is the standard notation for the rank 2 tensors $\mathbf{a}$ and $\mathbf{b}$ (further details can be found in [11]). The constitutive relationships that couple stresses, deformation gradients, temperature and heat fluxes have the following general form:

$$\Phi_1(\mathbf{s},\boldsymbol{\epsilon})=0\,,\quad\Phi_2(\mathbf{q},\theta)=0\,,\qquad(3)$$

where it is implicitly assumed that these relations may involve spatial and temporal derivatives of the functions. Particular forms for Φ_1 and Φ_2 are problem specific. In dealing with phase transformations, the approach adopted in this paper is based on the Landau criterion stating that any isothermal equilibrium configuration of the lattice corresponds to a minimum (global or local) of the free energy function. In our particular case, the analysis of the dynamics of ferroelastic materials involving the first order phase transformations is based on a low-dimensional reduction of the above model (1)-(3) leading to the modified Ginzburg-Landau type model [8]. To account for the first order phase transformations in the materials of interest, the above model of dynamic thermoelasticity must account for a nonconvex highly nonlinear character of the associated free energy function and in this case the basic model in the one-dimensional case can be represented in the following form [10, 8]:

$$\begin{aligned}&c_v\frac{\partial\theta}{\partial t}=k\frac{\partial^2\theta}{\partial x^2}+k_1\theta\epsilon\frac{\partial v}{\partial x}+G,\quad\frac{\partial\epsilon}{\partial t}=\frac{\partial v}{\partial x}\\&\rho\frac{\partial v}{\partial t}=\frac{\partial}{\partial x}\left(k_1\left(\theta-\theta_1\right)\epsilon-k_2\epsilon^3+k_3\epsilon^5\right)+\\&\nu\frac{\partial}{\partial t}\frac{\partial^2 u}{\partial x^2}-\delta\frac{\partial^3\epsilon}{\partial x^3}+F,\end{aligned}\qquad(4)$$

where u is displacement, θ temperature, ρ density, k_1, k_2, k_3, c_v, ν, δ and k are normalized material-specific constants, θ_1 is the reference temperature for 1D martensitic transformations, and F and G are distributed mechanical and thermal loadings, $\epsilon=\partial u/\partial x$ is the strain, and $v=\partial u/\partial t$ is the velocity. For the low dimensional reduction procedures of model (1)-(3) to models of the type (4), the interested reader can consult [9, 12].

The above model (4) for the dynamics of the first order phase transformation can also be constructed directly on the basis of the Landau free energy function which allows to characterize different stable phases at different temperatures [10, 8]:

$$W_L=\frac{k_1}{2}\left(\theta-\theta_1\right)\epsilon^2-\frac{k_2}{4}\epsilon^4+\frac{k_3}{6}\epsilon^6.\qquad(5)$$

Using W_L, from thermodynamics equilibrium conditions for the considered material, the constitutive law for the mechanical field is then obtained as:

$$\sigma=k_1\left(\theta-\theta_1\right)\epsilon-k_2\epsilon^3+k_3\epsilon^5,\qquad(6)$$

where σ is the stress.

In what follows, we consider the following boundary conditions [2]:

$$\frac{\partial\theta}{\partial x}=0,\ \frac{\partial\varepsilon}{\partial x}=0,\ v=0,\text{at }x=0,L,\qquad(7)$$

where L is the length of the material considered here in the one-dimensional case.

3 Application of the Chebyshev Collocation Method

The model (4), (7), supplemented by appropriate initial conditions, is solved numerically by approximating the solution with the linear combination

$$f^N(x,t)=\sum_{i=0}^{N}f_i(t)\phi_i(x),\qquad(8)$$

where $\phi_i(x)$ are the basis functions (trial functions), and $f_i(t)$ are expansion coefficients. $f^N(x,t)$ stands for the N^{th} order approximation to the solutions we are looking for. The governing equations can be cast in the form of evolution operator equation:

$$\frac{d\mathcal{U}}{dt}=\mathcal{M}(\mathcal{U}),\qquad(9)$$

where $\mathcal{U}$ is the solution and $\mathcal{M}(\mathcal{U})$ is an operator which contains all the spatial derivatives of $\mathcal{U}$, and

all the expansion coefficients are determined by the Galerkin method that requires the following condition to be satisfied:

$$\int_0^L \left(\frac{d\mathcal{U}^N}{dt} - \mathcal{M}(\mathcal{U}^N) \right) \psi_i(x) dx = 0, \qquad (10)$$

where $\psi_i(x)$ are test functions. This is supplemented by the Chebyshev collocation method where we choose the trial functions from the following conditions:

$$\phi_i(x_j) = \begin{cases} 1, & \text{i = j,} \\ 0, & \text{i} \neq \text{j .} \end{cases} \qquad (11)$$

and the test functions are chosen as:

$$\psi_i(x) = \delta(x_i) = \begin{cases} 1, & \text{x=}x_i, \\ 0, & x \neq x_i, \end{cases} \qquad (12)$$

where $\{x_i\}$ is a set of chosen discretization points in the computational domain with

$$x_i = L \left(1 - \cos(\frac{\pi i}{N}) \right) /2, \quad i = 0, 1, \ldots, N. \quad (13)$$

Finally, we are substituting corresponding approximations of the spatial derivatives to reduce our PDE-based model to a system of Differential Algebraic Equations (DAEs), from where (in a way similar to [10, 17]) we determine the temperature, stress, strain and displacement of the material.

4 Extended Proper Orthogonal Decomposition with Galerkin Projection

From the above described procedure, we obtain a collection of system states, so that the eigenmode series for the approximation to the system dynamics can be constructed using the extended POD method. First we obtain optimal basis functions for our dynamical system, and then its lower dimensional approximation can be obtained by projecting the full system orthogonally onto the subspace spanned by the chosen basis functions. For the current problem, the phase transformation can take place at different temperatures, by either mechanical or thermal stimulations. There may be no phase transformation if the temperature is sufficiently high. In order to model the dynamics of the ferroelastic material correctly, the empirical eigenfunctions have to take into account the temperature influence. Following [16], we choose a few (three) representative temperature values to demonstrate the analysis, in particular those for which the system has only martensite phase (low temperature θ_1), metastable austenite and martensite phases (medium temperature θ_2), or only austenite phase (high temperature θ_3), respectively. We denote the collection of snapshots with initial temperatures θ_i as $\boldsymbol{U}_i$, $i = 1, 2, 3$. If one employs the POD method directly to all the overall snapshots $\boldsymbol{U} = [\boldsymbol{U}_1, \boldsymbol{U}_2, \boldsymbol{U}_3]$ by putting all snapshots together, the characteristics of different blocks will be mixed and dispersed with each other, and that is why we are using the extended POD method to construct the eigenmodes using the snapshots collected in all the blocks. Taking all the blocks of snapshots simultaneously into account, the extended POD analysis can be formally represented in the following matrix form:

$$\boldsymbol{U} = \boldsymbol{\phi}\boldsymbol{C}, \qquad (14)$$

where

$$\boldsymbol{U} = [\boldsymbol{U}_1\, \boldsymbol{U}_2\, \boldsymbol{U}_3], \qquad \boldsymbol{\phi} = [\boldsymbol{\phi}_1\, \boldsymbol{\phi}_2\, \boldsymbol{\phi}_3] \qquad (15)$$

is a collection of snapshots and eigenmodes from each block, while the coefficient matrix is given as follows [4]:

$$\boldsymbol{C} = \begin{bmatrix} \boldsymbol{C}_1 & \boldsymbol{\phi}_1^T \boldsymbol{U}_2 & \boldsymbol{\phi}_1^T \boldsymbol{U}_3 \\ 0 & \boldsymbol{C}_2 & \boldsymbol{\phi}_2^T \boldsymbol{U}_3 \\ 0 & 0 & \boldsymbol{C}_3 \end{bmatrix}, \qquad (16)$$

where all the entries in the matrix can be obtained once the blocks of snapshots are provided. For those situations where more snapshot blocks are available, the extended POD can be carried out in a similar manner.

5 Computational Experiment: Modeling Hysteresis Effects

In what follows we analyze the performance of the developed low dimensional model by numerical experiments. First, we apply our one-dimensional PDE-based model to describe the dynamics of a shape memory alloy in order to extract the eigenmodes of the dynamics from the numerical results. Then, the phase transformations induced by either mechanical or thermal loadings can be modeled using the developed low dimensional model. The latter model can also be used to model mechanical and thermal hysteresis due to the martensitic phase transformation and some of the results are shown on the accompanying figures.

As an example, we carried out our computational experiments for a $Au_{23}Cu_{30}Zn_{47}$ rod of length $L =$ 1cm and with boundary conditions (7). All the physical parameters for this specific material are available in [11].

The numerical results, we present here as representative examples, have been obtained first by using the Chebyshev collocation methods for the PDE model (4). In the computation, there have been 15 nodes used for the Chebyshev approximation, the simulated time range is $t \in [0, 24]ms$ (two loading periods), and time step-size is set $1e^{-3}ms$. For each computation, there have been 200 snapshots of the system states collected in the block.

The first experiment is expected to be representative for the dynamics of SMA at low temperature. The snapshot block $\boldsymbol{U}_1$ is collected with the following input: $F = 1 \times 10^9$ kg/(s^{2}m^2), $G = 7 \times 10^7 \times \bar{g}(t)kg/(s^2m)$, where $\bar{g} = t/3$ for $t < 3$, $\bar{g} = (6-t)/3$ for $t < 9$, and $\bar{g} = (12-t)/3$ for $t < 12$, with the initial conditions as: $v = 0$, $\theta = 210^oK, \varepsilon = 0.01187 \times sign(x - 0.5)$. This numerical experiment involves thermally induced transformation [11], and it can be regarded as a representative case for thermally induced transformations, because the heat flux input used here is not a smooth function of time, and includes infinite number of frequency components.

The second numerical experiment with the PDE model is done with the following initial condition: $v = 0$, $\theta = 250^oK, \varepsilon = 0$. At this given temperature, there are metastable phases in the SMA rod, martensite and austenite might coexist under this temperature. The mechanical loading for this case is set: $G = 0$, $F = 7 \times 10^{10}$ for $0 < t < 3$, $F = 0$ for $3 < t < 6$ and $9 < t < 12$, $F = -7000$ for $6 < t < 9$ (all in kg/(s^{2}m^2)) which is sufficient to induce phase transformations mechanically. The snapshot block $\boldsymbol{U}_2$ is collected through this experiment.

The third block of snapshots $\boldsymbol{U}_3$ is collected using the numerical experiment with mechanical loading at high initial temperature, in which case there is no phase transformation to be induced. The initial temperature is set as: $v = 0$, $\theta = 310^oK, \varepsilon = 0$, and the mechanical loading is set the same as in the second experiment.

The developed low dimensional model has been employed to model the mechanical hysteresis when there are mechanically induced phase transformations and the numerical results (in Fig. 2) are compared to theoretical predictions (in Fig.1). Three different initial temperatures are chosen for the simulation. Because austenite is unstable when $\theta = 220^o$, so the mechanical loading will switch the material between martensite plus and minus, as indicated by the constitutive curve plotted in the top subplot of Fig. 1 (the transformation is $M+ \rightarrow M-$ or $M- \rightarrow M+$). In this case there is only one hysteresis loop which is sketched by the dashed line. The numerical simulation with this initial temperature (top subplot, Fig. 2) agrees well with this prediction. When initial temperature of the material is increased to $\theta = 240^o$, the constitutive curve is plotted in the middle subplot of Fig. 1, which encloses two separated hysteresis loops due to the metastable phases. The numerical results plotted in Fig. 2 demonstrate that the two hysteresis loops are successfully reproduced. If the initial temperature is increased further to $\theta = 320^o$, the constitutive curve (bottom, Fig. 1) indicates that there is no phase transformation because only austenite is stable. In this case, there is no hysteresis loop as confirmed by numerical results.

6 Conclusion

In the present paper, the dynamics of nonlinear thermomechanical materials has been successfully simulated using a low dimensional model constructed on the basis of the extended POD, which involves mechanically and thermally induced transformations. The dynamics has been first modelled and numerically analyzed by using a PDE model and the collections of snapshots of the system states have been constructed during the simulation. By using the extended proper orthogonal decomposition method, a set of common eigenmodes for the dynamics that covers the full temperature range has been obtained. The dynamics of material behavior has been then projected orthogonally onto the subspace spanned by a small number of eigenmodes, and a low dimensional model has been formulated. Numerical experiments have demonstrated that the dynamics of complex materials such as shape memory alloys can be successfully captured by the low dimensional model. Both thermally and mechanically induced phase transformations and related hysteresis effects have been successfully reproduced with the constructed model.

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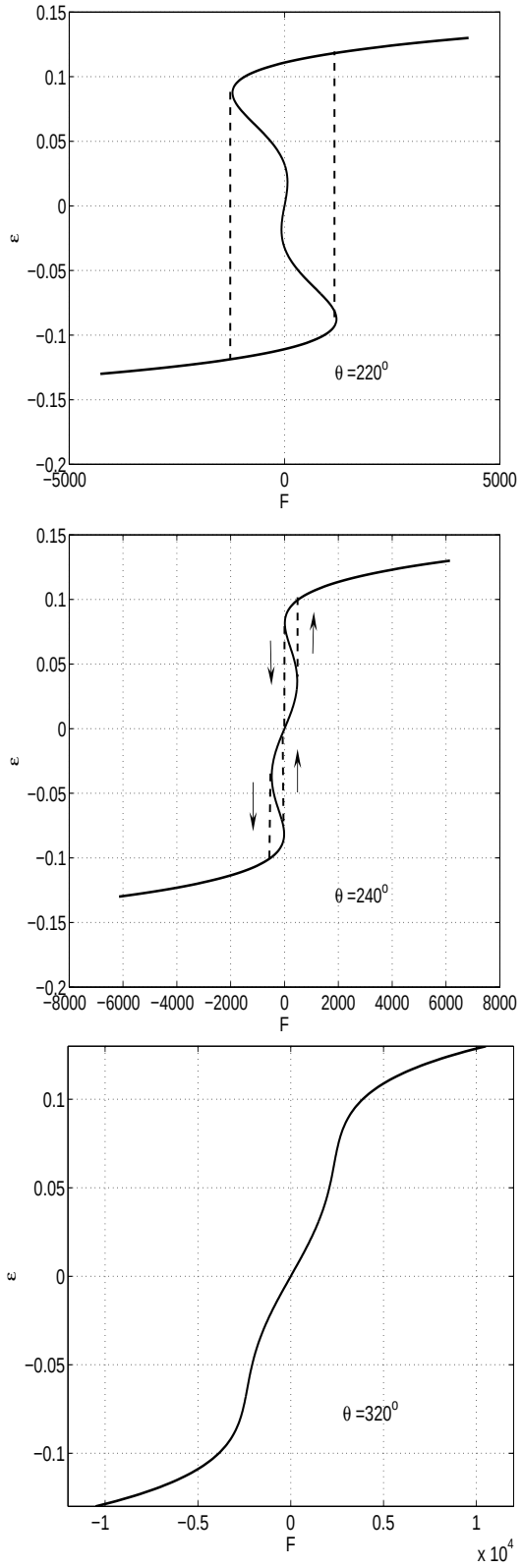

Figure 1: Hysteretic behaviour due to mechanically induced phase transformations: theoretical analysis, (top) $\theta = 220^o$, (middle) $\theta = 240^o$, (bottom) $\theta = 320^o$.

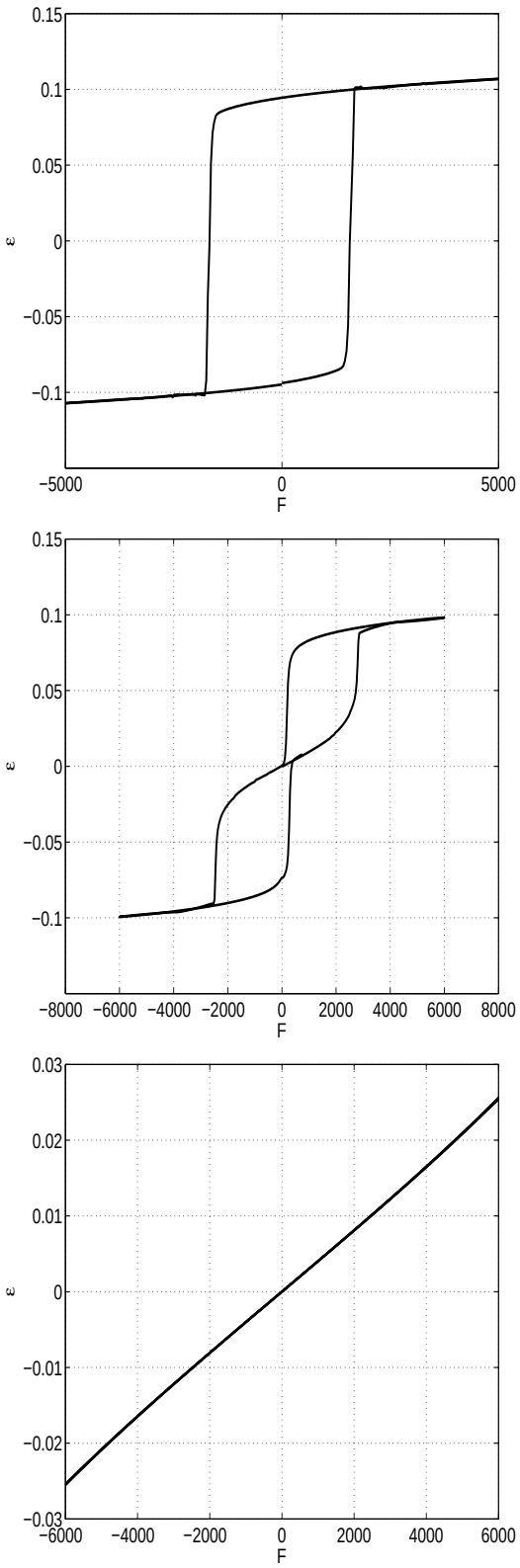

Figure 2: Hysteretic behaviour due to mechanically induced phase transformations: numerical analysis, $\theta = 220^o$ (top), $\theta = 240^o$ (middle), $\theta = 320^o$ (bottom).

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Table of Contents

Plenary Lecture 5

Low Dimensional Nonlinear Thermomechanical Models Describing Phase Transformations and their Applications

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Abstract: In this plenary talk we focus on the development of low dimensional approximations to coupled nonlinear systems of partial differential equations (PDE) describing phase transformations. The methodology is explained on the example of nonlinear ferroelastic/thermoelastic dynamics. We start from the general three-dimensional Falk-Konopka model and with the center manifold reduction obtain a Ginzburg-Landau-Devonshire one-dimensional model. The Chebyshev collocation method is applied for the numerical analysis of this latter model, followed by the application of an extended proper orthogonal decomposition. Finally, we present several numerical results where we demonstrate performance of the developed methodology in reproducing hysteresis effects occurring during phase transformations and provide a survey of related methodologies and applied mathematical problems arising in this context.
Current project is a joint work with O. Tsviliuk and L. Wang.

Brief Biography of the Speaker:
Roderick Melnik is a Full Professor at the Wilfrid Laurier University in Waterloo, Canada. He is a Tier I Canada Research Chair in Mathematical Modelling. Before moving to Canada, Professor Melnik held senior professorial and research positions in the USA, Europe, and Australia. He was also a visiting fellow at the Isaac Newton Institute of the University of Cambridge , at the Institute for Mathematics and its Applications of the University of Minnesota and other research institutions in Europe, North America, and Australia. Professor Melnik's major results are in the development, analysis and applications of mathematical models based on partial differential equations and computational mathematics, focusing on coupled dynamic phenomena, systems, and processes. The areas of his research contributions include computational physics, applied numerical analysis, chemistry, and biology, non-smooth control, and stochastic differential equations. Over the past years, some of his main contributions have been to the development and applications of mathematical models in the area nano- and bionano- sciences with particular emphasis on the analysis of coupled multiscale phenomena, processes, and systems. This includes his contributions to the analysis of coupled effects in low-dimensional nanostructures, such as quantum dots, in bio-inspired and in biological systems.