

LNCS 3039

Marian Bubak  
Geert Dick van Albada  
Peter M.A. Sloot  
Jack Dongarra (Eds.)

# Computational Science – ICCS 2004

4th International Conference  
Kraków, Poland, June 2004  
Proceedings, Part IV

4  
Part IV



Springer

*Commenced Publication in 1973*

Founding and Former Series Editors:

Gerhard Goos, Juris Hartmanis, and Jan van Leeuwen

## Editorial Board

Takeo Kanade

*Carnegie Mellon University, Pittsburgh, PA, USA*

Josef Kittler

*University of Surrey, Guildford, UK*

Jon M. Kleinberg

*Cornell University, Ithaca, NY, USA*

Friedemann Mattern

*ETH Zurich, Switzerland*

John C. Mitchell

*Stanford University, CA, USA*

Moni Naor

*Weizmann Institute of Science, Rehovot, Israel*

Oscar Nierstrasz

*University of Bern, Switzerland*

C. Pandu Rangan

*Indian Institute of Technology, Madras, India*

Bernhard Steffen

*University of Dortmund, Germany*

Madhu Sudan

*Massachusetts Institute of Technology, MA, USA*

Demetri Terzopoulos

*New York University, NY, USA*

Doug Tygar

*University of California, Berkeley, CA, USA*

Moshe Y. Vardi

*Rice University, Houston, TX, USA*

Gerhard Weikum

*Max-Planck Institute of Computer Science, Saarbruecken, Germany*

Marian Bubak Geert Dick van Albada  
Peter M.A. Sloot Jack J. Dongarra (Eds.)

# Computational Science - ICCS 2004

4th International Conference  
Kraków, Poland, June 6-9, 2004  
Proceedings, Part IV



Springer

## Volume Editors

Marian Bubak

AGH University of Science and Technology

Institute of Computer Science and Academic Computer Center CYFRONET

Mickiewicza 30, 30-059 Kraków, Poland

E-mail: bubak@uci.agh.edu.pl

Geert Dick van Albada

Peter M.A. Sloot

University of Amsterdam, Informatics Institute, Section Computational Science

Kruislaan 403, 1098 SJ Amsterdam, The Netherlands

E-mail: {dick,sloot}@science.uva.nl

Jack J. Dongarra

University of Tennessee, Computer Science Departement

Suite 413, 1122 Volunteer Blvd., Knoxville, TN-37996, USA

E-mail: dongarra@cs.utk.edu

Library of Congress Control Number: Applied for

CR Subject Classification (1998): D, F, G, H, I, J, C.2-3

ISSN 0302-9743

ISBN 3-540-22129-8 Springer-Verlag Berlin Heidelberg New York

This work is subject to copyright. All rights are reserved, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, re-use of illustrations, recitation, broadcasting, reproduction on microfilms or in any other way, and storage in data banks. Duplication of this publication or parts thereof is permitted only under the provisions of the German Copyright Law of September 9, 1965, in its current version, and permission for use must always be obtained from Springer-Verlag. Violations are liable to prosecution under the German Copyright Law.

Springer-Verlag is a part of Springer Science+Business Media

springeronline.com

© Springer-Verlag Berlin Heidelberg 2004

Printed in Germany

Typesetting: Camera-ready by author, data conversion by PTP-Berlin, Protago-TeX-Production GmbH  
Printed on acid-free paper      SPIN: 11009597      06/3142      5 4 3 2 1 0

# Thermomechanical Waves in SMA Patches under Small Mechanical Loadings

Linxiang Wang and Roderick V.N. Melnik

MCI, Faculty of Science and Engineering,  
University of Southern Denmark,  
Sonderborg, DK-6400, Denmark

**Abstract.** 2D thermo-mechanical waves in SMA (Shape Memory Alloys) patches are simulated with a model derived for a special case of material transformations. The mathematical model includes the coupling effect between thermal and mechanical fields. It is shown that the classical 1D Falk dynamical model of SMA is a special case of the formulated 2D model. The differential algebraic approach is adopted for the numerical analysis. Computational experiments are carried out with small distributed mechanical loadings to analyze thermo-mechanical waves and coupling effects. Numerical results from 2D structures are compared with its 1D analog which is already been verified.

**Keywords:** Nonlinear waves, thermo-mechanics coupling, differential-algebraic solver.

## 1 Introduction

A better understanding of the dynamics of SMA is an important task in many areas of applications. However, even for the one dimensional case, the analysis of this dynamics is quite involved due to martensitic phase transformation and a strongly nonlinear pattern of interaction between mechanical and thermal fields ([13,2] and references therein). It is not trivial either to analyze numerically the thermo-mechanical interaction even when the phase transformation is not included, because the strong nonlinearity and thermo-mechanical coupling are still there. For a number of practical applications, the understanding of the dynamics of SMA structures with dimensions higher than one is required, which makes the nonlinear thermo-mechanical waves in higher dimensions essential for the applications.

Many instructive investigations have been carried out to understand dynamics during the process of martensitic phase transition. They provided a firm background for the application development, in particular in the one-dimensional cases where the model for shape memory alloys is usually based on the Landau-Ginzburg free energy function ([12,3,5] and references therein). Although various approximations to the free energy function have been proposed in both one dimensional and three dimensional cases ([5,16] and references therein), results of two or three-dimensional cases are rarely available in the literature in the context

of modelling the thermo-mechanical waves and phase transformations in SMA. Recently, for the simulation of 2D microstructures in ferro-elastic materials, several free energy functions were proposed [6,7]. Although the authors proposed an interesting approach, no thermo-mechanical coupling was discussed and only static simulation of microstructures with a fixed temperature were presented in [6,7].

In this paper, we propose a two-dimensional dynamical model for modelling the thermo-mechanical coupling behavior. The model has been originally formulated to describe square-to-rectangular phase transformations in materials with shape memory effects. However, the phase transformations will not be discussed in this contribution. Our major emphasis here will be given to the first step in validation of the model: we will investigate the thermomechanical behavior of 2D SMA structures in the case of small mechanical loadings (not large enough to induce phase transformations). In this model, a similar free energy function as that used in [10,1,9] is employed to construct the 2D dynamical models.

## 2 The 2D Model for SMA Dynamics

Based on conservation laws for linear momentum and energy, the system describing coupled thermo-mechanical wave interactions for the first order phase transitions in a two dimensional SMA structure can be written as follows [16,14]

$$\begin{aligned} \rho \frac{\partial^2 u_i}{\partial t^2} &= \nabla_x \cdot \boldsymbol{\sigma} + f_i, \quad i, j = 1, 2, \\ \rho \frac{\partial e}{\partial t} - \boldsymbol{\sigma}^T : (\nabla \mathbf{v}) + \nabla \cdot \mathbf{q} &= g, \end{aligned} \quad (1)$$

where  $\rho$  is the density of the material,  $\mathbf{u} = \{u_i\}_{i=1,2}$  is the displacement vector,  $\mathbf{v} = \partial \mathbf{u} / \partial t$  is the velocity vector,  $\boldsymbol{\sigma} = \{\sigma_{ij}\}$  is the stress tensor,  $\mathbf{q}$  is the heat flux,  $e$  is the internal energy,  $\mathbf{f} = (f_1, f_2)^T$  and  $g$  are mechanical and thermal loadings, respectively. Let  $\phi$  be the free energy function of a thermo-mechanical system described by (1). Then, the stress and the internal energy are connected with the free energy function  $\phi$  by the following relationships:

$$\boldsymbol{\sigma} = \rho \frac{\partial \phi}{\partial \boldsymbol{\eta}}, \quad e = \phi - \theta \frac{\partial \phi}{\partial \theta}, \quad (2)$$

where  $\theta$  is the temperature, and the Cauchy-Lagrangian strain tensor  $\boldsymbol{\eta}$  is given by its components as follows (with the repeated-index convention used):

$$\eta_{ij}(\mathbf{x}, t) = \left( \frac{\partial u_i(\mathbf{x}, t)}{\partial x_j} + \frac{\partial u_j(\mathbf{x}, t)}{\partial x_i} \right) / 2, \quad (3)$$

where  $\mathbf{x}$  is the coordinates of a material point in the domain of interest.

In the two-dimensional case, the square-to-rectangular transformations could be regarded as a 2D analog of the cubic-to-tetragonal and tetragonal-to-orthorhombic transformations observed in general three-dimensional cases [6,

7]. It was established earlier for this kind of transformations that the free energy function  $\phi$  can be constructed by taking advantage of a Landau free energy function  $F_L$  [6,7]. Here, a simple free energy function is chosen for our purpose following the proposal in ([10,6,7,17,8] and references therein):

$$\phi = -c_v \theta \ln \theta + \frac{1}{2} a_1 e_1^2 + \frac{1}{2} a_3 e_3^2 + F_L, \quad F_L = \frac{1}{2} a_2 (\theta - \theta_0) e_2^2 - \frac{1}{4} a_4 e_2^4 + \frac{1}{6} a_6 e_2^6, \quad (4)$$

where  $c_v$  is the specific heat constant,  $\theta_0$  is the reference temperature for transformation,  $a_i$ ,  $i = 1, 2, 3, 4, 6$  are the material-specific coefficients, and  $e_1$ ,  $e_2$ ,  $e_3$  are dilatational, deviatoric, and shear components of strain, respectively. The later are defined as follows:

$$e_1 = (\eta_{11} + \eta_{22}) / \sqrt{2}, \quad e_2 = (\eta_{11} - \eta_{22}) / \sqrt{2}, \quad e_3 = (\eta_{12} + \eta_{21}) / 2. \quad (5)$$

By substituting the free energy function defined by Eq.(4) into the model (1)–(3), the following coupled system of equations are obtained. For the numerical analysis, the displacement are replaced by the strains in the governing equations:

$$\begin{aligned} \frac{\partial^2 u_1}{\partial t^2} &= \frac{\sqrt{2}}{2} \frac{\partial}{\partial x} (a_1 e_1 + a_2 (\theta - \theta_0) e_2 - a_4 e_2^3 + a_6 e_2^5) + \frac{1}{2} \frac{\partial}{\partial y} (a_3 e_3) + f_1, \\ \frac{\partial^2 u_2}{\partial t^2} &= \frac{1}{2} \frac{\partial}{\partial x} (a_3 e_3) + \frac{\sqrt{2}}{2} \frac{\partial}{\partial x} (a_1 e_1 - a_2 (\theta - \theta_0) e_2 + a_4 e_2^3 - a_6 e_2^5) + f_2, \\ c_v \frac{\partial \theta}{\partial t} &= k \left( \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} \right) + \frac{\sqrt{2}}{2} a_2 \theta e_2 \frac{\partial e_2}{\partial t} + g. \end{aligned} \quad (6)$$

The above mathematical model is expected be able to capture the thermo-mechanical interactions and phase transformations in the 2D SMA structures. However, as we have mentioned before, the phase transformations are excluded from our analysis here. We aim only at initial validation of the model with relatively simple model examples. For this purpose, only a small constant mechanical loading, which is not strong enough to induce phase transformations, is applied to the above model. Then, we compare our results to the results obtained with the corresponding 1D model. This 1D mathematical model is the well known Falk model [4,14]. As we pointed out in [18], this model can be obtained directly by a reduction of the above 2D model:

$$\begin{aligned} \rho \frac{\partial^2 u}{\partial t^2} &= \frac{\partial}{\partial x} \left( k_1 (\theta - \theta_1) \frac{\partial u}{\partial x} - k_2 \left( \frac{\partial u}{\partial x} \right)^3 + k_3 \left( \frac{\partial u}{\partial x} \right)^5 \right) + F, \\ c_v \frac{\partial \theta}{\partial t} &= k \frac{\partial^2 \theta}{\partial x^2} + k_1 \theta \frac{\partial u}{\partial x} \frac{\partial v}{\partial t} + G, \end{aligned} \quad (7)$$

where  $k_1$ ,  $k_2$ ,  $k_3$ ,  $c_v$  and  $k$  are re-normalized material-specific constants,  $\theta_1$  is the reference temperature for 1D martensitic transformations, and  $F$  and  $G$  are distributed mechanical and thermal loadings.

### 3 Numerical Methodology

For the convenience of numerical simulation, the 2D model is re-written in the following form in terms of the dilatational and deviatoric strains introduced above:

$$\begin{aligned}
\frac{\partial e_1}{\partial t} &= (\frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y})/\sqrt{2}, & \frac{\partial e_2}{\partial t} &= (\frac{\partial v_1}{\partial x} - \frac{\partial v_2}{\partial y})/\sqrt{2}, \\
\frac{\partial v_1}{\partial t} &= \frac{\partial \sigma_{11}}{\partial x} + \frac{\partial \sigma_{12}}{\partial y} + f_1, & \frac{\partial v_2}{\partial t} &= \frac{\partial \sigma_{12}}{\partial x} + \frac{\partial \sigma_{22}}{\partial y} + f_2, \\
c_v \frac{\partial \theta}{\partial t} &= k(\frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2}) + \frac{\sqrt{2}}{2} a_2 \theta e_2 \frac{\partial e_2}{\partial t} + g, \\
\sigma_{11} &= \frac{\sqrt{2}}{2} (a_1 e_1 + a_2 (\theta - \theta_0) e_2 - a_4 e_2^3 + a_6 e_2^5), \\
\sigma_{12} &= \sigma_{21} = \frac{1}{2} (a_3 e_3), \\
\sigma_{22} &= \frac{\sqrt{2}}{2} (a_1 e_1 - a_2 (\theta - \theta_0) e_2 + a_4 e_2^3 - a_6 e_2^5).
\end{aligned} \tag{8}$$

The above formulated model should be simulated together with the compatibility relations in terms of the strains [7]:

$$\frac{\partial^2 e_1}{\partial x_1^2} + \frac{\partial^2 e_1}{\partial x_2^2} - \sqrt{8} \frac{\partial^2 e_3}{\partial x_1 \partial x_2} - \frac{\partial^2 e_2}{\partial x_1^2} + \frac{\partial^2 e_2}{\partial x_2^2} = 0. \tag{9}$$

The 2D model given by Eq.(8) is a differential-algebraic system, it is obtained by keeping the constitutive relations as algebraic equations while the stress components are kept as independent variables to be solved for. The idea of simulating the thermo-mechanical waves by the differential-algebraic approach is stimulated by the idea of [12] where the same approach was adopted for the simulation of phase transformations in SMA. We note that to deal with a strong (cubic and quintic) nonlinearities, a smoothing procedure similar to that proposed in [15] has been employed. In particular, we have used the following expansions:

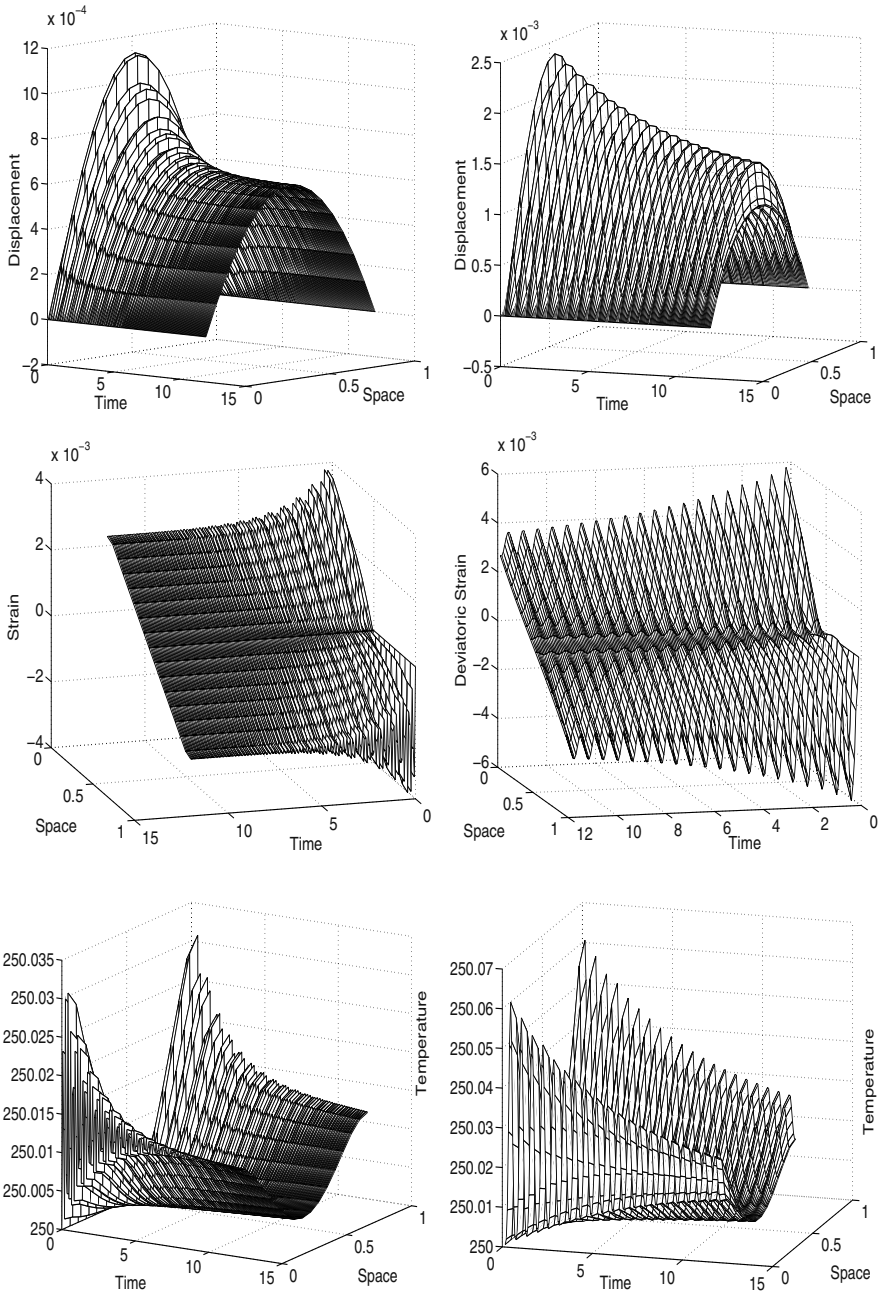
$$\epsilon^3 = \frac{1}{4} \sum_{i=0}^3 \epsilon_n^i \epsilon_{n-1}^{3-i}; \quad \epsilon^5 = \frac{1}{6} \sum_{i=0}^5 \epsilon_n^i \epsilon_{n-1}^{5-i}, \tag{10}$$

where  $\epsilon_n$  is the strain on the current time layer  $n$  while  $\epsilon_{n-1}$  is the strain on the previous time layer  $n-1$  (For 1D case,  $\epsilon = \partial u / \partial x$ , while for 2D problem,  $\epsilon = e_2$ ). We summarise this smoothing procedure as follows: Nonlinear terms are averaged here in the Steklov sense, so that for nonlinear function  $f(\epsilon)$  (in particular,  $\epsilon^3$  and  $\epsilon^5$ ), averaged in the interval  $[\epsilon_{n-1}, \epsilon_n]$ , we have

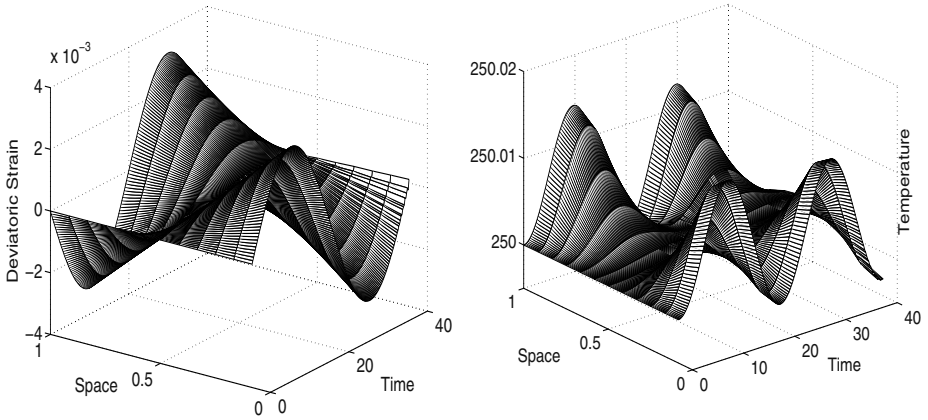
$$g(\epsilon_{n-1}, \epsilon_n) = \frac{1}{\epsilon_n - \epsilon_{n-1}} \int_{\epsilon_{n-1}}^{\epsilon_n} f(\eta) d\eta, \quad \epsilon_{n-1} = \epsilon(t_{n-1}), \quad \epsilon_n = \epsilon(t_n). \tag{11}$$

System (8) is discretized on a staggered grid. There are totally eight variables need to be solved for the two dimensional problems. The variables  $e_1$ ,  $e_2$ ,  $\theta$ ,  $\sigma_{11}$ ,  $\sigma_{12}$ ,  $\sigma_{22}$  are discretized at the same nodes, while velocity components  $v_1$  and  $v_2$  are computed at the flux points. For the time integration, the backward differentiation formula methodology is applied to obtain the numerical solution of the problem.





**Fig. 1.** Thermo-mechanical waves in SMA caused by small mechanical loadings. Left and right columns present the results obtained with the 1D and 2D models, respectively.



**Fig. 2.** Thermo-mechanical waves in SMA patch caused by varying mechanical loadings.

## 4 Numerical Results

Here, we demonstrate first the similarity of the response of 1D and 2D SMA structures under a small constant mechanical loadings, based on the numerical simulation. All simulations are carried out here on the same material, which is  $\text{Au}_{23}\text{Cu}_{30}\text{Zn}_{47}$ . For this specific material, all necessary physical parameters are taken the same as in [12].

The first simulation is performed in a long thin  $\text{Au}_{23}\text{Cu}_{30}\text{Zn}_{47}$  strip of length  $L = 1\text{cm}$  based on the 1D model given by Eq.(7). The initial conditions for this simulation are taken as:  $\theta^0 = 250^\circ\text{K}$ ,  $\epsilon^0 = v^0 = s^0 = 0$  where  $\epsilon = \partial u / \partial x$ ,  $s = k_1(\theta - \theta_1)\epsilon - k_2\epsilon^3 + k_3\epsilon^5$ ,  $v = \partial u / \partial t$ . Boundary conditions are taken as pinned-end mechanically and insulated thermally. The distributed mechanical loading is assumed constant as  $F = 100\text{g}/(\text{ms}^3\text{cm})$ , and there are no distributed thermal loadings. There are 17 nodes used for  $\epsilon$ ,  $s$  and  $\theta$  in the computational domain and 16 nodes are used for  $v$  approximated at flux points. Time span of the simulation is  $[0, 12]$  and time stepsize is set to 0.00025. Displacement, strain, and temperature distributions in the SMA strip are presented in Fig.1, from top to bottom on the left side. The MATLAB program for this case is already validated in [18,12], where the phase transformations are also investigated using the same model and algorithm.

The second simulation is performed in a  $\text{Au}_{23}\text{Cu}_{30}\text{Zn}_{47}$  patch with an area of  $1 \times 0.4\text{cm}^2$ . For this simulation, the coefficients in the 2D model are taken as follows:  $a_2 = k_1$ ,  $a_3 = k_2$ ,  $a_4 = k_3$ ,  $a_1 = k_1$ ,  $a_3 = 2k_1$ , and all other coefficients are taken the same value as those in the 1D case. The initial temperature is also

250° while all other variables are initially zero. Boundary conditions are taken as follows:

$$\begin{aligned} \frac{\partial \theta}{\partial x} = 0, \quad \frac{\partial u_2}{\partial x} = 0, \quad u_1 = 0, \quad \text{on left and right boundaries,} \\ \frac{\partial \theta}{\partial y} = 0, \quad \frac{\partial u_1}{\partial y} = 0, \quad u_2 = 0, \quad \text{on top and bottom boundaries.} \end{aligned} \quad (12)$$

Because the displacement components are already replaced by the strains in Eq.(8), the above boundary conditions are enforced in terms of velocities when the mechanical boundary conditions are concerned.

There are 17 nodes used in the x-direction and 7 in the y-direction in the computational domain. As before,  $v_1$  and  $v_2$  are computed at the flux points. The same time span and stepsize are used as those in the 1D case. The distributed mechanical loading is enforced only in the x-direction as:  $f_1 = 100\text{g}/(\text{ms}^3\text{cm})$ . Displacement, and strain, and temperature distributions on the line  $y = 0.2\text{cm}$  (the central horizontal line) in the SMA patch are presented in Fig.1, from top to bottom on the right side. It is shown clearly from the comparison of strain and temperature evolutions that, when the oscillations in the other direction can be neglected, the 2D SMA structure respond to the mechanical loadings in the same way as its 1D analog. It is also seen from the computation that the oscillations in 1D case are dissipated much faster than those in the 2D case. This implies that there might be a numerical instability problem in 2D simulations when the phase transformations take place due to the slow dissipation of oscillations. This comparison can be used as an initial validation of the 2D model.

The third numerical experiment is to investigate the dynamical thermo-mechanical response of the SMA patch under varying distributed mechanical loadings, but still small enough not to induce phase transformations. The SMA patch is now covers an area of  $1 \times 1\text{cm}^2$ , and there are 12 nodes in each direction. The loadings employed for this simulation are:  $f_1 = 200 \sin(20\pi t/40)\text{g}/(\text{ms}^3\text{cm})$  in the x-direction, and  $f_2 = f_1$  in the y-direction. The time span for this simulation is  $[0, 40]$  (one period of loading) and the time stepsize is set at  $4 \times 10^{-5}$ . All other simulation conditions and parameters are the same as those in the second case. The deviatoric strain and temperature distributions are presented in Fig.2. The simulation shows clearly that both temperature and strain field are driven periodically by the distributed mechanical loading because of the thermo-mechanical coupling. Under such a small loading, the SMA patch behaves just like a classical thermoelastic material.

Based on these three numerical experiments, we conclude that the formulated 2D model is able to capture the thermo-mechanical coupling in SMA. It gives the same prediction about the dynamical behavior of the SMA structure as that of the 1D model, when oscillations in one of the directions are negligible.

## References

1. Ball, R., James, M.: Fine phase mixtures as minimizers of energy. *Archive. Rat. Mech. Anal.* **100** (1988) 13-52.

2. Birman, V.: Review of mechanics of shape memory alloys structures, *Appl.Mech.Rev.* **50** (1997) 629-645.
3. Bunber, N.: Landau-Ginzburg model for a deformation-driven experiment on shape memory alloys. *Continuum Mech. Thermodyn.* **8** (1996) 293-308.
4. Falk, F.: Model free energy, mechanics, and thermomechanics of shape memory alloys. *Acta Metallurgica*, **28**, (1980) 1773-1780.
5. Falk, F., Konopka, p.: Three-dimensional Landau theory describing the martensitic phase transformation of shape memory alloys. *J.Phys.:Condens.Matter* **2** (1990) 61-77.
6. Ichitsubo, T., Tanaka, K., Koiva, M., Yamazaki, Y.: Kinetics of cubic to tetragonal transformation under external field by the time-dependent Ginzburg-Landau approach. *Phys. Rev. B* **62** (9) (2000) 5435-5441.
7. Jacobs, A.: Landau theory of structures in tetragonal-orthorhombic ferro-elastics. *Phys. Rev. B* **61** (10) (2000) 6587-6595.
8. Kartha, S.: Disorder-driven pretransitional tweed pattern in martensitic transformations. *Phys. Rev. B* **52** (2) (1995) 803-823.
9. Luskin, M.: On the computational of crystalline microstructure. *Acta Numerica* **5** (1996) 191-256.
10. Lookman, T., Shenoy, S., Rasmusseh, D., Saxena, A., Bishop, A.: Ferro-elastic dynamics and strain compatibility. *Phys. Rev. B* **67**(2003) 024114.
11. Matus, P., Melnik, R., Wang, L., Rybak, I.: Application of fully conservative schemes in nonlinear thermoelasticity: Modelling shape memory materials. *Mathematics and Computers in Simulation* (to appear)
12. Melnik, R., Roberts, A., Thomas, K.: Phase transitions in shape memory alloys with hyperbolic heat conduction and differential algebraic models. *Computational Mechanics* **29** (1) (2002) 16-26.
13. Melnik, R., Roberts, A., Thomas, K.: Coupled thermomechanical dynamics of phase transitions in shape memory alloys and related hysteresis phenomena. *Mechanics Research Communications* **28** 6 (2001) 637-651.
14. Melnik, R., Robert, A., Thomas, K.: Computing dynamics of Copper-based SMA via center manifold reduction models. *Computational Material Science* **18**(2000) 255-268.
15. Niezgodka, M., Sprekels, J.: Convergent numerical approximations of the thermomechanical phase transitions in shape memory alloys. *Numerische Mathematik* **58**(1991) 759-778.
16. Pawlow, I.: Three dimensional model of thermomechanical evolution of shape memory materials. *Control and Cybernetics* **29** (2000) 341-365.
17. Saxena, A., Bishop, A., Shenoy, S., Lookman, T.: Computer simulation of martensitic textures. *Computational Materials Science* **10** (1998) 16-21.
18. Wang, L., Melnik, R.: Nonlinear coupled thermomechanical waves modelling shear type phase transformation in shape memory alloys. in *Mathematical and Numerical Aspects of Wave Propagation*, Eds.G.C.Cohen, et al, Springer, 723-728 (2003).

---

## Workshop on Parallel Monte Carlo Algorithms for Diverse Applications in a Distributed Setting

---

Using P-GRADE for Monte Carlo Computations in a Distributed Environment.....	475
<i>V.N. Alexandrov, A. Thandavan, P. Kacsuk</i>	
Calculating Activation Energies in Diffusion Processes Using a Monte Carlo Approach in a Grid Environment.....	483
<i>M. Calleja, M.T. Dove</i>	
Using Parallel Monte Carlo Methods in Large-Scale Air Pollution Modelling .....	491
<i>V.N. Alexandrov, Z. Zlatev</i>	
Parallel Importance Separation for Multiple Integrals and Integral Equations .....	499
<i>S. Ivanovska, A. Karaivanova</i>	
Investigation of the Sensitivity of the Monte Carlo Solution for the Barker-Ferry Equation with Sequential and Parallel Pseudo-Random Number Generators .....	507
<i>T.V. Gurov, P.A. Whitlock</i>	
Design and Distributed Computer Simulation of Thin $p^+-i-n^+$ Avalanche Photodiodes Using Monte Carlo Model.....	515
<i>M. Yakutovich</i>	
Convergence Proof for a Monte Carlo Method for Combinatorial Optimization Problems .....	523
<i>S. Fidanova</i>	
Monte Carlo Algorithm for Maneuvering Target Tracking and Classification .....	531
<i>D. Angelova, L. Mihaylova, T. Semerdjiev</i>	

---

## Workshop on Modelling and Simulation of Multi-physics Multi-scale Systems

---

Coupling a Lattice Boltzmann and a Finite Difference Scheme .....	540
<i>P. Albuquerque, D. Alemani, B. Chopard, P. Leone</i>	
Accuracy versus Performance in Lattice Boltzmann BGK Simulations of Systolic Flows .....	548
<i>A.M. Artoli, L. Abrahamyan, A.G. Hoekstra</i>	

Mesoscopic Modelling of Droplets on Topologically Patterned Substrates .....	556
<i>A. Dupuis, J.M. Yeomans</i>	
Soot Particle Deposition within Porous Structures Using a Method of Moments – Lattice Boltzmann Approach .....	564
<i>B.F.W. Gschaider, C.C. Honeger, C.E.P. Redl</i>	
Numerical Bifurcation Analysis of Lattice Boltzmann Models: A Reaction-Diffusion Example .....	572
<i>P. Van Leemput, K. Lust</i>	
Particle Models of Discharge Plasmas in Molecular Gases .....	580
<i>S. Longo, M. Capitelli, P. Diomede</i>	
Fully Kinetic Particle-in-Cell Simulation of a Hall Thruster .....	588
<i>F. Taccogna, S. Longo, M. Capitelli, R. Schneider</i>	
Standard of Molecular Dynamics Modeling and Simulation of Relaxation in Dense Media .....	596
<i>A.Y. Kuksin, I.V. Morozov, G.E. Norman, V.V. Stegailov</i>	
Implicit and Explicit Higher Order Time Integration Schemes for Fluid-Structure Interaction Computations .....	604
<i>A. van Zuijlen, H. Bijl</i>	
Accounting for Nonlinear Aspects in Multiphysics Problems: Application to Poroelectricity .....	612
<i>D. Néron, P. Ladevèze, D. Dureisseix, B.A. Schrefler</i>	
Computational Modelling of Multi-field Ionic Continuum Systems .....	621
<i>J. Michopoulos</i>	
Formation of Dwarf Galaxies in Reionized Universe with Heterogeneous Multi-computer System .....	629
<i>T. Boku, H. Susa, K. Onuma, M. Umemura, M. Sato, D. Takahashi</i>	
A Multi-scale Numerical Study of the Flow, Heat, and Mass Transfer in Protective Clothing .....	637
<i>M.P. Sobera, C.R. Kleijn, P. Brasser, H.E.A. Van den Akker</i>	
Thermomechanical Waves in SMA Patches under Small Mechanical Loadings .....	645
<i>L. Wang, R.V.N. Melnik</i>	
Direct and Homogeneous Numerical Approaches to Multiphase Flows and Applications .....	653
<i>R. Samulyak, T. Lu, Y. Prykarpatsky</i>	