

# SERBIAN SOCIETY FOR COMPUTATIONAL MECHANICS

# **SEECCM 2017**

Fourth South-East European Conference on Computational Mechanics 3-4<sup>th</sup> July 2017 Kragujevac

# **BOOK OF PROCEEDINGS**

Editors Miloš Kojić, Manolis Papadrakakis and Nenad Filipović

Kragujevac, 2018

ISBN: 978-86-921243-0-3

## PREFACE

The success of many national and international conferences in the field of computational mechanics resulted in an initiative of National Associations of Computational Mechanics of the South-East European countries to organize South-East European Conference on Computational Mechanics (SEECCM).

The first one was held in Kragujevac, Serbia in 2006; the second one at the island of Rhodes, Greece in 2009 and the third one at the island of Kos, Greece in 2013. Previous three SEECCM conferences were extremelly successful and had a profound impact on the goals of the regional and world community of scientists to invent and apply computational methods in accordance with the continuously increasing demands in science, technology and medicine.

This year, following the path of tradition, the conference again took place in Kragujevac, Serbia on July 3<sup>rd</sup>-4<sup>th</sup>. The conference was organized by the *Serbian Society for Computational Mechanics, Bioengineering Research and Development Centar BioIRC* and *Faculty of Engineering, University of Kragujevac in Serbia*. Over 166 authors participated in the SEECCM 2017 Conference with more than 60 papers. The scientific field of papers mainly included the areas of computational mechanics, computational chemistry and applied biomedical engineering sciences.

The papers which fulfilled the reviewers' criteria were selected as the most significant ones and are included into this *Book of Proceedings* thematically divided into seven areas:

- 1. Mechanics
- 2. Biomechanics
- 3. Numerical Methods
- 4. Finite element modeling
- 5. Data mining
- 6. Computational Chemistry
- 7. Computational Biology

We firmly believe that the papers selected for the Proceedings reflect current trends and innovations in the field of computational mechanics and represent an outstanding base for all parties interested in this domain.

We would like to use this opportunity to thank one more time all the authors and keynote speakers who contributed to the quality of SEECCM2017 conference and the *Book of Proceedings* with hope that the tradition that we have built together will continue.

We would also like to express our deep appreciation to institutions who provided support – European Community on Computational Methods in Applied Sciences (ECCOMAS), Serbian Academy of Sciences and Arts and the Ministry of Education, Science and Technological Development of the Republic of Serbia.

# **ORGANISING BOARD**

## **Conference Chairs**

Miloš Kojić Manolis Papadrakakis Nenad Filipović

### **Organising Committee**

Dalibor Nikolić Đorđe Dimitrijević Milica Kaplarević Neda Vidanović

## **Scientific Committee**

Bathe Klaus-Jurgen USA, Beskos Dimitri, Greece Calo Victor, S Arabia Car Zlatan, Croatia Exarchos Themis. Greece Ferrari Mauro, USA Filipovic Nenad, Serbia Fotiadis Dimitrios, Greece Garbey Marc, USA Hajdin Nikola, Serbia Ibrahimbegovic Adnan, France Jeremic Boris, USA Jr Hughes Thomas, USA Kojic Nikola, USA Mang Herbert, Austria Matthies Hermann, Germany Mijailovic Srboljub, USA Mikic Borivoje, USA Nestorovic Tamara, Germany Onate Eugenio, Spain Ostrogorsky Aleksandar, USA Papadopulos Panos, USA Papadopulos Vissarion, Greece Papadrakakis Manolis, Greece Rosic Bojana, Germany Schrefler Bernhard, Italy Soric Jurica, Croatia

Stamenovic Dimitrije, USA Tsuda Akira, USA Ziemys Arturas, USA

# TABLE OF CONTENTS

Bursting Oscillations on Multiple Time Scales: Quantitative Techniques for Two Types of Systems with Cubic Nonlinearity8
Theory of Ambient Vibration Energy Harvester with Piezoelement18
Lifetime Prediction of Cardiovascular Stent Based on Fatigue to Fracture Approach
Analysis of Loads and Deformation of Valve Plate in Contact with Cylinder Block at Axial Piston Pump for Water Hydraulics
Interactive Software for Tracking Motion of Otoconia Particles in the Semicircular Canals of the Inner Ear42
Simulation of Aerosol Particle Flow Through Dry Powder Inhaler Aerolizer®
Finite Element Analysis of Femur During Gait Cycle61
Finite Element Analysis of Patient-Specific Bicuspid Aortic Valve67
Modelling Semicircular Canals Using DPD Method73
Virtual Surgery and Numerical Analysis of Dissected Aorta81
Optimal Selection of Morphometric Parameters for the Creation of Parametric Model of the Human Mandible Coronoid Process87
Biomechanical Analysis of Jumping Using Force Plate Measurements and Numerical Simulation94
Accuracy of Smeared Finite Element Model Improved by a Field of Correction Factors101
Convection–Diffusion Transport Model Using Composite Smeared Finite Element
Universal Service for Solving Systems of Linear Equations118
Parameter Estimation Using HPC on the Cloud Based Optimization Service
Multi-Scale Computational Homogenization of Graphene Polymer Nanocomposites
Aerodynamic Heating of Ballistic Missile Fin Configuration During Supersonic Flight Conditions151

Thermo-Mechanical Numerical Analysis of Transformation-Induced Stress Relaxation During Pseudoelastic Behavior of SMA
Solving Contact Problems Using One-Dimensional Finite Elements as Elastic Supports and Application in Angioplasty and Stent Deployment Modeling
Software Solution of Cupula's Membrane Deformation Shew for Use in Clinical Practice
Lifetime Prediction of the Car-Carrying Wagon's Axle Guard181
Finite Element Modelling of Rotary Transfer Machines
Investigating Low Velocity Impact on Biocomposites by MAT_54 Shell Modeling
Finite Element Modelling in Palletized Products Under Transportation 209
Elastic Post-Buckling Analysis of Rectangular Imperfect Plates Using the Semi-Analytical Finite Strip Method 220
Comparing Design Solutions by Harmonic Analysis in the Case of a Surface Finishing Machine
Finite Element Simulation of Turbulent Flow Using <i>k-w</i> Model and Rans Equations
Finite Element Modeling of Benign Paroxysmal Positional Vertigo Disease 
Geometry Optimization of Nitinol Stent Design and Effects on Mechanical Performance: Finite Element Analysis
Computational Fluid Dynamics (CFD) Modeling of the Fluid Flow Through Porous Structures
Automatic Main Pulmonary Artery Identification on Chest CT using Supervised Machine Learning
Framework for Creation of Customized Shape of the Shoe Insole
Analysis of Layer Recurrent Network to Estimate Nondimensional Velocity of the Dissociated Gas
Prediction of Second Primary Tumors in Patients with Oral Squamous Cell Carcinoma
Theoretical Investigation of Antioxidative Activity of Caffeic Acid 308
QSAR Analysis of Antioxidant Properties of Polyphenols by OH-related Molecular Descriptors

Antioxidant Activity of the Carboxylate Anions of the Selected Dihydroxybenzoic Acids
Thermodynamics of 2H <sup>+</sup> /2e <sup>-</sup> Free Radical Scavenging Mechanisms of 3-(4- Hydroxy-3-methoxyphenyl)propanoic Acid
Stability of Stoichiometric Networks with Conservation Constraints: the Case of Catalytic Carbonylation Model
Estimation of Antioxidative Capacity of Anthrarufin
Comparative Study of Antioxidant Activities of Catechol, Protocatechuic Acid and 3,4-Dyhydroxypiridine364
Computational Molecular Docking Studies of the Novel Coumarine Derivative towards Ubiquinol-Cytochrome C Reductase Binding Protein and Methylenetetrahydrofolate Reductase
Thermodynamic and Kinetic Aspects of the Electron-Transfer Reaction of Dopamine and its Metabolites towards Substituted Methylperoxy Radicals
378 Computational Molecular Docking Studies of Kaempferol-Procalcitonin Interaction
378         Computational Molecular Docking Studies of Kaempferol-Procalcitonin         Interaction       387         Protolytic and Tautomerization Reactions of Anthraquinone Dyes       393         Study of the Structure, Prooxidative, and Cytotoxic Activity of Some       402         Chelate Copper (II) Complexes       402         The Influence of Water Molecule Coordination to a Metal Ion on Water-       413         Computer Driven Bioavailability Analysis of Some Important Compounds       422
378         Computational Molecular Docking Studies of Kaempferol-Procalcitonin         Interaction       387         Protolytic and Tautomerization Reactions of Anthraquinone Dyes       393         Study of the Structure, Prooxidative, and Cytotoxic Activity of Some       402         Chelate Copper (II) Complexes       402         The Influence of Water Molecule Coordination to a Metal Ion on Water-       413         Computer Driven Bioavailability Analysis of Some Important Compounds       422         Mean-Field Approximation of Two Coupled Populations of Excitable Units       430

## Thermo-Mechanical Numerical Analysis of Transformation-Induced Stress Relaxation During Pseudoelastic Behavior of SMA

#### Vladimir Dunić<sup>1\*</sup>, Radovan Slavković<sup>1</sup>, Elżbieta Pieczyska<sup>2</sup>

<sup>1</sup>University of Kragujevac, Faculty of Engineering, 6 Sestre Janjić Street, Kragujevac, Serbia e-mail: dunic@kg.ac.rs, radovan@kg.ac.rs <sup>2</sup>Institute of Fundamental Technological Research, Polish Academy of Sciences, 5b Pawinskiego Street, Warsaw, Poland e-mail: epiecz@ippt.pan.pl

\*corresponding author

#### Abstract

A stress relaxation phenomenon is observed by coupled thermo-mechanical numerical analysis of SMA subjected to uniaxial test. The thermo-mechanical coupling is realized in the partitioned approach. The software components for the structural analysis (PAKS) and the heat transfer (PAKT) based on the Finite Element Method (FEM) have been used. The latent heat production is correlated with the amount of the martensitic volume fraction. The thermo-mechanical numerical analysis of a belt type specimen has been investigated for the strain controlled loading with the break during the martensitic transformation. The thermally induced martensitic transformation induced the significant stress change during the loading break what was expected according to the experimental results from literature.

**Keywords:** Shape memory alloys, stress relaxation, thermo-mechanical coupling, phase transformation, partitioned coupling

#### 1. Introduction

The thermo-mechanical coupling of Shape Memory Alloys (SMA) constitutive model has been investigated in previously published papers (Dunić et al. 2014, Dunić et al. 2016). The previous numerical tests verified that the influence of the temperature change during the martensitic phase transformation is significant on the stress magnitude (Dunić et al. 2014). Also, it was noticed that for the low strain rates, the temperature change is induced by the martensitic transformation but also by the convection and the thermoelastic effect. The idea of this paper is to describe numerically what happens if the loading process has a loading break in the middle of martensitic transformation for the pseudoelastic effect. The expected behavior based on experimental investigation is the monotonic stress and temperature drop (Pieczyska et al. 2006).

The paper will be organized as follows. In Section 2, the fundamental details about the SMA constitutive model implemented into the structure analysis program PAKS are given. In Section 3, the information about the heat transfer and the structure analysis FEM programs are given with

details about the partitioned coupling algorithm. In Section 4, the thermo-mechanical numerical analysis of the SMA belt type specimen is conducted to show stress relaxation phenomenon. At the end, in Section 5, conclusions about the achieved results are presented.

#### 2. A brief review of SMA constitutive model

The phenomenological constitutive model for SMA is derived from Gibbs free energy  $g(\sigma, T, \xi, \mathbf{e}_{tr})$  which depends on the stress  $\sigma$ , the temperature T and the internal state variables  $\xi$ ,  $\mathbf{e}_{tr}$  (Lagoudas 2010). The main relation which simplifies the model is the assumption that: "any change in the current microstructural state of the material is strictly a result of a change in the martensitic volume fraction" (Lagoudas 2010, Boyd, J., Lagoudas, D. 1996, Qidwai, M., Lagoudas, D. 2000):

$$\dot{\mathbf{e}}_{tr} = H\mathbf{n}_{tr}\dot{\boldsymbol{\xi}} \tag{1}$$

where H is the maximal transformation strain and  $\xi$  is the martensitic volume fraction. The direction of the strain tensor  $\mathbf{n}_{tr}$  depends on the transformation direction (forward or reverse):

$$\mathbf{n}_{tr} = \begin{cases} \frac{3\mathbf{S}}{2\overline{S}}; & \dot{\xi} > 0\\ \frac{\mathbf{e}_{tr}}{\overline{e}_{tr}} & \dot{\xi} < 0 \end{cases}$$
(2)

Using the second law of thermodynamics it was shown by Lagoudas, (2010) that:

$$\Pi \dot{\xi} \ge 0, \tag{3}$$

what leads to the transformation function in the following form (Lagoudas, 2010):

$$\Phi = \begin{cases} \Pi - Y; & \dot{\xi} > 0 \\ -\Pi - Y; & \dot{\xi} < 0 \end{cases}$$
(3)

where  $\Pi(\sigma, T, \xi)$  is the thermodynamic force and Y is the value which depends on transformation hardening functions (Lagoudas 2010). In the further evolution of the transformation function, the assumption of constant integration direction (deviatoric stress or transformation strain) of the stress integration procedure is used together with the separation of the total stress on deviatoric and mean part. This gives the possibility to solve only one equation on the integration point level (Kojić, Bathe 2005).

#### 3. Thermo-mechanical coupling

#### 3.1 Heat transfer program - PAK-T

The heat transfer program PAK-T (Kojić et al. 1999) computes heat transfer through the solids with the boundary conditions: convection on the part of the surface, prescribed surface flux, prescribed temperature, radiation, etc. From the Fourier's Law of heat conduction (Kojić 1998):

$$\mathbf{q} = -\mathbf{k}\nabla T \tag{4}$$

the energy balance equation is derived as (Lagoudas 2010, Dunić et al. 2016):

$$-\rho c \frac{\partial T}{\partial t} + \nabla^{T} \left( \mathbf{k} \nabla T \right) + q + \left( q_{dis} - T_{0} \alpha c_{m} \dot{e}_{m} \right) = 0$$
(5)

where q is the local heat source, **k** is the material's conductivity,  $\mathbf{T} = \nabla T$  is the temperature gradient and  $q_{dis}$  is the elementary dissipative energy. The term  $-T_0 \alpha c_m \dot{e}_m$  describes the Gough-Joule effect (Schweizer, Wauer 2001). The elementary dissipative energy  $q_{dis}$  of the martensitic transformation is given as (Lagoudas 2010, Dunić et al. 2016):

$$q_{dis} = \eta (\Pi - \rho \Delta s_0 T) \dot{\xi} \tag{6}$$

where  $\eta$  is the dissipative factor,  $\Pi$  is the thermodynamic force of the martensitic transformation,  $\xi$  denotes the martensite volume fraction rate, the product  $\rho \Delta s_0$  is the stress influence coefficient and  $\Delta s_0$  is the difference of effective entropy at zero stress for the martensitic and the austentic phase (Lagoudas, 2010).

#### 3.2 Structure analysis program - PAK-S

The structure analysis program PAKS (Kojić et al. 1999) solves linear and nonlinear structural problems. For the elastic and thermoelastic material, the stress can be determined by the constitutive relation:

$$\boldsymbol{\sigma} = \mathbf{C}_{el} \left( \mathbf{e} - \boldsymbol{e}_{th} \mathbf{I} \right) \tag{7}$$

where  $C_{el}$  is the elastic constitutive matrix and  $e_{th}$  is the thermal strain. The equilibrium equations can be derived in the following form (Matthies et al. 2006, Matthies, Steindorf 2002):

$$-\mathbf{div}(\tau) = \mathbf{r}_{s}, \qquad \tau = 2G\mathbf{h} + c_{m}(tr\mathbf{h})\mathbf{I}, \qquad \mathbf{h} = \mathbf{lnv}, \qquad \mathbf{b} = \mathbf{F}\mathbf{F}^{T} = \mathbf{v}^{2}$$
(8)

in which "tr" indicates the trace function,  $\tau$  is the Kirchhoff stress, **h** is the logarithmic strain, **F** is the gradient of deformation, **v** is the left stretch tensor, **b** is the left Cauchy-Green deformation tensor and **r**<sub>i</sub> is the body load. More details and possible formulations are given in (Bathe, 2006).

#### 3.3 The partitioned coupling approach for thermo-mechanical coupling

The thermo-mechanical coupling has very strong influence on SMA behavior (Pieczyska et al. 2013, Pieczyska et al. 2014, Dunić et al. 2014). There are two important advantages of partitioned coupling approach: easier implementation and reusing of existing software solutions (Matthies et al. 2006, Matthies, Steindorf 2002). This coupling approach can provide strong coupling, if the nonlinear Block-Gauss-Seidel numerical algorithm is used (Matthies et al. 2006). For the coupling realization (Dunić et al. 2016), the FEM programs for structural (PAKS) and the heat transfer analysis (PAKT) are connected using the CTL – Component Template Library developed by Niekamp (2005). The CTL is used as middleware interface necessary for communication between the components.

#### 4. Thermomechanical modeling of stress relaxation in the SMA

A belt type specimen (160 mm  $\times$  10 mm  $\times$  0.38 mm) is modeled by the FEM 3D elements (Dunić et al. 2014) (Pieczyska et al. 2014). The FEM mesh consists of 400 elements (80 $\times$ 5x1) with 972 nodes (Fig. 1). The specimen ends in the FEM model has a constant temperature because in the experimental setup presented in (Piecyzska et al. 2013, Dunić et al. 2014), the grips of the testing machine are very large in comparison to the specimen thickness. The rest of the model specimen has a possibility of free convection. The finite element mesh is the same for both PAKS and PAKT. The boundary and loading conditions are shown in Fig. 1.



Fig. 1. Finite element mesh with loading and boundary conditions (Dunić et al. 2014)

Material parameter	Value	Material parameter	Value
$E_A$ [GPa]	59.2	ν[-]	0.41
E <sub>M</sub> [GPa]	45	h[W m <sup>-2</sup> K <sup>-1</sup> ]	6.5
$lpha_{A.M}[\mathrm{K}^{-1}]$	$1.1 \times 10^{-5}$	$c_p c_p [J \text{ kg}^{-1} \text{ K}^{-1}]$	460
Η [-]	0.06	$\lambda_c  [\mathrm{W}  \mathrm{m}^{-1} \mathrm{K}^{-1}]$	18
$ ho\Delta s_0^{(A,M)}$ $ ho\Delta s_0^{(A,M)}$ [MPa K <sup>-1</sup> ]	-0.378	ρ[g cm <sup>-3</sup> ]	6.29
<i>M</i> <sub>0s</sub> [K]	213	$M_{0f}[K]$	209
<i>A</i> <sub>0s</sub> [K]	270	<i>A</i> <sub>0<i>f</i></sub> [K]	276

**Table 1.** Material parameters of the SMA (Dunić et al. 2014)

#### 5. Results and conclusions

The numerical stress relaxation test with a relaxation break in the branch of loading was introduced according to the experimental tests given in Pieczyska et al. (2006) in a following way - loading until a given strain value 0.36 and advanced martensitic transformation is obtained,

maintaining the strain value at the same level for 3 minutes, reloading and next unloading until the stress achieves zero.

The stress and the average temperature change vs. strain curves of the TiNi SMA, subjected to the loading-unloading tension tests at strain rate of  $10^{-2}$  s<sup>-1</sup> is presented in Fig. 2. As is seen, the proposed approach predicts decrease in stress if strain is kept constant during loading. Changes in the stress and in the average specimen temperature vs. time for the aforementioned relaxation tests, are presented in Fig 3. A monotonic stress drop 100 MPa is observed while the temperature of the specimen also drops monotonically towards its initial temperature.



Fig. 2. Stress and average temperature change as a function of strain for TiNi SMA tension test with 3min stress relaxation brake in the branch of loading



Fig. 3. Stress and average temperature changes vs. time for TiNi SMA tension test with 3min stress relaxation brake in the branch of loading

**Acknowledgements** The work presented in this paper is supported by the Ministry of Education, Science and Technological development, Republic of Serbia, Projects TR32036 and III41007.

#### References

Bathe KJ (2006). Finite Element Procedures. Cambridge, MA: K.-J. Bathe

- Boyd J, Lagoudas D (1996). A thermodynamical constitutive model for shape memory materials. part I. The monolithic shape memory alloy, *International Journal of Plasticity*, 12, 6, 805-842.
- Dunić V, Busarac N, Slavković V, Rosić B, Niekamp R, Matthies H, Slavković R, Živković M (2016). A thermo-mechanically coupled finite strain model considering inelastic heat generation, *Continuum Mechanics and Thermodynamics*, 28, 993-1007.
- Dunić V, Pieczyska E, Tobushi H, Staszczak M, Slavković R (2014). Experimental and numerical thermo-mechanical analysis of shape memory alloy subjected to tension with various stress and strain rates, *Smart Materials and Structures*, 23, 5, 055026.
- Kojić M, Bathe KJ (2005). *Inelastic Analysis of Solids and Structures*. Computational Fluid and Solid Mechanics, Berlin: Springer-Verlag Berlin and Heidelberg GmbH KG
- Kojić M, Slavković R, Živković M, Grujović N (1998). *Metod konačnih elemenata Linearna analiza, Kragujevac*: Mašinski fakultet Kragujevac, Univerzitet u Kragujevcu, Serbian.
- Kojić M, Slavković R, Živković M, Grujović N (1999). PAK-S: Program for FE Structural Analysis. Faculty of Mechanical Engineering, University of Kragujevac, Kragujevac
- Kojić M, Slavković R, Živković M, Grujović N (1999). PAK-T: Program for Heat Transfer Analysis. Faculty of Mechanical Engineering, University of Kragujevac, Kragujevac
- Lagoudas D (2010). Shape Memory Alloys: Modeling and Engineering Applications, Springer
- Matthies H, Niekamp R, Steindorf J (2006). Algorithms for strong coupling procedures, *Computer Methods in Applied Mechanics and Engineering*, 195, 17-18, 2028-2049.
- Matthies H, Steindorf J (2002). *Partitioned strong coupling algorithms for fluid structureinteraction*, Informatikbericht, Institute of Scientific Computing, Technische Universit at Braunschweig.
- Niekamp R (2005). *CTL Manual for Linux/Unix for the Usage with C++*. Institut fur Wissenschaftliches Rechnen TU Braunschweig, Germany.
- Pieczyska EA, Gadaj SP, Nowacki WK, Tobushi H (2006). Stress relaxation during superelastic behavior of TiNi shape memory alloy, *International Journal of Applied Electromagnetics* and Mechanics, 23, 3-8
- Pieczyska E, Staszczak M, Dunić V, Slavković R, Tobushi H, Takeda K (2014). Development of Stress-Induced Martensitic Transformation in TiNi Shape Memory Alloy, *Journal of Materials Engineering and Performance*, 23, 7, 2505-2514.
- Pieczyska E, Tobushi H, Kulasinski K (2013). Development of transformation bands in TiNi SMA for various stress and strain rates studied by a fast and sensitive infrared camera, *Smart Materials and Structures*, 22, 3, 035007.
- Qidwai M, Lagoudas D (2000). Numerical implementation of a shape memory alloy thermomechanical constitutive model using return mapping algorithms, *International Journal for Numerical Methods in Engineering*, 47, 6, 1123-1168.
- Schweizer B, Wauer J (2001). Atomistic explanation of the Gough-Joule-effect, *The European Physical Journal B Condensed Matter and Complex Systems*, 23, 3, 383-390.