SEECCM 2017

4th South-East European Conference on Computational Mechanics

03-04 July, Kragujevac, Serbia

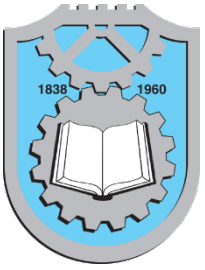
Organizers

Serbian Society for Computational Mechanics

Bioengineering Research and Development Center BioIRC

European Community on Computational Methods in Applied Sciences ECCOMAS

Department of Technical Sciences Serbian Academy of Sciences and Arts



Faculty of Engineering University of Kragujevac

Ministry of Education, Science and Technological Development of Republic of Serbia

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Contents

Welcome Address

Dear colleagues and students,

On behalf of the Organizing Committee, it is our great pleasure to welcome you to the 4th South East European Conference (SEECCM2017) in Kragujevac, Serbia.

The main objective of the SEECCM2017 is to summarize recent achievements in computational methods and their applications to industrial, technological and biomedical processes by bringing together leading scientists from all over the world and researchers from the South-East European (SEE) region. This goal is particularly important for the development in this field and motivation of young researchers and students in the SEE region.
The first SEECCM conference was held in 2006 in Kragujevac, Serbia and during this conference the Serbian Society for Computational Mechanics (SSCM) was founded. On the 10th-year anniversary of the SSCM we are happy to have new SEECCM conference in the same city. The previous three SEECCM conferences were successful and had a profound impact on the goals of the regional and the world community of scientists to invent and apply computational methods in the continuously increasing demands in science, technology and medicine. Today, Computational Mechanics is a very developed and integrative field which uses fundamental scientific laws and computer methods to study, predict and simulate material, engineering, physical, chemical and biomedical processes. Computer simulations are indispensable in testing hypotheses and assembling information in a quantitative context.

We have received more than 60 full papers and abstracts which were carefully reviewed before acceptance and we are thankful for such positive response. The topics of the papers fall into the area of: Solid Mechanics, Fracture Mechanics, Fluid Mechanics, Coupled Problems, Multiscale Modeling, Biomechanics, Nanomedicine, Cardiovascular Mechanics, Tissue Engineering, Dental Mechanics, Musculoskeletal Mechanics, Sport Biomechanics, Cellular and Molecular Mechanics, Medical Image Computing, Computational Chemistry, Medical Image Computing. The abstracts are included in this booklet, and some papers will be published in the Journal of the Serbian Society for Computational Mechanics, Vol. 11, Issue 1 – Special Issue – Proceedings of the 4th SEECCM, 2017.
We are delighted to announce the keynote speakers:

BURCZYNSKI Tadeusz | Institute of Fundamental Technological Research | Poland

ĐORĐEVIĆ Nenad | Brunel University London | UK

FERRARI Mauro | Houston Methodist Research Institute | USA

FOTIADIS Dimitrios | University of Ioannina | Greece

HELLMICH Christian | Institute for Mechanics of Materials and Structures | Austria

IBRAHIMBEGOVIĆ Adnan | University of Technology Compiègne | France

JEREMIĆ Boris | University of California at Davis | USA

KLEIN Erik | Slovak Technical University | Slovakia

MATTHIES Hermann | Braunschweig University of Technology | Germany

PEREGO Umberto | Polytechnic University of Milan | Italy

SCHREFLER Bernhard | University of Padova | Italy

We are thankful to the supporting organizations: Serbian Society for Computational Mechanics (the organizer) and our partners: Faculty of Engineering University of Kragujevac, Bioengineering R&D Center BIOIRC; and ECCOMASS and Serbian Academy of Sciences and Arts as auspice organizations. Also, we are thankful to the Organizing Committee and collaborators of BIOIRC and Faculty of Engineering for extraordinary efforts in solving many tasks regarding Conference preparation and support of the authors. We are grateful to the members of the Program and Scientific Committee for their dedication and support.

On behalf of the Organizing Committee we wish you a pleasant stay in the City of Kragujevac – in the heart of Serbia, and hope that you will be satisfied with the Conference achievements and enjoy Kragujevac's hospitality.

Conference Chairs:
Miloš Kojić, Manolis Papadrakakis and Nenad Filipović

Program at a Glance

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Computational Chemistry
Mechanics
Biomechanics
Numerical Methods
Data Mining
Computational Biology
Finite Element Modelling

Technical Program

MONDAY, 03 JULY 2017

08:00 - 09:00	Registration

09:00 - 09:30	Opening Ceremony

09:30 - 10:00	Keynote speaker: **"Engineering Mechanics for Medicine and Biology: News on the "Cement Line" in Osteonal Bone."** **Prof. Christian Hellmich** *Institute for Mechanics of Materials and Structures, Austria*

10:00 - 10:30	Coffee Break

10:30 - 11:00	Keynote speaker: **"Simulation of fracture and delamination in layered shells due to blade cutting"** **Prof. Umberto Perego** *Polytechnic University of Milan, Italy*

Session M.1 - 11:00-12:30
Biomechanics
Chair: Velibor Isailović

M.1.1 - *Interactive Software for Tracking Motion of Otoconia Particles in the Semicircular Canals of the Inner Ear*
Tijana Đukić, Igor Saveljić, Nenad Filipović

M.1.2 - *Simulation of Aerosol Particle Flow Through Dry Powder Inhaler Aerolizer®*
Tijana Šušteršič, Aleksandra Vulović, Sandra Cvijić, Svetlana Ibrić, Nenad Filipović

M.1.3 - *Finite Element Analysis of Femur During Gait Cycle*
Aleksandra Vulović, Tijana Šušteršič, Nenad Filipović

M.1.4 - *Finite Element Analysis of Patient-Specific Bicuspid Aortic Valve*
Smiljana Đorović, Aleksandar Milosavljević, Lazar Velicki, Nenad Filipović

M.1.5 - *Modelling Semicircular Canals Using DPD Method*
Milica Nikolić, Nenad Filipović

M.1.6 - *Virtual Surgery and Numerical Analysis of Dissected Aorta*
Igor Saveljić, Nenad Filipović, Lazar Velicki

M.1.7 - *Optimal selection of Morphometric Parameters for the Creation of Parametric Model of the Human Mandible Coronoid Process*
Jelena Mitić, Miloš Madić, Nikola Vitković, Miodrag Manić, Miroslav Trajanović

M.1.8 – *Biomechanical Analysis of Jumping Using Force Plate Measurments and Numerical Simulation*
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15:00 - 15:30	Keynote speaker: **"A multiphase porous media model for transport oncophysics"** **Prof. Bernhard Schrefler** *University of Padova, Italy*

15:30 - 16:00	Keynote speaker: **"Computational models and Data – a Possible Fusion"** **Prof. Hermann Matthies** *Braunschweig University of Technology, Germany*

16:00 - 16:30	Coffee Break

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17:30 - 18:00	Keynote speaker: **"Coupled Probability-Multiscale-Mechanics Method for Heterogeneous Composites: Formulation, Computations and Probability-Based Explanation of Size Effect"** **Prof. Adnan Ibrahimbegović** *University of Technology Compiègne, France*

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20:00 - 24:00	Cultural Program and Gala Dinner

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11:00 - 11:30	Coffee Break

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15:00 - 15:30	Keynotespeaker: **"Computational Intelligent Design of 2D Nanostructures Based on Carbon"** **Prof. Tadeusz Burczyński** *Institute of Fundamental Technological Research, Poland*

15:30 - 16:00	Keynote speaker: **"Localization and Damage Induced Softening using Finite Element and Smooth Particle Hydrodynamics methods"** **Prof. Nenad Đorđević** *Brunel University London, UK*

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18:30 - 19:00	Closing Ceremony

Book of Abstracts

Session M.1 - 11:00-12:30
Biomechanics

Chair: Velibor Isailović

M.1.1 - *Interactive Software for Tracking Motion of Otoconia Particles in the Semicircular Canals of the Inner Ear* **-** Tijana Đukić, Igor Saveljić, Nenad Filipović

One of balance disorders is called benign paroxysmal positional vertigo (BPPV) and one of the pathological conditions that can cause BPPV is called canalithiasis. Canalithiasis occurs when otoconia particles enter the semicircular canal (SCC) of the inner ear, cause a disturbance in the flow of the fluid within the canal and affect the displacement of the cupula, that is located within the canal and that sends information to the brain about registered movements.
In this paper, a numerical model is presented, that includes a three-dimensional simulation of endolymph flow, free motion of otoconia particles within the SCCs, deformable cupula and full interaction between all the elements. This model was implemented in a software that performs real time simulation and visulization of the motion of the whole domain and immersed free-moving otoconia particles and its effect on the cupular displacement. This software can be used to study the influence of many factors in the process of canalithiasis and as an assistive tool for treatment planning in clinical practice.

M.1.2 - *Simulation of Aerosol Particle Flow Through Dry Powder Inhaler Aerolizer®* - Tijana Šušteršič, Aleksandra Vulović, Sandra Cvijić, Svetlana Ibrić, Nenad Filipović

The aim of this study was to analyze aerosol particle dispersion in a Dry Powder Inhaler (DPI). These types of inhalers are widely used for disease treatments due to easy delivery of drug to the patient's lungs. Analysis was done by combining computation fluid dynamics (CFD), for simulation of fluid flow (air), with discrete phase model (DPM) for particles simulation. CFD analysis provided us with information about the maximum velocity in the barrel (46.54 m/s) for the flow rate of 28.3 L/min. From the use of DPM we obtained information about particle trajectories from the capsule chamber to the end of mouth piece. Based on those information, we were able to calculate the number of particles that are transported into patient's throat. Considering the used boundary conditions this percentage is low, about 5%. Knowledge obtained in this way can help us better understand how particles move until they reach the mouth and throat of patients and can be used in order to improve performance of different types of inhalers.

M.1.3 - *Finite Element Analysis of Femur During Gait Cycle* - Aleksandra Vulović, Tijana Šušteršič, Nenad Filipović

The aim of the present study was to better understand stress distribution during gait cycle in femur. Hip joint is an important element that is greatly responsible for our ability to walk. In this paper we have analyzed one element of the hip joint. A patient-specific three-dimensional model of the femur was developed from medical scans, while material characteristics and boundary conditions were adopted from the literature. The considered model included the cortical and cancellous femur bone. The finite element analysis was used for numerical calculation of the stress distribution of the femur bone during gait cycle. Results presented are for the initial phase of gait cycle at 0% and at 50% of gait cycle. Maximum Von Mises Stress was calculated to be about 24.5 MPa at 50% of gait cycle. Maximum Principal Stress was 21 MPa.

M.1.4 - *Finite Element Analysis of Patient-Specific Bicuspid Aortic Valve* - Smiljana Đorović, Aleksandar Milosavljević, Lazar Velicki, Nenad Filipović

The main purpose of this study was to examine biomechanical characteristics of a patient-specific bicuspid aortic valve (BAV) model using computational analysis based on finite element method. Full patient-specific geometry was reconstructed based on Computed tomography (CT) scan images, in order to obtain three-dimensional (3D) finite element mesh. Dynamic computational analysis, with applied equivalent material characteristics and boundary conditions, was performed. The initial results for this single case, displacements and Von Mises stress distribution, were quantified concerning anatomical patient's structures. Patient-specific geometry results in regions of abnormal stresses on the leaflets and the aortic root, with asymmetrically open bicuspid valve. Due to the difficulty in obtaining such parameters experimentally, computational analysis gives better insight into the aortic root biomechanics that is needed to achieve advancements in surgical repair techniques.

M.1.5 - *Modelling Semicircular Canals Using DPD Method* - Milica Nikolić, Nenad Filipović

Semicircular canals are part of the inner ear. Each ear has three canals, filled with fluid. Primary function of the semicircular canals is to secure balance, specifically rotational motion. Translational motion is regulated by utricle. Utricle is a sort of fluid chamber, placed in vestibule and in front of the semicircular canals. Both utricle and semicircular canals are containing hair cells in contact with the sensory cells, providing information about translational or rotational movement to the brain. Semicircular canals are positioned in three planes orthogonally to each other. Each canal at one end has extension called ampulla, in which a membrane called cupula is placed. During the rotational motion, fluid moves inside the canals, exposes pressure on the cupula, which

activates nerves and sends information about the change of the position to the brain. Dissipative Particle Dynamics (DPD) method was used for modeling behavior of the fluid inside the semicircular canal, together with membrane - cupula. That is a pioneer application of this kind of discrete method in the inner ear models, concretely semicircular canals. Deformation of the cupula during rotational maneuver can be found in the literature - analytical solution for the cupula displacement. Deformation of the cupula, its displacement, is measured and compared with analytical solution. Way of cupula deformation is observed as well and, finally, force acting on the cupula was calculated and compared to analytically derived value of the force. Compared results show good matching and confirm application of the discrete method in this subject of investigation.

M.1.6 - *Virtual Surgery and Numerical Analysis of Dissected Aorta* - Igor Saveljić, Nenad Filipović, Lazar Velicki

Aorta is the largest human blood vessel and continuously exposed to high blood pressure and shear forces. Aortic dissection is a very serious condition which leads to cleavage of the inner layer of the aortic wall, and further fragmentation. The mortality rate in untreated dissection was 75% in the first two weeks. Hemodynamic properties of blood flow through the newly created false lumen, and its dominance over the true lumen, has a significant impact on the outcome of the surgery and the patient's life. Virtual operations, as well as numerical methods for solving fields of physical quantities obtained model, gives a clear picture how the operation affects the flow through the branches affected dissection. The patient used in this paper had an aortic dissection of type I according to DeBakey. Results are presented for the case before surgery and after the virtual surgery.

M.1.7 - *Optimal selection of Morphometric Parameters for the Creation of Parametric Model of the Human Mandible Coronoid Process* - Jelena Mitić, Miloš Madić, Nikola Vitković, Miodrag Manić, Miroslav Trajanović

3D parametric models of human bones are of immense importance in the design of personalized osteofixation materials. They are widely used in cases of incomplete geometrical data of human bones, caused by a trauma or disease of the bone. Parameter model of human mandible created using the Methods of Anatomical Features (MAF), enables the creation of geometric precise and anatomically accurate models of human bones. The accuracy of the 3D model depends on the number and quality of parameters, which are conditioned by morphometric parameters. The aim of this paper is optimization of number of the basic central and bilateral mandibular morphometric parameters when creating a parametric model of the human mandible. Applied regression methods are "best subsets" and "stepwise", which allow solving the problems of multicollinearity and eliminating independent variables that are of little significance, and the identification of the best regression model with a smaller number of independent variables in relation to the entire model.

M.1.8 - *Biomechanical Analysis of Jumping Using Force Plate Measurments and Numerical Simulation* - Radivoje Radaković, Nikola Mijailović, Aleksandar Peulić, Nataša Petrović-Zdravković, Aleksandra Nikolić, Vladislava Stojić, Nenad Filipović

In this study biomechanical analysis of human body stiffness and stress distribution in the knee during vertical jump analysis has been investigated. Ten professional football players performed ten periodic jumps while vertical ground reaction force was measured using a force plate with one axial load cell force sensor. The stiffness calculation was based on the analogy of the periodic jumping and oscillation movement of the system which consists of spring and body appropriate mass. The frequency of oscillation is obtained using Fourier transform. Detailed knee stress obtained with finite element analysis with boundary condition for force has been presented. A biomechanical analysis of jumping using force plate measurement and finite element method for assessment of specific athlete knee can become a future standard for assessment of athelete capability.

Session M.2 - 12:30-13:10
Mechanics

Chair: Milica Nikolić

M.2.1 - *Simulation of Fracture and Delamination in Layered Shells Due to Blade Cutting* - Federica Confalonieri, Umberto Perego

A new isotropic damage cohesive model for the simulation of mixed-mode delamination is presented. The model is based on consideration of the interface internal friction, naturally leading to coupled opening and shear damage mechanisms. Mixed-mode fracture energy turns out to be a direct outcome of the model and does not require the definition of an empirical law, additional to pure Mode I and II fracture energies. The model has been developed to account for delamination processes promoted by blade cutting of carton packages.

M.2.2 - *Theory of Ambient Vibration Energy Harvester with Piezoelement* - Livija Cvetićanin, D. Cvetićanin

In this paper we consider the theory of the ambient vibration energy harvester. After explanation of the procedure of vibration energy harvesting, the mathematical model is formulated. The influence of parameters of the system on the level of the harvested

power is specified. A device which contains a piezoelectric element is used for vibration energy harvesting. The interaction between mechanic and electric part of the system is taken into consideration. Two types of piezoelectric elements are analyzed: linear and nonlinear. Motion is described with a system of two coupled equations. In the paper the equations are solved numerically. Advantages and disadvantages of the ambient vibration energy harvester with piezoelectric element are presented. The direction for future investigation to eliminate the lack of the harvester is suggested.

M.2.3 - *Lifetime Prediction of Cardiovascular Stent Based on Fatigue to Fracture Approach* - Gordana Jovičić, Arso Vukicević, Dalibor Nikolić, Nenad Filipović

The principal aim of this study was to define and apply numerical procedures to assess the durability of coronary stents based on the estimation of safety from fatigue to fracture. This procedure is carried out within three phases: a) initial fatigue analysis based on S-N approach; b) fatigue lifetime assessment based on fatigue crack growth simulation using Paris-power law, and c) safe-operation i.e., no-fatigue failure (based on forming of Kitagawa-Takahashi diagram) as well as immediate fracture event predictions of the stent. The results indicated that the presented numerical algorithm gave an estimation of structural survival/durability on the side of safety that can be combined efficiently with other experimental procedures during the phase of stent design.

M.2.4 - *Analysis of Loads and Deformation of Valve Plate in Contact with Cylinder Block at Axial Piston Pump for Water Hydraulics* - Nenad Todić, Snežana Vulović, Miroslav Živković, Slobodan Savić, Vesna Ranković

This paper focuses on mathematical modeling of axial piston pump for water hydrailucs. The cylinder block-valve plate plays an important role in the axial piston pump because its failures predominate in maintenance. Through analyzing the surface morphology of the worn valve plate, its eccentric wear in the high-pressure area occupies the primary position. Since the axial piston pump is full of fluid, its normal operation depends on the lubrication between the friction pairs. Based on the tribology theory, most of abrasive wear of the axial piston pump is caused by fluid damage between the friction pair surfaces. Under ideal condition, there is a layer of fluid between the valve plate and the cylinder block, which lubricates the operation of the friction pair. Tribological problems with the axial piston pumps for water hydraulics are particularly pronounced because of temperature load and wear. This paper analyzes the load of the contact block and the plate in the phases of suction and pressure and interaction between the fluid and the contact surface of the plate.

Session M.3 - 13:10-14:00
Data Mining

Chair: Bojana Anđelković Ćirković

M.3.1 - *Automatic Main Pulmonary Artery Identification on Chest CT using Supervised Machine Learning* - Daniel A. Moses, Laughlin Dawes, Claude Sammut, Tatjana Zrimec

The pulmonary arterial system can be affected by many pathological processes with potentially lethal consequences. Automatic detection and extraction of the pulmonary arteries can significantly speed up the diagnosis and intervention. In this paper we present a method for automatic seed point detection within the main pulmonary artery (MPA) in CT data to aid its segmentation. We used supervised machine learning to train models that can accurately predict images that contain the MPA in 3 orthogonal anatomical planes: axial, coronal and sagittal. Through intersection of these predicted images we triangulate the likely position of the seed point in the MPA on each of the 3D data sets. Experiments were performed on CT datasets from fifty patients and with different machine learning algorithms: ANN, SVM, naïve Bayes and kNN. The best performance for accurate main pulmonary artery localization (92%) was seen at the models tarnished with the SVM with Radial Basis Function kernel.

M.3.2 - *Framework for creation of customized shape of the shoe insole* - Suzana Petrović Savić, Zoran Jovanović, Goran Devedžić

Foot is the body part which is in constant contact with the ground. Since foot has to adjust to the ground and transfer body weight properly, it is very susceptible to injuries and deformities. One of the most common deformities is flat foot that implies fallen arches. These deformities influence non-amenity during walking and irregular body weight transfer. In order to return foot mechanics in normal acting, it is necessary to wear corrective insoles. This study presents methodology aiming at speeding up the customized insole manufacturing process through creation of so-called “digital chain”. Patients with flat foot leave footprint in polyurethane foam, which is later scanned and transferred into digital model. Selecting the appropriate points of the acquired scanned image data set defines input parameters for creating spatial insole shape. These parameters, consequently, define boundary spatial curves, which in turn rule the insole’s free form shape. This is the basis for upgrading and setting up the initial shape with corrective elements.

M.3.3 - *Multiscale Microstructural Optimization of Carbon Nanotube/Polymer Structures using Genetic Algorithms* - Maria Tavlaki, Odysseas Kokkinos, Vissarion Papadopoulos, Manolis Papadrakakis

The current work proposes a novel three-level multiscale optimization technique to optimize the orientation and dispersion of nanotubes in several benchmark carbon nanotube-polymer structures: a) At the atomic level, a nanotube was modeled as a space-frame structure using mMSM. b) At the microscopic level, a Representative Volume Element consisting of a straight nanotube embedded in polymer was analyzed using a first-order homogenization technique. c) Finally, at the highest level, a macroscopic structure was analyzed concurrently with the previous level using a nested solution scheme. One RVE corresponding to a nanotube orientation and diameter was assigned to every element of the macroscopic structure. Using the NSGA-II multi-objective optimization algorithm, a set of nanotube angles and diameters was calculated so that the energy for each macroscopic structure was minimized, under the constraint that the mean nanotube volume fraction over the structure has to remain constant.

M.3.4 - *Analysis of Layer Recurrent Network to Estimate Nondimensional Velocity of the Dissociated Gas* - Vesna Ranković, Slobodan Savić, Nenad S. Todić

In this paper a layer recurrent neural network has been used to predict the nondimensional velocity of the gas that flows along a porous wall. Equations were analyzed using finite difference method and data has been obtained from a CFD-based computer code. The activation functions of the hidden nodes are hyperbolic tangent sigmoid transfer function. Results of simulations show that the application of the layer digital recurrent neural network to predict the velocity of the gas gives satisfactory results. The performance of the network model has been assessed through the correlation coefficient.

M.3.5 - *Prediction of Second Primary Tumors in Patients with Oral Squamous Cell Carcinoma* - Bojana Anđelković Ćirković, Daniela Elena Costea, Nenad Filipovic

Oral squamous cell carcinoma (OSCC) is the most common malignant head tumor. Patients with OSCC are at increased risk for the development of a second primary malignancy, which is defined as a second malignancy that presents either simultaneously or after the diagnosis of an index tumor. This study aimed to develop data mining prediction model for the occurrence of second primary tumors (SPT) for OSCC patients. Methodology approach based on genetic algorithm (GA) and artificial neural network (ANN) was used to perform automatic feature selection as well as design of the classifier structure and tuning of classifiers' parameters. The algorithms were successfully applied to the novel data set of 95 patients with OSCC. Our results suggest that we developed the optimized ANN model for prediction of second primary tumors in OSCC patients with high accuracy. The model could help clinicians to tailor the treatment plan and adopt follow - up strategy to efficiently manage the OSCC disease.

Session M.4 - 18:00-19:30
Finite Element Modelling

Chair: Aleksandra Vulović

M.4.1 - *Finite Element Modelling of Rotary Transfer Machines* - Alberto Martini, Marco Troncossi, Nicolò Vincenzi

Vibration monitoring and control are central topics for machine tools, since high vibration levels reduce the quality of machined surfaces and shorten the tool life. In order to predict potential vibration issues since the early design stage, it is necessary to implement ad hoc numerical models for modal analysis. This requires significant efforts and possible conflicts with tight production scheduling of companies. This work focuses on a specific family of rotary transfer machines for the manufacturing of parts related to lock&keys industry. It investigates the possibility to achieve an acceptable estimation of the elastodynamic behavior of the machine tools through limited modifications of the Finite Element (FE) models used for structural analysis, which are generally available in the early phases of the design process. The structural FE model of a new machine tool is implemented and validated through experimental tests performed on a prototype. Then, the elastodynamic FE model is derived and simulated, and the numerical results are presented.

M.4.2 - *Investigating Low Velocity Impact on Biocomposites by MAT_54 Shell Modeling* - Felipe Vannucchi de Camargo, Ana Pavlović

Biocomposites have risen as an alternative for supplying the sustainability concern in the composites field, and as in any emergent structural technology, there is a need to quantify the characteristics of such materials by experimental testing and numerical simulations. Among the important tests required to provide a wide comprehension of the material properties, the evaluation of low-velocity impact resistance is essential for allowing its application on structural components. Given the explicit shell material MAT_54 of LS-DYNA used in simulations of such kind to represent the slave part, the present work thoroughly studies the influence of some of its most important immeasurable parameters that demand calibration to understand their influence on a low-velocity impact condition.

M.4.3 - *Finite Element Modeling in Palletized Products Under Transportation* - João Pedro Teixeira Peixoto de Queiroz, Antonio Carlos de Figueiredo Silveira, Felipe Vannucchi de Camargo

Being palletized products are one of the most common means of goods transportation, recent studies show that there is still room for improvement on the packaging technology for achieving a more profitable process. Given the current overview, packaging optimization techniques are a prolific area of study for generating money saving, improving safety and reducing merchandise losses, being potentially profitable for all those involved in the supply chain. In order to figure out how to improve this process, it is necessary to understand all technical branches embraced by the subject as well as being capable of measure its damaging mechanisms; thus, the present work thoroughly lists the most important factors to be considered in palletized products transportation through a state-of-the-art review, including the qualification of the principal forces acting on the packs during transport as well as the quantification by numerical modeling techniques through random vibrations, sloshing and shock simulations.

M.4.4 - *Finite Element Analysis of Patient-Specific Bicuspid Aortic Valve Elastic Post-Buckling Analysis of Rectangular Imperfect Plates Using the Semi-Analytical Finite Strip Method* - Aleksandar Borković, Saša Kovačević, Dragan D. Milašinović, Gligor Radenković

Elastic post-buckling analysis of imperfect rectangular plates subjected to a uniform compression stress along one direction is presented. The semi-analytical finite strip method is improved by generalization of its nonlinear formulation through inclusion of various types of strips and boundary conditions. The equations of balance are derived via incremental formulation of virtual work, while the Newton-Raphson and arc-length methods are implemented into a solver. Geometric initial imperfections are modeled as a scaled buckling mode of a structure. The presented theory is verified via comparison of results with the ones from literature and Abaqus. The semi-analytical finite strip method is ideally suited for this type of analysis due to good convergence properties.

M.4.5 - *Comparing Design Solutions by Harmonic Analysis in the Case of a Surface Finishing Machine* - Ana Pavlović, Cristiano Fragassa, Francesco Ubertini, Giuseppe Lucisano

This paper investigates the dynamic response of a large production machine, used in surface finishing by tool machining in the case of wide dimension ceramic tiles. In particular, the study aims at improving this phase of the industrial process, relatively mysterious inside the ceramic manufacturing, and the overall quality of the final products. A harmonic analysis has been preferred for this scope respect to other numerical approaches, while two different basements of cutting machine have been considered as alternative design solutions. The response in frequency and phase has been observed and compared. Stresses and deformation have been also considered in comparison. This numerical computation permitted to select a convenient design solution for the basement.

M.4.6 - *Finite Element Simulation of Turbulent Flow Using Model and Rans Equations* - Aleksandar Nikolić, Nenad Filipović, MarkoTopalović, Miroslav Živković

Turbulent flow is largely unstable and divergent. For this reason, the turbulent problems are treated through statistical rather than deterministic methods. Analysis of turbulent fluid flow in this paper is performed using two-equation statistical model that can calculate values in the viscous sublayer. Implicit integration of the equations is used for determining the fluid velocity, pressure, turbulence, kinetic energy, and dissipation of turbulent kinetic energy. These values are calculated in the finite element nodes for each step of incremental-iterative procedure. Turbulent model is verified on an example of fluid flow in backward facing step channel. Analysis results correspond well with the experimental results from the literature and developed model can be used for more complex problems that are experiencing turbulent flow.

M.4.7 - *Finite Element Modeling of Benign Paroxysmal Positional Vertigo Disease* - Žarko Milošević, Velibor Isailović, Igor Saveljić, Dalibor Nikolić, Vladislava Stojić, Nebojša Zdravković, Dušan Pavlović, Nenad Filipović

Benign paroxysmal positional vertigo (BPPV) is the most commonly diagnosed vertigo disease. Thera are three semicircular canals (SCC) system located in inner ear which are employed for indicating rotational movements. Most common test for indicating BPPV is video head impulse test (vHIT). BPPV is diagnosed by tracking the eye movements or nystagmus. Three-dimensional biomechanical model of the SCC is simulated with full 3D fluid-structure interaction of wall, cupula deformation and endolymph fluid flow was developed. The otoconia particles are coupled with fluid and solid domain. A full Navier-Stokes equations and continuity equations are used for fluid domain with Arbitrary-Lagrangian Eulerian (ALE) formulation for mesh motion. We compared results of simulation with real patient data for right anterior vHIT test. This technology can be used for prediction and better understanding of BPPV disease.

M.4.8 - *Geometry Optimization of Nitinol Stent Design and Effects on Mechanical Performance: Finite Element Analysis* - Dalibor Nikolić, Nenad Filipović

The Finite element methods was used for evaluation of the geometry optimization on mechanical performance of Nitinol stent old design vs new optimized design for the Z-shaped closed-cell self-expanding stent. Stent made by laser cutting from Nitinol tube form, by application of expanding and crushing force. The behavior of stent tested by two different models, old model Palmaz- Schatz design and optimized design using suggestion from topology optimization (modern design form). Models

calculation show that modern design has better clinical behavior due to lower chronic outward force, better superplastic behavior and higher radial resistive strength. In the paper was comparison results between two stent designs, old design and modern design obtained by optimizing old stent designs.

M.4.9 - *Computational Fluid Dynamics (CFD) Modeling of the Fluid Flow Through Porous Structures* - Varun Sharma

Open cell metallic foam hydrodynamics were studied using computational fluid dynamics (CFD) in view of thermal engineering applications with a major focus on the heat exchanger. Very latest Voronoi tessellation 3D effects based techniques were used for foam creation as well as for the computational domain. Latest analytical formulas were also discussed covering the recent development. For CFD modelling, steady state incompressible laminar flow model was investigated. Finite difference methods based on commercial pre and post processing software was used for iteration solving. Three different inlet velocities 2 m/s, 4 m/s, 6 m/s were chosen to pass through the pore channel. The sole purpose of the investigation was to observe the velocity regime effects under different rate, pressure exertion on the strut length, pressure drop and geometrical influence on the dynamics behavior. Due to highly chaotic behavior, CFD helps us in understanding of the inner pore field. Results showed that with the increase in velocity there is an upsurge in pressure drop under different inlet flow rate. The geometrical parameter is mainly responsible for the fluid behavior.

Session T.1 - 09:00-09:40
Computational Biology

Chair: Marko Živanović

T.1.1 - *Mean-Field Approximation of Two Coupled Populations of Excitable Units Modeled by FitzHugh-Nagumo Elements* - Kristina Todorović, Igor Franović, Nebojša Vasović, Srđan Kostić

In this study, the focus lies with the two delay-coupled populations of identical excitable units modeled by the Fitzhugh-Nagumo elements. The analysis on stability and bifurcations in the macroscopic dynamics exhibited by the system of two coupled large populations comprised of N stochastic excitable units each is performed by studying an approximate system, obtained by replacing each population with the corresponding mean-field model. The aim is to demonstrate that the bifurcations affecting the stability of the stationary state of the original system, governed by a set of 4N stochastic delay-differential equations for the microscopic dynamics, can accurately be reproduced by a flow containing just four deterministic delay-differential equations which describe the evolution of the mean-field based variables. We show how analytically tractable bifurcations occurring in the approximate model can be used to identify the characteristic mechanisms by which the stationary state is destabilized under different system configurations, like those with symmetrical inter-population couplings.

T.1.2 - *microRNA Based Methodology for Early Cancer Detection* - Marko Živanović, Danijela Cvetković, Nenad Filipović

Nowadays, cancer is increasingly widespread disease. Early diagnosis is very important because it increases the survival rate of patients and if cancer is detected in early stage a complete healing is not negligible. In these circumstances, cancer is becoming a chronic disease. Speaking of detection, numerous tumor markers are followed, including the growing use of detection microRNA. Our methodology is based on precise, fast, accurate and inexpensive detection of microRNAs as tumor markers. We chose the establishment of the methodology for determining the microRNA-21, which can be considered a breast cancer marker.

T.1.3 - *Computer Driven Bioavailability Analysis of Some Important Compounds Found in Anticancer Herbs* - Draško Tomić, Miroslav Puškarić, Zlatan Car

There is a mounting evidence that some herbs can slow down the spread of cancer, and in some cases even cure it. In the Eastern medicines like Chinese and Ayurveda, and in the South America, the evidence for this is present for centuries. Western medicine is slow in adopting this evidence. There are several reasons for that, among them the lack of clinical trials, the chemical complexity of anti-cancer herbs consisting of dozens of compounds like polyphenols, tannins, saponins, quinones etc., and the concern about the safety of their use. In opposite to in-vivo clinical trials, a large number of in-vitro experiments with anti-cancer herbs was performed, showing us that these herbs alone, or in the combination with other herbs, can effectively kill various types of cancer cells. Other experiments have shown that these herbs can enhance the effectiveness of chemotherapy and lessen the side effects of it and the radiotherapy. Moreover, mouse model experiments proved the toxicity of most anti-cancer herbs is bellow the dosage required for the effective cancer-killing dose. However, in-vivo animal experiments are not so convincing, and in most cases, reasons for that is the poor bioavailability of the herbal compound that fights cancer. Especially in the case when a certain compound is poorly soluble in water, it can hardly reach cancer cells within the body. In vitro and in vivo experiments are costly, last a while, and results are highly dependent on the experimental environment. Besides, there are important ethical questions when using animals in such experiments. For these reasons, we decided to perform the computer driven water solubility analysis of

some compounds found in a certain anticancer herbs. Results derived from this analysis show that some of them like curcumin and artemisinin have poor water solubility, thus limiting their use, at least in their native form. At the same time, we found that computer driven molecular conformation between these compounds may help to show the way of increasing their bioavailability, thus enhancing their anticancer activity.

T.1.4 - *Modification of Polysaccharides with Phenols for Hydrogels fFormation and Electrospinnig* - Nikolina Popović, Olga Prodanović, Ivana Gađanski, Danijela Cvetković, Marko Živanović, Vladimir Pavlović, Nenad Filipović, Radivoje Prodanović

Carboxymethylcellulose (CMC) and alginate (ALG) are water-soluble polysaccharides used in food and cosmetics industry. They have big potential for use in pharmaceutical products due to their high biocompatibility, biodegradibility, low immunogenicity and low price. When crosslinked they can absorb large amounts of water and swell to form hydrogels with great physical properties. The need for new biomaterials and hydrogels is growing daily, due to their use in tissue engineering, drug delivery and cell and enzyme immobilization studies. In this study we modified ALG and CMC, in order to get a cross-linkable polymer that can make hydrogels by chemical and enzymatic means. After periodate oxidation we obtained polysaccharides with different degrees of oxidation: 2.5, 5, 10, 15 and 20 mol%. Further modification using reductive amination in the presence of different phenolic compounds like tyramine, was done. This modification was confirmed by UV–VIS and FT-IR spectroscopy, while concentration of phenol and ionizable groups was determined using absorbance at 275 nm and acid–base titration. All CMC and AlG tyramines were able to form hydrogels after cross-linking with horse radish peroxidase (HRP) and hydrogen peroxide. Both derivatives have been successfully electrospun and crosslinked afterwards. Due to the introduction of amino groups and decrease in molecular weight, they were significantly more soluble in water up to 30 % (w/w) compared to native polysaccharides and their electrospinability also improved. We aim to make nanofibers using tyramine-polysaccharides that will be more stable in cell culture media after cross-linking covalently and with calcium/barium ions. Diameter of nanofibers was determined by scanning electron microscopy (SEM). Cross-linked nanofibers that we obtained will be used for tissue engineering of blood vessels.

Session T.2 - 09:40-10:30
Coputational Chemistry (part I)

Chair: Dejan Milenković

T.2.1 - *Theoretical Investigation of Antioxidative Activity of Caffeic Acid* - Izudin Redžepović, Svetlana Marković, Jelena Tošović

Caffeic acid (CA) is one of the most abundant dietary polyphenols, which exhibits significant antioxidative activity. However, its antioxidative mechanisms are not fully elucidated. This work reports the results of mechanistic research of the hydrogen atom transfer (HAT), radical adduct formation (RAF), sequential proton loss electron transfer (SPLET), and single electron transfer – proton transfer (SET-PT) mechanisms of CA in benzene and water solutions. Our results revealed that HAT and RAF are competitive antioxidative mechanisms of CA, because HAT pathways lead to more stable radical products, and RAF pathways require smaller activation barriers. In polar basic media SPLET is a probable antioxidative mechanism of CA, and extremely fast, while SET-PT is not a favorable antioxidative pathway of CA in any medium.

T.2.2 - *QSAR Analysis of Antioxidant Properties of Polyphenols by OH-Related Molecular Descriptors* - Nenad Raos, Ante Miličević

For the theoretical modeling of radical scavenging activity (RSA) and the first oxidation potential (Epa) of the three sets of polyphenolic compounds we used two models based on the number of OH groups in molecules. The first model distinguishes vicinal (Nv) and non-vicinal (Nnv) OH groups. The second model is based on two variables, the number of OH-bearing moieties (Nm) and the total number of OH groups (NOH). All models gave fairly good agreement with the experiment (r = 0.91- 0.98).

T.2.3 - *Antioxidant Activity of the Carboxylate Anions of the Selected Dihydroxybenzoic Acids* - Jelena Đorović, Svetlana Jeremić, Edina Avdović, Ana Amić, Jasmina M. Dimitrić Marković

In the present study the M05-2X/6-311++G(d,p) theoretical model was used to evaluate scavenging potency of the carboxylate anions of 2,3-, 2,6-, and 3,4-dihydroxybenzoic acids. Reaction enthalpies related to the antioxidant mechanisms of the investigated species were calculated in water and benzene. The single electron transfer followed by proton transfer is not favorable reaction pathway under any conditions. Hydrogen atom transfer is the preferred reaction pathway in benzene, while sequential proton loss electron transfer is the predominant reaction pathway in polar solvent, water, for all examined compounds. The approach, based on the reactions enthalpies related to the examined radical scavenging mechanisms, shows that thermodynamically favoured mechanism depends on the polarity of the reaction media and properties of free radical reactive species.

T.2.4 - *Thermodynamics of 2H+/2e- Free Radical Scavenging Mechanisms of 3-(4-Hydroxy-3-*

Methoxyphenyl)Propanoic Acid - Ana Amić, Zoran Marković, Jasmina Dimitrić Marković, Svetlana Jeremić, Bono Lučić, Dragan Amić

The thermodynamic preference of different free radical scavenging mechanisms of 3-(4-hydroxy-3-methoxyphenyl)propanoic acid (HMPPA), a colon catabolite of dietary (poly)phenols, was studied using density functional theory. The role of guaiacyl moiety and carboxyl group of HMPPA in double (2H+/2e) processes of inactivation of free radicals was theoretically investigated in polar and nonpolar media using Gaussian 09 software package. Obtained results indicate that HMPPA possesses potential for inactivating free radicals of different characteristics (HO•, HOO•, CH3O•, CH3OO•, PhO•, Cl3COO• etc.) via double hydrogen atom transfer (dHAT) and double sequential proton loss electron transfer (dSPLET) mechanisms. Concentration of HMPPA in serum may reach very low M values and may contribute to health benefits associated with regular intake of polyphenol-rich diet by direct scavenging of reactive oxygen species.

Session T.3 - 12:00-14:00
Coputational Chemistry (part II)

Chair: Jelena Đorović

T.3.1 - *Stability of Stoichiometric Networks with Conservation Constraints. The Case of Catalytic Carbonylation Model* - Željko Čupić, Ljiljana Kolar-Anić, Stevan Maćešić, Katarina Novaković

Stability analysis of stoichiometric networks with conservation constraint is described aiming to underlain specificities of this family of dynamic systems and to ofer the procedure for their treatment. The main goal of this work is to highlight complications and common mistakes, which may occur in stoichiometric network analysis of such systems. The model of catalytic carbonylation of alkyne-functionalized poly(ethylene glycol) is used as an example for the illustration of proper stability analysis. After several simplifications of the model, source of instability is determined.

T.3.2 - *Estimation of Antioxidative Capacity of Anthrarufin* - Svetlana Jeremić, Zana Dolićanin, Jelena Đorović, Ana Amić, Marijana Stanojević Pirković, Zoran Marković

Anthrarufin is a derivate of anthraquinone with hydroxyl groups in positions 1 and 5. It is already evaluated as potential antioxidant. In this paper, we estimated thermodynamical possibility of anthrarufin to form stable radical, and to scavenge free radicals. Due to it, optimal geometries of all reactive species that can be obtained during radical reactions, were calculated using M06-2X/6-311++G(d,p) level of theory. Based on enthalpy values, it was estimated that, among three possible conformers of anthrarufin, the most stable is the one with two intramolecular hydrogen bonds. It is found that anthrarufin can form radical and diradical moieties in gas phase by homolytic cleavage of O–H bond. To investigate scavenger potency of anthrarufin in reaction with free radicals, :$^{\bullet}OH_2$ $^{\bullet}OCH_3$, $^{\bullet}OOH_2$ $CH_3OO^{\bullet}$ and $O_2^{\bullet-}$ are chosen to be inspected. It is found that anthrarufin scavenge $^{\bullet}OH$ and $^{\bullet}OCH_3$ following HAT and SPLET mechanisms. Toward residual free radicals, anthrarufin is inactive.

T.3.3 - *Comparative Study of Antioxidant Activities of Catechol, Protocatechuic Acid and 3,4-Dyhydroxypiridine* - Žiko Milanović, Dejan Milenković, Zoran Marković

Density Functional Theory (DFT) was used to evaluate the free radical scavenging potency of Catechol, Protocatechuic acid and 3,4-Dihydroxypyridine. The M06-2X/6-311+G(d,p) theoretical model was applied. The HAT mechanism is the most favorable reaction pathway for antioxidative action of CA, PA and 3,4-DHP in the benzene, as non-polar solvent. On the other hand, the SPLET mechanism is the most favorable reaction pathway for antioxidative action of investigated compounds in the aqueous phase. SET-PT is not a favorable mechanism of antioxidative action of CA, PA and 3,4-DHP in any solvent. The predicted values of VCEAC for 3,4-DHP imply that this compound has good antioxidant properties.

T.3.4 - *Computational Molecular Docking Studies of the Novel Coumarine Derivative Towards Ubiquinol-Cytochrome C Reductase Binding Protein and Methylenetetrahydrofolate Reductase* - Edina Avdović, Srećko Trifunović, Dejan Milenković, Zana Dolićanin, Marijana Stanojević Pirković, Zoran Marković

Molecular docking analysis was carried out in order to identify the potency of inhibition of the novel coumarine derivative 3-(1-(phenylamino)ethylidene)-chroman-2,4-dione against Ubiquinol-Cytochrome C Reductase Binding Protein and Methylenetetrahydrofolate reductase. The ligand was prepared for docking by minimizing its energy at B3LYP-D3BJ/6-311+G(d,p) level of theory. The inhibition activity was obtained for ten conformations of ligand inside protein. This study proved that the molecular docking analysis is very important for the interactions of coumarine derivatives with biologically important proteins.

T.3.5 - *Thermodynamic and Kinetic Aspects of the Electron-Transfer Reaction of Dopamine and its Metabolites Towards Substituted Methylperoxy Radicals* - Dušan Dimić, Dejan Milenković, Dragan Amić, Jasmina Dimitrić Marković

The thermodynamic parameters of the reaction of

dopamine, 3,4-dihydroxyphenylacetic acid, 3-methoxytyramine and homovanillic acid towards differently substituted methylperoxy radical are calculated. The preferability of the mechanisms is discussed based on the enthalpies of reactions and it was proven that different mechanisms are plausible for different radicals. The reactivity of radicals is dependent on the number of chlorine atoms, as proven by NBO and QTAIM analyses. Hydrogen Atom Transfer (HAT) is the most probable mechanism for reaction with trichloromethylperoxy radical, while for methylperoxy HAT and Sequential Proton Loss Electron Transfer (SPLET) are competitive. The kinetic parameters for the electron-transfer reaction, calculated by Marcus theory, are also discussed for the reaction with these two radicals. It was proven that both thermodynamic and kinetic parameters are needed in order to establish the order of the antiradical potency of the investigated molecules.

T.3.6 - *Computational Molecular Docking Studies of Kaempferol-Procalcitonin Interaction* - Marijana Stanojević Pirković, Svetlana Jeremić, Jasmina M. Dimitrić Marković, Dušan Dimić, Dragan Amić, Dejan Milenković

Molecular docking analysis was carried out in order to identify the inhibition potency of the kaempferol and its coorresponding anion against human Procalcitonin. The ligands were prepared for docking by minimizing their energy using B3LYP-D3/6-311+G(d,p) level of theory. The inhibition activity was obtained for ten conformations of ligands inside the protein. This study proved that the molecular docking analysis is very important tool in analyzing the interactions of biologically important molecules, kaempferol and human procalcitonin in this case.

T.3.7 - *Protolytic and Tautomerization Reactions of Anthraquinone Dyes* - Peter Poliak, Vladimir Lukeš

The two most abundant anthraquinone derivatives in natural dyes, alizarin (1,2- dihydroxyanthraquinone) and purpurin (1,2,4-trihydroxyanthraquinone) were studied using the density functional theory (DFT). The complete protolytic and tautomeric reaction paths were mapped using the B3LYP/6-311++G(d,p) approach and corresponding reaction energetics were calculated. The electronic spectra of all studied species were obtained using the time dependent DFT. Solvation model based on the quantum mechanical charge density of a solute molecule interacting with a continuum (SMD model) was used to take solvent effect into account. Calculated data allowed the identification of the individual protonated/deprotonated tautomeric forms in the experimental systems.

T.3.8 - *Study of the Structure, Prooxidative, and Cytotoxic Activity of Some Chelate Copper(II) Complexes* - Vladimir P. Petrović, Marko N. Živanović, Dušica Simijonović, Jelena Đorović, Zorica D. Petrović, Snežana D. Marković

The six chelate N,O-copper(II) complexes were synthetized starting from salicylaldehyde anil Schiff bases, as ligands. Their structure is elucidated using experimental and theoretical tools. In vitro biological activities, i.e. cytotoxic and prooxidative effects against human epithelial mammary gland/breast metastatic carcinoma MDA-MB-231, epithelial colorectal carcinoma HCT-116, and fetal lung fibroblast healthy MRC-5 cell lines of investigated compounds are determined, also. Complexes Cu-1, Cu-6, and especially Cu-7 showed significant cytotoxic effects, with IC50 values comparable with effects of positive control CisPt. In addition, investigated complexes induced extreme oxidative and nitrosative stress in all treated cell lines. The most prominent effect is observed on HCT-116 cells, and on MRC-5 cells, while MDA-MB-231 cells showed higher resistance to the investigated cell lines, giving us direction towards the substances with more specific selectivity.

T.3.9 - *The Influence of Water Molecule Coordination to a Metal Ion on Water-Nucleic Base Hydrogen Bonds* - Jelena M. Andrić, Ivana M. Stanković, Snežana D. Zarić

The hydrogen bond interactions of nucleic bases with noncoordinated and coordinated water molecule were studied by analyzing data in the Protein Data Bank (PDB) and by quantum chemical calculations. The analysis of the hydrogen bond interactions in the crystal structures from the PDB indicates that hydrogen bonds of nucleic bases and water molecule are stronger when water is coordinated to a metal ion. The results of the calculations are in accordance with the PDB data and show that the hydrogen bond interactions for doubly charged $[Mg(H_2O)_6]^{2+}$ complex (-12.94 to -49.96 kcal/mol) and for singly charged $[Na(H_2O)_6]^{+}$complex (-6.66 kcal/mol to -19.63 kcal/mol) are stronger than for noncoordinated water (from -4.63 to -8.93 kcal/mol).These calculated values for hydrogen bond interactions are similar to the strength of hydrogen bonds between nucleic bases.

Session T.4 - 16:30-18:30
Numerical Methods

Chair: Miljan Milošević

T.4.1 - *Accuracy of Smeared Finite Element Model Improved by a Field of Correction Factors* - Miljan Milošević, Miloš Kojić, Vladimir Simić

Recently introduced smeared finite element provides a new methodology of modeling complex diffusion transport of molecules and drugs in coupled capillary and tissue domain (Kojic et al. 2017). The transport from

capillary system is smeared to continuous mass sources within tissue, under the assumption of uniform concentration within capillaries. The fundamental relation between capillary surface area and volumetric fraction is derived as the basis for modeling transport through capillary walls. Despite adequate theoretical considerations, there are still differences in overall mass transport when comparing detailed 3D model and smeared model. We investigated effects on the smeared model accuracy of different parameters of the smeared model such as: ratio of thickness vs. diameter of capillary wall, ratio of diffusion coefficient in capillary wall vs. surrounding tissue, and volume fraction of capillaries within tissue domain. As a result, using numerical procedure, we established a field of correction factors needed to improve accuracy of smeared model. Field of correction factor is implemented in our PAKT FE solver (Kojic et al. 2008, 2010), and used for various calculations. Example of a real 3D configuration of capillary networks showed applicability of correction factors, enhanced accuracy of smeared models, and encouraged use of smeared model in real problems such as models of drug transport in tumor or human organs.

T.4.2 - *Convection–Diffusion Transport Model Using Composite Smeared Finite Element* - Miloš Kojić, Miljan Milošević, Vladimir Simić, Nikola Kojić, Arturas Ziemys, Mauro Ferrari

The mass exchange from blood vessels to tissue and vice versa occurs through blood vessel walls. Due to geometrical complexity and heterogeneity of capillary systems, it is not feasible to model in silico individual capillaries for whole organ domains. Hence, there is a need for simplified and robust computational models that address mass transport in capillary-tissue systems. We here generalize a smeared modeling concept for gradient-driven mass transport introduced in (Kojic et al. 2017) where the basic composite smeared finite element (CSFE) was formulated. An outline of the generalization is presented by considering the tissue as a composite medium consisting of cells and extracellular space. The generalized CSFE has the following nodal variables (degrees of freedom - DOF): pressure for the capillary and tissue domain (taken for convection as a homogenous medium), and concentration for capillary domain, extracellular space and cells. Here, cells can be of different types – healthy, cancer, immune, etc. The domains are coupled by connectivity elements at each node. The smeared concept is implemented into our implicit-iterative FE scheme and into FE package PAK (Kojic et al. 2010). A numerical example given in this study illustrates accuracy of the CSFE element, robustness of the introduced methodology and its applicability to real physiological conditions.

T.4.3 - *Universal Service for Solving Systems of Linear Equations* - Bogdan Milićević, Miloš Ivanović

In this paper, EqSolver, the service for solving systems of linear equations, is presented. This service runs on a computing cluster and is also able to use graphics processing units. Software with built-in interface for communication with EqSolver, can send data regarding systems of equations, and EqSolver will return the solutions. EqSolver provides several solvers. User can choose which solver will be used for solving certain systems of equations.

There are three main advantages of using this service. In order to use solvers provided by EqSolver, user doesn't have to change his development environment. Some equation systems require a lot of memory and can not be solved on regular desktop computers. Since EqSolver runs on a HPC cluster, memory is distributed amongst nodes, which enables solving large systems of equations. In most cases, certain speedup can be achieved by using EqSolver. Achieved speedup depends on chosen solver, number of nodes EqSolver runs on and the time spent in communication between EqSolver and the client.

T.4.4 - *Parameter Estimation Using HPC on the Cloud Based Optimization Service* - Boban Stojanović, Miloš Ivanović, Višnja Simić, Filip Radovanović, Nikola Milivojević

Most computer models are defined using parameterized mathematical relations. The parameters describe an underlying physical setting, but their values are often unknown or uncertain. Parameter estimation can be considered as an optimization process which searches for parameter values that minimize difference between the model results and measurements. In this paper, we present a HPC in the cloud based optimization service that provides a robust on-demand parameter estimation using remote computing resources. The service is intended for solving complex parameter estimation problems in the distributed computing environment. The solution is PaaS that hides details of the implementation, enabling user to employ single- and multi-criteria optimization for the estimation of model parameters, without knowing (1) the optimization theory and (2) specific HPC and IaaS techniques. Performance of the service is benchmarked on the real-world example of "Iron gate" hydraulic-hydropower model parameter estimation.

T.4.5 - *Multi-Scale Computational Homogenization of Graphene Polymer Nanocomposites* - Gerasimos Sotiropoulos, Vissarion Papadopoulos, Manolis Papadrakakis

Graphene, due to its extraordinary mechanical properties, has attracted interest as a filler material in polymer composites. The present work, aims to provide an effective way for the modeling of the mechanical behavior and properties of graphene nanocomposites in multiple scales. Two distinct points in the modeling process of graphene nanocomposites are presented in detail, first the method of simulation of graphene and second the

load transferring mechanism between the matrix and the filler. Single layer graphene sheets (SLGS) can be modeled using atomistic simulation techniques that are computationally expensive and cannot be used effectively for assessing the properties of graphene reinforced nanocomposites. In the present work a continuum mechanics approach is followed for the modeling of graphene. A methodology, proposed in our previous work, is used for the calculation of the effective properties of an equivalent shell element (ESE) that can accurately represent both the membrane and the plate behavior of the SLGS, regardless its size. The interfacial load transferring mechanism between the SLGS and the polymer matrix is simulated by use of a cohesive zone model (CZM) that successfully captures delamination and debonding phenomena. The parameters' values of the traction separation law implemented in the CZM cannot be uniquely chosen due to the dispersion of the available experimental data and their effect on the mechanical properties of the nanocomposite is investigated through an extensive parametric study. Representative volume elements subjected to cyclic loading are used for the estimation of expected nanocomposite properties.

T.4.6 - *Aerodynamic Heating of Ballistic Missile Fin Configuration During Supersonic Flight Conditions* - Stevan Maksimović, Ognjen Ognjanović, M. Maksimović, I. Vasović

This work considers aerodynamic heating and aero-thermo-mechanical analysis of fin type structures on the missile at supersonic flight. At high Mach number the heat due to friction between body and flow, i.e. viscous heating must be taken into account because the velocity field is coupled with the temperature field. The flow field around the fins of the missile and especially the temperature distribution on its surface, as well as aerodynamic-thermal/structural analyses are numerically modeled in ANSYS Workbench environment. Detail investigation was carried out for two Mach numbers at supersonic flight. Available structural experimental results have been used for computational structural mechanics validation and verification, in order to assure credibility of numerical fluid-thermal-structure interaction. In this work a multidisciplinary framework for numerical aerodynamic-thermal/structural analyses, based on only one multi-module software, was used to analyse thermal effects on fin structure during supersonic flights conditions.

T.4.7 - *Thermo-Mechanical Numerical Analysis of Transformation-Induced Stress Relaxation During Pseudoelastic Behavior of SMA* - Vladimir Dunić, Radovan Slavković, Elżbieta Pieczyska

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.

T.4.8 - *Solving Contact Problems Using One-dimensional Finite Elements as Elastic Supports and Application in Angioplasty and Stent Deployment Modeling* - Velibor Isailović, Nenad Filipović, Miloš Kojić

Solving contact problem of two or more solid bodies is a very challenging issue. Contact problems occur very often in engineering, for instance: collision of two cars in crash tests, tire rolling, metal forming processes, coupled engineering parts with clearance, transition or interference fit, etc. There are several approaches that can be implemented in order to solve this problem (Wriggers 2008). This paper shows procedure how simple one-dimensional finite elements can be used as an elastic supports with a goal to provide specific boundary condition between two or more solid bodies. The basic idea is to analyze positions of nodes placed on outer body surface according to the other body surfaces and to add additional stiffness in nodes which are in contact with certain faces of some other solid body. This methodology is general and can be applied to modeling of angioplasty endovascular procedure or modeling of medical stent deployment problem. Initial results of angioplasty numerical model are given in the results section.

T.4.9 - *Bursting Oscillations on Multiple Time Scales: Quantitative Techniques for Two Types of Systems with Cubic Nonlinearity* - Ivana Kovačić

This work is concerned with bursting oscillations – a kind of mixed-mode oscillations in which fast flows occur along periodically changeable slow flows. The corresponding governing equation stems from a non-autonomous oscillator, with a harmonic external excitation that has a low-valued angular frequency. Two cases regarding the existence and influence of cubic geometric nonlinearity are considered: a bistable one and a pure cubic case. Their distinctive characteristics in terms of the corresponding S-curve and the related slow and fast flows are discussed first. Then, two different quantitative techniques are presented to obtain their slow and fast flows as well as the overall response.

T.4.10 - *Software Solution of Cupula's Membrane Deformation Shew for Use in Clinical Praxis* - Radun

Vulović, Milica Nikolić, Nenad Filipović

Human detects angular motion thanks to the excitation that is happening inside the semicircular canals (SCCs) of the inner ear. Afferent hair cells inside the SCCs are the ones that actually play the main role in detecting fluid flow inside those canals.
The present work briefly presents the mechanical and mathematical model behind the cupula membrane deformation during head rotation. Numerical solutions of the full model and a thorough analytical study of the linearized model reveal the principal mechanisms of canalithiasis.
Canalithiasis is a condition where small particles (small calcite particles, i.e. otoconias, syn. otoliths) disturb the flow in the SCCs. That can cause benign paroxysmal positional vertigo (top-shelf vertigo) and in our software we visualise the the membrane deformation for such conditions.

T.4.11 - *Lifetime Predictions of the Car-Carrying Wagon's Axle Guard* - Vladimir Milovanović, Gordana Jovičić, Miroslav Živković

This study focuses on the estimation of lifetime wagon structure's mechanical part. The mechanical part chosen for this investigation is an axle guard of running gear elements of the Hccrrs 2x2 axle car-carrying wagon. The observed axle guard is exposed to low cycle fatigue. Lifetime estimation procedure, based upon experimental and numerical methods has been introduced and applied. A complete cyclic characterization of the material is obtained, including new experimental ε–N fatigue curves for uniaxial tension–compression. The work has been developed using the experimental equipment and procedures available in Centre for engineering software and dynamic testing at Faculty of Engineering University of Kragujevac. According to the obtained experimental investigation and results performed by numerical calculations, the number of cycles until failure of axle guard is obtained.

75th Birthday of Miloš Kojić

This year (2017) we celebrate the 75th birthday of professor Miloš Kojić. Here are briefly presented his personal data and main scientific, professional and educational achievements.

Professor Kojić grew up in the village of Zakuta near Kragujevac, where he finished primary school and then high school in the city of Kragujevac. He graduated in 1964 from the Mechanical Engineering Department in Kragujevac (University of Belgrade), as the first in his generation, and completed MS studies at the Faculty of Natural Sciences of the University of Belgrade in 1969. He obtained his PhD degree in Mechanical Engineering from Rice University, Houston, in 1972.

The professional career of professor Kojić started in 1964, as an assistant for Mechanics at Mech Eng Dept in Kragujevac, and ended by retiring as a full professor in 2007. He was teaching various courses in Mechanics and Computational Methods at the undergraduate and graduate level at the University of Kragujevac, and others, including Univ Sarajevo and Belgrade Metropolitan University. He is the author of more than 10 textbooks.

He was a Visiting Scholar at Mech Eng Dept of MIT, a Research Scientist at Harvard School of Public Heath (10 years); a Research Engineer at ADINA R&D in Watertown, USA (4 years); and a Senior Scientist at Automobile Institute "Zastava" Kragujevac (1/3 of working time, 1975-1990). In 2006 he was elected as the first president of the Serbian Society for Computational Mechanics and the editor of the Journal of the Serbian Society for Computational Mechanics. From 2008 he serves as the director of the Bioengineering R&D Center BIOIRC, which he co-founded. From 2009 he serves as the Senior Member at Houston Methodist Research Institute. In 2009. he became a Corresponding Member of the Serbian Academy of Sciences and Arts.

The main research interest of professor Kojić is computational mechanics and the Finite Element Method in particular. He has over 250 publications, among which are a large number (~150) of scientific papers published in world leading journals. In the first period of his career his research was focused on nonlinear material problems in FEM, where he introduced the effective-stress-function, later generalized to governing parameter method for stress integration. His achievements were reported in a number of papers and summarized in the book: M. Kojić and K. J. Bathe, Inelastic Analysis of Solids and Structures, Springer, 2005. From 1995 his research was mainly oriented to bioengineering problems, particularly related to modeling nonlinear behavior of biologic materials. Results were published in various journals and summarized in the book: M. Kojić, N. Filipović, B. Stojanović, N. Kojić, Computer Modeling in Bioengineering, J. Wiley and Sons, 2008. More recently, from 2009, professor Kojić has been focused on the development of methods and software for modeling convective-diffusive transport of particles and molecules within the capillary system and tissues, particularly related to cancer. Here, he is leading the development of novel computational methodology, resulting finally into smeared models for general biomedical applications.

Professor Kojić is the founder and PI of the general-purpose FE program PAK (abbreviation in Serbian for Program for Structural Analysis), initiated in 1975. The PAK program is today composed of many moduli, including: structural analysis with geometrical and material nonlinearities (with large number of material models), fracture mechanics, field problems (fluid mechanics, heat transfer, flow through porous media), coupled problems (solid-fluid interaction, heat transfer and mechanics, flow through deformable porous media); biomechanics with tissue models, muscle

models, plaque growth models coupled with blood flow, convective-diffusive transport within capillary and tissue systems, multiscale hierarchical diffusion models, smeared models with composite finite element formulation. Based on the development of the computational methodology and PAK software (with modern pre-and post-processing) a large number of national and international (EU, USA) projects, as well as industrial, have been realized over the past several decades. Also, a significant number of MS and PhD theses (around 50) have been completed, and around 40 researchers are currently engaged in Kragujevac (University of Kragujevac – Faculty of Engineeing Sciences and Faculty of Sciences, and R&D Center BIOIRC) within several groups in the engineering and biomedical engineering fields. It can be said that a Serbian school of computational mechanics has been established in Kragujevac (currently with 15 professors and more than 30 researchers).

For his overall achievements in science, engineering, education and contribution to the Serbian society, a number of distinguished awards have been given to professor Kojić, including Diploma of the City of Kragujevac and Gold Medal of the Serbian Engineering Society.