

COMPUTATIONAL MECHANICS IN SCIENCE,
APPLICATIONS AND TEACHING

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According to: *Tib Journal Abbreviations (C) Mathematical Reviews*, the abbreviation TEOPM7 stands for TEORIJSKA I PRIMENJENA MEHANIKA.

COMPUTATIONAL MECHANICS IN SCIENCE, APPLICATIONS AND TEACHING

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Abstract. *We express our opinion about the role of Computational Mechanics (CM) in science, applications and education. The presented thoughts rely on our experience gained by working over decades (first author in particular) in the field of CM.*

First, as a challenge of an opinion that computational mechanics is rather a tool, not the science, we give our view that computational mechanics is a complex interdisciplinary scientific field where new methods and solutions are sought, new hypotheses are tested, and events in material world are elucidated or predicted. It is quite an art to achieve the goal that general analytical formulations or experimental findings become useful and practical numbers, graphs, and even simulations of living systems response.

Second, we would like to emphasize the enormous impact of CM in applications; ranging from the support of experimental investigations, to everyday engineering in design and industry, to bioengineering and medicine. Giant steps have been undertaken by invention of the finite element method in the 6th decade of last century. From that time on, a huge number of researchers have opened new frontiers, introducing new computational methods, improving the algorithms and incorporating achievements in computer technology.

Third, we want to address the issue of the CM participation within university programs. We believe that the CM methods, software development and application should be a significant part of the overall education in engineering departments, but also (to appropriate extent) in other departments of natural and biomedical sciences, technology and medicine. All courses should be accompanied by the corresponding software. We here cite our experience where around 40 PhD and MS theses have been completed at University of Kragujevac, with the CM topics, development of engineering software (our system of programs PAK) and applications in engineering and bioengineering. This approach in education will result in preparing students to use modern CM tools and software in their work after university studies.

Key words: *methods of computational mechanics, finite element method, discrete particle methods, computer application, education*

1. INTRODUCTION

Mechanics is the branch of applied science concerned with the study of mechanical phenomena: the behavior of solids, fluids, and complex materials under the action of forces. CM is that sub-discipline of mechanics dealing with the use of computational methods and devices to study events governed by the principles of mechanics. It is fundamentally important part of computational science and engineering based on the use of computational approaches to characterize, predict, and simulate physical events and engineering systems governed by the laws of mechanics (Oden, 1987).

It can be considered that CM has three aspects (Felippa, 1994). The first one is engineering application; this is mainly in the fields of classical and recently developing new engineering disciplines. The second one, the backbone of the field, is the theoretical mechanics which uses continuum approach. The third one is the numerical solution of the analytical equations.

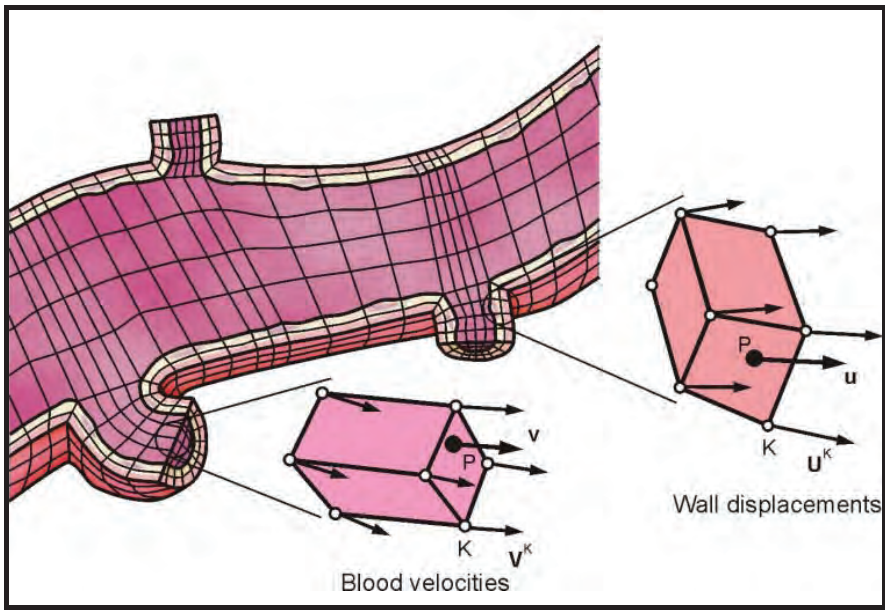


Fig. 1 Fluid and solid finite elements used in modeling blood flow with blood vessel deformation (according to Kojic et al. 2008)

The main goals of CM are directed to the development and application of computational methods based on the principles of mechanics. With the use of these

computational methods CM has had a profound impact on science and technology. It has effectively transformed much of classical Newtonian theory into practical and powerful tools for prediction and understanding of complex systems and for creating optimal designs. Active research topics include improvements of classical (Figs. 1 and 2) and development of new finite element methods (e.g. discontinuous Galerkin method), computational acoustics and fluid-structure interaction, algorithms for dynamical and transient transport phenomena, adaptive solution schemes using configurational forces, modeling the behavior of complex materials and biological tissue, and coupled problems (multiphysics) where multiple interacting physical fields are modeled. Methods and algorithms for high performance computing including massively parallel computing (Morton, 1976) are important for complex applications are currently in development stage. A recent research in CM is focused on multiscale methods to solve problems involving mutually dependent events occurring on different time and length scales.

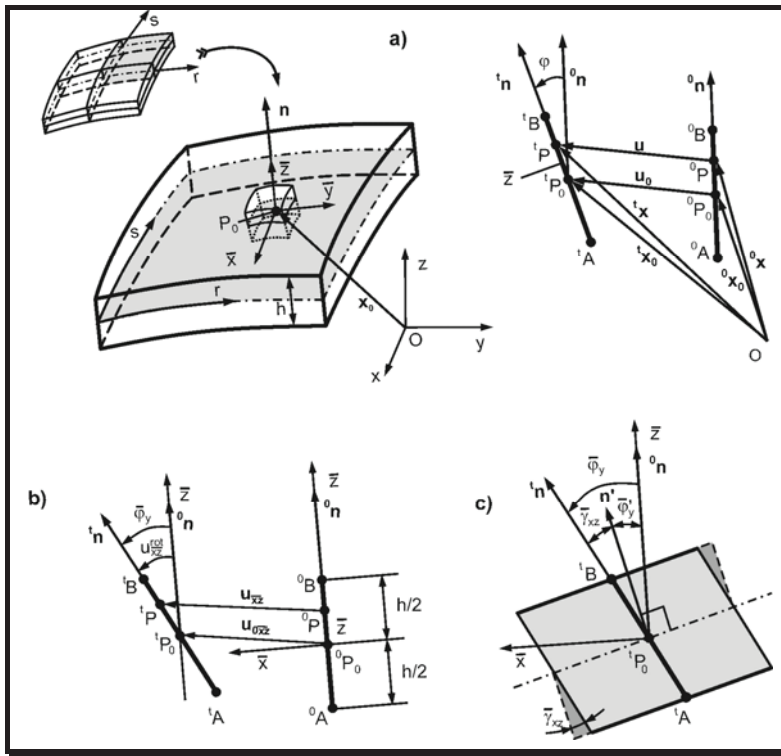


Fig. 2 Shell finite element which relies on the classical theory of shells, used in structural mechanics (according to Kojic et al. 2008)

In the next sections we present several examples to illustrate the role of CM in various fields, ranging from treating the fundamental problems in mechanics to applications to practical problems which could not be addressed without the CM

methods. Then, a brief discussion regarding the role of CM in education is given, followed by concluding remarks.

2. SELECTED EXAMPLES OF USE OF CM METHODS

Applications of CM methods in science, engineering and medicine are so broad that it is very hard to select the most representative examples. Based on our experience, we here give a few examples in which we and our collaborators have been involved, which may illustrate complexity and variety of CM methods.

2.1. Flamant problem in solid mechanics

The famous Flamant problem in solid mechanics (Flamant 1892) represent the problem of finding the solution of the stress distribution when an elastic semi-space is loaded by concentrated force normal to the free surface. It is known from experiments that tensional stresses develop in the vicinity of the force action point, but which cannot be obtained by classical continuum mechanics theory. Use of a microstructural doublet mechanics (DM) theory (Ferrari et al 1997) is illustrated graphically in Fig. 3. A challenge was to develop a computational procedure to include the DM so that it can be used for general analyses of problems involving microstructural material description.

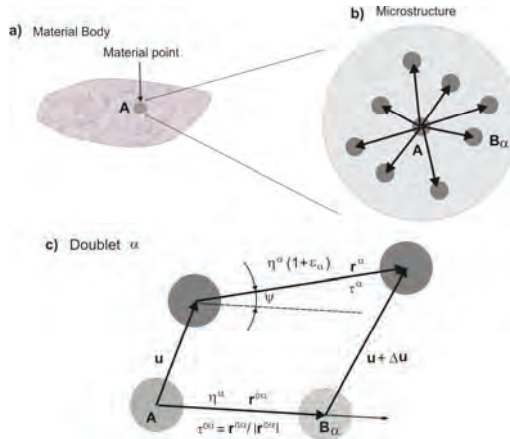


Fig. 3 Microstructural kinematics of deformation described according to doublet mechanics theory (Ferarri et al. 1997)

The basic equation expressing elongation strain of a “doublet” (a pair of neighboring particles used for microstructure representation) is given as

$$\epsilon^\alpha = \sum_{\chi=1}^M \frac{\eta_\alpha^{(\chi-1)}}{\chi!} \tau_j^\alpha T_{k_1 k_2 \dots k_\chi}^\alpha \frac{\partial^{k_1 k_2 \dots k_\chi} u_j}{\partial x_{k_1} \partial x_{k_2} \dots \partial x_{k_\chi}} \approx T_{jk}^\alpha \frac{\partial u_j}{\partial x_k} + \frac{\eta_\alpha}{2} T_{jkm}^\alpha \frac{\partial^2 u_j}{\partial x_k \partial x_m} \tag{1}$$

sum on $j, k, m = 1, 2, 3$; no sum on α

where T_{jk}^α are coefficients as products of directional cosines of the doublet, u_i are displacements and η_α is the microstructural scaling factor. This equation has been built into the FE framework and the correctness of the methodology and software (PAK, Kojic et al. 1998, 2010) is illustrated in Fig. 4.

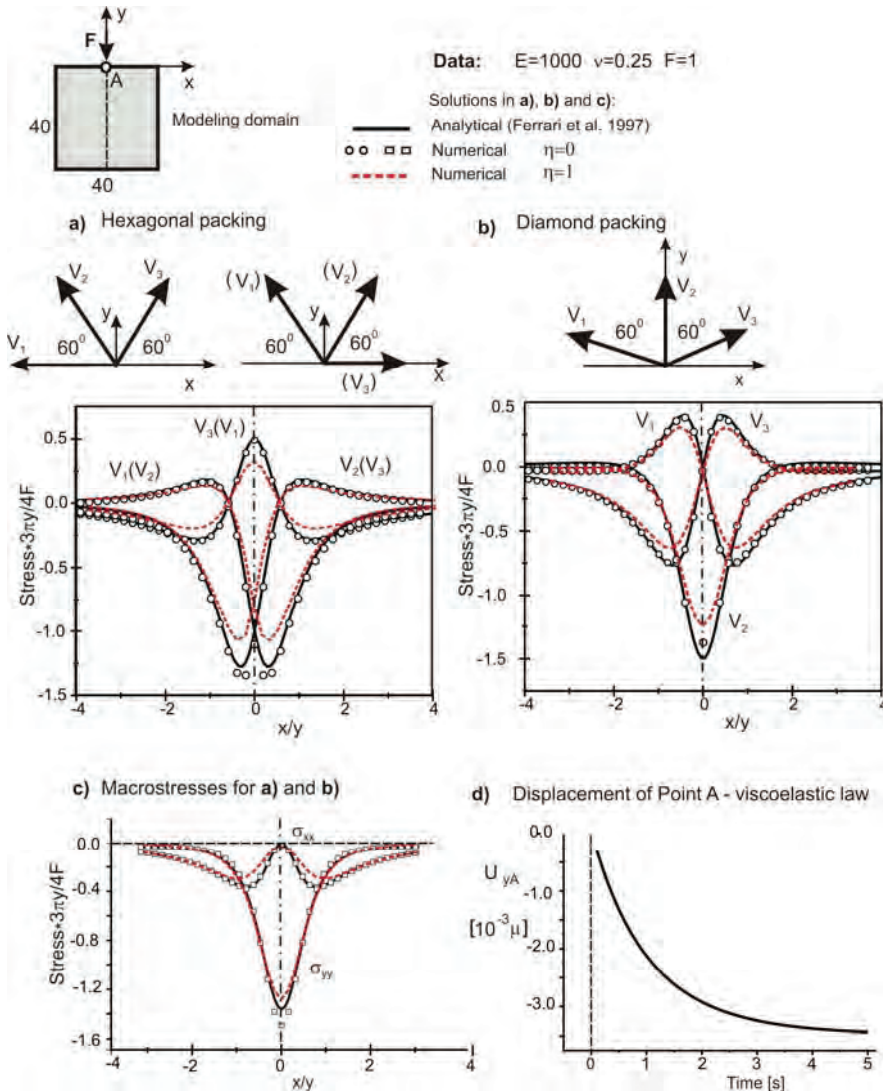


Fig. 4 Flamant problem. Microstresses for the three doublets: a) Hexagonal packing (two orientations); b) Diamond packing. c) Macrostresses for both packings a) and b). d) Displacement of the point A where the constant force is acting during time for the viscoelastic constitutive relations (according to Kojic et al. 2011).

2.2. Modeling of inelastic deformation of material

Material response to mechanical or other loadings (such as thermomechanical) is described by a constitutive law which relates the stress vs. deformation measures. The constitutive law can be simple, as linear elastic, but it can be very complex, described by complex functions and parameters, and can include the material history of deformation. Examples of these constitutive laws are those used for elastic-plastic or creep deformation of engineering materials, or for biological materials. Constitutive relationships are usually established by simple experiments (e.g. for metal plasticity, Kojic and Bathe 2005). However, it has been a challenge to find material response in real conditions of loading within structures or in biological systems, and generally represents a scientific task and art to develop adequate computational methods. We here show one concept, known as the governing parameter method (GPM), introduced in Kojic (1996) for modeling inelastic material deformation; and its application to a real engineering problem.

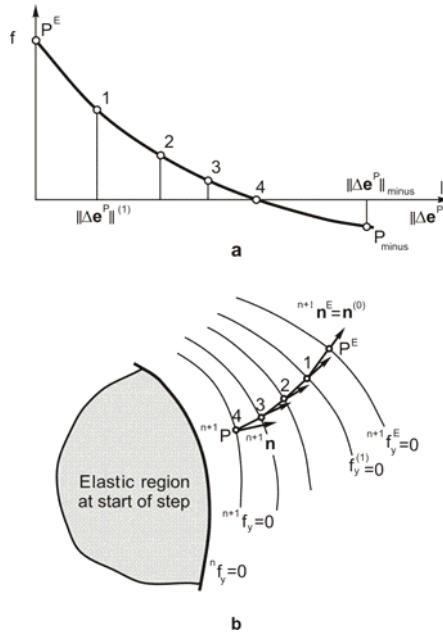


Fig. 5 Return mapping according to the GPM. a) A bisection procedure in finding zero-value of the governing function – solution is between points P^E and P_{minus} . b) Graphical interpretation of search the final point ^{n+1}P starting from P^E (according to Kojic and Bathe 2005).

Using the GPM it is possible to implicitly integrate constitutive law (providing the best solution accuracy) within a load step and to satisfy the yield condition at end of the step, see Fig. 5. In case of plasticity, the problem of calculation of stresses and plastic strains is reduced to finding the zero of a monotonic function,

$$f\left(\|\Delta\mathbf{e}^P\|\right) = {}^{n+1}f_y\left({}^{n+1}\boldsymbol{\sigma}^E - \|\Delta\mathbf{e}^P\|\mathbf{C}^E {}^{n+1}\hat{\mathbf{n}}, {}^n\boldsymbol{\beta} - \|\Delta\mathbf{e}^P\|\hat{\mathbf{C}}^P {}^{n+1}\mathbf{n}_\beta\right) \quad (2)$$

where $\Delta\mathbf{e}^P$ are increments of plastic strains, $\boldsymbol{\sigma}^E$ are elastic stresses, \mathbf{C}^E is elastic constitutive matrix, $\hat{\mathbf{C}}^P$ is the matrix related to internal parameters $\boldsymbol{\beta}$, $\hat{\mathbf{n}}$ and \mathbf{n}_β are normals to corresponding to yield surface f_y and internal parameters; and the left upper index $n+1$ indicate that evaluation of quantities is performed at end of load step. This solution procedure is illustrated in Fig. 5, generally termed as the return mapping.

Figure 6 shows FE solution and comparison with experiment for large deformation of a car joint, based on the GPM within the program PAK.

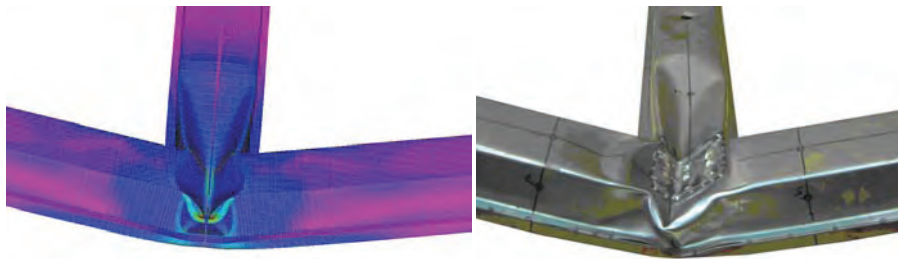


Fig. 6 Finite element solution (large strain elastic-plastic analysis) and experimentally determined deformation of a joint of car structure (Zivkovic and collaborators 2006)

2.3. Muscle model

Modeling of biological materials remains a big challenge and requires further experimental data and specific computational methods. Some solution concepts are presented in Kojic et al. (2008). Here, we show a model of tongue using a relatively simple Hill’s model and imaging technique to simulate motion of tongue produced by internal excitation which is governed by the nervous system and biochemical processes within the tongue tissue.

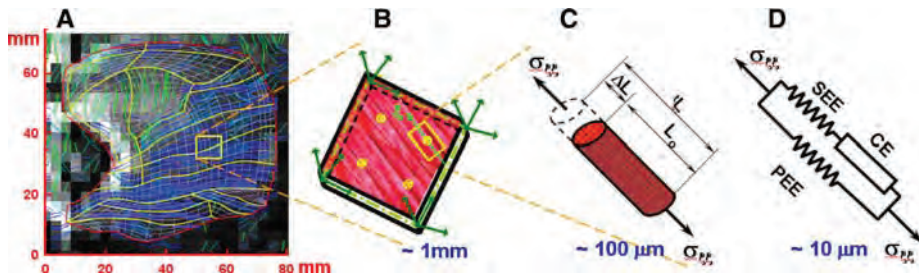


Fig. 7 Multiscale model of tongue contraction. Muscle fibers are determined using a DTI tractography images (the left panel), the domain is discretized into finite elements with fibers, and material behavior is described by Hill’s model for fibers deformation (according to Mijailovic et al. 2010)

Computational procedure form muscle modeling introduced in Kojic et al. (1998) and further generalized in Stojanovic et al. (2007), is implemented to tongue model (Mijailovic et al. 2010), Fig. 7.

Field of active stresses for two specific times is shown in Fig. 8.

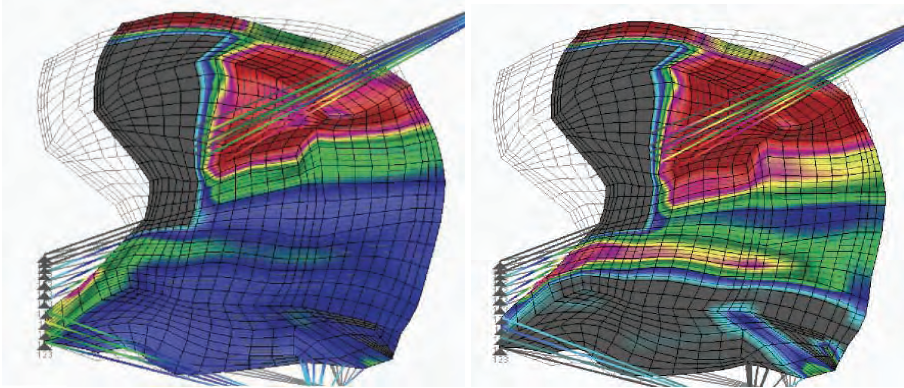


Fig. 8 Active stress distribution within the tongue for: a) $t=370\text{ms}$ and b) $t=500\text{ms}$ (according to Mijailovic et al. 2010)

2.4. Mass transport of LDL through blood flow and plaque growth model

Fluid flow problems and transport phenomena have been the subject of investigations over centuries. Many problems have been solved in analytical form for simple boundary conditions. However, those analytical methods are practically of no use for complex flows and mass transport. Methods of computational mechanics enable us today to treat the real engineering, scientific and medical problems. Here we select few of those of interest in medicine. The first one is related to transport of the LDL proteins within the blood, which cause plaque initiation and growth.

The model of plaque formation include the following processes: a) transport of the LDL within blood (fluid domain); b) transport of LDL within tissue (solid domain); and plaque formation within the tissue.

The governing equations for blood flow are described by the Navier-Stokes equations and continuity equation (here for incompressible fluid), while the mass-balance diffusion equation (with diffusive and convective terms) is the governing equation for the concentration field of the LDL within the blood. Those equations can be transformed to the FE balance equations and further used for general boundary conditions, today in a routine manner.

Specifics for this problem are first related to mass transfer of LDL within the arterial wall, which coupled with the transmural flow. This mass transport is modeled by a convection-diffusion-reaction equation as follows

$$\nabla \cdot (-D_w \nabla c_w + k c_w u_w) = r_w c_w \quad (3)$$

in the wall domain, where c_w is the solute concentration in the arterial wall, D_w is the solute diffusivity in the arterial wall, K is the solute lag coefficient, and r_w is the

consumption rate constant. Second, the LDL transport in lumen of the vessel is coupled to these equations by Kedem-Katchalsky equations (details are given in (Filipovic et al 2010)).

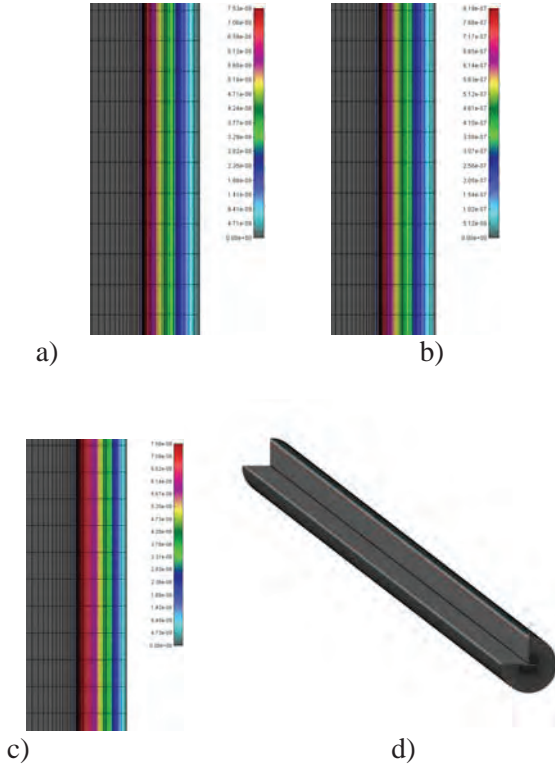


Fig. 9 a) Oxidized LDL distribution 0.37%; b) Macrophages distribution 4.2% from media; c) Cytokines distribution 0.39%; d) three-dimensional representation of the model

Finally, the model of plaque formation includes the inflammatory process. This process is described by three additional reaction-diffusion partial differential equations (Calvez et al 2008), (Boynard et al 2009):

$$\begin{aligned}
 \partial_t Ox &= d_1 \Delta Ox - k_1 Ox \cdot M \\
 \partial_t M + \text{div}(v_w M) &= d_2 \Delta M - k_1 Ox \cdot M + S / (1 - S) \\
 \partial_t S &= d_3 \Delta S - \lambda S + k_1 Ox \cdot M + \gamma (Ox - Ox^{thr})
 \end{aligned} \tag{4}$$

where Ox is the oxidized LDL in the wall, M and S are concentrations in the intima of macrophages and cytokines, respectively; d_1, d_2, d_3 are the corresponding diffusion coefficients; λ and γ are degradation and LDL oxidized detection coefficients; and v_w is the inflammatory velocity of plaque growth, which satisfies Darcy's law and continuity equation (Filipovic et al 2010). Since geometry of the blood vessel changes during inflammation, a 3D mesh moving algorithm and ALE (Arbitrary Lagrangian Eulerian) formulation for fluid dynamics was applied (Filipovic et al 2006).

The above models are incorporated into a FE scheme and solved using massive computational procedures, as well as experimental data for material constants and imaging technique for geometry of blood vessels. The computed results are verified by experimental observations using histology analysis and image processing. Figure 9 shows the computed distributions of the three model constituents within a blood vessel wall, while in Fig. 10 are given graphs of distributions within the media of the wall.

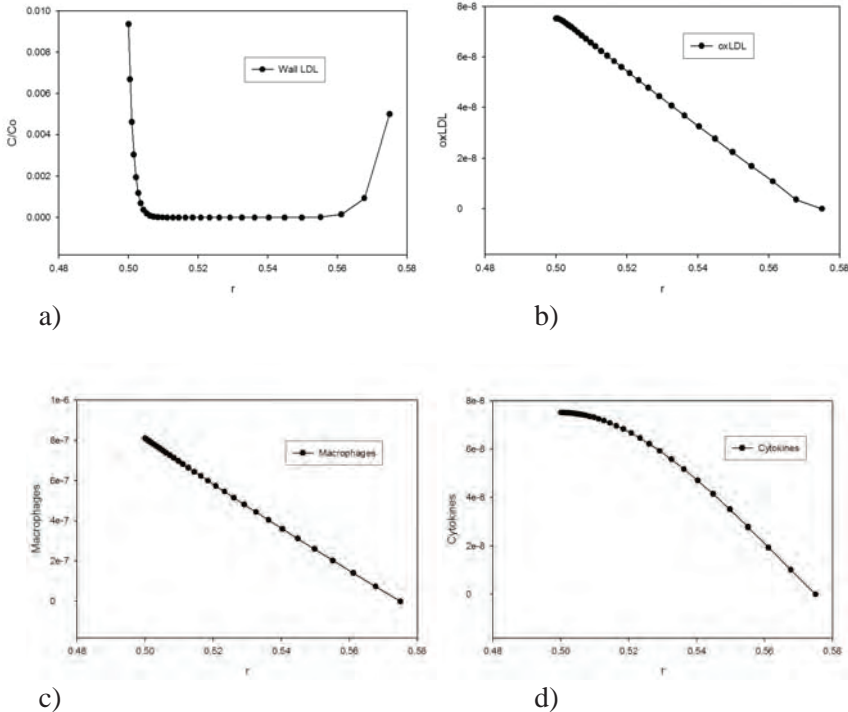


Fig. 10 a) Dimensionless wall LDL concentration profile in the media; b) Oxidized LDL concentration profile in the media c) Macrophages profile in the media d) Cytokines profile in the media

2.5. Self-healing material model using Dissipative Particle Dynamics (DPD)

A self-healing material is used to cover surfaces of vital parts of structures in order to prevent corrosion. When a nanoscopic scratch occurs, a healing material follows from nanocontainers into scratches. This process can be modeled using molecular dynamics (Tyagi et al 2004). Another approach to this problem is a mesoscopic modeling using the DPD method (Groot and Warren 1997, Filipovic et al. 2008a,b). Here we show how the DPD can be applied in modeling the self healing process.

Motion of each DPD particle (further called “particle”) is described by the following Newton law equation:

$$m_i \dot{\mathbf{v}}_i = \sum_j (\mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R) + \mathbf{F}_i^{ext} \quad (5)$$

where m_i is the mass of particle “ i ”; $\dot{\mathbf{v}}_i$ is the particle acceleration as the time derivative of velocity; \mathbf{F}_{ij}^C , \mathbf{F}_{ij}^D , and \mathbf{F}_{ij}^R are the conservative (repulsive), dissipative and random (Brownian) interaction forces, that particle “ j ” exerts on particle “ i ”, respectively, provided that particle “ j ” is within the radius of influence r_c of particle “ i ”; and \mathbf{F}_i^{ext} is the external force exerted on particle “ i ”, which usually represents gradient of pressure or gravity force as a driving force for the fluid domain. The total interaction force $\mathbf{F}_{ij} = \mathbf{F}_{ij}^C + \mathbf{F}_{ij}^D + \mathbf{F}_{ij}^R$ (Fig. 11). Description of these forces is given in literature (e.g. Groot and Warren 1997).

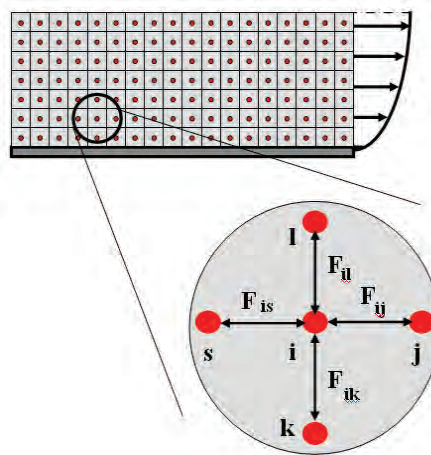


Fig. 11 Interaction forces in the DPD method.

The additional interaction forces between particles of inhibition agents, which are placed in the primer layer and metal substrate particles, are added similarly as it was done in a model of thrombosis in Filipovic et al. (2008a) (also in Jovanovic and Filipovic 2006, Filipovic et al. 2008c). These attractive forces are expressed as

$$F_a = k_{sf} \left(1 - \frac{L_{sf}}{L_{sf}^{\max}} \right) \quad (6)$$

where L_{sf} is the distance of the inhibition particle from the substrate, k_{sf} is the effective spring constant, and L_{sf}^{\max} is the maximum length of inhibition particle attractive domain.

Solution example is shown in Fig. 12. This DPD model, with inhibitors in the primer layer with thickness of 4 μm , consists of a 2D rectangle crack domain with depth of 0.1 mm. Total number of DPD particles was 24 000 (240x100). Diameter of nanocontainer

was 100 nm and concentration of nanocontainers inside the primer layer was 10%. The total number of time steps for simulation was 100 000.

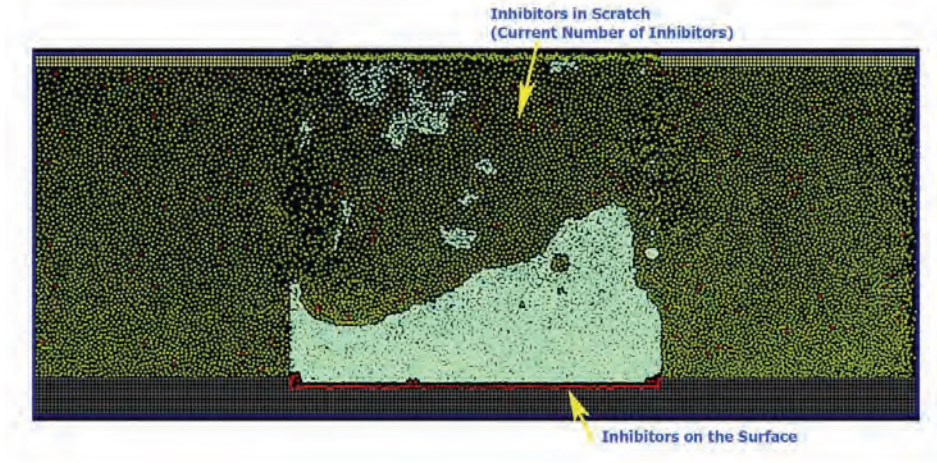


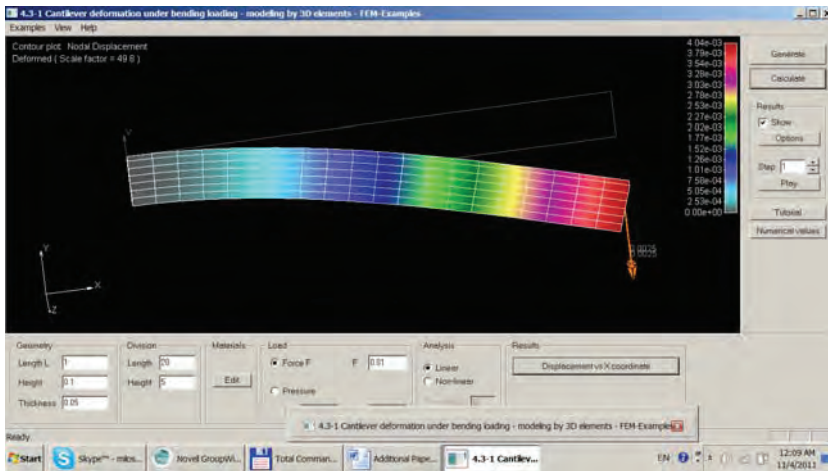
Fig. 12 The DPD model after 100 000 time steps (200s). Red particles represent the inhibition particles, green particles make primer layer, grey particles (substrate) are considered to be fixed in space domain. The surrounding particles are shown with light blue color and represent the fluid.

3. COMPUTATIONAL MECHANICS IN EDUCATION

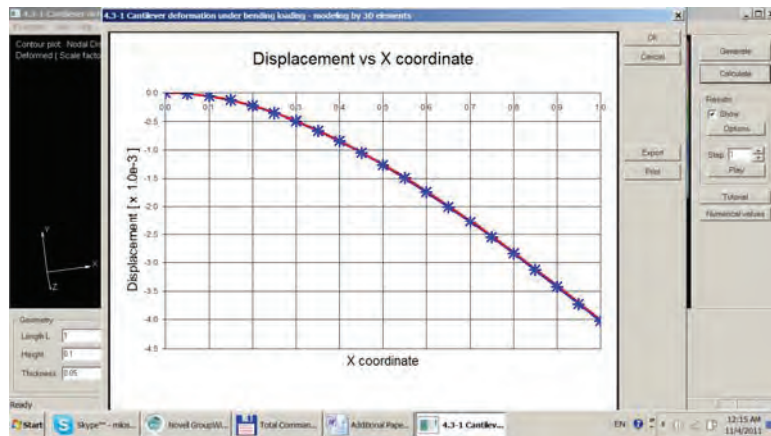
Courses in Mechanics has a tradition in Serbia as solid, well designed and lectured, supported by exercises and literature. Those courses refer to mechanics of rigid and deformable bodies and fluid mechanics. On the other hand, due to development of computer technology new courses in informatics emerged at almost all departments in natural and technical sciences and medicine.

However, courses in computational mechanics are quite rear in any of the current level of education. Based on the current stage of CM, its use in various fields of science, technology and medicine, illustrated above through several examples, and from our experience, we offer the following ideas.

- There should be special at departments in technical sciences and mathematics devoted to computational mechanics. The courses should be accompanied by use of various software packages within exercises. Example of use of such software is shown in Fig. 13.



a)



b)

Fig. 13 Use of software in Kojic et al. (2008) to parametrically model beam bending. a) Displacement field; b) Comparison of analytical (solid line) and FE (dots) solutions.

- Advances courses in mechanics should include parts related to CM as an extension of the classical analytical methods.
- Within courses in medicine there should be sections devoted to computer modeling. There, without going to deep into theoretical considerations, it is possible to connect the basic procedures in medicine with the possibilities of modeling using computational methods and software. Figure 14 illustrates blood flow through an aneurism can be modeled by using a software package.

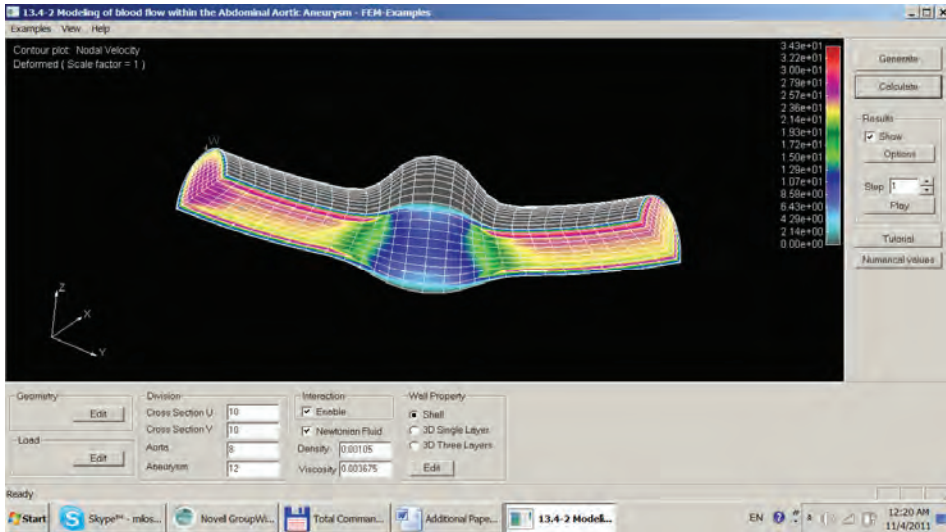


Fig. 14 Computed velocity field of blood within an aneurism (software accompanying book Kojic et al. 2008)

The above ideas are particularly of interest in the Ph.D. programs, within courses and research.

4. CONCLUDING REMARKS

The main goals of this discussion are to outline the role of CM in research and education. This discussion is based on experience of the authors and their collaborators.

In modern research it is simply a necessity to use methods of CM and software to be able to elucidate problems in various fields of science, technology and medicine.

Teaching courses in Computational Mechanics should be designed for students to become familiar with modern methods of computational mechanics and various applications. The courses may contain theoretical background, with details usual for any other branch of scientific disciplines, for students of mathematically or technically oriented studies. For students in the fields where CM and software are used as a tool for modeling purpose, the courses should be oriented to applications, with an outline of the theoretical background.

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RAČUNSKA MEHANIKA U NAUCI, PRAKTIČNOJ PRIMENI I OBRAZOVANJU

M. Kojic **N. Filipovic**

U radu pokazujemo ulogu računске mehanike u nauci, praktičnoj primeni i obrazovanju. Izlaganje se oslanja na naše iskustvo stečeno dugogodišnjim radom (posebno prvog autora) u oblasti proračunske mehanike.

Prvo, kao odgovor na mišljenje da je računska mehanika radije alat, a ne nauka, dajemo naš pogled da je računska mehanika kompleksna interdisciplinarna naučna oblast gde se traže nove metode i rešenja, testiraju nove hipoteze, i razjašnjavaju i predviđaju pojave u materijalnom svetu. Prava je umetnost postići da uopštene analitičke formulacije ili eksperimentalni rezultati budu pretvoreni u praktične brojeve, grafike, ili čak simulacije odziva živih sistema. Drugo, želeli bismo da naglasimo ogroman uticaj računске mehanike, počevši od podrške eksperimentalnim istraživanjima, svakodnevnih inženjerskih poslova u dizajnu i industriji, bioinženjeringu i medicini. Preduzeti su ogromni koraci otkrivanjem metode konačnih elemenata u šestoj deceniji predhodnog veka. Od tada, ogroman broj istraživača je pomerio granice, otkrivajući nove računске metode, poboljšavajući algoritme i povezujući nauča dostignuća sa kompjuterskom tehnologijom.

Treće, želimo da se pozabavimo pitanjem uključivanja računске mehanike u univerzitetske programe. Verujemo da računska mehanika, razvoj i primena softvera moraju zauzimati značajnu ulogu u ukupnom obrazovanju na inženjerskim smerovima, ali takođe (u odgovarajućoj meri) i na ostalim smerovima prirodnih i biomedicinskih nauka, tehnologiji i medicini. Sva predavanja treba da imaju softversku podršku. Naše iskustvo se ogleda u približno 40 odbranjениh doktorskih i magistaskih teza na Univerzitetu u Kragujevcu, na temu proračunske mehanike, razvoja inženjerskog softvera (naš softver PAK) i primena u inženjerstvu i bioinženjeringu. Ovakav pristup će rezultovati osposobljavanjem studenata da rukuju modernim alatima i softverima računске mehanike u njihovom poslu posle studija.

Ključne reči: metode računске mehanike, metoda konačnih elemenata, diskretna čestična metoda, kompjuterska aplikacija, obrazovanje

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