Convergence analysis and validation of a discrete element model of the human lumbar spine

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ABSTRACT

Degenerative diseases of the spine can lead to or hasten the onset of additional spinal problems that significantly reduce human mobility. The spine consists of vertebral bodies and intervertebral discs. The most degraded are intervertebral discs. The vertebral body consists of a shell (cortical bone tissue) and an internal content (cancellous bone tissue). The intervertebral disc is a complex structural element of the spine, consisting of the nucleus pulposus, annulus fibrosus, and cartilaginous plates. To develop numerical models for the vertebral body and intervertebral disc, first, it is necessary to verify and validate the models for the constituent elements of the lumbar spine. This paper, for the first time, presents discrete elements-based numerical models for the constituent parts of the lumbar spine, and their verification and validation. The models are validated using uniaxial compression experiments available in the literature. The model predictions are in good qualitative and quantitative agreement with the data of those experiments. The loading rate sensitivity analysis revealed that fluid-saturated porous materials are highly sensitive to loading rate: a 1000-fold increase in rate leads to the increase in effective stiffness of 130 % for the intervertebral disc, and a 250-fold increase in rate leads to the increase in effective stiffness of 50 % for the vertebral body. The developed model components can be used to create an L4-L5 segment model, which, in the future, will allow investigating the mechanical behavior of the spine under different types of loading.

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1. Introduction

The problem of treatment of patients with degenerative-dystrophic lesions in the lumbar spine still remains unsolved. The intervertebral disc undergoes the greatest degenerative changes, which requires replacement with an artificial element. The structure of intervertebral disc is rather complex that ensures the redistribution of stresses in the vertebral body (Nikkhoo et al., 2018). Degenerative-dystrophic changes in the lumbar spine significantly affect the spine mobility. The parts of the spine in the lumbar region (L3-S1) are subject to the greatest damage. Experimental studies based on in-vitro and in-vivo methods are used to study the influence of various factors on the spine biomechanics. Ex-vivo studies focus mainly on histological data and the results of magnetic resonance imaging, radiography, which determine degenerative-dystrophic changes in the structure of vertebral body, intervertebral discs (Lao et al., 2015), (Kaya Ayvaz et al., 2021), changes in geometric characteristics of the elements of the spine and assess the kinematics of the system (Liu et al., 2016). Testing machines are used to study the mechanical properties of the spine (Mantell et al., 2016). The purpose of their use is to determine the stiffness of the systems (Daniels et al., 2013) and the critical force characterizing the onset of fracture in the spine (Xiang et al., 2021). The above-described methods of experimental research provide important information about the kinematic and structural parameters of the spine. However, they are not capable to determine a strain/stress distribution pattern under dynamic loading, for example such as impact. Moreover, empirical research on some issues is time-consuming, costly, and ethically constrained. Computer modeling makes it possible to determine the influence of different factors on the material behavior at different scales (Konovalenko et al., 2009, Balokhonov et al., 2021). Concerning the biomechanical processes in the spine, most of computer simulations were carried out on the basis of the finite element method utilizing the commercial software packages such as ANSYS and ABAQUS (Naoum et al., 2021). The methods based on the continuum representation of the material provide a good understanding of the kinematics of the process and the patterns of the stress and strain fields. However, modeling fracture and discontinuities in materials in these methods is debatable and a rather laborious process. Therefore, it is urgent to develop numerical models that allow describing material discontinuities, cracking, etc., to predict the mechanical behavior of the spine under various loading conditions, as well as to predict the service life during arthroplasty. Before numerical study of the mechanical behavior of the spine, it is necessary to carry out verification and validation of the developed model (Mengoni, 2021). One of the important aspects of modeling in biomechanics is determining the velocity sensitivity of the developed model (Bezci et al., 2015).

The aim of this work is to develop a numerical model of the mechanical behavior of the vertebral body and intervertebral disc under dynamic loads based on the method of computational particle mechanics. Validation, verification, and sensitivity analysis of the developed models are also performed in this study.

2. Materials and Methods

2.1. Method of movable cellular automata

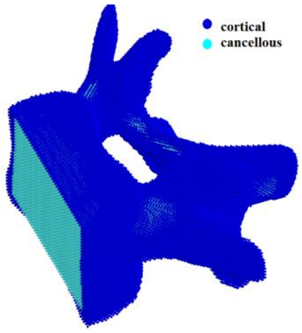
To describe the mechanical behavior of biological tissues, herein we used the model of a poroelastic body implemented in the method of movable cellular automata (MCA) (Psakhie et al., 2001), (Shilko et al., 2015), which is an efficient method of computational particle (discrete) mechanics. It has been established that discrete methods have proven themselves to be very promising for modeling contact loading of different materials at the macro and mesoscale (Psakhie et al., 2001), (Smolin et al., 2014). In the MCA method, a solid is considered as an ensemble of discrete elements of finite size (cellular automata) that interact with each other according to certain rules, which, within the particle approach and due to many-body interaction forces, describe the deformation behavior of the material as an isotropic elastoplastic body. The motion of the ensemble of elements is governed by the Newton-Euler equations for their translation and rotation. Within the framework of the MCA method, the value of averaged stress tensor in the volume of an automaton is calculated as a superposition of forces that act to the areas of interaction of the automaton with its neighbors (Shilko et al., 2015). It is assumed that stresses are homogeneously distributed in the automaton volume. Knowing the components of the averaged stress tensor allows adapting to MCA different models of plasticity and fracture of classical mechanics of solid.

The description of the fluid-saturated material in the MCA method is based on the use of such effective (implicit) characteristics as the volume fraction of interstitial fluid, porosity, permeability, and the ratio of the macroscopic bulk modulus of elasticity to the bulk modulus of the solid skeleton of the material (Psakhie et al., 2016). The fluid filtration in the material is governed by Darcy's law. The mechanical effect of pore fluid on stress and strain of the solid skeleton of the automaton is described using Biot's linear poroelasticity model, therefore, pore fluid pressure affects only the diagonal components of the stress tensor (Basniev et al., 2012). Herein, to describe the strength properties of the sold skeleton of the bone tissues, we used the model of elastic-brittle medium with von Mises' criterion of fracture. Previously, the verification and validation of poroelastic models of tissues of the femur and tibia based on the MCA method were carried out by Shilko et al. (2021), Eremina et al. (2019), and Chirkov et al. (2020).

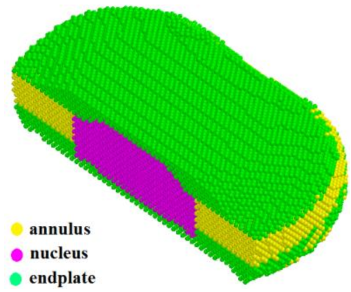
2.2. Models of the vertebral body and intervertebral disc

The lumbar spine consists of such elements as the vertebral body (Figure 1, a) and the intervertebral disc (Figure 1, b). In its turn, the vertebral body of the spine consists of a cortical shell and an inner part of cancellous tissue (Figure 1, a). The intervertebral disc has a three-component structure: nucleus, annulus, and cartilaginous plates (endplate) (Figure 1, b). The solid CAD model of the vertebral body was taken from the

Internet (L4 vertebral body, 2021). The CAD models for other components (cortical shell, nucleus, endplates, and annulus) were created by the authors using the FreeCAD software.



a)



b)

Figure 1. Parts of the models with their cross-sections for (a) vertebral body L4 and (b) intervertebral disc L4-L5.

The properties of biological tissues used herein and presented in Table 1 correspond to the data provided by Schmidt et al. (2010) and Fan et al. (2018). Cortical tissue serves as a hard shell; it has low porosity and permeability (Xu et al., 2016). The spongy tissue has both high porosity and high permeability. The material of the cartilaginous plates is of great importance for its high porosity and relatively low permeability. Cancellous and cartilage tissues have different elastic characteristics at different scales (Wolfram et al., 2010). Thus, compression experiments (macroscale) show the value of the elastic modulus for spongy tissue within 100 MPa (Garo et al., 2009, Ogurkowska & Błaszczyk, 2020). At micro- and nano-indentation (the penetration depth of the indenter corresponds to the size of the matrix cells), the elastic modulus reaches 10-15 GPa for spongy tissue (Haj-Ali et al., 2017) and 7-10 GPa for cartilaginous tissue (Dall'Ara et al., 2013).

Table 1. Poroelastic parameters of the lumbar spinal tissues.

Tissue	Density ρ, kg/m^3	Young's modulus E, MPa	Poisson's ratio ν	Porosity, θ	Permeability k, m^2
Annulus	1060	2.5	0.20	0.8	$3{\cdot}10^{-19}$
Nucleus	1060	1.5	0.30	0.8	$3{\cdot}10^{-19}$
Endplate (cartilage)	1000	5.0	0.46	0.8	$7{\cdot}10^{-18}$
Cortical	1850	1000	0.30	0.04	$1{\cdot}10^{-16}$
Cancellous	700	100	0.20	0.7	$1{\cdot}10^{-19}$

2.3. Loading and boundary conditions

At uniaxial compression of the model of lumbar spine, the mechanical load was applied by setting the same displacement velocity in the vertical direction to the upper layer of the automata while fixing the automata of the lower layer of the sample (Figure 2 a, 3 a). At the initial stage, the velocities of the automata of the upper layer increased smoothly from 0 to V m/s (where V differs for different tests, and its particular value is given below), and then remained constant. This scheme was used to eliminate artificial dynamic effects and ensure a smooth and fast transition of the sample deformation process to a quasi-static regime (Romanova et al., 2019, 2019a). For the automata of the upper and lower layers of the sample, horizontal displacements were allowed, and the lateral surfaces of the sample were free.

3. Results of simulation

3.1. Verification

The purpose of verification is to check the effectiveness of the scheme for numerical integration of the equations embedded in the method. The main method used for model verification is convergence analysis.

For example, Jones & Wilcox (2008) consider the object discretization as optimal when the further increase in mesh resolution gives less than 5% of the accuracy.

In this work, in order to analyze the convergence of a three-dimensional model of the vertebral body and intervertebral disc, we studied the difference in the model stiffness with a varying discretization of the solid CAD model under consideration (Figures 2, 3).

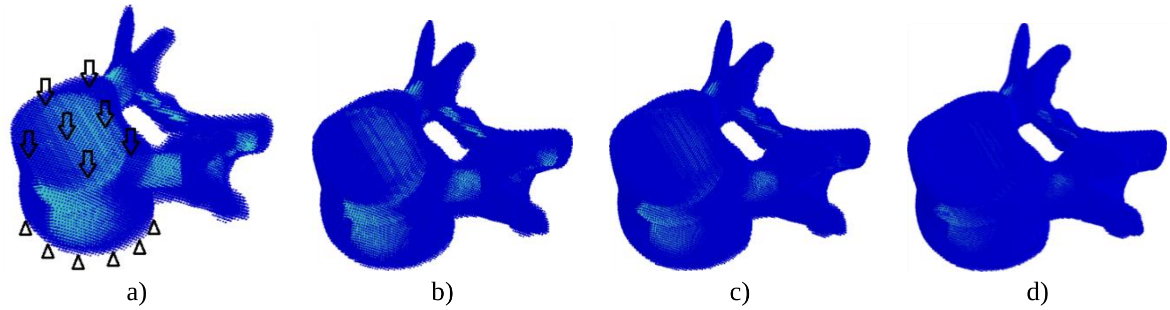


Figure 2. Model samples of the vertebral body L4, presented as a package of automata with different number of elements: a) 99340 (with loading scheme), b) 189564, c) 387209, d) 444287.

For the model samples of the vertebral body and intervertebral disc, the loading was set by choosing the velocity value of *V* equal to 10 mm/s and 25 mm/s, respectively (Figures 2, a and 3, a).

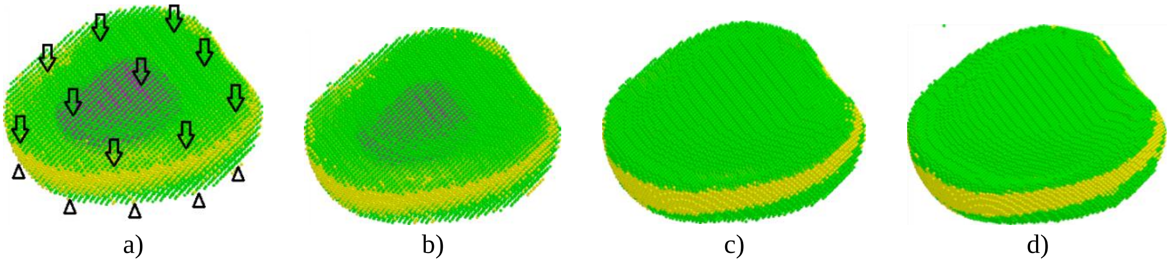


Figure 3. Model samples of the intervertebral disc L4-L5, presented as a package of automata with different number of elements: a) 23549 (with loading scheme), b) 435692, c) 89319, d) 105287.

The models were verified by changing the model discretization. Based on the calculated data, we analyzed convergence of the model stiffness (global parameter) with an increase in the number of automata *n* and a corresponding decrease in the automaton size (Figure 4).

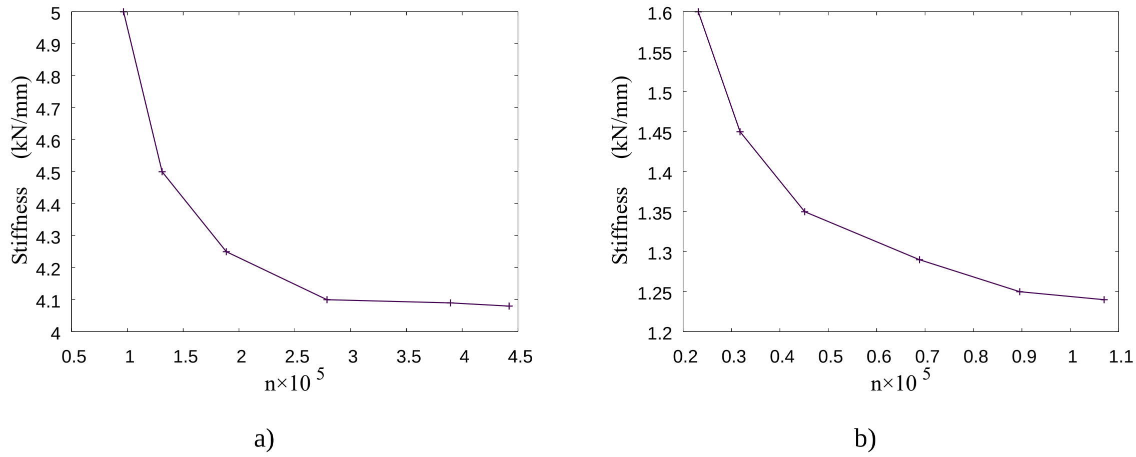


Figure 4. Stiffness versus number of elements in the model for: a) vertebral body L4, b) intervertebral disc L4-L5.

The results of the convergence of the stiffness values with increasing the number of elements showed that the maximum difference in stiffness between the minimum sampling and the maximum sampling does not exceed 20 % (Figure 4). In the case of the vertebral body, the difference in the stiffness values of the model samples with the number of automata equal to 387209 and 444287 is less than 5 %. In the case of the intervertebral disc, it was shown that the difference between the stiffness values of the model sample with the numbers of automata 89319 and 105287 is also less than 5 %. Thus, the analysis results showed that samples with the number of automata 387209 and 89319 for the vertebral body and intervertebral disc, respectively, can be considered to be representative.

3.2. Validation

Model validation is a test of the effectiveness of the equations embedded in the method to simulate real behavior and properties of the subject of the study. That is why a model validation is based on comparing the simulation results with experimental data. The model is never "right" for every possible scenario and application; the validation process focuses on a specific case of interest (Mengoni, 2021). Herein, the validation of the developed model for the vertebral body was performed by comparing the simulation results for the model stiffness with the experimental data by Garo et al. (2011). The loading velocity according to the literature data was chosen equal to 10 mm/s. The results obtained (Figure 5, a) demonstrate good agreement with the literature data by Garo et al. (2011) but they are also close to the data by Stemper et al. (2015).

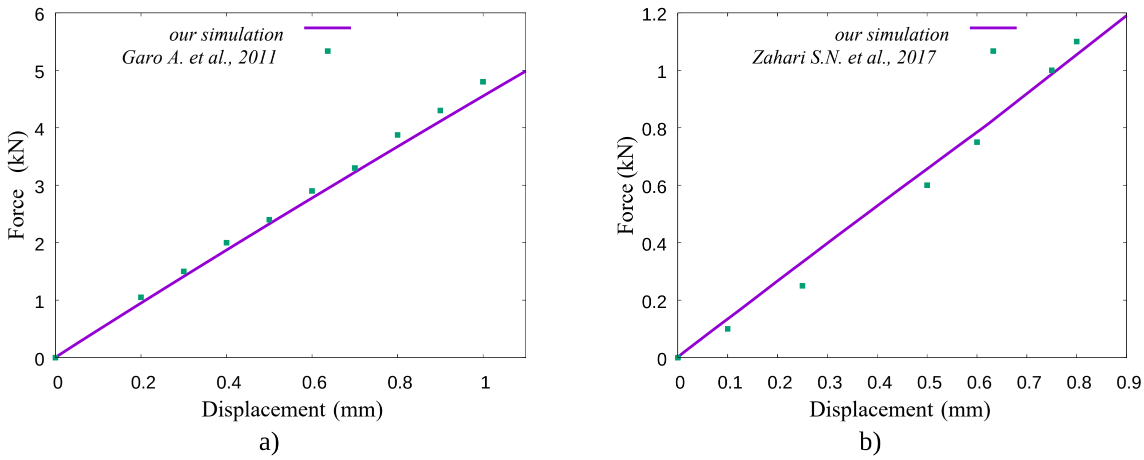


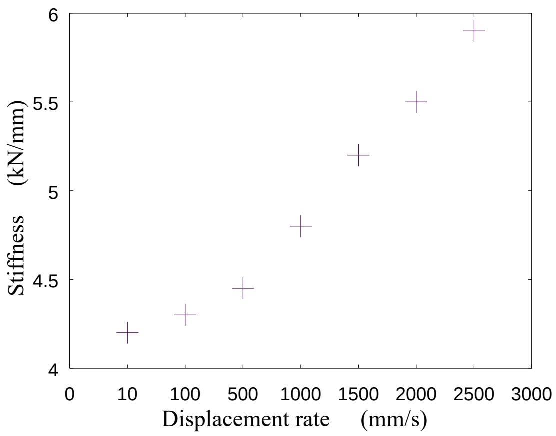
Figure 5. Compressive force versus displacement at different loading rates for (a) vertebral body (L4) and (b) intervertebral disc (L4-L5).

Then, the stiffness validation for the intervertebral disc model was carried out by comparing the simulation results with the experiments by Zahari et al. (2017). The displacement rate was chosen 25 mm/s in accordance with the procedure for carrying out the corresponding experiments. The results obtained are presented in Figure 5 b, they also show good agreement with the literature data; it is worth noting that our data are also very close to other experiments by Markolf & Morris (2001) and Konz et al., (2001).

The results of the validation of three-dimensional models of the vertebral body (L4) (Figure 5 a) and intervertebral disc (L4-L5) (Figure 5 b) showed that the use of poroelastic models allows us to account for loading rate influence on the response of the biological tissues of the elements of the lumbar spine. Thus, using the proposed models it is possible to correctly describe the mechanical behavior of the vertebrae and intervertebral discs under dynamic loading.

3.3. Sensitivity analysis

It is known that the segments of the spine are fluid-saturated bodies and are highly sensitive to the loading rate. Based on the results of the verification and validation, it was found that the stiffness of the vertebral body L4 is 4200 N/mm. Next, the effect of the loading rate on the stiffness of the model vertebral body in the range from 10 to 2500 mm/s was investigated. With a 250-fold change in speed, the increase in effective stiffness is about 50 % (Figure 6 a). It should be noted that the obtained values of the stiffness at different loading rates are consistent with the data presented by Ochia et al. (2003), Stemper et al. (2015), and Garo et al. (2011).



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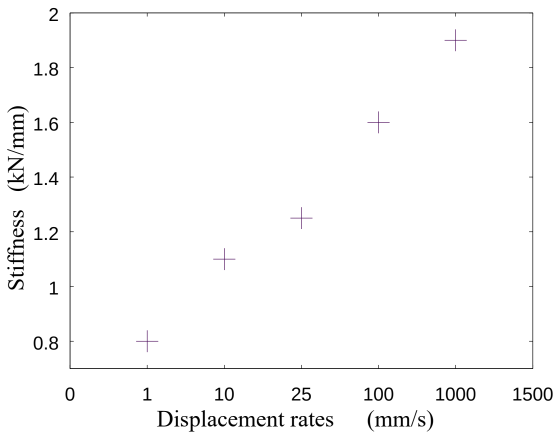

b)

Figure 6. Stiffness versus displacement rate for (a) lumbar vertebral body (L4) and (b) intervertebral disc (L4-L5)

The intervertebral disc is highly porous (its total porosity is about 80%) and fluid-saturated body sensitive to loading rate (Bezci et al., 2015), (Nikkhoo et al., 2018). In this work, we investigated the effect of the displacement rate in the range from 1 to 1000 mm/s under uniaxial compression of the disk. With a 1000-fold change in speed, the increase in effective stiffness is about 130% (Figure 6 b). The resulting trend of the stiffness dependence on the loading rate is consistent with the data presented by Jacobs et al. (2014), Strange et al. (2010), Amin et al. (2016), Jamison et al. (2013), and Newell et al. (2017).

The results of the analysis of the loading rate sensitivity of the elements of the lumbar spine showed that the intervertebral disc is the most sensitive to this parameter. Such difference in the loading rate sensitivity is most likely related to the high porosity of all materials that make up the disk. In the case of the vertebral body, the cortical shell, which has low porosity, promotes a protective function.

4. Conclusion

This article presents the verification, validation, and velocity sensitivity analysis of the 3D models of the basic elements of the lumbar spine. For the analysis, the method of movable cellular automata was used.

Verification, as it always should be, precede validation to ensure that errors associated with the discretization of the object under study can be distinguished from errors caused by the incorrect choice of physical and mechanical parameters of the model. The convergence analysis showed that the model samples of the lumbar vertebral body (L4) and intervertebral disc (L4-L5) are representative ones if the number of discrete elements in them exceeds 387209 and 89319, respectively.

The models of the elements of the lumbar spine were validated using uniaxial compression experiments. For this, the results obtained from numerical calculations were compared with experimental data from the literature. The analysis of such a comparison showed a good quantitative agreement of the calculated data with the experimental results.

It is known that fluid-saturated porous materials are very sensitive to loading rate. The analysis of the loading rate sensitivity showed that with an increase in the loading speed, the value of the effective elastic characteristics increases, which, in turn, is consistent with the experimental data.

Based on the results of the work, it was established that the developed numerical poroelastic models of the spine elements based on the MCA method could be successfully used in the future to construct three-dimensional models of the segment of the lumbar spine to predict the stress and strain fields in the system and assess the risk of its injuries under dynamic loads.

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