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DEVELOPMENT OF SUBSYSTEM SOFTWARE FOR RESEARCH OF EXPERIMENTAL CONSTRUCTIONS FOR THE FEMUR REINFORCING

І.В. Прокопович, О.В. Савєльєва, Т.І. Старушкевич. **Розробка підсистеми дослідження експериментальних конструкцій для армування стегнової кістки.** Армування кістки є одним з самих ефективних хірургічних втручань, а розробка, вдосконалення і виробництво імплантатів спрямовано на створення якісних, надійних конструкцій, здатних зберігати свої функціональні властивості упродовж тривалого часу. Одним з найважливіших етапів розробки і проектування силових конструкцій, що імплантуються, є біомеханічне обгрунтування їх працездатності і надійності. В статті наведено розробку та апробацію програмної підсистеми дослідження експериментальних конструкцій для превентивного армування стегнової кістки, вивчення особливостей створення таких систем. Підсистема проектування, запропонована в статті, є допоміжним модулем для програмного забезпечення Ansys, написаний на мові програмування Python в середовищі PyScripter. Він дозволяє побудувати якісну картину напружено-деформованого стану в деякому вибраному об'ємі шийки стегна, провести уточнення сітки кінцевих елементів та завдання крайових умов, що в свою чергу використовується для проведення математичного розрахунку напруженого стану. Дослідження включає розрахунок напружених станів у інтактній двошаровій кісці для виявлення критичних точок – точок початку руйнування кортикального слою кістки. Розрахунковий модуль, що створено, полегшує взаємодію с програмним забезпеченням, дозволяючи більш точно вказувати необхідні умови проведення експерименту. На основі отриманих в ході експериментів результатів, можна зробити висновок о корисності використання як створеного модулю, так і створених моделей. Результати проведення експерименту чисельне демонструють ліпші характеристики армованої кістки на відміну від інтактної.
Ключові слова: тривимірне моделювання, система ANSYS, мова програмування Python, профілактичне армування, імплантати, метод кінцевих елементів, аналіз на міцність, розрахунок навантажень

I. Prokopovich, O. Savelyeva, T. Starushkevych. **Development of subsystem software for research of experimental constructions for the femur reinforcing.** Bone reinforcement is one of the most effective surgical interventions. In addition, development, improvement and production of implants aimed at creating high quality, reliable structures that can retain their functional properties for a long time. One of the most important stages in the development and design of implantable power structures is the biomechanical justification of their performance and reliability. The article presents the development and testing of a software subsystem for the study of experimental structures for preventive reinforcement of the femur, as well as the study of the peculiarities of the creation of such systems. The design subsystem, which is proposed in the article, is an auxiliary module for Ansys software, written in the Python programming language in the PyScripter environment. It allows you to build a qualitative picture of the stress-strain state in a selected volume of the femoral neck, to refine the grid of finite elements and set boundary conditions, which in turn used for mathematical calculation of the stress state. The study includes the calculation of stress states in the intact bilayer bone to identify critical points of onset of destruction of the cortical layer of bone. The created calculation module facilitates interaction with the software, allowing specifying more precisely necessary conditions of carrying out experiment. Based on the results obtained during the experiments, we can conclude about the usefulness of using both the created module and the created models. The results of the numerical experiment show better characteristics of the reinforced bone in contrast to the intact.
Keywords: three-dimensional modeling, ANSYS system, Python programming language, preventive reinforcement, implants, finite element method, strength analysis, load calculation

Introduction

Bone reinforcement is one of the most cost-effective surgical interventions. In addition the development, improvement and production of implants is aimed at creating high-quality, reliable structures that can retain their functional properties for a long time**.** In this regard, one of the most important stages in the development of implants is the biomechanical justification of their performance and reliability, ie the ability of implant materials to resist destruction or irreversible deformation under the action of functional loads of different nature and size [1, 2].

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Today, the capabilities of modern computer technology and software are widely used to solve this problem. The most common method of solving this problem is mathematical (computer) modeling of mechanical behavior of the system “Implant - body structures” in the process or as a result of load [3]. Extensive capabilities of modern computer technology and software and a powerful universal mathematical apparatus provide sufficient reliability, efficiency and flexibility in predicting the behavior of such systems. It takes into account the influence of many internal (system structure, material properties, conditions of interaction of system components at the interface, etc.) and external (type, magnitude, points of application of loads, limiting the movement of points and volumes of the system, etc.) factors [4].

Analysis of the main achievements and literature (Materials and research methods)

As shown by studies of designed implants using computer simulations, as well as experience in technical and clinical trials, changes to the design of the implant or its properties are appropriate at the level of the calculated mechanical parameters of 70…80 % of the critical. This is due to many reasons and their possible unfavorable combination [5, 6]. First, the accuracy of the calculation results is limited both by the capabilities of the most commonly used mathematical method and the modeling technique. With an acceptable time to calculate the option, determined by the complexity of the created model, the absolute error of the result can be 5…10 %. In addition, it is necessary to take into account the possibility of exceeding the actual load on the implant compared to the calculated, the mismatch of the actual position of the implant with its “ideal” installation in the model, differences in anatomy and properties of body structures from the average values and many other factors [7, 8 , 9].

The combined effect of these factors should be “compensated” by the coefficient of safety margin, which is equal to the ratio of the “critical” parameter of mechanical behavior of this component of the system (stress or deformation, maximum allowable displacement, etc.) to the corresponding design value. Ideally, this ratio should be at least 1.3…1.5 [9, 10]. The very achievement of this coefficient was set as a task in this work. Due to the complex geometry of the femur and femoral neck, mathematical modeling of bone tissue in the work will be carried out only on the basis of numerical approaches, for example, on the basis of the finite element method (FEM). Therefore, in addition to geometry and internal structure for numerical experiments, it is important to choose the size of the finite element, so as not to lose the main features of the structure of bone tissue.

If in metallic materials the finite element can be reduced to the size of a crystal lattice, the size of which is very small, then the bone does not have a crystal lattice. Moreover, the more precisely the finite element grid specifies the volume of the structural element, the more accurate the solution we get in terms of mathematics. Thus, it is necessary to determine the size of the structural element of bone tissue, which will justify the choice of the size of the final element [10].

Bone tissue is a complex multistage biocomposite material. Due to the lack of scientific materials and research on the mechanical characteristics of this natural composite, the construction of the model will use known data at the level of macromechanics (effective average characteristics) [11, 12].

For a full-fledged study within the model of macromechanics of continuous media, it is most optimal to use the minimum linear size $d = 0.3$ mm, which represents the distance between the centers of osteons. Osteon is a structural unit of compact matter. Osteocyte bone cells are arranged concentrically, forming circular systems (osteons) and consist of 5 to 20 cylindrical plates inserted into each other. In the center of each osteon is a channel in which blood vessels and nerves are located.

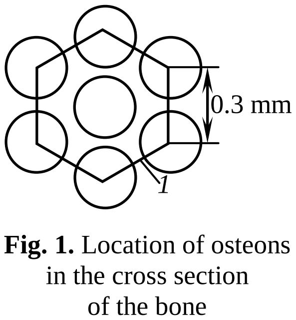

Fig. 1. Location of osteons in the cross section of the bone

Osteons are close to each other, forming a strong structure. This value ($d = 0.3$ mm) is used as the minimum allowable linear size of the bulk finite element in the numerical solution of boundary value problems to assess the stress-strain state in bone tissue, because osteon is the minimum bulk unit of biocomposite material at the level of macromechanics of solid media (Fig. 1) [13, 14].

By static processing of a series of X-rays, the “average” parameters of the femur were determined, which correspond to the average human weight of 75…80 kg. The length of such an average femur was 400…420 mm, the offset distance from the longitudinal axis of the femur to the center of the femur (or the center of rotation of the joint) was 40…43 mm, and the diameter of the bone marrow canal in the isthmus was 12…13 mm [13, 14].

In [15, 16, 18], when constructing a finite element model of the bone, it was experimentally shown that to model the stress-strain state of the femoral neck, it is sufficient to use the upper 2/3 of the femur in the calculations. This fact significantly simplifies the geometric complexity of the femur and, accordingly, saves CPU time of the numerical experiment.

The purpose of the study, problem statement

The purpose of the research presented in this article is to develop and test a software subsystem for the study of reinforced femur. The relevance of the topic is to study the features of creating systems and tools for the study of experimental structures for preventive reinforcement of the femur. The research methods considered in the work are a synthesis of the analysis of the scientific literature and the experimental approach both for creation of three-dimensional models, and for writing of the subroutines (modules) intended for research of these models. Mathematical modeling can also provide useful information about the behavior of the implant and the interacting structures of the body in “abnormal” situations due to, for example, errors in the planning and technique of the operation itself. This information allows you to formulate additional (to medical) “technical” justification for the correct choice and exact installation of the implant.

Femoral implant design subsystem

Design subsystems implement the concept of a software component. According to the purpose of the subsystem, computer-aided design systems are divided into those that design and maintain. Designers include subsystems that perform design procedures and operations. For example, the subsystem of logical design, the subsystem of design, the subsystem of technological design, the subsystem of design of parts and assembly units, etc. The service subsystems include subsystems designed to maintain the performance of design subsystems. For example, the subsystem of information retrieval, the subsystem of documentation, the subsystem of graphical display of the design object, etc. [17]. Subsystems at the level of formalization of tasks are separate units. Their main functions are automation of individual sections of the most time-consuming design processes, including input and output of information, production of documentation, etc. Subsystems at the level of the computer-aided design system considered at this stage are complex design complexes aimed at automating the design of individual components of complex products.

The femoral implant design subsystem is a design system that is responsible for automating the method of numerical solution of the problem of calculating the stress-strain state in the femoral neck. The main task of using this subsystem is to determine the influence of the location of the implant, the angle of its inclination in the bone on the stress-strain state. The design subsystem proposed in the article is an auxiliary module for Ansys software [17], written in the Python programming language. The main functions of the proposed module are to set the boundary conditions for the imported model according to the scheme proposed in the figure, to determine the critical points of the highest voltage and derive the results.

Algorithm for numerical solution of the problem:

1. Research using the developed module of the intact bone model:
   1.1. Establishment of boundary conditions;
   1.2. Initial construction of a grid of finite elements;
   1.3. Definition of critical points;
2. Study of options for placement of the implant in the bone:
   2.1. Tasks of boundary conditions for the system “Bone – implant”;
   2.2. Study of changes in voltage in the areas of critical points
3. Output of the voltage tensor component in the OZ direction.
4. Calculation of the evaluation of the effectiveness of reinforcement of different implant placement.

In order to accurately calculate in Ansys software, it is necessary to clearly indicate the physical characteristics of the material and boundary conditions. In this study, the mechanical characteristics of

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Table 1

Mechanical characteristics of materials: E is the Young's modulus, v is the Poisson's ratio

Material	E, Pa	v
Cortical bone	$1.7 \cdot 10^{10}$	0.32
Spongy bone	$3.25 \cdot 10^{8}$	0.29

the bone in the elastic region were used under the assumption of isotropic and homogeneity of titanium implants. Numerical values of the Young's modulus and Poisson's ratio are presented in Table 1. Hereinafter, the Young's modulus for the cortical bone is denoted by Ek, and for the spongy bone - Es. The data in the Table 1 indicate that the "stiffness" of the spongy tissue is almost 2 orders of magnitude lower than that of the cortical bone.

One of the most important steps of the study is the choice of kinematic and force boundary conditions when setting boundary value problems in extreme conditions of load (fall).

In [18], an experiment was described that allows to determine the magnitude of the loads acting on the body. The experiment involved 14 subjects (men and women) under the age of 35 weighing from 49 to 92 kg. During the experiment, the person was in a supine position on the platform (Fig. 2). The man with the platform was brought up and then released.

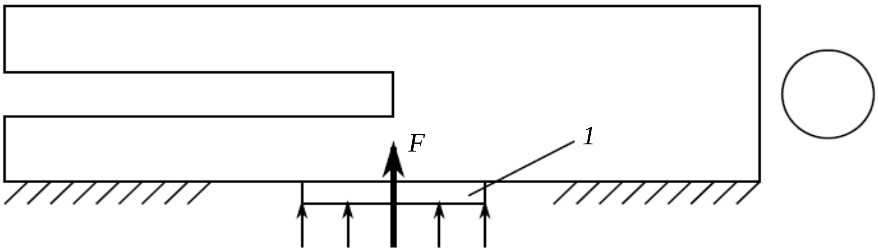

Fig. 2. Apparatus for conducting experiments in the conditions of "pelvic release": F is the resulting force of the distributed load acting on the platform *1* for high-precision load measurement

The rate of fall of the subject was set by calculating the rate of fall of the body from a height of 0.55 m from the amount of growth (corresponding to the center of gravity in the standing position). To determine the typical load acting on the proximal thigh, when falling, the concept of "Effective mass" was introduced, which presses at the moment of falling on the proximal region.

"Effective mass" takes into account the soft tissues in the thigh and depends on whether the muscles are tense or not. On average, it is 55 kg of human weight.

As a result of the experiment, it was found that the impact force corresponded to 6100 N with relaxed muscles and 12000 N with tense muscles in men. In women, the figures are 5050 N and 6370 N, respectively.

Different studies use the same principle of fixation of the studied bone. Therefore, the kinematic and force boundary conditions can be set as shown in Fig. 3.

From the point of view of the mechanics of a deforming rigid body, there is no fundamental difference between applying a load to the femoral head and fixing a large skewer, and a mirror image when the load is applied to a larger skewer and the head is fixed.

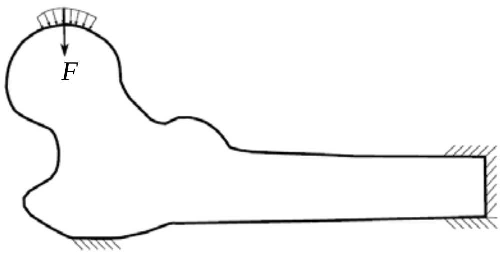

Fig. 3. Kinematic and force boundary conditions in the fall of man: F is the resulting force of the distributed load acting on the head of the femur

The principle of operation of the created software module

The designed module consists of a set of modules written in Python in the PyScripter environment. It allows you to build a high-quality picture of the stress-strain state in some selected volume of the femoral neck. The commands.py module allows you to interact with the standard set of commands offered in Ansys. The module implements the AnsysCommander class, which contains the numbers of the last points, lines, surfaces and volumes, as well as commands in the text representation.

When calling different methods of a class in the text representation the next set of commands is written down. The class implemented a small set of commands required for this study. Once a class is created and methods are called to compose the desired sequence of commands, a string representation can be obtained through the getOut () method.

Example of using the AnsysCommander class:

Listing 1. Example of using the AnsysCommander class

```
cmd = AnsysCommander (10 ,20 ,30 ,40)
cmd .k (3.5 ," −1.7" ,0)
cmd .k (3.5 ," −1.7" ,0 , 10)
cmd . getOut ()
# return :
# K ,11 ,3.5 , −1.7 ,0
# K ,10 ,3.5 , −1.7 ,0
```

The core.py module is used by almost all routines because it implements the basic functions required by most programs, namely:

– getCurrentPath () – returns the current directory;

– readFile () \ saveFile () – read / write file;

– readFormattedSigmas () – reading the values of voltage components in nodes in the list format (n, sx, sy, sz, sxy, syz, szx, sint);

– readFormattedNodes () – read the coordinates of nodes in the list format (*n*, *x*, *y*, *z*);

– readNodes () – reading the coordinates of nodes in ANSYS format, ie dividing the nodes into 20 lines and ANSYS signatures;

– equalsDouble () – comparison of non-integers with a certain accuracy;

– distance () – calculation of the distance between points, the coordinates of which are represented as arrays.

The specialCommands.py module generates ANSYS commands to run the calculation in the createSolveCommands () method.

The delta.py module determines the average distance between the specified point and the nearest nodes. The coordinates of the point and the number of nearest nodes are specified in the program parameters.

The areadist.py module determines the minimum distance between the two nodes closest to a given point.

The first function of the module used is to refine the finite element grid. The ANSYS software package allows for “intelligent” finite element (FE) partitioning, the algorithm of which is adapted to complex geometry. Implemented FE splitting for the femur demonstrates that the distance between the nodes of the FE of this grid is greater than the required distance of 0.3 mm. Clarification of the FE grid in the entire femur is unjustified, because this study examines the stress-strain state in the neck of the femur, as well as due to increased requirements for PC due to a sharp increase in the complexity of the task. Therefore, a module for local refinement of the FE grid in the vicinity of the points specified in the program was developed.

Before starting the calculation, a code is generated to obtain the coordinates of the nodes. Subsequently, the search for voltage values is performed on these coordinates. It is necessary to receive coordinates before performance of calculation as after the decision coordinates of knots will change. The result of running the specialCommands.py module to get a list of nodes is seen in Listing 2:

Listing 2. Commands for displaying the coordinates of all nodes in the file

```
*get , NNUMMAX ,node ,,num , max
*del , NARRAY
```

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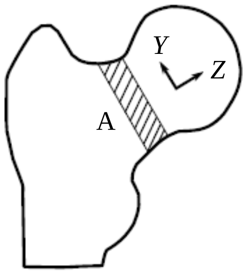

Fig. 4. Area and local coordinate system for refining the FE grid

```
*dim , NARRAY ,array , NNUMMAX ,11
*vget , NARRAY (1 ,2) , node ,,loc ,x
*vget , NARRAY (1 ,3) , node ,,loc ,y
*vget , NARRAY (1 ,4) , node ,,loc ,z
*vfil , NARRAY (1 ,1) , ramp ,1 ,1
* cfopen , nodesLoc , txt
* vwrite
(‘NODE ‘ ,10x,’X ‘ ,10x,’Y ‘ ,10x,’Z ‘)
* vwrite , NARRAY (1 ,1) , NARRAY (1 ,2) , NARRAY (1 ,3) , NARRAY (1 ,4)
(F8 .0,tl1 ,’ ‘,E12 .5,’ ‘,E12 .5,’ ‘,E12 .5)
* cfclos
```

In the sectionmesh.py module the refinement of a grid of finite elements in the set area is implemented, for example, as it is shown in Fig. 4. To do this, set the parameter of the section - the coordinate on the axis and the thickness of the region A (located between two flat sections) in the coordinate system shown in Fig. 4. The coordinates of the nodes are also displayed in this coordinate system. All nodes in this area are selected and ANSYS commands are generated for them to refine the grid. In addition, the program can specify the refinement level and scope for the ANSYS-command NREFINE. The result of the program is a set of calls to commands for execution in ANSYS.

Clarification of the grid FE in the area does not allow you to create a grid FE acceptable sampling area for calculations on a desktop PC, because a large number of nodes leads to memory overflow.

This program was applied to the cross section and points AA′ of Fig. 5, or more precisely, to the cross section of the plane containing AA′ and the O*X* axis in the local coordinate system.

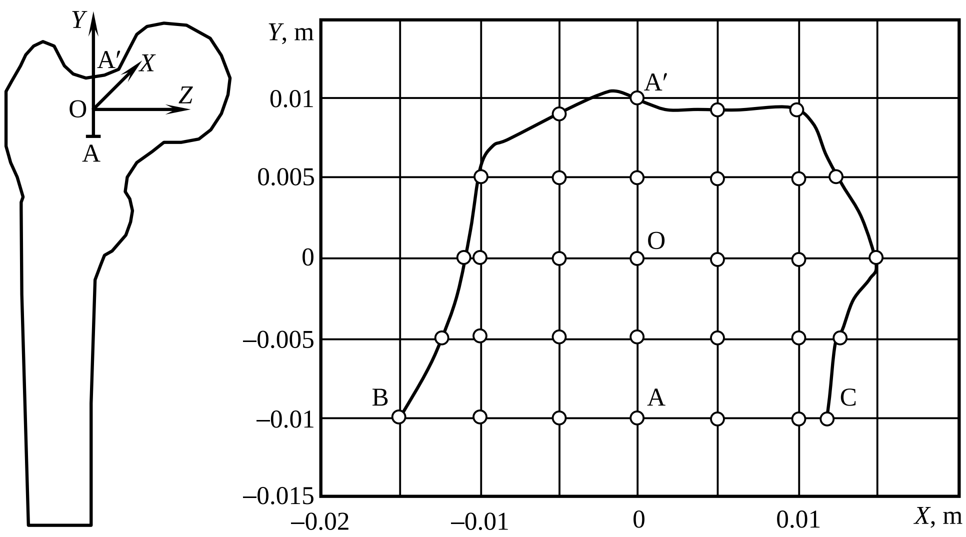

Fig. 5. Location of the section

Fig. 5 shows the nodes of FE in the cross section AA′ depending on the required distance between the nodes at given points in the cross section of the bone, where in Fig. 6, *a* – primary FE division; in Fig. 6, *b*, *c* – sequential refinement of the FE grid by reducing the finite element by 2 times in the areas of Fig. 5.

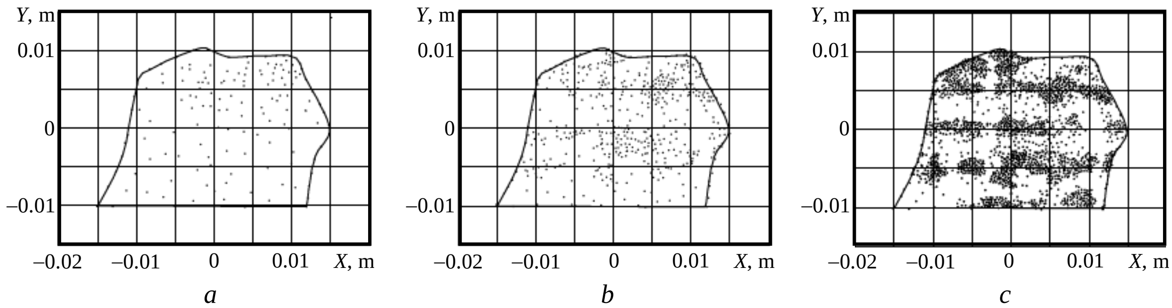

Fig. 6. Finite-element partitioning in local areas: *a* – primary FE division; *b*, *c* – sequential refinement of the FE grid by reducing the finite element by 2 times in the areas of Fig. 5

The second function of the module is to set boundary conditions under instantaneous loads. Boundary conditions are generated in the forceRight.py module.

Force ("instantaneous") loads are set in the form of pressure on the surface of the femoral neck. To do this, the program must provide a list of points, lines, surfaces from ANSYS. The coordinates of the points are displayed in the global and local coordinate systems shown in Fig. 7. Surfaces in ANSYS consist of lines, and lines, in turn, are defined by a set of corresponding points. In order to enter the position of each point in the module, the model was exported in .obj format.

Having obtained the connection between surfaces and points, we can discard those surfaces that lie to the right of section A. To do this, the method genPres () passes the parameter – the coordinate on the axis O*Z* – which determines the position of the section A. The surface is considered to be to the right of the section A-A, if the sum of the differences between the *z* coordinate of the point and the section parameter the condition is fulfilled:

$$\sum_{i=1}^{n}(z_i - Z_\mathrm{A}) > 0,$$

where z_i is the component of the surface point with index i; Z_A is the coordinate of the section on the axis z in the local coordinate system; n is the number of points on the surface, usually $n = 3$, because in the vast majority of cases triangular flat surfaces are used to create any geometric model.

External pressure is set for the selected sections. To do this, calculate the total area of the selected surfaces. Data on surface areas are present in ANSYS, if the usual elemental partitioning is performed in advance. Then the pressure is calculated by dividing the load parameter set by the user in the program by the total area:

$$P = \frac{F}{\sum_{i \in U} S_i},$$

where P is the pressure; F – a priori given external force; S_i – surface area with index i; U – many surfaces that satisfy the previous condition.

Similarly, in the genDof () method, the task of fixing on surfaces below the section B-B is realized (Fig. 7). Fastening is rigid, ie the vector of displacements in the corresponding nodes is zero. Fastening is set using the ANSYS command DA.

Commands to run the calculation are quite simple. Here the final time of calculation and a step so that only one iteration of calculation was carried out, and then calculation is started are exposed. The result of run-

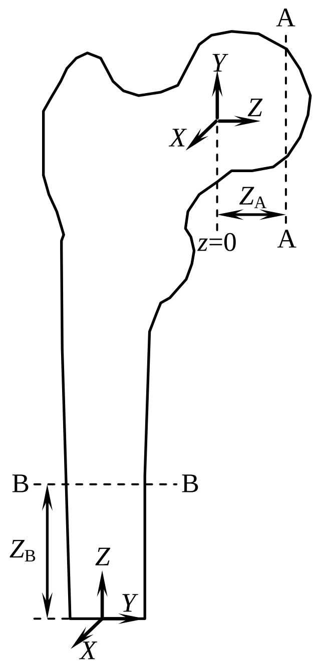

Fig. 7. Sections and coordinate systems for setting boundary conditions corresponding to the process of impact when a person falls

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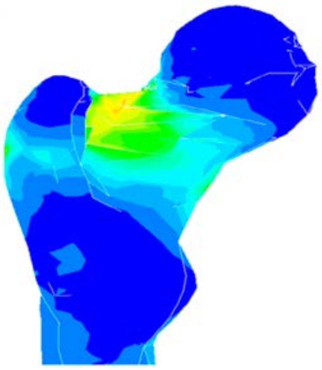

Fig. 8. Distribution of tension intensity in the area adjacent to the femoral neck

ning the specialCommands.py module to get the numerical solution of a linear problem running is shown in Listing 3:

Listing 3. Starting the calculation of a linear problem

```
/ SOLU
DELTIM ,0 ,1 ,1
TIME ,1
!/ STATUS , SOLU
SOLVE
```

A system of common linear equations compiled in the process of FE partitioning and can be solved by a direct or iterative method. The direct method is a Gaussian transformation, the application of which is a vector of unknown displacement components from the relation:

$$Ku = F \,,$$

where K – extended stiffness matrix, u – extended vector of unknowns; F – extended vector of loads.

The direct solution method uses the decomposition of the matrix into two triangular matrices (lower triangular and upper triangular). Thus, the matrix can be represented as:

$$K = LU \,,$$

where L is the upper triangular, U is the lower triangular matrix, respectively. Then by means of direct and inverse substitutions there is a vector u. A typical iterative method uses the initial approximation u_1. At each iteration, the vector is calculated so that the following relationship holds:

$$\lim_{i \to \infty} u_i = u \,,$$

where u_i is the vector of the solution on the i-th iteration, the i-th solution. The iterative process is stopped after reaching the specified accuracy after a finite number of iterations.

This work used a sparse direct method, which is usually used to solve 95 % of the problems encountered. The method has the optimal ratio of memory consumption and solution speed.

The calculation of the instantaneous voltage in the intact bone is created according to the following algorithm in the software application ANSYS:

1. Creating a new project that will contain all subsequent calculation files;
2. Editing the library of materials: creating two materials for the cortical and cancellous bone;
3. Import a bone model saved in .obj format;
4. Opening the model in the subroutine of calculation Mechanical, assigning to each layer of bone the corresponding material by editing the project bodies;
5. Assigning the dependence of the model layers;
6. Tasks of boundary conditions by means of the command of the created module;
7. Clarification of the grid of finite elements using the command of the created module;
8. Start the calculation with the Solve function;
9. Analysis of results and identification of critical points.

The largest values of stress intensity are really concentrated in the neck of the femur. This is observed in real life, according to fracture statistics, which show that a neck fracture is most likely when a person falls (Fig. 8).

There is a concentration of stress in a small area adjacent to the surface. In this regard, we can conclude that this critical point (area) is the source of bone destruction.

Conclusions

The main purpose of the study was to develop and test the software subsystem for the study of reinforced femur. The problem of developing a subsystem – a module to facilitate mathematical calculation was solved.

As a result, a module was created to refine the grid of finite elements and set boundary conditions, which in turn was used to perform a mathematical calculation of the stress state. The study includes the calculation of stress states in the intact bilayer bone to identify critical points of onset of destruction of the cortical layer of bone. The calculation was performed for different locations of the implant in the bone. After calculations, the results of both experiments - intact and reinforced system - were compared. Based on the comparison of the results, the most rational location of the implant for reinforcement and further studies of the two-layer bone model was selected.

The created calculation module facilitates interaction with the software, allowing to specify more precisely necessary conditions of carrying out experiment.

Based on the results obtained during the experiments, we can conclude about the usefulness of using both the created module and the created models. The results of the numerical experiment show better characteristics of the reinforced bone in contrast to the intact.

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