Simulation of mechanical behaviour of the proximal femur as a poroelastic solid using particles

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Abstract. Full understanding of the mechanical behaviour of living bone is the key to solving many important problems of modern orthopaedics and arthroplasty. An important role in the study of the mechanical behaviour of living bone belongs to the development and use of comprehensive numerical models. In this work, we model the mechanical behaviour of the proximal femur as a 3D poroelastic solid consisting of the interior cancellous part and the outer cortical part. For simplicity, both parts are assumed isotropic linear poroelastic material. However, they have different values of porosity, fluid content and elastic properties, which are taken from literature. For computer simulation, we used the so-called movable cellular automaton method, which is a representative of simply deformed discrete elements i.e. computational particle mechanics. The method allows simulating dynamics of the elastic skeleton deformation and viscous fluid flow in the skeleton pores according to Biot’s theory of linear poroelasticity. Using the model developed we study the mechanical behaviour of the proximal part of the femur in compression with different rate of loading and different permeability. The results obtained for both saturated and drained bones are discussed.

1. Introduction
Traditionally bone tissues are modelled as homogenous elastic bodies [1]. However, this is the simplest case, which does not account for specific multiphase structure of the bone. There are two main approaches that consider the bones more realistically. The first approach considers the bone consisting of cortical and cancellous tissues and takes into account the structure of both tissues [2]. This way uses the mechanics of anisotropic elastic body. The second approach puts main attention to the influence of the interior fluid on the mechanical behaviour of living bone [3,4]. This way uses the theory of poroelasticity of Boit.

Mainly, the poroelastic approach is aimed at getting values that are more realistic for elastic moduli of different bone tissues. For this purpose, the authors try to solve analytically the problem of sound waves propagation in poroelastic medium and then use it for the analysis of experimental data. Some papers are devoted to building the numerical poroelastic models based on finite element simulation software, which may face specific problems in computational accuracy and stability.

In this paper, we use poroelastic theory for numerical simulation of mechanical behaviour of the proximal part of femur under different loading conditions. For the sake of simplicity, in this study,

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material properties are assumed to be isotropic. First, we consider data about poroelastic properties of bone found in the literature for simulation of uniaxial compression of small cubic specimens for both cortical and cancellous bone tissues with different rate of loading. These test simulations allowed us to verify the chosen parameters for both materials and to study the influence of these parameters on the mechanical behaviour of the materials. After that, we numerically studied the peculiarities of mechanical behaviour of the standard model for the proximal part of femur under compression loading.

2. Movable cellular automaton method for poroelastic body

For simulating the mechanical behaviour of the bone materials, we use the particle-based method of movable cellular automata [5–7]. A simulated body is represented by an ensemble of bonded equiaxial discrete elements of the same size (called movable cellular automata), which position, orientation, and state can change due to interaction with neighbours. Automata interact among each other through their contacts. The initial value of the contact area is determined by the size of automata and their packing.

When describing the kinematics and dynamics of an automaton motion, its shape is approximated by an equivalent sphere. This approximation is the most widely used in the discrete element method and allows one to consider the forces of central and tangential interaction of elements as formally independent. This makes also possible to use the simplified Newton-Euler equations of motion.

Movable automata are treated as deformable. Strains and stresses are assumed to be uniformly distributed in the volume of each automaton. Within the framework of this approximation, the values of averaged stresses in the automaton volume may be calculated as the superposition of forces applied to different parts of the automaton surface. In other words, averaged stresses are expressed in terms of the interaction forces [6, 7]:

$$\bar{\sigma}_{i\alpha\beta} = \frac{R_j S_y^0}{\Omega_i^0} \sum_{j=1}^{N} \left[ f_{ij} (\vec{n}_{ij})_\beta + \tau_{ij} (\vec{t}_{ij})_\beta \right]$$

(1)

where $i$ is the automaton number, $\bar{\sigma}_{i\alpha\beta}$ is the component $\alpha\beta$ of averaged stress tensor, $\alpha, \beta = x, y, z$ (XYZ is the global coordinate system), $\Omega_i^0$ is the initial volume of the automaton $i$, $S_y^0$ is the initial value of the contact area of the automaton $i$ and $j$, $R$ is the radius of equivalent sphere (semi-size of the element $i$), $f_i$ and $\tau_i$ are specific values of central and tangential forces of interaction between the automata $i$ and $j$, $\vec{n}_{ij}$ and $\vec{t}_{ij}$ are the projections of unit normal and unit tangent vectors onto the $\alpha$-axis, $N$ is the number of interacting neighbours.

Invariants of the averaged stress tensor $\bar{\sigma}_{i\alpha\beta}$ are used to calculate central interaction forces ($f_i$, $\tau_i$) and criterion of an inter-element bond break (criterion of local fracture). The components of the averaged strain tensor $\bar{\epsilon}_{i\alpha\beta}$ are calculated in increments using the specified equation of state of the simulated material and the calculated increments of averaged stresses [6, 7].

The authors previously showed that the relation for the force of central interaction of automata is formulated based on the constitutive equation of the material for the diagonal components of the stress tensor, while the force of tangential interaction is formulated on the basis of similar equations for non-diagonal stresses [6]. When implementing the linear elastic model, the expressions for specific values of central and tangential forces of the mechanical response of the element $i$ to mechanical action from the neighbouring automaton $j$ are written as follows:

$$\begin{align*}
\Delta f_{ij} &= 2G_i \Delta \epsilon_{ij} + D_i \Delta \sigma_{ij} \text{mean} \\
\Delta \tau_{ij} &= 2G_i \Delta \gamma_{ij}
\end{align*}$$

(2)
where the symbol $\Delta$ means increment of the corresponding variable during time step $\Delta t$ of the numerical scheme of integration of motion equations, $\Delta \varepsilon_{ij}$ and $\Delta \gamma_{ij}$ are increments of normal and shear strains of the automaton $i$ in $i$-$j$ pair, $G$ is the shear modulus of the material of the automaton $i$, $K$ is the bulk modulus, $D_i = 1 - 2G_i/K_i$.

Due to the necessity of the third Newton's law ($\sigma = \sigma_t$ and $\tau = \tau_t$), the increments of the reaction forces of the automata $i$ and $j$ are calculated based on the solution of the following system of equations:

$$
\begin{align*}
\Delta f_{ij} &= \Delta f_{ji} \\
R_i \Delta \varepsilon_{ij} + R_j \Delta \varepsilon_{ji} &= \Delta r_{ij} \\
\Delta \tau_{ij} &= \Delta \tau_{ji} \\
R_i \Delta \gamma_{ij} + R_j \Delta \gamma_{ji} &= \Delta f^t_{ij}
\end{align*}
$$

(3)

where $\Delta r_i$ is the change in the distance between the centres of the automata for a time step $\Delta t$, $\Delta f^t_{ij}$ is the value of the relative shear displacement of the interacting automata $i$ and $j$ [6, 7]. The system of equations (3) is solved for the increments of strains. This allows calculation of the increments of the specific interaction forces. When solving the system (3), the increments of mean stress and the values of specific forces in the right-hand sides of relations (2) are taken from the previous time step or are evaluated and further refined within the predictor-corrector scheme.

Automata that model fluid-saturated material are considered as porous and permeable. Pore space of such an automaton can be saturated with liquid. The characteristics of the pore space are taken into account implicitly through the specified integral parameters, namely, the porosity $\phi$, permeability $k$, the ratio $a = 1 - K/K$ of the macroscopic value of bulk modulus $K$ to the bulk modulus of the walls of porous skeleton $K$. The mechanical influence of the pore fluid on the stresses and strains in the solid skeleton of an automaton is taken into account on the basis of the linear Biot’s model of poroelasticity [8, 9]. Within this model, the mechanical response of a “dry” automaton is assumed linearly elastic and is described based on the above-sown relations. The mechanical effect of the pore fluid on the automaton behaviour is described in terms of the local pore pressure $P$ (fluid pore pressure in the volume of the automaton). In the Biot model, the pore pressure affects only the diagonal components of the stress tensor. Therefore, it is necessary to modify only the relations for the central interaction forces in (2):

$$
\Delta f_{ij} = 2G_i \left( \Delta \varepsilon_{ij} - \frac{a_i \Delta P_{ij}^{\text{pore}}}{K_i} \right) + D_i \Delta \sigma_{ij}^{\text{mean}}.
$$

(4)

Interstitial fluid is assumed to be linearly compressible. The value of fluid pore pressure in the volume of a discrete element is calculated on the basis of relationships of Biot’s poroelasticity model with the use of the current value of pore volume [9, 10]. The pore space of discrete elements is assumed to be interconnected and provides the possibility of redistribution (filtration) of interstitial fluid between the interacting elements. A pore pressure gradient is considered as the “driving force” of filtration. The redistribution of fluid between elements is carried out by numerical solution of the classical equation of transfer of fluid density [11]. This equation is solved by the finite volume method on an ensemble of discrete elements.

3. Simulation of cubic specimens of cortical and cancellous bones  

The aim of this section is to choose the correct values of the model for both cortical and cancellous bone tissues. The first who considered bones like poroelastic bodies was Cowin [3]. In his paper [4] he also provided the values of the main parameters of poroelastic body for cortical and cancellous tissues.
of the human bone. These parameters are as follows: Young’s modulus, Poisson’s ratio, the permeability, Biot’s coefficient (or bulk modulus of the solid phase), the porosity, densities of the solid grain and the fluid. Later, several authors have made experimental and theoretical studies aimed to get the values of poroelastic parameters for some specific bones of humans and animals [12–16]. Based on data published in the literature one may conclude that there is a large scatter of the main poroelastic properties of the bone tissues. For example, permeability estimates span across several orders of magnitude \((10^{-6}–10^{-1} \text{ m})\), and values for Young’s modulus vary from 1 up to 25 GPa [16]. That is why it is of special interest to study the peculiarities of the mechanical behaviour of small model specimens in compression depending on the variation of these properties.

Basic values of the poroelastic properties chosen for our numerical models for both cortical and cancellous bone tissues are shown in table 1. The fluid in both bone tissues is assumed to be the same and equivalent to salt water, with a bulk modulus \(K = 2.4 \text{ GPa}\), and density \(\rho = 1000 \text{ kg/m}^3\).

| Bone tissue | Bulk modulus of the solid phase, \(K\), GPa | Bulk modulus of the matrix, \(K\), GPa | Shear modulus of the matrix, \(G\), GPa | Density of the matrix, \(\rho\), kg/m\(^3\) | Porosity \(\phi\) | Permeability, \(m\) |
|-------------|----------------------------------------|--------------------------------------|----------------------------------|-----------------------------------|----------------|------------------|
| Cortical    | 17.0                                   | 14.0                                 | 5.55                             | 1850                              | 0.04           | 1.0 \times 10^{-6} |
| Cancellous  | 17.0                                   | 3.3                                  | 1.32                             | 600                               | 0.80           | 3.5 \times 10^{-6} |

The developed model was applied to study the dynamic mechanical behaviour of the fluid-saturated porous materials under uniaxial compression at a constant speed. We studied and analysed the dependences of the effective Young's modulus of fluid-saturated materials on the strain rate and the characteristic time of fluid redistribution in the pore space. In our calculations, the material parameters and the strain rate varied within wide limits: the permeability of the material varied within 4 orders of magnitude, the viscosity of the fluid varied within 2 orders of magnitude, the sample size changed within the order of magnitude and the strain rate varied within 3 orders of magnitude.

We simulated uniaxial compression of 3D cubic specimens along the vertical axis (Z). The size of the automata for all models in this study was equal to 2 mm. The base size of the cubic specimens was chosen to be 5 cm. The initial pore pressure of interstitial fluid was assumed to be equal to atmospheric. Fluid could freely flow out from the compressed specimen through the side surface.

Analysis of the simulation results showed that under compression, the values of the mechanical characteristics of the fluid-saturated material are determined by the balance of two competing processes [17, 18]:

- deformation of the solid skeleton, providing compression of the pore space and a corresponding increase in the pore pressure of the interstitial fluid;
- outflow of the interstitial fluid through the side surface, which leads to the inverse effect of lowering pore pressure.

We revealed a key control parameter that determines the specific dynamic value of the mechanical characteristics of fluid-saturated materials, namely the dimensionless Darcy number:

\[
Da = \frac{T_{\text{Darcy}}}{T_{\text{load}}} \sim \frac{\eta \dot{\varepsilon}_{\text{def}} L^2}{k \Delta P} \dot{\varepsilon}_{\text{def}},
\]

where \(T_{\text{Darcy}}\) is the characteristic time of fluid filtration (Darcy time scale), \(T_{\text{load}} \sim 1/\dot{\varepsilon}_{\text{def}}\) is the time scale of the specimen deformation, \(\dot{\varepsilon}_{\text{def}}\) is the specimen strain rate, \(\eta\) is the dynamic viscosity of the pore fluid, \(L\) is the characteristic length of the pore pressure difference \(\Delta P\) (a half of length of the cubic side in the considered case). The parameter \(Da\) characterizes the ratio of the timescales of deformation of the fluid-saturated porous specimen and filtration of the pore fluid.
The simulation results showed that the effective Young's modulus of fluid-saturated bone tissues non-linearly depends on the strain rate $\dot{\varepsilon}_{def}$, the specimen size $L$, the dynamic viscosity of pore fluid $\eta_f$, and the permeability of solid skeleton $k$. In particular, Young's modulus of a fluid-saturated sample is minimal (equal to $E_{min}$) at infinitely small strain rates and tends to the maximum value (Young's modulus of undrained sample $E_{max}$ [9]) at large ones. The key result is the established ability to build single “gauge” dependence applicable to specimens of porous materials of various sizes, characterized by different permeability of solid skeleton, different fluid viscosities and deformed at different strain rates. An argument of such a “master curve” is the dimensionless Darcy number $Da$ (figure 1):

$$E = E_{max} + \frac{E_{min} - E_{max}}{1 + (Da/Da_0)^p},$$

where $E_{min}$ corresponds to $Da \rightarrow 0$ (“dry” specimen), $E_{max}$ corresponds to $Da \rightarrow \infty$ (undrained specimen), $Da$ and $p$ are the fitting constants. This master curve has a logistic (sigmoidal) form but the fitting values of $Da$ and $p$ (as well as $E_{min}$ and $E_{max}$) are different for cortical and cancellous bones.

![Figure 1](image_url)

**Figure 1.** Dependences of the normalized Young's moduli of the modelled specimens of cortical (a) and cancellous (b) bone tissues with different poroelastic properties on the Darcy number. Crosses show numerically obtained values, lines are approximating curves.

Based on the presented results we chose the values of the poroelastic parameters for both bone tissues applied to the model proximal femur corresponding to Darcy numbers about 50, i.e. the middle of the plots range shown in figure 1. This means that at the loading rate of the model femur the effect of interstitial fluid flow is expected to be well pronounced.

4. **Simulation of proximal femur**

The geometry of the model is based on the so-called 3rd generation composite femur [19], which provides geometries of the cortical and cancellous parts as different solid bodies. General view of the model represented as fcc packing of automata and its cross-section are shown in figure 2. At the bottom of the model we place a disk with properties of the cortical bone; the automata of this disk are fixed. For compressing the femur, we place a special cylindrical “cap” on the femur head. This “cap” is shown in blue colour in figure 2. Automata of the “cap” have the properties corresponding to cartilage. Loading is applied by setting the constant velocity $V = 1$ m/s to the automata of the upper face of the “cap”. The velocity vector is directed along the face normal. Note, that this loading results in both compression and small bending of the bone.

To reveal the role of the interstitial fluid flow in the model femur under compression we studied three different cases. In the first case, all bone tissues contained no fluid, i.e. were “dry” (drained test). In the second case, we used the chosen poroelastic parameters from table 1. In the third case, all pores
containing fluid were assumed to be closed, which means no permeability of the materials (undrained test). Then we analysed the distributions of mean stress, equivalent stress and pore fluid pressure at the final point at the total strain about 2%.

**Figure 2.** General view of the model for proximal femur (left) and its cross-section (right).

**Figure 3.** Distribution of mean stress in cross-section of the model femur at drain test (a), test with chosen poroelastic parameters (b), and undrained test.

**Figure 4.** Distribution of equivalent stress in cross-section of the model femur at drained test (a), test with chosen poroelastic parameters (b), and undrained test.
Distributions of mean stress in the cross section of the model for all three cases are shown in figure 3. One can see that fluid filtration cause the increase in mean stress in the cortical part of the femur head, especially in the area of its contact with the loading “cap”. At the same time, the drained and undrained tests do not differ from each other. However, distributions of equivalent stress in the cross section of the model for these cases shown in figure 4 clearly demonstrate that shear stress in the same area is much smaller for the undrained test while for the two other cases are practically the same.

It can be clearly seen from figures 3 and 4 that the maximum stresses occur in the cortical part of the femur. Figure 5 shows the 3D view of both equivalent and mean stresses distribution in the model (actually, the outer part of the cortical bone). It is obvious that the main stresses are localized in the femoral neck. The shear stresses propagate along the loading direction into the main part of the bone up to the supporting plate. But the most dangerous seems the tensile mean stress in the upper part of the femoral neck (figure 5, b).

Figure 5. Distribution of equivalent stress (a) and mean stress (b) in the model femur with chosen poroelastic parameters.

Figure 6 shows distributions of the pore pressure in the cases with interstitial fluid. It can be seen that ability to flow results in filtration of the fluid to the regions of large tensile and shear stresses of the cortical bone, but not the maximum tensile mean stress (upper part of the femoral neck). At the same time, one can see negligible pore pressure in the cancellous bone in case of fluid filtration (figure 6, c).

Conclusion
Based on the movable cellular automaton method we developed a 3D numerical model for mechanical behaviour of cortical and cancellous bone tissues as an isotopic linear poroelastic material. Using the data from literature and the results of numerical compression tests, we chose the values of the model parameters for both tissues. We revealed the Darcy number as a key control parameter that determines the dynamic mechanical characteristics of fluid-saturated materials. Using the model developed we studied the mechanical behaviour of the proximal part of the femur with different permeability in compression. The results obtained allow us to conclude that presence of the interstitial fluid and its ability to flow in the bone tissue pores can dramatically change the stress field in the bone subjected to mechanical load, especially in the area of the femoral neck.
Figure 6. Distribution of pore pressure in the model for the test with chosen poroelastic parameters (a, c) and undrained test (b, d), (c) and (d) are corresponding cross-sections.

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References

[1] Evans F G 1957 Stress and strain in bones, their relation to fractures and osteogenesis (Springfield, Ill: Charles C. Thomas)
[2] Kutz M 2003 Standard Handbook of Biomedical Engineering & Design. Bone mechanics, (New York: McGraw-Hill)
[3] Cowin S C 1999 J. Biomech. 32 217
[4] Smita T H, Huygheb J M, Cowin S C 2002 J. Biomech. 35 829
[5] Psakhie S G, Moiseyenko D D, Smolin A Yu, Shilko E V, Dmitriev A I, Korostelev S Yu, Tatarintsev E M 1999 Comp. Mater. Sci. 16 333–343
[6] Shilko E V, Psakhie S G, Schmauder S, Popov V L, Astafurov S V and Smolin A Yu 2015 Comp. Mater. Sci. 102 267–285
[7] Smolin A Yu, Shilko E V, Astafurov S V, Kolubaev E A, Eremina G M, Psakhie S G 2018 Defence Technology 14 643–656.
[8] Biot M A 1957 *J. Appl. Mech.* **24** 594–601
[9] Detournay E and Cheng A H-D 1993 *Comprehensive Rock Engineering: Principles, Practice and Projects* vol 2, ed. J A Hudson (Oxford: Pergamon Press) p 113
[10] Psakhie S G, Dimaki A V, Shilko E V and Astafurov S V 2016 *Int. J. Num. Meth. Engng.* **106** 623–643
[11] Basniev K S, Dmitriev N M, Chilingar G V, Gorfunkle M and Mohammed Nejad A G 2012 *Mechanics of Fluid Flow* (Hoboken: John Wiley & Sons)
[12] Lim T-H, Hong J H 2000 *J Orthop. Res.* **18** 671–677
[13] Kohles S S, Roberts J B 2002 *J. Biomech. Eng.* **124** 521–526
[14] Cardoso L, Schaffler M B 2015 *J. Biomech. Eng.* **137** 011008
[15] Sandino C, McErlain D D, Schipilow J, Boyd S K 2015 *J. Mech. Behav. Biomed. Mater.* **44** 1–9
[16] Le Pense S, Chen Y 2017 *J. Mech. Behav. Biomed. Mater.* **65** 90–101
[17] Shilko E V, Dimaki A V, Smolin A Yu and Psakhie S G 2018 *Procedia Structural Integrity* **13** 1508–1513
[18] Shilko E V, Dimaki A V, Psakhie S G 2018 *Scientific Reports* **8** 1428
[19] Cheung G, Zalzal P, Bhandari M, Spelt J K, Papini M 2004 *Medical Engineering & Physics* **26** 93–108