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HIERARCHICAL MULTISCALE MODELLING OF POROUS MEDIA WITH APPLICATIONS IN BIOMECHANICS

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Abstract: *We consider materials with different levels of porosity at different scales. Homogenization theory provides a natural way of upscaling fluid-structure interaction problem posed at the smallest scale to higher levels of porosities in a sense that effective material coefficients (stiffness, permeability, Biot coefficients etc.) at a higher level are obtained by applying homogenization to the lower level. This approach leads to a convenient hierarchical description of the porous medium, suitable for multiscale modelling - in the contribution we present numerical examples motivated by bone tissue poromechanics.*

Keywords: ***poroelasticity, homogenization, multiscale modelling, double porosity.***

1. Introduction

Porous fluid saturated materials with different levels of porosities are abundant in nature and can be engineered as well to conform with requirements in technical practice. This paper describes one approach to modeling of the mechanical behavior of fluid-saturated cortical bone tissue. The multiscale model presented here is based on the theory of homogenization and provides an efficient computational tool which can be used firstly to study influence of the bone structure on the mechanical properties, namely on the stiffness and on the overall strength, secondly to study the mechano-transduction: how the macroscopic loading determines local deformation and microflows in the hierarchical porous structure. The latter phenomenon is tightly related to evolutionary processes which on a longer time scale lead to tissue remodeling and growth.

In the present study we focus on one sub-topic of the homogenization-based bone modelling. Namely, we provide homogenization-based formulae which enable to compute the poroelasticity coefficients for a given geometry and topology of micro- and mesoscopic levels. We describe an arrangement of porosities, each one forming a separate connected system, which are connected by a quasipermeable, or an impermeable interface; then the homogenized problem results in two different pressures. At the mesoscopic scale we take into account the Darcy flow in the poroelastic matrix, although in the mesoscopic channels the fluid is assumed to be static with no pressure gradients.

Only the main results relevant for computer implementation are reported here, as the derivation of the homogenization formulae is beyond the scope of this paper. In Section 2. we discuss modelling assumptions and introduce all formulae and equations constituting the two-level homogenized model. The hierarchical homogenization is implemented in our in-house finite element code; in Section 3. we illustrate the hierarchical upscaling procedure using a numerical example.

2. Hierarchical model of double porosity

We consider a poroelastic medium saturated by fluid. The porosity of the medium is formed at two levels, distinguishable by different sizes of pores, see Fig. 1. These are connected by a weakly permeable interface, so that the model also describes a situation of disconnected porosities, see Rohan and Cimrman (2012).

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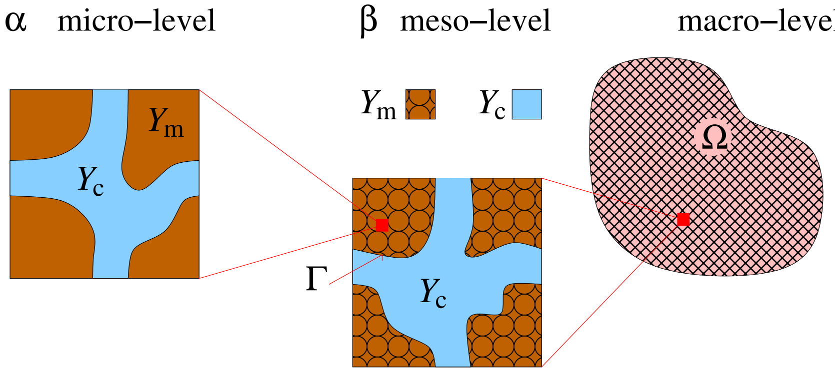


Fig. 1: The two-level heterogeneous structure: α-level is formed by a single connected porosity Y_c^α; the matrix Y_m^α is formed by the solid. At the β-level, the homogenized structure of the α-level forms the material situated in the matrix Y_m^β. Representative periodic cells are depicted.

The two levels, further labeled by superscripts α and β are associated with the "microscale" and the "mesoscale", respectively. In bone modelling, the two levels correspond to the canaliculo-lacunar and the Haversian porosities.

At the microscale level, we consider an elastic solid phase forming a porous skeleton filled with fluid. We assume only moderate pressure gradients at the mesoscopic scale, such that the fluid is static. The pores can form a connected porosity, or mutually separated inclusions: in the first case only one scalar pressure value represents the pressure field in the porosity. By homogenizing this two-phase medium we obtain a Biot-type model describing at the mesoscale the upscaled poroelastic microstructure α, cf. Auriault and Sanchez-Palencia (1977).

At the mesoscale the above mentioned α-poroelasticity model describes the material occupying the matrix of the meso-structure β; at this "higher" level the canals can exchange the fluid with the microscopic pores of the α level due to a weakly permeable interface. For upscaling from the meso- to the macroscopic scale, we take into account a slow flow in the "dual porosity" associated with the microscopic scale.

In this paper we only report the main results relevant for a computer implementation. Homogenization at each scale level proceeds in two steps:

1. Find effective (homogenized) coefficients by solving auxiliary problems for several characteristic (or corrector) functions, cf. Rohan et al. (2012b); Rohan and Cimrman (2011);
2. Compute the homogenized coefficients that can be used for the higher level and/or "global" (homogenized) model of the current level. Due to linearity of the problems, those steps are decoupled in a sense that the computation of the homogenized coefficients for the global level is valid for any point having the corresponding "microstructure".

Let us consider the scale parameter ε, describing the ratio of the characteristic sizes, L^α and L^β, of the two levels, i.e. $\varepsilon = L^\alpha/L^\beta$. By superscript $^\varepsilon$ we indicate dependence of functions and other parameters on ε. We use the same symbol also for upscaling from meso- to macro-scale: $\varepsilon = L^\beta/L^{macro}$.

Let us denote Ω^ℓ the domain at level $\ell = \alpha, \beta$. We assume that the domain Ω^ℓ is obtained from a periodic microstructure generated by a representative unit cell Y^ℓ decomposed as follows

$$Y^\ell = Y_m^\ell \cup Y_c^\ell \cup \Gamma_Y^\ell\,, \quad Y_c^\ell = Y^\ell \setminus Y_m^\ell\,, \quad \Gamma_Y^\ell = \overline{Y_m^\ell} \cap \overline{Y_c^\ell}\,, \quad \ell = \alpha, \beta\,, \tag{1}$$

where Y_m^ℓ is the matrix, Y_c^ℓ are the channels and Γ_Y^ℓ is the matrix–channels interface. Without loss of generality we can define $Y = (]0,1[)^3$ to be the unit cube, so $|Y| = 1$. As a result of (1), the domain Ω^ℓ is defined by $\bigcup_{k\in\mathbb{K}^\varepsilon} \varepsilon(Y^\ell + k)$ with $\mathbb{K}^\varepsilon = \{k \in \mathbb{Z}^3, \varepsilon(Y^\ell + k) \subset \Omega^\ell\}$.

The homogenization procedure starts with a model at the microscale, see Rohan and Cimrman (2012), written in terms of the displacement vector $\boldsymbol{u}^{\alpha,\varepsilon}$ of the matrix and the fluid pressure $p^{\alpha,\varepsilon}$ in pores, and the following material parameters, which form the input of the model:

- $\mathbb{D}^\varepsilon$: the elasticity fourth-order tensor of the matrix,
- γ: the fluid compressibility,
- ν: the fluid viscosity.

For each microstructure we also compute the porosities (volume fractions of pores) $\phi^\ell = |Y_c^\ell|/|Y^\ell|$, $\ell = \alpha, \beta$.

The upscaling procedure of the heterogeneous continuum consists in the limit analysis of the ε dependent model with respect to $\varepsilon \to 0$. For this we use the periodic unfolding method Cioranescu et al. (2008); Griso and Rohan (2007).

2.1. Homogenization results for level α

The two steps of the solution algorithm involve:

Corrector problems First, let us introduce some notation:

$$
\begin{aligned}
a_m^\alpha\left(\boldsymbol{w},\, \boldsymbol{v}\right) &= \fint_{Y_m^\alpha} (\mathbb{D}\boldsymbol{e}_y(\boldsymbol{w})) : \boldsymbol{e}_y(\boldsymbol{v})\;, \\
\boldsymbol{\Pi}^{ij} &= (\Pi_k^{ij})\;, \quad i,j,k = 1,2,3 \text{ with } \Pi_k^{ij} = y_j \delta_{ik}\;,
\end{aligned} \tag{2}
$$

where denotes $\boldsymbol{e}_y(\boldsymbol{w})$ is the small strain tensor (derivatives w.r.t. Y domain coordinates y). By $\mathbf{H}^1_\#(Y_m)$ we mean $\mathbf{H}^1$ space of vector functions periodic in Y_m. The problem for the characteristic responses then reads: Find $(\boldsymbol{\omega}^{ij}, \boldsymbol{\omega}^P) \in \mathbf{H}^1_\#(Y_m) \times \mathbf{H}^1_\#(Y_m)$ satisfying

$$
\begin{aligned}
a_m^\alpha\left(\boldsymbol{\omega}^{ij} + \boldsymbol{\Pi}^{ij},\, \boldsymbol{v}\right) &= 0\;, \quad \forall \boldsymbol{v} \in \mathbf{H}^1_\#(Y_m)\;, \\
a_m^\alpha\left(\boldsymbol{\omega}^P,\, \boldsymbol{v}\right) &= \fint_{\Gamma_Y} \boldsymbol{v}\cdot\boldsymbol{n}^{[m]}\,\mathrm{dS}_y\;, \quad \forall \boldsymbol{v} \in \mathbf{H}^1_\#(Y_m)\;.
\end{aligned} \tag{3}
$$

Homogenized coefficients Using the characteristic responses (3) obtained at the microscopic scale the effective properties of the deformable porous medium are given by

$$
A_{ijkl}^\alpha = a_m^\alpha\left(\boldsymbol{\omega}^{ij} + \boldsymbol{\Pi}^{ij},\, \boldsymbol{\omega}^{kl} + \boldsymbol{\Pi}^{kl}\right)\;, \quad B_{ij}^\alpha = -\fint_{Y_m} \mathrm{div}_y \boldsymbol{\omega}^{ij}\;, \quad M^\alpha = a_m^\alpha\left(\boldsymbol{\omega}^P,\, \boldsymbol{\omega}^P\right)\;, \tag{4}
$$

where $\mathbb{A}^\alpha$ is the skeleton stiffness corresponding to the dried medium, $\boldsymbol{B}^\alpha$ are the Biot-type stress coefficients associated with pressure in channels Y_c^α and M^α is effective Biot compressibility modulus. Obviously, the tensors $\mathbb{A}^\alpha = (A_{ijkl}^\alpha)$ and $\boldsymbol{B}^\alpha = (B_{ij}^\alpha)$ are symmetric; moreover $\mathbb{A}^\alpha$ is positive definite and $M^\alpha > 0$.

2.2. Homogenization results for level β

The two steps of the solution algorithm involve:

Corrector problems To define the local problems for corrector functions, we need the following bilinear forms which involve the homogenized coefficients computed in (4):

$$
\begin{aligned}
a_m^\beta\left(\boldsymbol{w},\, \boldsymbol{v}\right) &= \fint_{Y_m^\beta} \mathbb{A}^\alpha \boldsymbol{e}_y(\boldsymbol{w}) : \boldsymbol{e}_y(\boldsymbol{v})\;, \\
b_m^\beta\left(p,\, \boldsymbol{v}\right) &= \fint_{Y_m^\beta} p\hat{\boldsymbol{B}}^\alpha : \boldsymbol{e}_y(\boldsymbol{v})\;, \quad \hat{\boldsymbol{B}}^\alpha := \boldsymbol{B}^\alpha + \phi^\alpha \mathbf{I}.
\end{aligned} \tag{5}
$$

It is worth noting that upscaling from the meso- to the macro-level does not lead to any fading memory terms involving time convolutions, in contrast with upscaling of the double porosity media, cf. Rohan et al. (2012b); Rohan and Cimrman (2010). As a counterpart to the α level, see (3), the characteristic responses, i.e., displacement modes at the mesoscopic level, satisfy the following problems: find $\boldsymbol{w}^{ij}, \hat{\boldsymbol{w}}, \bar{\boldsymbol{w}} \in \mathbf{H}^1_\#(Y^\beta_m)$ such that

$$\begin{aligned} a^\beta_m\left(\boldsymbol{w}^{ij} + \boldsymbol{\Pi}^{ij},\, \boldsymbol{v}\right) &= 0 \quad \forall \boldsymbol{v} \in \mathbf{H}^1_\#(Y^\beta_m)\,, \\ a^\beta_m\left(\hat{\boldsymbol{w}},\, \boldsymbol{v}\right) &= b^\beta_m\left(1,\, \boldsymbol{v}\right) \quad \forall \boldsymbol{v} \in \mathbf{H}^1_\#(Y^\beta_m)\,, \\ a^\beta_m\left(\bar{\boldsymbol{w}},\, \boldsymbol{v}\right) &= -(1-\phi^\alpha) \fint_{\Gamma^\beta_Y} \boldsymbol{v}\cdot\boldsymbol{n}^{[m]} \quad \forall \boldsymbol{v} \in \mathbf{H}^1_\#(Y^\beta_m)\,. \end{aligned} \tag{6}$$

The pressure fluctuation associated with the α-level porosity is driven by the characteristic pressure response: find $\eta^1 \in H^1_\#(Y^\beta_m)/\mathbb{R}$ such that

$$\fint_{Y^\beta_m} \boldsymbol{K}\nabla_y(\eta^i + y_i)\cdot\nabla_y\psi = 0 \quad \forall \boldsymbol{v} \in H^1_\#(Y^\beta_m)\,. \tag{7}$$

The permeability $\boldsymbol{K}$ can be computed using the standard homogenization of the Stokes flow considered in a connected α-porosity generated by Y^α_c, see e.g. Hornung (1997); Sanchez-Palencia (1980).

Homogenized coefficients The homogenized coefficients describing the material behaviour at the β level are computed as follows:

$$\begin{aligned} \mathbb{A}^\beta &= (A^\beta_{ijkl}), \quad A^\beta_{ijkl} = a^\beta_m\left(\boldsymbol{w}^{ij} + \boldsymbol{\Pi}^{ij},\, \boldsymbol{w}^{kl} + \boldsymbol{\Pi}^{kl}\right)\,, \\ \boldsymbol{B}^\beta &= (B^\beta_{ij}), \quad B^\beta_{ij} = b^\beta_m\left(1,\, \boldsymbol{w}^{ij} + \boldsymbol{\Pi}^{ij}\right)\,, \\ \bar{\boldsymbol{B}}^\beta &= (\bar{B}^\beta_{ij}), \quad \bar{B}^\beta_{ij} = (1-\phi^\alpha)\phi^\beta\delta_{ij} + a^\beta_m\left(\boldsymbol{w}^{ij},\, \bar{\boldsymbol{w}}\right)\,, \\ \boldsymbol{K}^\beta &= (K^\beta_{ij}), \quad K^\beta_{ij} = \fint_{Y^\beta_m} \boldsymbol{K}\nabla_y(\eta^i + y_i)\cdot\nabla_y(\eta^j + y_j)\,, \end{aligned} \tag{8}$$

where $\mathbb{A}^\beta$ is the skeleton stiffness corresponding to the dried medium, $\boldsymbol{B}^\beta$ and $\bar{\boldsymbol{B}}^\beta$ are the Biot-type stress coefficients associated with two pressures, p^α pressure field in the matrix (in the α-level pores) and $\bar{p}^\beta$ a single scalar pressure in the β-level channels, respectively, and $\boldsymbol{K}^\beta$ is the effective permeability. There are three effective Biot compressibility modulae

$$M^\beta = a^\beta_m\left(\hat{\boldsymbol{w}},\, \hat{\boldsymbol{w}}\right)\,, \quad \bar{M}^\beta = a^\beta_m\left(\bar{\boldsymbol{w}},\, \bar{\boldsymbol{w}}\right)\,, \quad N^\beta = a^\beta_m\left(\hat{\boldsymbol{w}},\, \bar{\boldsymbol{w}}\right)\,, \tag{9}$$

which constitute the following compressibility matrix:

$$\mathbb{M}^\beta = \begin{bmatrix} M^\beta + M^\alpha + \gamma\phi^\alpha & N^\beta \\ N^\beta & \bar{M}^\beta + \gamma\phi^\beta \end{bmatrix}\,. \tag{10}$$

Macroscopic equations The macroscopic behaviour of the double porosity fluid saturated medium is described by the triplet $(\boldsymbol{u}, p^\alpha, \bar{p}^\beta) \in \mathbf{H}^1(\Omega^\beta)\times L^2(\Omega^\beta)\times\mathbb{R}$ which satisfies the macroscopic equations (we use the abbreviation $\Omega = \Omega^\beta$)

$$\begin{aligned} \int_\Omega \mathbb{A}^\beta\boldsymbol{e}(\boldsymbol{u}):\boldsymbol{e}(\boldsymbol{v}) - \int_\Omega \boldsymbol{e}(\boldsymbol{v}):\left[\boldsymbol{B}^\beta, \bar{\boldsymbol{B}}^\beta\right][p^\alpha, \bar{p}^\beta]^T &= \int_{\partial\Omega}(1-\phi^\beta)\hat{\boldsymbol{g}}^\alpha\cdot\boldsymbol{v}\,\mathrm{dS}_x \\ &\quad + \int_\Omega (1-\phi^\beta)\hat{\boldsymbol{f}}^\alpha\cdot\boldsymbol{v}\,, \\ \int_\Omega [q^\alpha, \bar{q}^\beta]\left[\boldsymbol{B}^\beta, \bar{\boldsymbol{B}}^\beta\right]^T &: \boldsymbol{e}(\dot{\boldsymbol{u}}) \\ + \int_\Omega \boldsymbol{K}^\beta\nabla p^\alpha\cdot\nabla q^\alpha + \int_\Omega \kappa^\beta(p^\alpha - \bar{p}^\beta)(q^\alpha - \bar{q}^\beta) & \\ + \int_\Omega [q^\alpha, \bar{q}^\beta]\cdot\mathbb{M}^\beta[\dot{p}^\alpha, \dot{\bar{p}}^\beta]^T &= -J^\beta_{\mathrm{ext}}\bar{q}^\beta + \int_{\partial\Omega}(1-\phi^\beta)q^\alpha\bar{w}_n\,\mathrm{dS}_x\,, \end{aligned} \tag{11}$$

for all triplets $(\boldsymbol{v}, q^\alpha, \bar{q}^\beta) \in \mathbf{H}^1(\Omega^\beta) \times L^2(\Omega^\beta) \times \mathbb{R}$, where $\kappa^\beta = \fint_{\Gamma_Y^\beta} \bar{\kappa}$ is the average interface permeability, $\hat{\boldsymbol{f}}^\alpha, \hat{\boldsymbol{g}}^\alpha$ are given forces, $\bar{w}_n$ is a draining flux outwards the α porosity and $J^\beta_{\rm ext}$ is a given overall drainage of the β-level connected pores. Obviously, the data must satisfy some solvability conditions.

If $\boldsymbol{K}^\beta$ or κ^β are nonvanishing, initial conditions must be supplied; one may consider the unloaded and undeformed state, or a steady state characterized by a single pressure value, i.e. $p^\alpha(x, \cdot) = \bar{p}^\beta(\cdot)$, $x \in \Omega^\beta$.

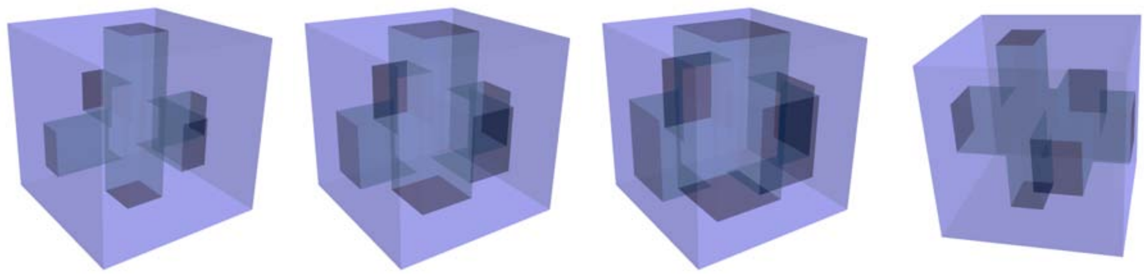
3. Numerical example

The homogenization results presented in previous sections were discretized by the finite element method and implemented in a standalone computer code based on our code SfePy, see Cimrman and contributors (2012). In this section we show some results obtained by this code.

For numerical illustration of effects of geometry of connected porosities on the level α we used the reference periodic cells of the micro structures shown in Fig. 2. Three cases were considered:

- **#1**: α-level porosity in Fig. 2 (a), β-level porosity in Fig. 2 (d),
- **#2**: α-level porosity in Fig. 2 (b), β-level porosity in Fig. 2 (d),
- **#3**: α-level porosity in Fig. 2 (c), β-level porosity in Fig. 2 (d),

that is, the diameters of α-level channels increased with the case number. The following material/geometrical



(a) (b) (c) (d)

Fig. 2: (a)-(c): reference cells for level α, case #1, #2 and #3. (d) reference cell with connected porosity for level β for all cases.

parameters were used:

coefficient	units	where	level	values
stiffness $\mathbb{D}$	GPa	Y_m	α	$\lambda = 17$, $\mu = 1.7$
kinematic fluid viscosity ν	m^2/s	Y_c	α	$\nu = 10^{-6}$
fluid compressibility γ	GPa^{-1}	Ω^β	macro β	$\gamma = 1.0$
interface permeability κ^β	m / (GPa s)	Ω^β	macro β	$\kappa^\beta = 10^{-6}$
porosity ϕ	1	case #1	α	$\phi = 0.119$
	1	case #2	α	$\phi = 0.236$
	1	case #3	α	$\phi = 0.376$
	1	all cases	β	$\phi = 0.185$

where the Lamé parameters defined the stiffness tensor as follows:

$$\mathbb{D} : D_{ijkl} \equiv \mu(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) + \lambda\delta_{ij}\delta_{kl} \; .$$

Because a practical computation has to be related to a real scale of an existing microstructure, and because of scaling assumptions for fluid viscosity and interface permeability, we assumed the real value of $\varepsilon = 10^{-3}$ and scaled the values given above accordingly, when solving for the homogenized coefficients

coef.	$\boldsymbol{K}^\alpha$	$\boldsymbol{K}^\beta$
#1	$\begin{bmatrix} 4.44 \cdot 10^{-5} & 0 & 0 \\ 0 & 4.44 \cdot 10^{-5} & 0 \\ 0 & 0 & 1.40 \cdot 10^{-4} \end{bmatrix}$	$\begin{bmatrix} 3.62 \cdot 10^{-5} & 0 & 0 \\ 0 & 3.62 \cdot 10^{-5} & 0 \\ 0 & 0 & 1.14 \cdot 10^{-4} \end{bmatrix}$
#2	$\begin{bmatrix} 2.95 \cdot 10^{-4} & 0 & 0 \\ 0 & 2.95 \cdot 10^{-4} & 0 \\ 0 & 0 & 5.91 \cdot 10^{-4} \end{bmatrix}$	$\begin{bmatrix} 2.40 \cdot 10^{-4} & 0 & 0 \\ 0 & 2.40 \cdot 10^{-4} & 0 \\ 0 & 0 & 4.82 \cdot 10^{-4} \end{bmatrix}$
#3	$\begin{bmatrix} 1.06 \cdot 10^{-3} & 0 & 0 \\ 0 & 1.06 \cdot 10^{-3} & 0 \\ 0 & 0 & 1.74 \cdot 10^{-3} \end{bmatrix}$	$\begin{bmatrix} 8.63 \cdot 10^{-4} & 0 & 0 \\ 0 & 8.63 \cdot 10^{-4} & 0 \\ 0 & 0 & 1.42 \cdot 10^{-3} \end{bmatrix}$

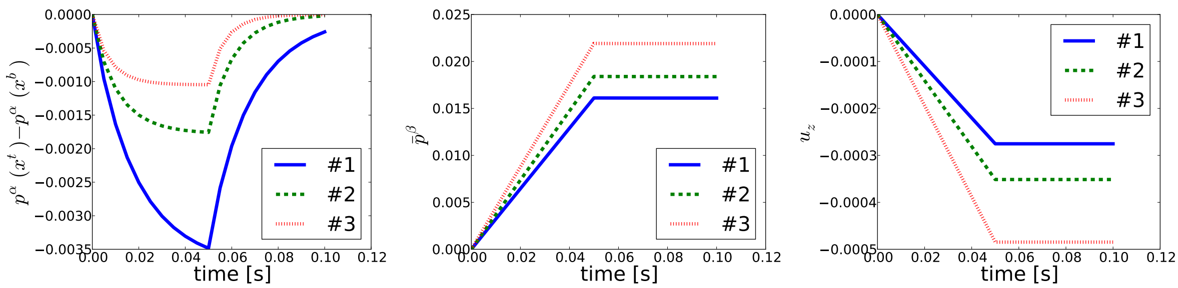
Tab. 1: Homogenized permeability coefficients on levels α, β for cases #1, #2 and #3.

($\nu \to \nu/\varepsilon^2$, $\kappa^\beta \to \kappa^\beta/\varepsilon$). The computations resulted in the homogenized coefficients. Here we report only the permeabilities that are summarized in Tab. 1 for the three cases.

The macroscopic equations of level β (11) were solved on a cube domain with the following initial and boundary conditions:

- $\boldsymbol{u}(0,\cdot) = 0$, $p^\alpha(0,\cdot) = 0$, $\bar{p}^\beta(0,\cdot) = 0$,
- $\boldsymbol{u}(t,x) = 0$ for x in bottom face,
- pressure traction load on the top face, with magnitude equal to time step $\times 10^{-2}$ [GPa] up to step 10, then held on the value 10×10^{-2}, for 20 time steps, $t \in [0, 0.1]$.

In Fig. 3 we compare time histories of macroscopic solutions for the three cases and in Fig. 4 several snapshots of macroscopic solutions are shown. It can be seen that the connected porosity behaves in a viscoelastic manner because of the fluid flow in the interconnected pores. The influence of the pore geometry (radius) is clearly demonstrated.



(a) (b) (c)

Fig. 3: Comparison of time histories of macroscopic solutions for the three cases: (a) difference between p^α in a point on the top face x^t and bottom face x^b; (b) $\bar{p}^\beta$, (c) z-displacement in x^t.

4. Conclusion

We have developed a two-level homogenized model of poroelastic media with weakly permeable interface between the two porosities. The two upscaling levels allow representing three scales which, however, should be separated in the sense of different enough characteristic lengths. As an advantage, the poroelastic coefficients can be computed for a given geometrical arrangement of micro- and meso-structures.

Since the model is intended to describe hierarchical structure of pores in the canaliculo–lacunar porosity of bone, we consider two "microscopic" levels with connected pores (Rohan et al., 2012a).

The homogenization procedure reported in this paper makes possible to treat an arbitrary geometry and topology of the pores, whereby the localization tensors and coefficients can be calculated as the response of the autonomous microscopic problems; this was demonstrated using a numerical example computed by our code (Cimrman and contributors (2012)). The assumption of the weakly permeable

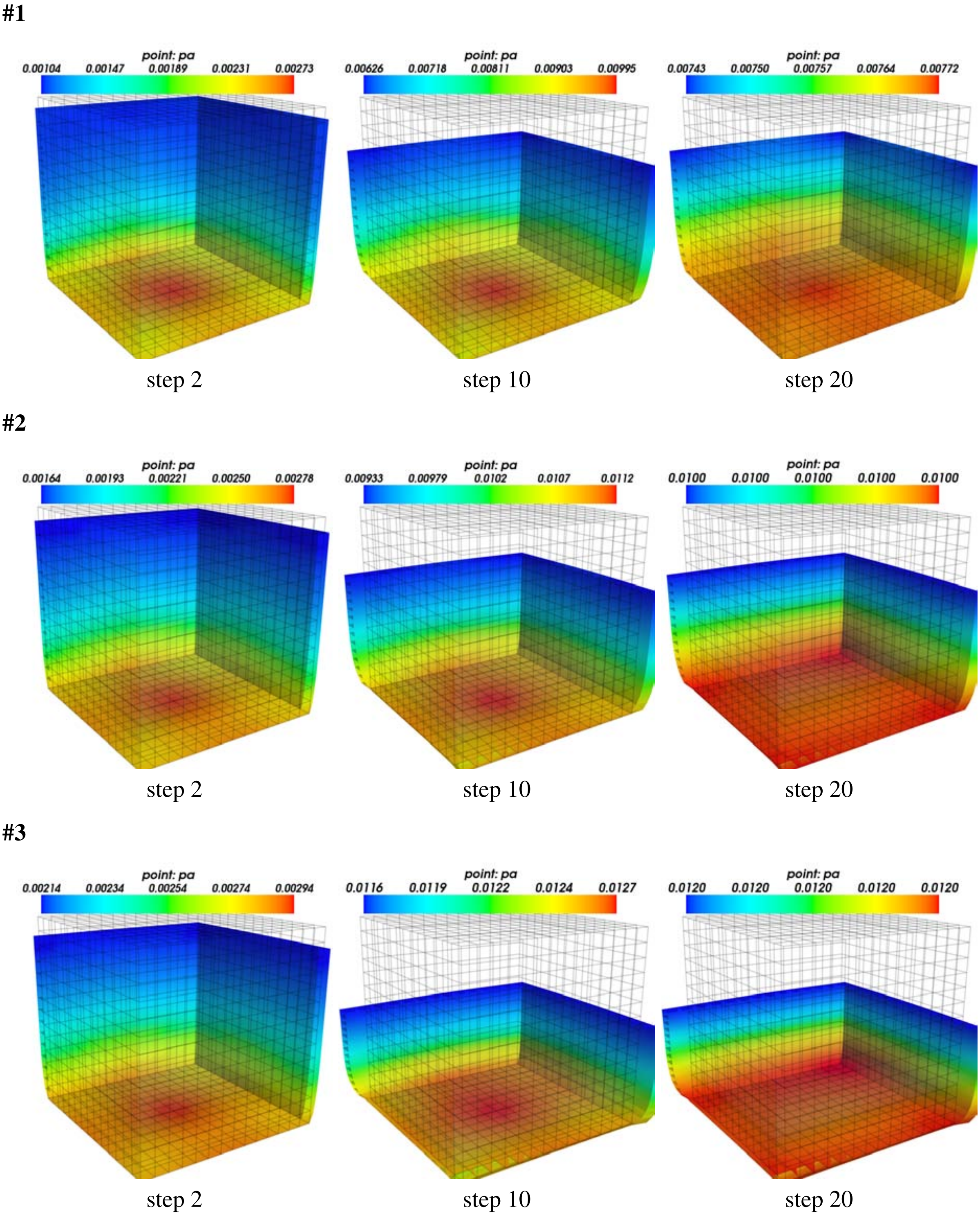


Fig. 4: Snapshots of macroscopic solutions ($10\times$ magnified $\boldsymbol{u}$, color = p^α) in time steps 2, 10 and 20 for the case #1 (top), #2 (middle) and #3 (bottom).

interface disables full connection of the two porosities; this situation is treated in a separate paper Rohan et al. (2012a), cf. Rohan et al. (2012b) for related issues of the double porous materials.

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