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PARAMETERIZED ORTHOTROPIC CELLULAR MICROSTRUCTURES AS MECHANICAL MODELS OF CANCELLOUS BONE

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Abstract. *Constitutive properties of cancellous bone depend on microstructural geometry. Evaluation of the interrelationship is a crucial issue in analysis of stresses and strains in bone tissues and simulation of their remodelling. Known limitations of experimental methods as well as of the micro-FE techniques make the analysis and homogenization of 'equivalent' trabecular microstructures an advantageous tool for this task. In this study, parameterized orthotropic constitutive models of cancellous bone are derived from finite element analysis of repeatable microstructure cells. The models are fully three-dimensional, have realistic curvilinear shapes and are parameterized with four shape parameters. Variation of the parameters allows to imitate most of the typical microstructure patterns observed in real bones, along with variety of intermediate geometries. The models are a geometrically enhanced version of those presented in the author's previous work [1]. Static numerical tests are performed with the finite element method for an exhaustive number of parameter value sets (microstructure instances). Repeatability of the microstructure allows to test only a sigle cell with appropriate boundary conditions. Values of computed stresses and strains allow to determine all coefficients of elastic orthotropic stiffness matrix. Results have a form of tabularized functions of elastic constants versus the shape parameters. Comparison of the results with micro-FE data obtained for a large set of cancellous bone specimens [2] proves a good agreement.*

1 INTRODUCTION

Constitutive properties of cancellous bone are necessary data in any reliable analysis of stress and strain distribution in bone. Besides, in view of the nature of adaptive bone remodelling as well as of pathological changes in bone microstructure due to e.g. osteoporosis, the constitutive properties should be related to certain geometric parameters of bone microstructure.

Material properties of cancellous bone may be assumed elastic orthotropic [3]. Input data to the analysis must thus contain nine independent elastic constants and three angle values defining the spatial orientation of principal axes of orthotropy. This makes twelve constants altogether, each of them being a function of spatial location, as the tissue is strongly heterogeneous.

The necessary data is thus very extensive. Three methods of their acquirement can be distinguished

- mechanical tests (see e.g. [4, 5, 6, 7, 8, 9]) — the most ‘traditional’ method, suffering from numerous limitations (fragmentary character, errors due to size effects, preparation-induced damage, support conditions, arbitrary preparation directions, limited number of measurable elastic constants) which make their results unsatisfactory for computational engineers,

- computer simulation of mechanical tests consisting in the finite element analysis of cancellous bone specimens digitized with micro-CT techniques (see e.g. [10, 11, 12, 13, 14, 16, 15, 17] — the method provides the complete set of elastic constants and orientation angles for each specimen, under the assumption that microscopic elastic constants of trabecular tissue are known. The results are, however, still prone to the above mentioned errors, although to a lesser extent,

- mechanical analysis of equivalent repeatable cellular microstructures believed to imitate cancellous bone [19, 20, 21, 22, 23, 1] — overcomes all drawbacks of the former two methods, at a price of worse compatibility to real bone morphology. The models simplify, to a lesser or larger extent, trabecular geometry and thus they usually fail to describe at a satisfactory accuracy a full variety of types of cancellous bone.

The common disadvantage of the first two methods is that the data provided are not systematic, i.e. not directly related to any geometric parameters of the microstructure. Thus, it is not possible to directly extrapolate them to other tissue instances. Such relationships can be estimated by the correlation analysis between the measured constants and certain directional morphometric parameters of the geometrically anisotropic microstructure [12, 13], the results are, however, merely statistical graphs and do not explain the dependence mechanism. Besides, the relation between e.g. the loss or growth of trabecular tissue and evolution of anisotropic morphometric parameter values is not straightforward, which makes it still difficult to employ such results in simulation of bone remodelling. The third method provides results that are parameterized by certain geometric parameters.

This paper follows the third concept and extends ideas presented in the author’s previous publication [1]. The objective is to numerically derive a parameterized family of repeatable cellular microstructures whose numerically derived constitutive properties could describe with good accuracy mechanical behaviour of as many kinds of cancellous bone as possible. In particular, the model can imitate, for different values of geometric parameters, the four basic types of microstructure distinguished by Gibson and Ashby [18]: (i) equiaxed bar network (spatial frame), (ii) equiaxed plate network (spatial cluster of thin-walled boxes), (iii) honeycomb tube, and (iv) array of parallel plates with spacer bars. The enhancement to the model presented in [1] consists in introduction of a new design of repeatable cell geometry that allows to model full orthotropy of material and overcome the problem of systematic right angles between trabeculae (which may result in unrealistic relationships between e.g. the anisotropic Poisson ratio values). Three different geometric families of equivalent microstructures are investigated. The results are compared to experimental-numerical data [2] obtained for a large set of actual cancellous bone specimens. The models provide exhaustive information on how stiffness and anisotropy of bone depends on cross-sectional parameters of trabecular bars and plates of different spatial orientations. The data can thus be used to e.g. qualitative studies of bone anisotropy or to simulations of bone remodelling processes with anisotropic microstructure evolution laws.

2 GEOMETRIC MODEL

The equivalent trabecular microstructure model consists of repeatable cells arranged in rows and layers so as to completely fill the 3-D space. Figure 1 presents the general geometry of three cell types analysed in the paper. Each of them is inscribed into a space-filling polyhedron: a cube, a triangular prism (wedge), and an irregular dodecahedron, further referred to as the "qcs polyhedron" (for roughly resembling a quartz crystal shape). The first two of them were analysed in [1]; the third one is developed in order to overcome some drawbacks of the former. Pink areas are the cross-sections at which the cell is connected to identical neighbouring cells. The size of the entire cell (the *unit* length) is not essential – it does not affect the macroscopic mechanical properties of the repeatable structure constituted by the cell. Directions of the x_i axes correspond to local principal directions of mechanical orthotropy of cancellous bone and do not imply orientation of microstructure in the real space.

Four dimensionles shape parameters, t_c, t_h, t_v and t_e, define different repeatable microstructural instances. The first three of them are defined in Fig. 1; they take values from the interval (0,1) (additionally $t_h \geq t_c$ and $t_v \geq t_c$) and they define mutual proportions between trabecular thicknesses and plate widths in different difrections. The fourth parameter, t_e, is the extension ratio of the entire cell in the x_1 direction. In Fig. 1, $t_e = 1$ which corresponds to transverse isotropy in the (x_1, x_2) plane; other values of t_e result in fully orthotropic microstructures.

Figure 2 displays examples of microstructures built up of the three basic cells for various sets of parameter values. It can be seen that the models can simulate a wide variety of microstructural patterns of cancellous bone, including the typical patterns reported by Gibson and Ashby [18].

3 COMPUTATIONS

Macroscopic mechanical properties of the equivalent microstructures are determined with finite element analysis. A specific code is written to discretize a single cell with finite elements for arbitrary values of the shape parameters t_c , t_h , t_v , t_e . Figure 3 presents an example of a finite element mesh.

Since the microstructure is repeatable, only one cell needs to be actually analysed, with appropriate boundary conditions that ensure fitting of all deformed neighbouring cells to each other. Such arbitrary definition is possible, without knowing the stress and strain distributions, because of multiple types of symmetry assumed in the geometric designs of the microstructural cells.

Six static load cases are considered: pure stretching in three orthogonal directions x_1 , x_2 , x_3 and pure shear in three orthogonal planes (normal to the three directions). Loads are imposed cubic cell

wedge cell

qcs cell

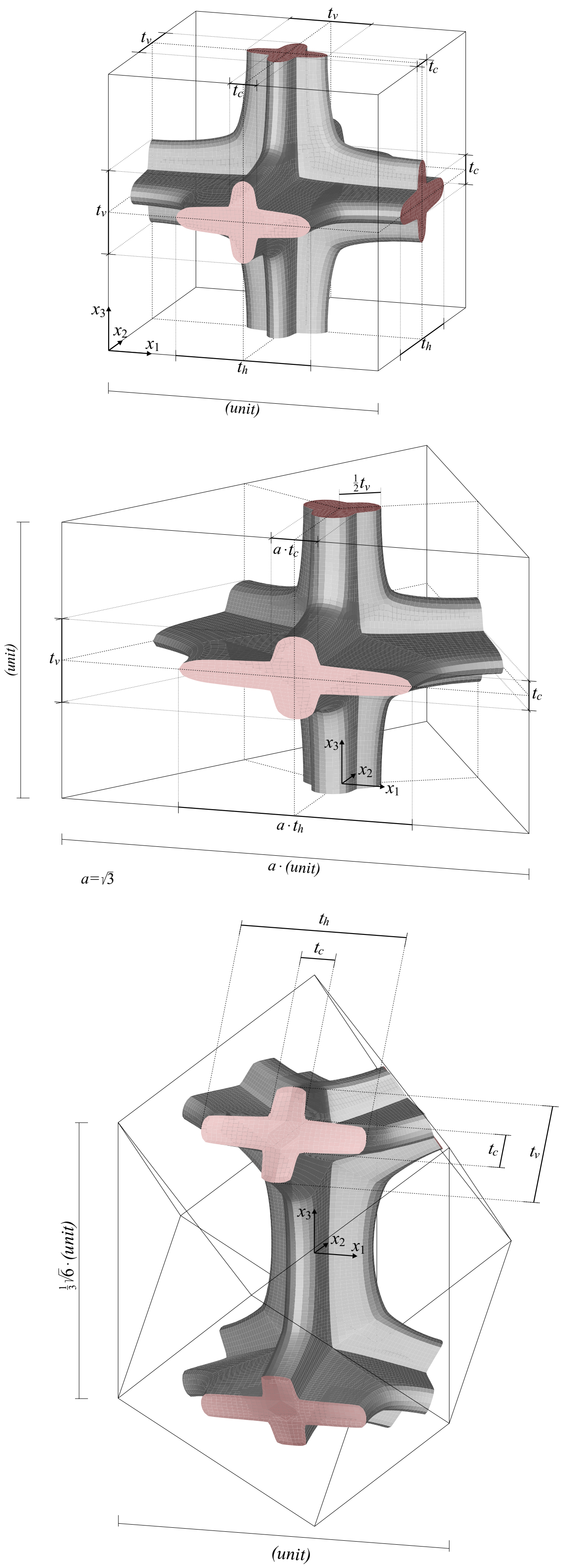

Figure 1: Geometry of a repeatable structural cell

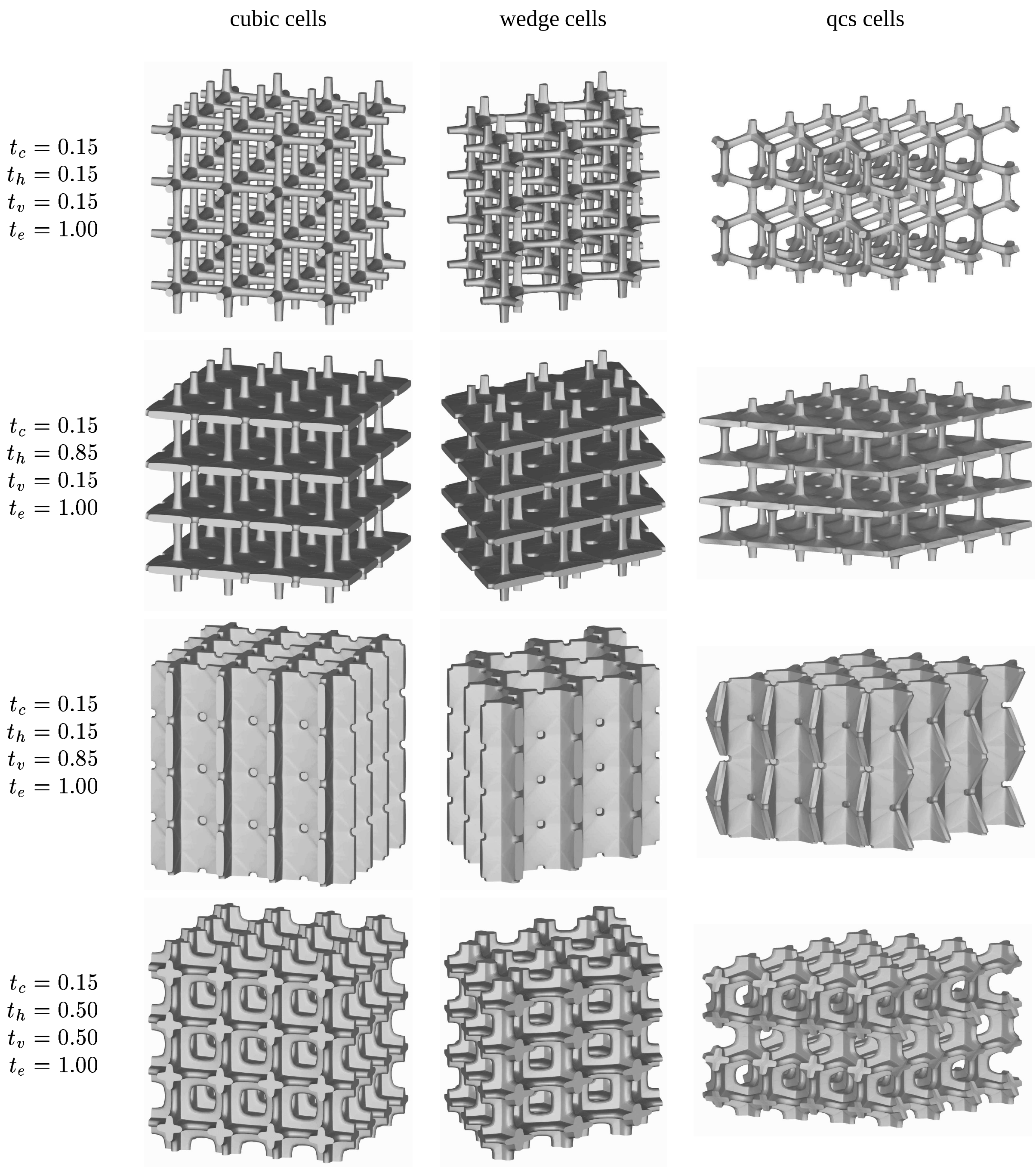

Figure 2: Examples of typical microstructures generated with repeatable cells of the three types for different values of geometric parameters

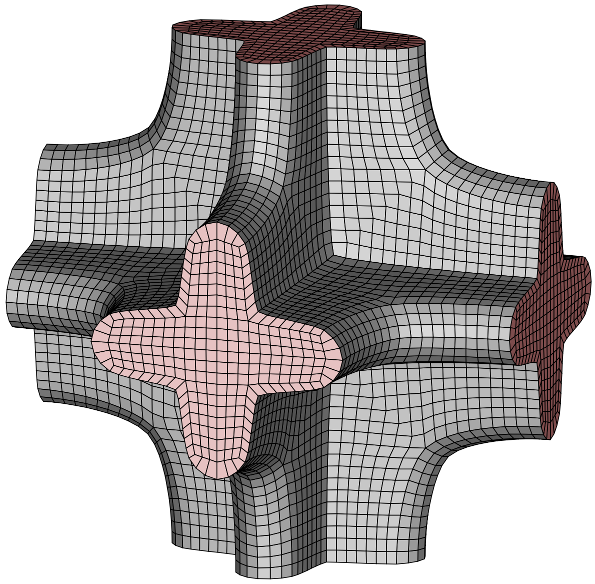

Figure 3: Example of a finite element mesh (cubic cell, $t_c = 0.15$, $t_h = 0.50$, $t_v = 0.50$, $t_e = 1.00$)

by assumed displacements of certain nodes (corresponding to uniform macroscopic strains) and, for each case, reaction forces are measured. The forces, when divided by appropriate macroscopic cross-sectional areas, give six macroscopic stress components for each load case. Assuming the constitutive equation in the form

$$\boldsymbol{\sigma} = \mathbf{C}\,\boldsymbol{\varepsilon} \tag{1}$$

we can compute all the 36 coefficients of the constitutive stiffness matrix $\mathbf{C}$,

$$[\mathbf{C}] = \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{21} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{31} & C_{32} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{41} & C_{42} & C_{43} & C_{44} & C_{45} & C_{46} \\ C_{51} & C_{52} & C_{53} & C_{54} & C_{55} & C_{56} \\ C_{61} & C_{62} & C_{63} & C_{64} & C_{65} & C_{66} \end{bmatrix} \tag{2}$$

one column per load case. Due to geometric symmetries of the model the matrix appears to actually have the form

$$[\mathbf{C}] = \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ & C_{22} & C_{23} & 0 & 0 & 0 \\ & & C_{33} & 0 & 0 & 0 \\ & & & C_{44} & 0 & 0 \\ & sym. & & & C_{55} & 0 \\ & & & & & C_{66} \end{bmatrix} \tag{3}$$

(this is not a prerequisite in the computational scheme, but the numerical results described below in this section yield the form (3) of $\mathbf{C}$ with the accuracy of at least five decimal digits). Thus, there are only 9 elastic constants that need to be determined for each microstructural instance, i.e. for each set of shape parameter values t_c , t_h , t_v , t_e, and for assumed one of the three cell geometry types. Having them, we are also able to determine the engineering constants appearing in the inverse form of the constitutive equation (1)

$$\boldsymbol{\varepsilon} = \mathbf{D}\,\boldsymbol{\sigma}, \tag{4}$$

with

$$[\mathbf{D}] = \begin{bmatrix} \frac{1}{E_1} & -\frac{\nu_{12}}{E_1} & -\frac{\nu_{31}}{E_3} & 0 & 0 & 0 \\ & \frac{1}{E_2} & -\frac{\nu_{23}}{E_2} & 0 & 0 & 0 \\ & & \frac{1}{E_3} & 0 & 0 & 0 \\ & & & \frac{1}{G_{23}} & 0 & 0 \\ & sym. & & & \frac{1}{G_{31}} & 0 \\ & & & & & \frac{1}{G_{12}} \end{bmatrix}. \tag{5}$$

In order to determine the family of elastic properties parameterized by the shape parameters t_c , t_h , t_v , t_e, the finite element analysis described above has to be repeated for a sufficiently large number of microstructural instances. The stiffness coefficients C_{ij} and corresponding engineering elastic constants are thus determined as tabularized functions of the shape parameters for a wide spectrum of their values, for each of the three cell geometries separately.

In our study, numerical tests have been performed for a representative number of $(t_c\,, t_h\,, t_v\,, t_e)$ quadruplets. The value of t_c varied from 0.05 to 0.95 with the increment 0.05 while the values of $t_h\,,\ t_v$ varied independently from t_c to 0.95 with the same increment. Independently, t_e was assigned values 0.6, 0.8, 1.0, 1.2 and 1.4. This extensive set of ‘discrete’ results enables to extrapolate them on the entire domain $t_c \in (0,1)$, $t_h \in [t_c\,, 1)$, $t_v \in [t_c\,, 1)$, $t_e \in [0.6, 1.4]$. The domain of geometric data is much wider than the reality of cancellous bone types — thus many of the analysed combinations of the shape parameter values may not correspond to any real trabecular architecture. However, in order to make the results comprehensive, computations were performed for all of them.

The ABAQUS 6.4 general purpose finite element system [24] was used to perform the analysis. 8-node linear brick elements with selectively reduced Gauss integration were used. Depending on particular geometry, the number of elements in a cell model ranged between 11 000 and 133 000.

Certain mechanical properties had to be assigned to the trabecular bone at the microscopic level. Isotropy has been assumed. The Young modulus was set to unity — the resulting macroscopic stiffness matrix coefficients C_{ij} are thus dimensionless and have to be scaled by the actual trabecular stiffness. The Poisson ratio had to be assigned an arbitrary value ($\nu = 0.3$ has been assumed).

Tabularized values of elastic constants obtained as results of the analysis, are very extensive. Full comprehensive set of results for each cell geometry in the form of formatted ASCII files is available in the WWW [25]. Figure 4 displays an example set of graphs for the qcs cell, for $t_e = 1$ (transverse isotropy) and for selected values of t_c .

4 DISCUSSION

Validation of the FEA results obtained for equivalent microstructures is not easy, because of the lack of comprehensive experimental evidence. One can find, however, published results of finite element analysis of CT-scanned microstructural segments of different kinds of cancellous bone. Complete sets of orthotropic material constants were computed this way for several hundreds of samples of human cancellous bone, cf. [26]. Van Rietbergen and Huiskes [2] report these results depicted versus the volume fraction (dimensionless density) for each sample.

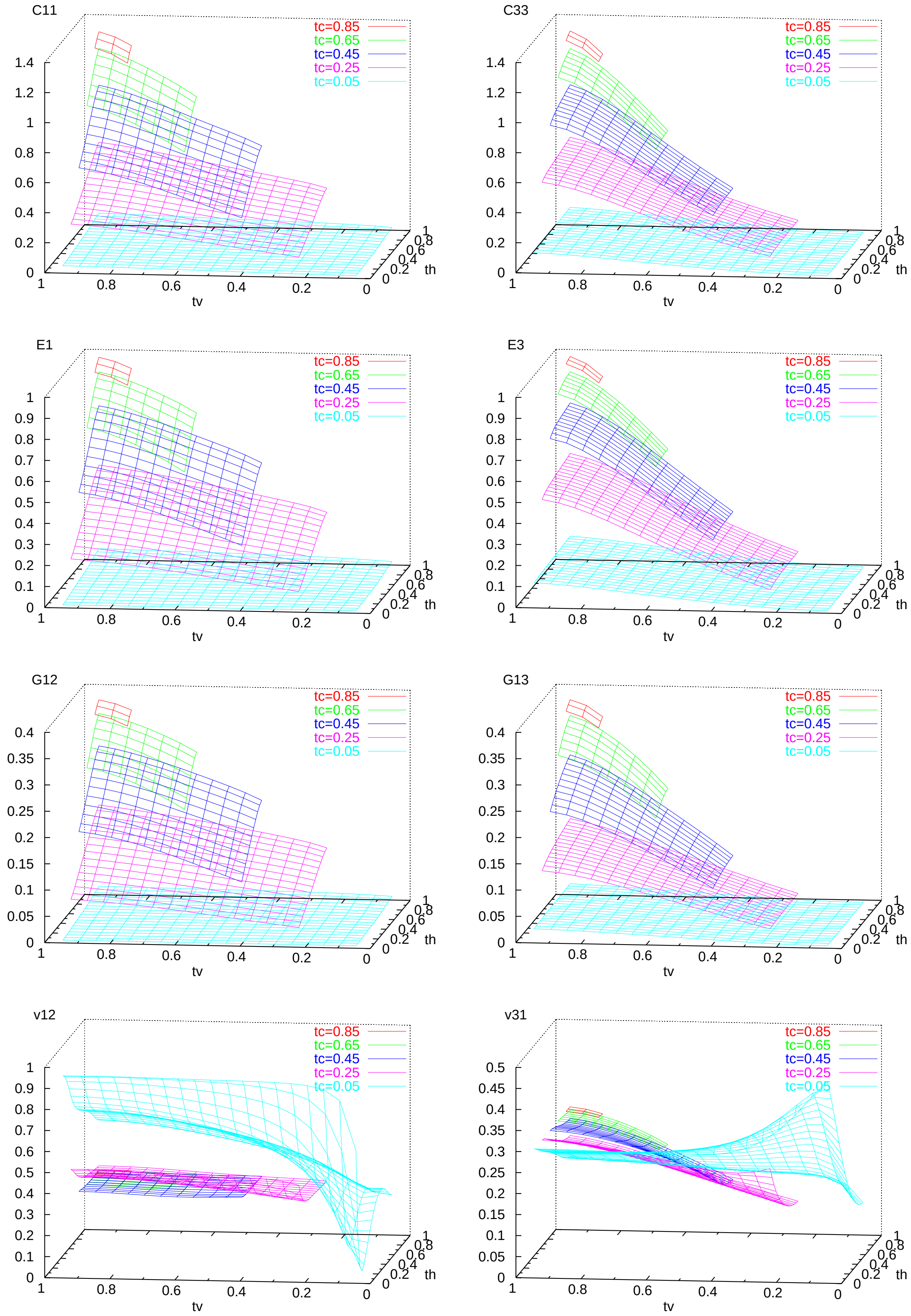

Figure 4: Elastic constants computed as functions of shape parameters, qcs cell, $t_e = 1$

Figures 5–7 present comparison of these data with our model results. For better compatibility, only results for volume fractions $\rho < 0.40$ are considered and, for the sake of legibility, results for only selected values of t_h , t_v and t_e are displayed. Note that there is a difference in definition of directions x_1 , x_2 , x_3 between the two studies – in the cited data the axis x_1 corresponds to the highest value of stiffness modulus (i.e. $E_1 \geq E_2 \geq E_3$) while in this study there is no such rule so that the directions had to be redefined in Figs. 5–7 to make the two sets of results comparable.

Comparing the areas covered by clouds of points obtained for actual bone (bullets) and for the equivalent microstructures (crosses), we can see that in most cases the latter 'include' the former, i.e. the equivalent model results cover wider areas than the results for actual bone specimens. This is a good result, indicating that, as it has already been mentioned, the equivalent microstructures can model much wider spectrum of possible morphologies than those occurring in physiological reality of various cancellous bone types. However, in some cases differences between experimental and model results can be observed. It is seen, for instance, in Fig. 5 that longitudinal moduli obtained for cubic cell family visibly overestimate the experimentally determined values. To some (although much lesser) extent, this phenomenon can be observed for wedge cells (E_1 and E_3) and for qcs cells (E_3). For shear moduli, cf. Fig. 6, compatibility of model and experimental results is very good. The most signifiocant differences can be observed for the Poisson ratio values (Fig. 7). Cubic cells exhibit a systematic property $\nu_{ij} \leq 0.3$ (where 0.3 is the value of ν assumed for isotropic trabecular tissue. For prismatic cells we have $\nu_{13} \leq 0$ while ν_{23} takes either values higher than 0.3 or very close to zero. In both the cases the properties can be qualitatively deduced from specific features of the cells' geometry and connectivity. It can be seen, however, that the systematic properties do not conform to the experimental results for Poisson ratios. In view of the latter, only the qcs cell family corresponds reasonably to reality, although one can point some isolated experimental values of Poisson ratios (especially in the range $\nu_{ij} < 0.15$) that are not represented in the cloud of model results. Summarizing, the equivalent microstructure based on the qcs model seems to be the one best conforming to real cancellous bone from the point of view of its mechanical properties.

The four geometric parameters characterizing the microstructure are convenient from the point of view of the equivalent microstructure definition and description, however, in an actual sample of bone they may not be easily measurable. There are other quantities like histomorphometric coefficients frequently reported in description of cancellous bone (Tb.Th, Tb.Sp, Tb.N, BV/TV, BS/TV), as well as various anisotropic fabric tensors (MIL, SVD, SLD, VO). Some of them may be associated with the parameters defined in this study, for example apparent density (BV/TV) is directly measured here and there is a full conceptual analogy between the parameter t_c and the Tb.Th ratio. However, the other parameters do not lend themselves to be easily expressed by known measurable quantities. Further studies are necessary to correlate the shape parameters t_c , t_h , t_v , t_e , and, indirectly, also the measured elastic constants, with the morphometric parameters, particularly with principal values of fabric tensors which are possible to be measured for equivalent cells. Results are to be published in [27].

The concept of parameterization of orthotropic material properties by orthotropic geometric quantities allows to better estimate full mechanical properties of actual bone in cases we have only partial information about the properties and geometry. Besides, the concept allows to better understand correlation between orthotropic mechanical properties and adaptive remodelling of trabeculae as well as their pathological changes (e.g. due to osteoporosis). It can also enable new anisotropic formulations of bone remodelling laws.

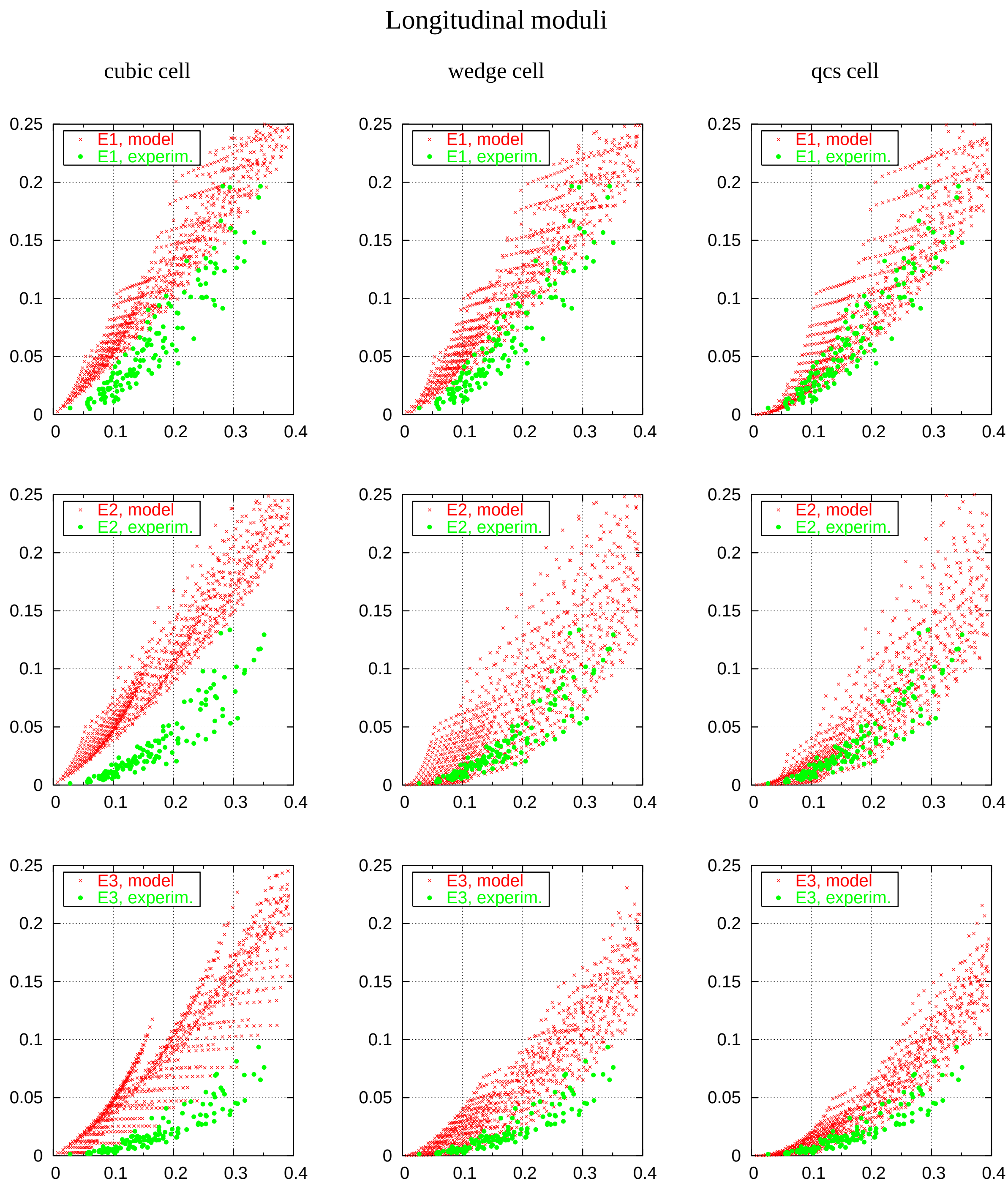

Figure 5: Material constants vs. apparent density graphs for various trabecular geometries: comparison of this study model results with micro-FE results for actual cancellous bone samples [2]. This study results are limited to $\rho < 0.40$ and to only selected values of shape parameters. Part 1: Longitudinal moduli E_1 , E_2 , E_3

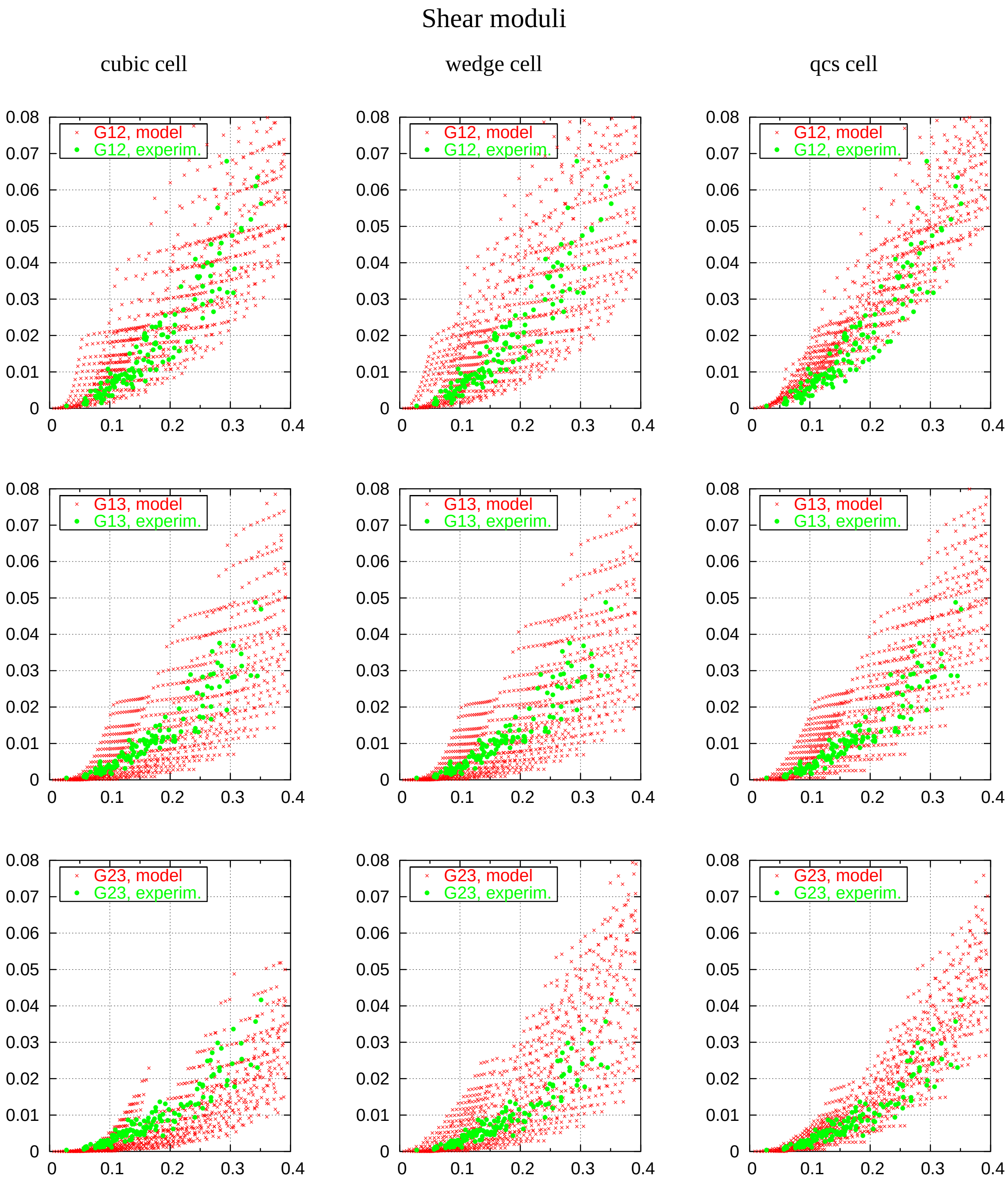

Figure 6: Material constants vs. apparent density graphs for various trabecular geometries: comparison of this study model results with micro-FE results for actual cancellous bone samples [2]. This study results are limited to $\rho < 0.40$ and to only selected values of shape parameters. Part 2: Shear moduli G_{12} , G_{13} , G_{23}

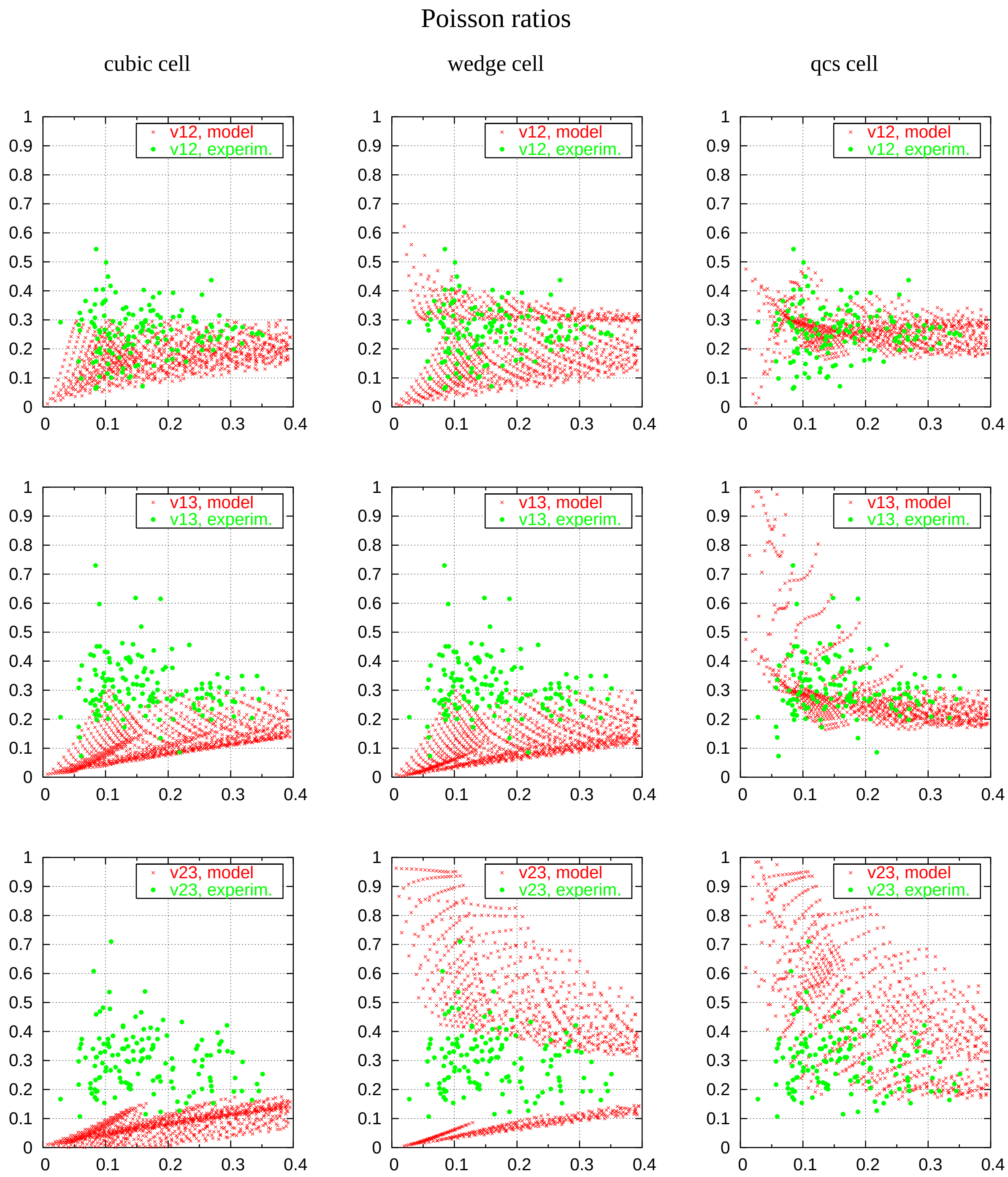

Figure 7: Material constants vs. apparent density graphs for various trabecular geometries: comparison of this study model results with micro-FE results for actual cancellous bone samples [2]. This study results are limited to $\rho < 0.40$ and to only selected values of shape parameters. Part 3: Poisson ratios ν_{12} , ν_{13} , ν_{23}

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