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Modeling of Vertebrae Bone Growth by Topology Optimization ⋆

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1. INTRODUCTION

It is widely known that trabecular bones of vertebrates are constantly being remodeled in response to the corresponding local stresses and strains Boyle (2011). This is called Wolff's law. On the other hand, it has yet to be understood how the outer shape of a vertebrae bone is formed. In this study, based on the observation of zebrafish vertebrae bones, we hypothesize that a vertebrae bone is composed of the two regions: one is formed a priori, while the other is formed a posteriori against external loading like trabecular bones. Assuming that Wolff's law can be expansively applied to the formation of the outer shape of a vertebrae bone, we introduce a mathematical model using topology optimization.

2. ZEBRAFISH AS A MODEL ORGANISM

In this research, we focus on zebrafish as a model organism. Zebrafish backbone is consist of 32 vertebrae (Fig. 1). The vertebrae bones significantly change their shapes as zebrafish is growing up from juvenile to adult (Fig. 2).

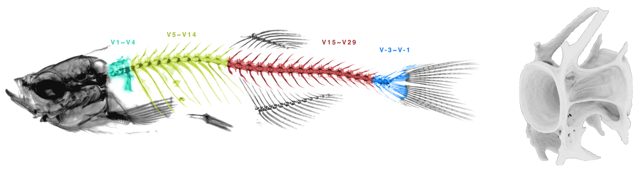

Fig. 1. Zebrafish skeleton (left) and V15 single vertebra(v15) scanned with micro-CT (right)

3. MATHEMATICAL MODELING

Based on the observation of zebrafish vertebrae bones, we hypothesize that a vertebrae bone is composed of two regions: one is formed a priori, while the other is formed a posteriori against external loading. To simulate the growth of such a vertebrae bone we first divide the computational domain into some subdomains as shown in Fig. 3. Regardless of external loading the white parts always have bones, while the green parts have no bones

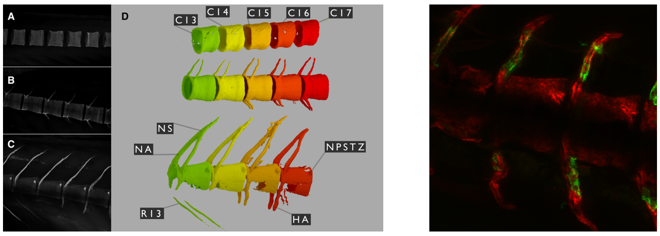

Fig. 2. Vertebra development (left) and visualization of osteoblast (right)

because the regions are occupied by nerves and blood vessels. These parts form a congenital basic structure. Assuming that loading acts on the two ends of the two cones, we apply distributed load on the red and orange parts with 1 and 0.5, respectively. In response to these mechanical stimuli, the bone shape in the purple parts is determined based on the following mathematical model.

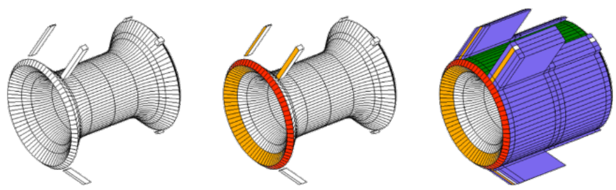

Fig. 3. Computational domain for simulating the growth of vertebrae bone.

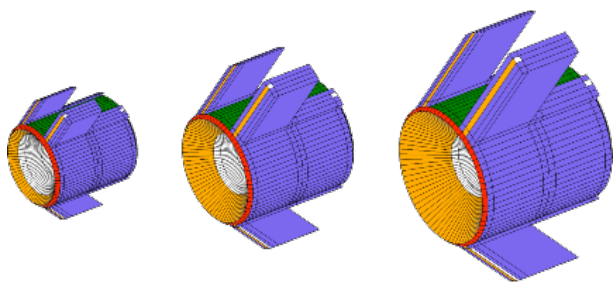

Fig. 4. Parameterization for the growth of computational domain

We first define bone density ρ by the following regularized Heaviside function of a scalar function ϕ:

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$$\rho(\phi) = \begin{cases} d & (\phi < -h) \\ (1-d)H(\phi) + d & (-h \leq \phi \leq h) \\ 1 & (h < \phi) \end{cases} \tag{1}$$

where h is the half bandwidth between the bone domain ($h < \phi$) and the void domain ($\phi < -h$). d is a very small positive lower bound set for avoiding singularity of the stiffness matrix. $H(\phi)$ is defined as

$$H(\phi) = \frac{1}{2} + \frac{15}{16}\left(\frac{\phi}{h}\right) - \frac{5}{8}\left(\frac{\phi}{h}\right)^3 + \frac{3}{16}\left(\frac{\phi}{h}\right)^5 \tag{2}$$

With this representation, we assume that the bone structure in the purple part is obtained as a solution to the following optimization problem:

$$\begin{aligned} &\underset{\phi}{\text{minimize}} \quad f := \int_{\Gamma_\mathrm{N}} \boldsymbol{t} \cdot \boldsymbol{u} \, \mathrm{d}\Gamma \\ &\text{subject to } g := \int_{\mathrm{D}} \rho(\phi) \, \mathrm{dD} - \overline{V} \leq 0, \end{aligned} \tag{3}$$

where $\overline{V}$ is the upper bound of total volume, $\boldsymbol{t}$ is the external surface traction, $\boldsymbol{u}$ is the displacement vector. Since the optimization problem (3) takes the nested form, the displacement vector $\boldsymbol{u}$ is given by solving the following force equilibrium problem.

Assuming the deformation is infinitesimal, the stress tensor σ and the strain $\boldsymbol{\epsilon}$ can be expressed with linear isotropic elasticity tensor $\mathbf{E}$ as

$$\sigma = \mathbf{E} : \boldsymbol{\epsilon}(\boldsymbol{u}), \qquad \boldsymbol{\epsilon}(\boldsymbol{u}) = \frac{1}{2}\left(\nabla \boldsymbol{u} + \nabla \boldsymbol{u}^\top\right). \tag{4}$$

Bone density ρ is embedded in the elasticity tensor as

$$\mathbf{E} = \rho^P \mathbf{E}_0, \tag{5}$$

where $\mathbf{E}_0$ is the elasticity tensor when $\rho = 1$. $P(= 3)$ is introduced for penalizing the intermediate values [0,1]. Finally, the force equilibrium problem is formulated as

$$\left.\begin{aligned} -\nabla \cdot \sigma = \mathbf{0} & \text{ in } \mathrm{D} \\ \boldsymbol{u} = \mathbf{0} \quad & \text{ on } \Gamma_\mathrm{D} \\ \sigma \cdot \boldsymbol{n} = \boldsymbol{t} \quad & \text{ on } \Gamma_\mathrm{N} \end{aligned}\right\}. \tag{6}$$

In order to set up the time evolution equation for topology optimization (3), we introduce the Lagrangian $L := f + \lambda g$ and pursue the following optimality condition Kawamoto (2013):

$$\frac{\mathrm{d}L}{\mathrm{d}\phi} = \frac{\mathrm{d}f}{\mathrm{d}\phi} + \lambda \frac{\mathrm{d}g}{\mathrm{d}\phi} = 0, \quad \lambda g = 0, \quad \lambda \geq 0, \quad g \leq 0, \tag{7}$$

where λ is the Lagrange multiplier. Finally, we update the scalar function ϕ by the following reaction diffusion equation:

$$\frac{\partial \phi}{\partial t} = \kappa \nabla^2 \phi - \alpha \frac{\mathrm{d}L}{\mathrm{d}\phi} \tag{8}$$

where, κ is the diffusion factor and α reaction factor.

4. NUMERICAL EXAMPLES

We implement the above mentioned method using COMSOL Multiphysics COMSOL (2015). The reaction diffusion equation (8) can be solved by the PDE mode (weak form) in the mathematics module in COMSOL Multiphysics. Also, the force equilibrium problem (6) can be solved by the solid mechanics module. The parametrized domain can be controlled by the parameter sweep function. When updating the parameter, the final configuration at the previous stage is used as the initial configuration for the next stage. At each stage, the upper bound of the volume fraction is set to 20%. Fig. 5 shows the representative five stages out of 10 stages. As the vertebrae bone growing, additional strengthening structures are formed on the both sides. Fig. 6 compares the measured shape of a zebrafish vertebrae bone and the shape produced by the proposed mathematical model. The calculated shape seemed to capture the basic structure but the shape has more roundish struts.

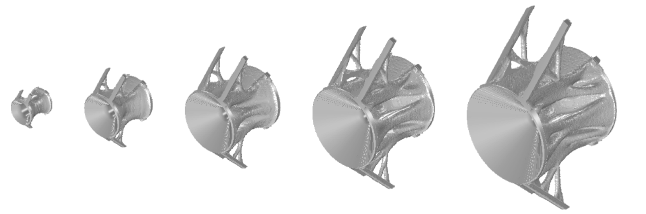

Fig. 5. Simulation of the growth of a vertebrae bone using topology optimization with a parametrized computational domain

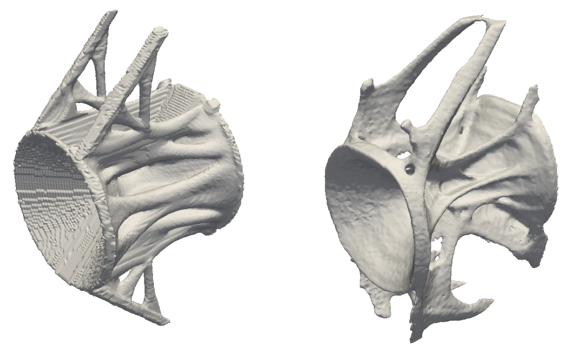

Fig. 6. Simulation (left) and measurement (right)

5. CONCLUSION

We have proposed a mathematical model for simulating the zebrafish vertebrae bone growth using topology optimization. Numerical results show the proposed model can capture the basic feature of vertebrae bone, while there still remain some discrepancies between the calculated shape and the measured shape.

REFERENCES

C. Boyle, Y.Y. Kim. Computational Simulation of Bone Remodeling using Design Space Topology Optimization. Proc. Appl. Math. Mech. 11, 97-98, 2011.

A. Kawamoto, T. Matsumori, T. Nomura, T. Kondoh, S. Yamasaki, S. Nishiwaki. Topology optimization by a time-dependent diffusion equation. International Journal for Numerical Methods in Engineering. 93(8):795-817, 2013.

COMSOL Multiphysics User's Guide, 2015. COMSOL AB.