Results and Data: Significant Changes to Model

By Dallin Fairbourn

This document describes changes I have made to my model during implementation. I have adjusted equations as well as updated the unified modeling language (UML) diagram to reflect the current program.

To model collagen formation, I adjusted the equation for creating naïve collagen to be the following:

$$\frac{dx_1}{dt} = k_1 - k_2 x_1$$

This equation assumes the formation of collagen is not dependent on its own concentration, but the density of naïve collagen is decreased as the collagen is assembled as shown in the second term of the equation. The equation to model the formation of assembled collagen was also adjusted to be the following:

$$\frac{dx_2}{dt} = k_2 x_1$$

Cell movement was assumed to take place when the naïve collagen density at their location reached 5.85×10^{-5} mg/μm^3 of collagen. The collagen was then assumed to take 10 days to fully mature, so the constant k_2 was set to 0.1 days^{-1}.

The equation to model the creation of hydroxyapatite was adjusted to be the following:

$$\frac{dH}{dt} = k_3[Ca^{2+}]^5[PO_4^{3-}]^3 H$$

This allows us to relate hydroxyapatite formation to calcium concentration. One of my goals for this project was to model how calcium concentration affects bone mineralization. Using this equation allows us to explore that relationship. The equations relating hydroxyapatite formation to inhibitor and nucleator concentration were omitted for the time-being for simplicity.

The program was built using 6 separate files. These files are all ultimately utilized by the main.py file. The simulation is run from main.py file, and all 6 files must be in the same directory in order for the simulation to run properly.

Data extracted from the model created by Komarova et al was imported into main.py to compare the models for bone mineralization [1]. The model currently reflects how long it takes for an fibrocartilaginous callus to form (about 11 days) after which hydroxyapatite begins to crystallize in the osteoid matrix [2].

The program was updated to have two additional classes: Simulation and Matrix. These classes help to split up the workload of the BoneMatrix class, and they help to streamline the adjustment of the simulation and data visualization. The UML diagram was updated, and is displayed in Figure 1:

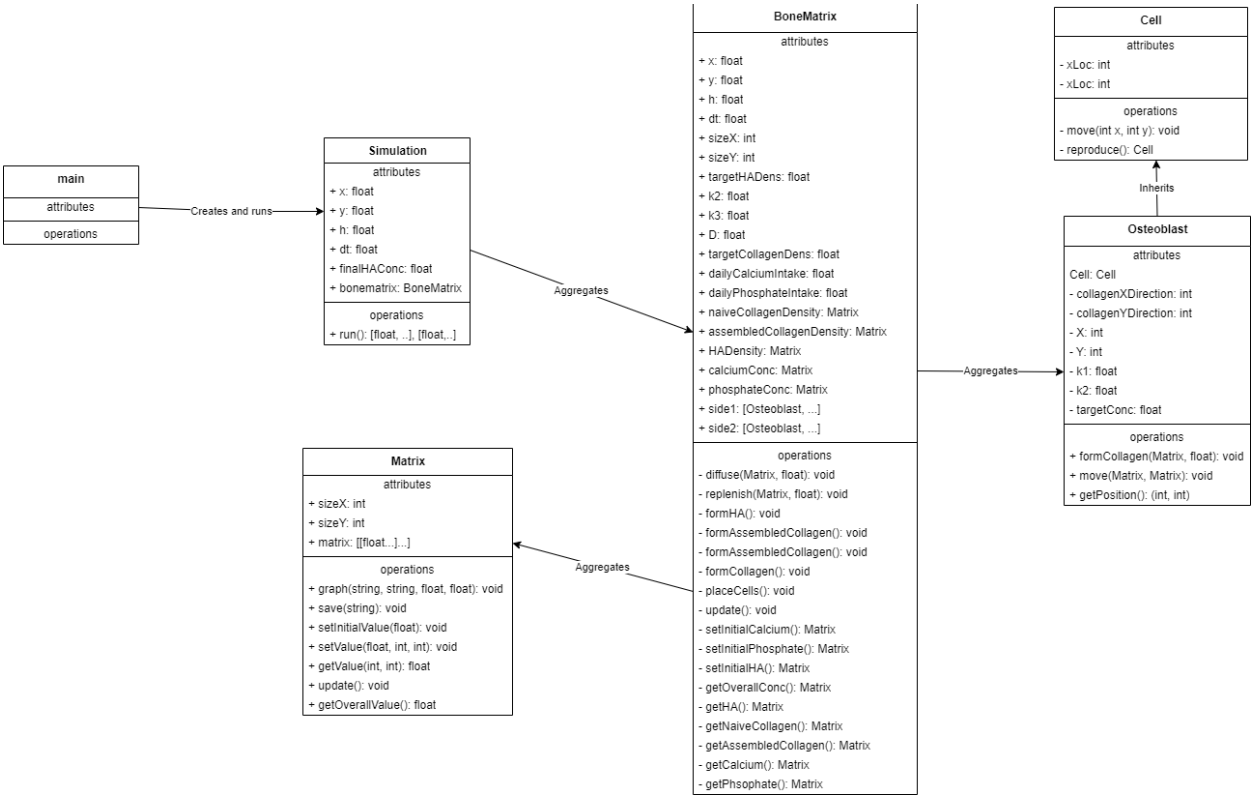

Figure 1. An image of the updated UML diagram.

1. Komarova S, Safranek L, Gopalakrishnan J, Ou M, Mckee M, Murshed M, et al. Mathematical model for bone mineralization. Frontiers in Cell and Developmental Biology [Internet]. 2015 [cited 2022 Nov 6];3. Available from: https://www.frontiersin.org/articles/10.3389/fcell.2015.00051

2. Sheen JR, Garla VV. Fracture Healing Overview. StatPearls [Internet]. Treasure Island (FL): StatPearls Publishing; 2022 [cited 2022 Nov 7]. Available from: http://www.ncbi.nlm.nih.gov/books/NBK551678/