MORPHOGENESIS MODELING OF CONICAL STROMATOLITES

An Undergraduate Research Scholars Thesis

by

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Submitted to the Undergraduate Research Scholars program at
Texas A&M University
in partial fulfillment of the requirements for the designation as an

UNDERGRADUATE RESEARCH SCHOLAR

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May 2017

Major: Geophysics

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ABSTRACT

Morphogenesis Modeling of Conical Stromatolites

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Stromatolites are the oldest macroscopic fossils that record the interaction between sediments and microbes. The question that remains is why do microbial mats tend to give a conical geometry to stromatolites. Prior researches on the diffusive gradients that occur around such structures have supplied an analytical view onto how microbial mats develop such conical shapes. Numerical modeling of diffusion has shown how the process of diffusion acts within the microbial mat and leads to the formation of a stromatolite. Moreover, past research has found that in order to study a stromatolites growth, one has to utilize many other factors and functions, not just look at the diffusion equation. Present models have been made but also have some assumptions to them due to the time span that stromatolites have been existence for.

DEDICATION

I would like to dedicate this to my parents, Andres and Natalia Montalvo, along with the rest of my family. I would also like to dedicate this to my advisor, for giving me the opportunity to work under him and continue working under him in such a great project.

CHAPTER I

INTRODUCTION

Stromatolites are attached, laminated, lithified, sedimentary rocks accreting from a point or limited surface (Petroff et al. 2010). Physical, chemical, biological-are all processes that produce stromatolites. It has been shown through past research that the topographic reliefs of such stromatolites were shaped from microbial mats: bacterial communities that form in layers growing on different rough surfaces (Tice et al. 2011). As the mat grows it will eventually need way of attaching and sticking together. In order to stick together, bacteria produce exopolymers, or EPS, that allow for the adhesion of the microbial mat (Tice et al. 2011). Nevertheless, it can be said that stromatolites are the structures made due to mat growth (biological), the trapping and lithification of sediments (physical), and or mineral encrustation (chemical) (Tice et al. 2011).

These structures are not uniform in shape. They can form domes, mounds, cones, and even columns. However, the shape and texture of a stromatolite can tell us about the kind of microbial metabolism that caused such structure (Petroff et al. 2010). The primary purpose for this research is to understand what mechanisms allow for the creation of conical stromatolites by comparing some existing models. Recent studies on modern stromatolites have shown that the diffusion of metabolites along with the process of photosynthesis, allow for the spatial organization of modern stromatolites (Petroff et al. 2010). Nevertheless, it is also believed that conical stromatolites were not built through the influence of biological or environmental factors. Rather, they were created through a geometric feature defined by diffusion through a thin film (Petroff et al. 2013). The process of diffusion produces a diffusive gradient that causes minerals to precipitate at different speeds in respect to curvature: higher curvature leads to faster precipitation (Petroff et al. 2013). The diffusion equation shows that the concentration of the chemical species changes in time. Moreover, there exist 3 time scales that account for the growth of stromatolites. First you have the time for the diffusion of small molecules; defined as T_d – (d_o^2/D), where T_d = the time for diffusion, d_o =microbial mat thickness=, and D=diffusive coefficient of small molecules (Petroff et al. 2013). Secondly, you have the time scale over which the microbial mat grows (T_g). The last time scale is the rate at which a stromatolite grows due to the precipitation of minerals; defined as T_s –(d_o /c_o)>>T_g (c_o is the accumulation rate of carbonate platforms, must be <<1cm/yr) (Petroff et. al 2013). Since the time scales of both microbial mat and stromatolite growth are significantly longer than the diffusive time scale, the concentration is always at a steady state, thus defining the Laplace equation (Petroff et al. 2013).

CHAPTER II

PAST RESEARCH AND ANALYSIS

The geometric features of stromatolite deal directly with the dynamics common to the process of diffusion through a thin film. Such processes have to be studied by how the laminas in the structure are formed, which are affected due to the chemical changes in precipitating minerals as they change depending on the chemical and physical conditions. However, even though lamina can differ from stromatolite to stromatolite, their conical shape infers that they were formed by the same class of dynamics defined by diffusion through a thin film. Past research has produced mathematical models showing the functions that go along side these diffusive processes, which have not only allowed for the previous study of the shape of such structures but also have allowed for a quantitative prediction of what future or past stromatolites may look like (Petroff et al. 2013). Moreover, the inefficiency in the molecular diffusion within the microbial mat couples the growth of a stromatolite with the overlying mat geometry of the structure therefore defining that a stromatolite grows at a rate proportional to the diffusive gradient at the base of the microbial mat. For such reasons, the largest diffusive gradients tend to be normal to the surface of the stromatolite, therefore defining the rate at which stromatolite grows as a process influenced by the thickness of the microbial mat.

Stromatolites have three relevant time scales that breakdown their growth into three parts and make for a steady state system. τ_d, $\tau_d \sim {d_0}^2/D$, represents the typical time for diffusion of small molecules in a microbial mat (Petroff et al. 2013). The time is a function of microbial mat thickness d_0, and the diffusion coefficient of small molecules or ions in the mat D. The second time scale τ_g, time over which a microbial mat grows, has to be estimated but can be said to range between tens of hours and weeks (Petroff et al. 2013). The last time scale, τ_s, is the rate at which the stromatolite grows through the precipitation of minerals. Although it still difficult to estimate very old samples, the scale is much greater than τ_g and can be defined as $\tau_s \sim \frac{d_0}{c_0}$, c_0 being the rate of precipitation. The separation of time scales only holds if c_0 is much less than 1cm/yr (Petroff et al. 2013).

In his paper, Petroff assumed that the rate of mineral precipitation is limited by diffusion through a thin microbial mat. Two processes have been said to create this diffusion-limited growth. The first process states that stromatolite growth could be limited by the diffusive flux of ions related to the precipitation of minerals. The second states that the rate of mineral precipitation could be limited by the rate at which the degradation of bacteria provides nuclei for heterogeneous precipitation. Even though two possible processes cause diffusion-limited growth, the rate of mineral precipitation and the diffusive flux will scale with each other at the base of the microbial mat.

In order to understand how the shape of a stromatolite is affected by the process of diffusion through a thin film we must look at the diffusion equation

$$\frac{\partial \psi}{\partial t} = D\nabla^2\psi \quad (1)$$

where D is the coefficient in the microbial mat. However the concentration of ψ is always at steady state due to the time scale difference of the diffusive timescale when compared to the microbial mat and stromatolite growth time scales. For such reasons we must solve the function $\nabla^2\psi = 0$ in order to find the rate at which minerals precipitate in the microbial mat. In order to do this, the function must be evaluated in a coordinate system that expresses the shape of a simple stromatolite. After making the switch to this coordinate system and after applying the Laplacian, the function, close to the surface of a stromatolite, can be expressed as

$$\frac{\partial^2 \psi}{\partial n^2} + 2H\frac{\partial \psi}{\partial n} + \nabla_s^2 \psi = 0 \quad (2)$$

where H is the mean curvature of the stromatolite surface.

Petroff also states, that the largest diffusive gradients tend to form normal to the surface of the stromatolite. In order to show this, a rescaling of every quantity in equation (2) must be done. The concentration ψ is rescaled by taking the difference in concentrations between the surface mat and the surface of the stromatolite therefore yielding a dimensionless concentration $\phi = \frac{\psi - \psi_0}{\psi_1 - \psi_0}$. The typical radius of curvature R_0 must rescale the curvature H giving a dimensionless curvature $\eta = R_0 H$. We also must rescale the coordinates, therefore defining the dimensionless coordinates $\sigma_i = \frac{s_i}{R_0}$. Moreover, due to the variance of ψ over the thickness of the microbial mat d_0 we must also define another dimensionless coordinate $v = \frac{n}{d_0}$. After rescaling all quantities we get

$$\frac{\partial^2 \phi}{\partial v^2} + 2\left(\frac{d_0}{R_0}\right)\eta\frac{\partial \phi}{\partial v} + \left(\frac{d_0}{R_0}\right)^2 \nabla_s^2 \phi = 0 \quad (3)$$

However, when the mat is much thinner that the stromatolite ($d_0 << R_0$), the concentration ϕ becomes a one-dimensional solution equation

$$\frac{\partial^2 \phi}{\partial v^2} + 2\epsilon\eta\frac{\partial \phi}{\partial v} = 0 \quad (4)$$

where $\epsilon = \frac{d_0}{R_0} << 1$. The one-dimensional function defines the rate of precipitation as being influenced by the local geometry of the microbial mat and not by shape of the mat. It is important to note that equation (4) requires two boundary conditions; concentration of the diffusing species reaching a constant value at the base of the mat ($\phi(0) = 0$) and at the surface of the mat ($\phi(1+\epsilon\eta d_1)$=1). After applying the boundary conditions to the equation we find that

$$\phi(v) = v + \epsilon\eta(1 - d_1 - v)v + O(\epsilon^2) \quad (5)$$

Some derivation of the function finds a diffusive flux $j \sim D(\psi_1 - \psi_0)$, which implies that wherever the overlying mat is thick, mineral precipitation will be slow. In other words, increasing the thickness of the mat in regions of high curvature will slow down the growth process of the stromatolite. Overall, the stability of a stromatolite shape depends on how the microbial mat reacts to the shape of the underlying surface.

When studying stromatolite growth and their shape one must always keep in mind the relationship between the shape of the underlying stromatolite and the geometry of a microbial mat. However, due to their long time period of existence, and even going through both oxygenic phases of earth, there are difficulties in establishing a growth equation. As time progressed most stromatolites lived in different hydrodynamic environments therefore also implying a difference in the dynamics by which the stromatolite grew. Even though such conditions were true, it can be assumed that there is a nonsingular relationship between the curvature of the mat and the thickness of its growth. Moreover, the thickness is a function of the dimensionless curvature $\epsilon\eta$, and because $\epsilon \ll 1$ the thickness of the mat can be approximated by a Taylor series

$$d(\epsilon\eta) \approx d(0) + \frac{\partial d}{\partial \eta} \quad (6)$$

or can also be expressed as

$$d = d_0(1 + \epsilon\eta d_1) \quad (7)$$

where $d_1 = (\frac{\partial d}{\partial \eta})/d_0$ (Petroff et al. 2013).

The process of stromatolite translational growth relates the orientation of a point on the surface to the curvature of that point, as seen in the function below

$$\frac{c_t}{c_0} cos\theta = 1 + (1 - d_1) d_0 H(\theta) \quad (9),$$

where H(θ) is the dependence on curvature on orientation. The function can be reexpresed as a differential equation for the shape of the translating stromatolite

$$\frac{\chi^{-1}}{\sqrt{1 + f'^2}} = 1 - \Delta \frac{rf'' + f'(1 + f'^2)}{2r(1 + f'^2)^{\frac{3}{2}}} \quad (10)$$

where the derivatives are with respect to r, the distance of a point on the surface from the central axis, and where the dimensionless precipitation rate $\chi = c_0/c_t$ (Petroff et al. 2013). Moreover, in order to determine the shape of the growth under the influence of diffusion we must establish two boundary conditions, *f*(0)=0 specifying the coordinate system and *f* ‘(0)=0 (considering smooth stromatolites) specifying the slope of the stromatolite near the apex (Petroff et al. 2013). It is important to note that the function for the shape of a translating stromatolite does not have a unique solution, therefore giving a number of distinct ways a stromatolite may grow.

The two main processes that influence the growth of a stromatolite are mineral precipitation and the diffusive gradients within the mat. Such processes can happen in so many ways that there could be various geometries to a stromatolite. The conical shape of a stromatolite just represents a balance between both processes where that slope of the walls record the rate of mineral precipitation relative to the speed of vertical growth and the curvature records the thickness of the microbial mat.

CHAPTER III

RESULTS

Petroff's (Petroff et al. 2013) analytical methodology for stromatolite growth was replicated in deal.II, a C++ based FEM library that supports the creation of finite element codes. deal.II has very well-documented tools to build finite element codes for a broad variety of PDEs. The stromatolite growth was simulated using deal.II's finite element model of diffusion process that is solved on a mesh, which resembles microbial mat geometry that overlies a stromatolite. Since stromatolite grows on geologic time scales (Petroff et al. 2013), we solved the diffusion equation (1) as a two-dimensional steady state or Laplace equation.

The finite element mesh (Figure 1) was generated using *GridGenerator :: hyper_rectangle* function in deal.II, followed by mesh transformation using *GridTools :: transform* function. The top boundary of the mesh for this model is described by a non-homogeneous boundary condition. The concentration or ψ values for this boundary condition are proportionate to the y-coordinate of each vertex of the mesh cell on that boundary. Since the mesh is a curved rectangular or parabolic shape, the center-top vertices have the highest ψ values. The bottom boundary of the mesh is set to a constant using the *ConstantFunction* in deal.II. The left and right boundary of the mesh are set to zero using *ZeroFunction* in deal.II.

The set up and assemble procedure necessary to solve the system for this problem are similar to the one described in step-6 of the deal.II tutorials. The only exception is adaptive mesh refinement (AMR) algorithm; even though AMR approach is applied in step-6 of the deal.II tutorial, it not used for mesh refinement. The linear system of equations described by this model is solved using a SSOR Preconditioned Conjugate Gradient algorithm. Direct methods for solving set of linear equations such as Gaussian elimination and LU decomposition are not very efficient solvers for such problems.

After solving the Laplace equation or steady-state diffusion equation on mesh for current time step, the mesh is deformed by moving each vertex based on the displacement gradient (growth gradient) for that vertex in the current time step times a small deformation constant. This is done through the *move_mesh* function. For this model, the mesh was deformed for 1000 timesteps.

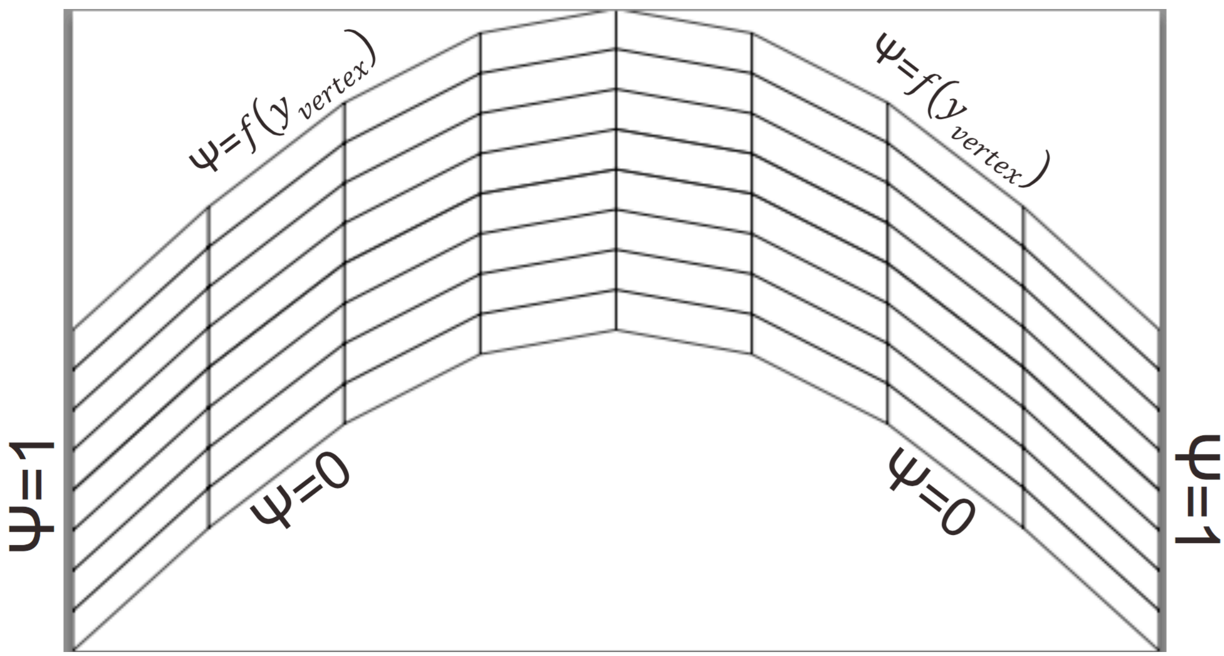

Figure 1: Geometry of the microbial mat/stromatolite structure represented by a mesh in deal.II along with appropriate boundary and initial conditions for this model.

Figures 2(a, b, c, and d) show the stromatolite growth using a time-lapse series; each figure in the series is also overlaid by the original grid (timestep 0) when there is no deformation. The color bar next to the stromatolite shows the concentration scale, which can be used to compare the diffusion concentration and gradient over time.

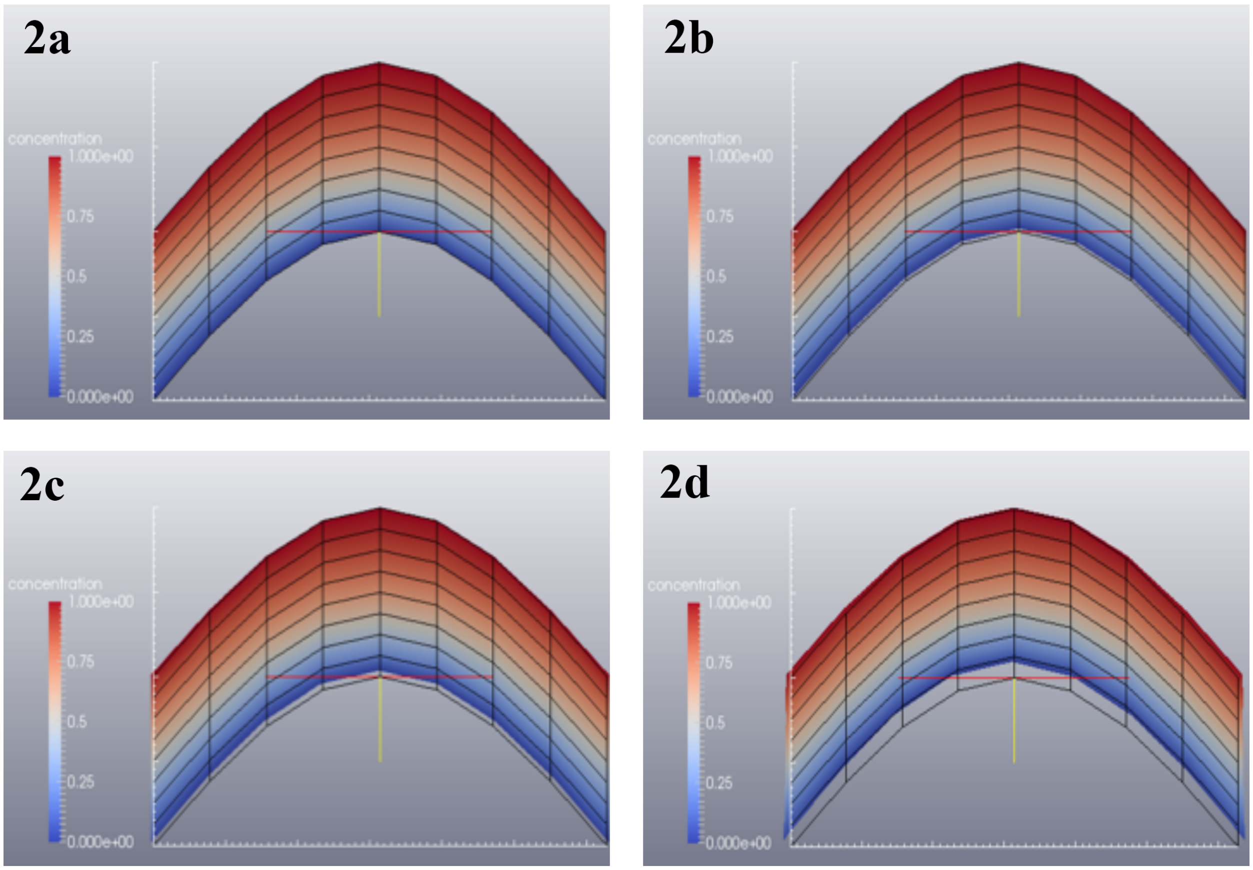

Figure 2: Stromatolite growth at timestep = 0 (2a), timestep = 100 (2b), timestep = 200 (2c), and timestep = 500 (2d).

CHAPTER IV

CONCLUSION

Results from Petroff et al. 2013's paper were replicated in deal-II, a C++ software library that supports the creation of finite element models. However, in their paper, Petroff et al. does not include the hydrodynamic influence on stromatolite growth, a factor that would affect the growth rate and time due to constant shear and high-energy tidal environment. In order to simulate this growth, further research in COMSOL Multiphysics must be applied. COMSOL Multiphysics is a professional simulation package that supports multiple physics, described by different physics, and allows co-simulation with these physics. Nol et al. 2017 successfully used COMSOL Multiphysics to simulate coral growth; similar workflow will be applied to simulate stromatolite growth.

REFERENCES

Chindapol, Nol et al. “Modelling Growth and Form of the Scleractinian Coral *Pocillopora Verrucosa* and the Influence of Hydrodynamics.” Ed. Edmund J. Crampin. *PLoS Computational Biology* 9.1 (2013): e1002849. *PMC*. Web. 2 Mar. 2017.

Tice, Michael M., Thornton, D.C.O, Pope, M.C., Olszewski, T.D., & Gong, J. "Archean microbial mat communities." *Annual review of earth and planetary sciences* 39 (2011): 297-319.

Petroff, Alexander P., Beukes, N.J., Rothman, D.H., & Bosak,T. "Biofilm growth and fossil form." *Physical Review X* 3.4 (2013): 041012.

Petroff, Alexander P.,Sim, M.S., Maslov, A., Krupenin, M., Rothman, D.H., & Bosak, T. "Biophysical basis for the geometry of conical stromatolites." *Proceedings of the National Academy of Sciences* 107.22 (2010): 9956-9961.

Pitt-Francis, Joe, and Jonathan Whiteley. *Guide to Scientific Computing in C*. London: Springer-Verlag, 2012. Print.