

# 1. STATEMENT OF WORK: CHAOS AND CRYSTALS: STUDENT RESEARCH OPPORTUNITIES.

**1.1. Objectives and Significance.** In some ways pure mathematical research is not very different from any other sort of scientific research. It consists of conducting experiments, observing patterns of cause and effect, and testing predictions made based upon those observations. With mathematics, however, there is a fourth required step of logical proof. Another difference is that the objects of study are abstract—you can't touch them—and even the rules of behavior for those objects are chosen arbitrarily. Experiments in mathematics are actually calculations, all on paper.

However, once a concept and its rules (together called a theory) become the subject of many experiments and proven patterns, concrete examples are often found in the physical world of real objects and real rules (physical, chemical, biological, economical) that correspond nearly perfectly to that abstract theory. Then the patterns proven by the mathematicians can be used (together with observed physical laws) to help predict what the outcome of a physical experiment will be. This is called mathematical modeling. The amazing thing is that mathematical beauty and utility so often coincide. A theory that is applicable often turns out to be elegant, and vice versa.

In 2003 a group of material scientists led by Jack Douglas of the National Institute of Standards and Technology observed for the first time certain features of the strange way in which a crystal grows. They studied both *self similar* and *chaotic* crystals.

Self similarity of an object is demonstrated by the ability to zoom in on a part only to see the same picture as when viewing the whole. You can sometimes find this kind of symmetry in the grocery store in the art on a carton label, where a smiling mascot is pictured holding the very same carton, which in turn bears a picture of a miniature mascot holding a tiny carton, and so on. The branches of some crystals exhibit the familiar self-similarity of ferns and pine trees, where a branch has the same form as the whole tree.

Under slightly different conditions crystal branching becomes chaotic; more like the growth of frost on a windowpane, or like seaweed. When mathematicians speak of chaos, they do not mean random behavior. Rather they refer to a completely determined pattern of events, but one that becomes more and more complex over time, so that there is no shortcut to predicting its outcome. Imagine dropping a teaspoon of purple dye into a plate of warm water. All the initial variables such as temperature and speed

of the dye will determine the swirling pattern you observe. However, there is no quick formula for calculating the shape of the swirl after an hour. This is quite different from the case of calculating the path of a rocket to the moon, for instance, since we can predict that flight almost perfectly.

Ferreiro, Douglas, Warren and Karim made nearly continuous observations as their snowflake-like structures formed and branched out in a solution, and then measured each with great precision. Immediately they noticed several key facts. The first was that at certain temperatures the usual regular increase in size of the crystal became a pulsating, rhythmic growth. The researchers made several guesses at the cause of this pulsation but the state of knowledge about the driving forces here is incomplete. Upon even more de-

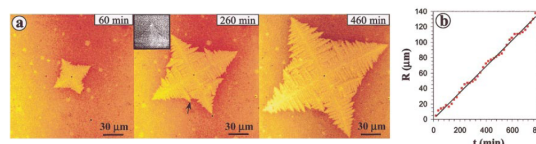


FIGURE 1. Oscillating crystal growth.

tailed inspections the crystal investigators were able to pinpoint another oscillation. The first growth variable which they had already measured was the radial length from the center of the crystal to the tip of a main arm of the crystal. Now they extended their approach to the thickness of an arm of the crystal, measuring the length from the main arm axis to the tip of one of its sub-branches. Interestingly, this growth measurement oscillated with the same period as the radius, but was perfectly out of phase with the radius. In other words, the radius and the arm thickness take turns growing, one after the other.

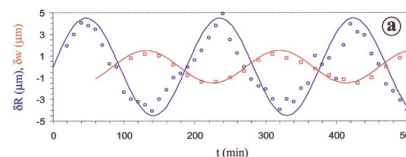


FIGURE 2. Out of phase.

In 2007 the principal investigator (S. Forcey) discovered a new set of ideas in pure mathematics which bears remarkable similarity to some of the observed characteristics of crystals, both self similar and chaotic. The research being proposed here is the mathematical development of the new theory, as well as investigation into the possibility of applications to crystal growth.

Our primary objective is to thoroughly research and publish results about the mathematical theory involved in these applications, in preparation for a federal grant effort. Two main avenues of pure mathematics will be further developed if this proposal is funded. They are: A) research into the abstract properties of a foundational family of mathematical theories called *categories of Young diagrams*; and B) research into classification of a second level of theories called *operads* built upon that foundation. These terms will be defined shortly. Then these pure mathematical results will be applied to the modeling of crystal growth. Some of this work has already been done by the principal investigator, presented at various conferences and published in a collaborative paper.

Our secondary objective is to engage undergraduate math majors and masters degree candidates in this area of research. It is elementary enough to allow students to quickly participate in the actual research, designing and conducting experiments, looking for patterns in the collected data, and helping to formulate and prove conjectures. The principal investigator has directed three masters theses and three senior research projects. Two of those theses each resulted in collaboratively published papers. Two of the masters theses and one of the senior projects were in this precise area, and the others in closely related topics. The third thesis, in the area of research proposed here, is currently in the process of becoming a publication. Also the senior project most recently completed in this area is being extended further by the student, with intention of publication. The future funding requested of the NSF will include tuition and stipend money for students.

**1.2. Plan and Methods A: Structure.** The mathematical objects we plan to study are *combinatorial* in nature. This means that they are made of simple building blocks put together according to simple rules. Here the building blocks will be cubes of various dimension as illustrated in Figure 3. We will al-

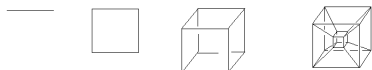


FIGURE 3. Segment, square, cube, hypercube.

low squares or cubes to be stacked in columns and then several columns to be placed together. The placement rule for squares is that the columns must

get shorter from left to right. The result forms what is called a *Young diagram*. Here are a couple of examples:

$$A = \begin{array}{|c|c|c|c|c|} \hline \square & \square & \square & \square & \square \\ \hline \square & & & & \\ \hline \end{array} \text{ and } B = \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \square & \\ \hline \end{array}$$

Two diagrams can be added together in several ways, all described as “combining two stacks of boxes.” In the 2-dimensional case we let  $\otimes_1$  denote horizontal stacking, or adding the lengths of the rows of two diagrams. We let  $\otimes_2$  denote vertical stacking, or adding the heights of columns. If  $A$  and  $B$  are as above then:

$$A \otimes_1 B = \begin{array}{|c|c|c|c|c|c|c|} \hline \square & \square & \square & \square & \square & \square & \square \\ \hline \square & \square & & & & & \\ \hline \square & & & & & & \\ \hline \end{array} \text{ and } A \otimes_2 B = \begin{array}{|c|c|c|c|c|} \hline \square & \square & \square & \square & \square \\ \hline \square & \square & \square & \square & \square \\ \hline \square & \square & \square & \square & \square \\ \hline \square & \square & \square & \square & \square \\ \hline \square & \square & \square & \square & \square \\ \hline \end{array}$$

Next we describe “vertical and horizontal multiplication,” denoted  $\boxtimes_1$  and  $\boxtimes_2$ . These both begin by packing each box of diagram  $B$  with a copy of  $A$ . Then the two kinds of multiplication are the two ways of collapsing all the boxes to form a new Young diagram (horizontally then vertically or vice versa). If

$$A = \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \text{ and } B = \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \dots \text{then here is the packing:}$$

$$\begin{array}{|c|c|} \hline \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} & \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \\ \hline \end{array} \quad \begin{array}{|c|c|} \hline A & A \\ \hline A & \\ \hline A & \\ \hline \end{array} = \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \quad \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array}$$

and so:

$$A \boxtimes_1 B = \left( \begin{array}{|c|c|} \hline \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \\ \hline \otimes_2 \\ \hline \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \\ \hline \otimes_2 \\ \hline \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \\ \hline \end{array} \right) \otimes_1 \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} = \begin{array}{|c|c|c|c|} \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \end{array}$$

and

$$A \boxtimes_2 B = \left( \begin{array}{|c|c|} \hline \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \\ \hline \otimes_1 \\ \hline \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \\ \hline \otimes_2 \\ \hline \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \\ \hline \otimes_2 \\ \hline \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \end{array} \\ \hline \end{array} \right) = \begin{array}{|c|c|c|c|} \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \square \\ \hline \end{array} .$$

The current state of knowledge about the mathematical structures embodied by the various ways of combining stacks of boxes includes many unknowns.

Some of the structures we will be looking for are *semi-groups*, *rigs*, *rig categories*, *iterated monoidal categories*, and *globular monoidal categories*. The detailed definitions of all these structures are not given here; rather we point out that the value of looking for the structures is that there are already theorems about them that will be of use in applications. We will explain a little of the next to last term in the list. The *iterated monoidal* structure has to do with how the products interact. For instance, when starting with 4 diagrams we can always get a higher stack of boxes by combining horizontally first and then vertically. We say one Young diagram is less than another if its first column is shorter than the other's. If the first few pairs of columns are the same height in each diagram then the first pair of unequal columns is used to decide which diagram is greater. Let four Young diagrams be as follow:

$$A = \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \square & \\ \hline \end{array} \quad B = \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \\ \hline \square & \square & \\ \hline \end{array} \quad C = \begin{array}{|c|} \hline \square \\ \hline \square \\ \hline \square \\ \hline \end{array} \quad D = \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \square & \\ \hline \end{array}$$

Then the fact that  $(A \otimes_2 B) \otimes_1 (C \otimes_2 D) \leq (A \otimes_1 C) \otimes_2 (B \otimes_1 D)$  appears as follows:

$$\begin{array}{|c|c|c|c|} \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \\ \hline \square & \square & \square & \\ \hline \square & \square & \square & \\ \hline \end{array} \leq \begin{array}{|c|c|c|c|} \hline \square & \square & \square & \square \\ \hline \square & \square & \square & \\ \hline \square & \square & \square & \\ \hline \square & \square & \square & \\ \hline \end{array}$$

Figure 4 shows this same *interchange* inequality but with colors to indicate how it came about. Higher

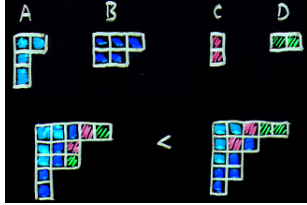


FIGURE 4. Interchange.

dimensions are also described in our first paper. It is shown that the category of  $n$ -dimensional Young diagrams with stacking products in each dimension constitutes an  $n$ -fold monoidal category. The structure of the multiplications of 2-d Young diagrams is described in a Masters thesis which is also to be prepared for publication as part of the project time-line.

**1.3. Plan and Methods B: Growth.** The second focus area of the pure math is on recursively growing sequences of Young diagrams, known as *operads*. Given any Young diagram  $B$  we can construct a unique sequence of growing diagrams that is minimal

in each term with respect to ordering of the diagrams. By minimal we mean that the principle which determines each of the later terms in succession is that of choosing the minimal next term out of all possible such terms.

**1.1. Definition.** The 2-fold operad in the category of Young diagrams generated by a Young diagram  $B$  is denoted by  $\mathcal{C}_B$  and defined as follows:  $\mathcal{C}_B(1) = 0$  and  $\mathcal{C}_B(2) = B$ . Each successive term is defined to be the maximum of all the products of prior terms which compose to the term in question; for  $n > 2$  and over  $\sum j_i = n$ :

$$\mathcal{C}_B(n) = \max\{\mathcal{C}_B(k) \otimes_1 (\mathcal{C}_B(j_1) \otimes_2 \cdots \otimes_2 \mathcal{C}_B(j_k))\}.$$

Here are the first few terms of the operad thus generated by  $B = \begin{array}{|c|} \hline \square \\ \hline \end{array}$ .

$$0, \begin{array}{|c|} \hline \square \\ \hline \end{array}, \begin{array}{|c|c|} \hline \square & \square \\ \hline \square & \\ \hline \square & \\ \hline \end{array}, \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \\ \hline \square & \square & \\ \hline \end{array}, \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \\ \hline \square & \square & \\ \hline \end{array}, \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \\ \hline \square & \square & \\ \hline \end{array}, \begin{array}{|c|c|c|} \hline \square & \square & \square \\ \hline \square & \square & \\ \hline \square & \square & \\ \hline \end{array}, \dots$$

Notice that the growth of the first column is periodic—it grows by a single box at every other step. The growth of the number of boxes in the remaining columns all to the right of the first one is also periodic, but precisely out of phase with the first column's growth. This matches the growth pattern of a crystal.

In fact, it is easy to find example sequences which do even better at precisely modeling a given crystal. The first step is to simplify the problem by considering Young diagrams with only one column. This is a simple enough problem to introduce directly to undergraduates. They can program it and then design and run experiments by choosing various starting sequences and computing their long term behavior. In Figure 5 we show how a given experimental run is nearly the same as a sinusoidal model of the radial growth in a crystal. There is in fact very lit-

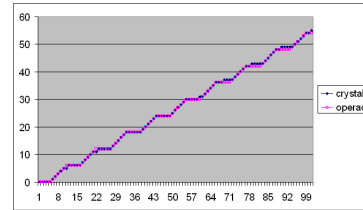
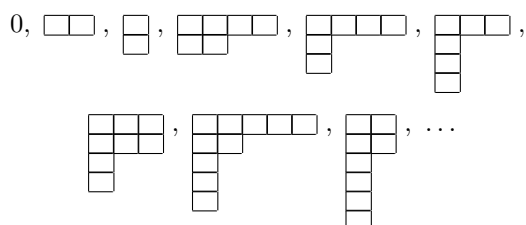


FIGURE 5. Crystal models: Sinusoidal vs operad.

tle known about these sequences. Some of them are easily reduced to a simple “shortcut” formula. The main open question which made up both the content

of the experimentation module of our Research Experience class and one student's senior project was indeed: just when is a shortcut possible?

Even less is known about the sequences which are generated by a starting sequence of  $k$  Young diagrams. These are where the behavior of the sequence can approach chaos. For example, if the starting sequence is  $0, \begin{smallmatrix} \square & \square \end{smallmatrix}, \begin{smallmatrix} \square \\ \square \end{smallmatrix}$  then the sequence proceeds like this:



Notice that the first column still grows linearly, but the other columns grow with ever more complicated patterns. The overall mass, or number of blocks in each term, appears to grow chaotically:

$$0, 2, 2, 6, 6, 6, 8, 10, 8, 14, 12, 14, 14, 16, \dots$$

The theoretical side of our research will include classifying sequences based upon their starting terms, into those with various shortcut formulas and those displaying varieties of chaos.

In chaotic situations, such as the growth of some crystals, we often turn to computer simulations to attempt to guess the future. One purpose of our diagram sequences is to serve as building blocks in such a simulation. We plan to experiment with combinations of Young diagrams to make virtual crystals, and try to match these to actual crystal growth.

Another use of high performance computing will be in the theoretical research. To work towards classifying sequence behavior based upon starting terms,

we will need to do extensive mathematical experimentation. The calculation of many terms in a sequence of Young diagrams is highly recursive, and programs already written to do this job usually run for longer than is desirable. Students can participate in every stage of this process—helping to design experiments, writing faster programs to run the experiments, and analyzing results. Faster computers would of course also be of assistance, and so this project would benefit from the realization of the supercomputing center currently being planned as a joint effort between TSU and IBM.

Since the growth is in multiple dimensions, it suggests applications to studies of *allometric* measurements. This refers to multiple characteristics of a system which grow in tandem. These measurements are often used in biological sciences to try to predict values of one characteristic from others, such as tree height from trunk diameter, or skeletal mass from total body mass. There are also potential applications to networks, where the growth of diameter or linking distance of a network is related logarithmically to the growth in number of nodes.

The multiplications of Young diagrams also support operads. These sequences however, grow exponentially rather than linearly. Again there is much theoretical work to be done in classifying these sequences. There is also the opportunity to look for applications to real world exponential growth.

The following time-line shows past and future actions in pursuit of this research project. It includes mention of the integration of this research into the Research Experience course required of all math majors at TSU. Opportunities for future funding are listed at the end. These include the National Science Foundation's programs in Applied Mathematics, Ceramics (CER) and Electronic Materials (EM).

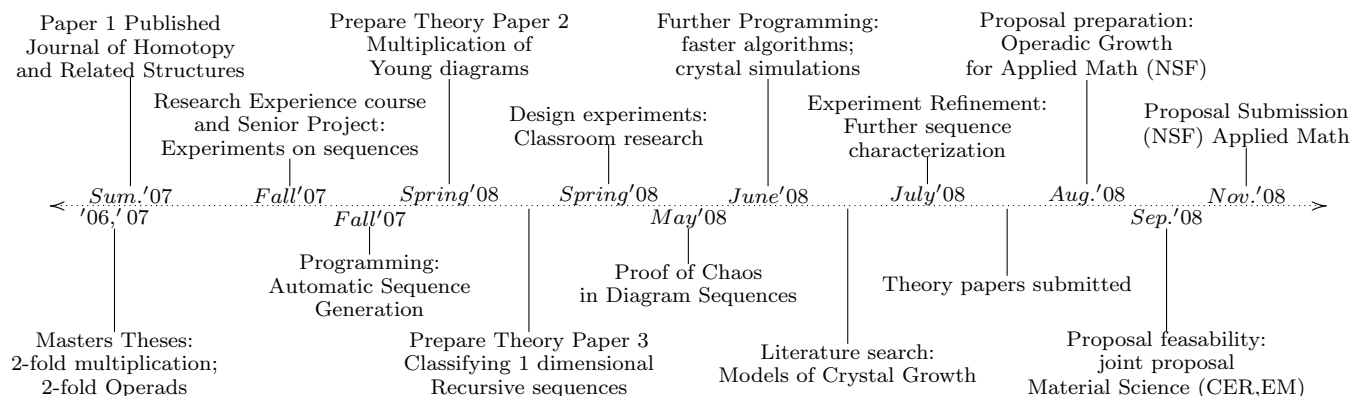


FIGURE 6. Timeline.