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Self-healing tile sets: rates of regrowth in damaged assemblies

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Self-Healing Tile Sets: Rates of Regrowth in Damaged Assemblies

by

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Abstract

This thesis looks into rates of growth within holes in self-assembled tile structures. Specifically, we are interested in whether the hole will regrow or decay further under a certain set of conditions. Tile sets have the ability to assemble themselves (including regrowing damaged sections of an assembly) when under good conditions, chiefly whether the ratio of monomer concentration to bond strength is below a certain threshold. Inside a hole, however, regrowth may or may not occur even when this threshold is exceeded.

Introduction

An emerging field in the computer sciences is the notion of self-assembly. This is the process by which pre-existing, simple, disorganized components, without external interference, naturally come together to form complex assemblies. These components assemble themselves based on some rule set that governs interactions between each of the elements. [1] Systems involving self-assembling components can be found in many places in the real world, giving a very practical application for modeling systems in a lab setting. [2][3]

As early as 1998, the kinetic Tile Assembly Model (the kTAM) was created to model self-assembling systems in a lab. This model takes into account relations between tiles (the self-assembling components), in addition to rates of association and dissociation of the tiles. Finally, the kTAM is concerned with the reversibility of assemblies (assuming a process is indeed reversible); that is, based on a given structure, the process can be run in reverse to determine what elements could be used to produce the structure. [1][3][4]

It is this final property that allows users of the kTAM to study self-healing. If a self-assembled structure is damaged (for example, if tiles are removed), the assembly can use its ability to self-heal to determine what elements were inside the hole. It is important that this is done correctly; that is, that the assembly is able to find the correct elements to rebuild the structure. The process of proofreading is used to ensure that there are no errors within a structure; therefore, using self-healing and proofreading, a damaged assembly can be correctly reconstructed. [3]

The growth or decay of a tile system can be predicted using two environmental factors, called G_{mc} (monomer concentration) and G_{se} (sticky-end bond strength). The kTAM model allows these parameters to be adjusted, causing a variety of different behaviors based on the value of τ, defined as $\tau = \frac{G_{mc}}{G_{se}}$. It is well-documented that certain values of τ result in different behaviors of the system as a whole. If, for example, τ is greater than 2 (so $G_{mc} > 2G_{se}$), no growth occurs (and the system will, in fact, shrink). However, if τ is less than 2 (so $G_{mc} < 2G_{se}$), conditions are sufficient for new tiles to attach to existing ones, causing growth to the system. In situations where τ is significantly less than 2 (certainly if τ is less than 1, where $G_{mc} < G_{se}$), errors begin to appear in the system, and tiles become mismatched. In this case, the system is too "cold" (G_{se} is too high) and proofreading breaks down, causing improper tiles to be attached to the system. Optimal growth occurs when τ is just under 2. [4][5] This can be observed in Figure 1.

While proofreading may seem like a complicated process, it is quite brilliant in its simplicity. Tiles are added at a rate $k_f = ke^{-G_{mc}}$ and removed at a rate $k_{r,b} = ke^{-bG_{se}}$, where b is the total bond strength of a tile to the assembly. If $k_f \geq k_{r,b}$, the tiles remain, while they fall off if $k_f \leq k_{r,b}$. When τ is close to 2 (when $G_{mc} \approx 2G_{se}$), properly added tiles result in a k_f greater than $k_{r,b}$, resulting in continued growth. If the tile is mismatched, then the value of k_f is less than that of $k_{r,b}$, causing the mismatched tile to fall off. [1][3][4][5] This ensures that, with the proper proportion of G_{mc} and G_{se}, there is a very low error rate ε for the system. If a particular value of ε is desired, low values for G_{mc} and G_{se} can be selected, though this will exponentially decrease the rate at which the system grows. [3][5] Figure 1 shows the regions defined above, while Figure 2 and Figure 3 show sierpinski2x2.tiles, a rendering of the Sierpinski triangle, at optimal and poor values of τ, respectively.

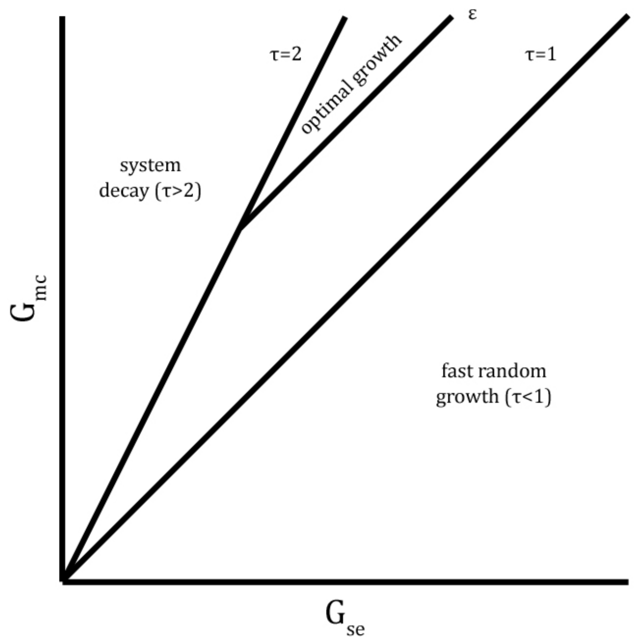

Figure 1: Graph explaining growth and error rates for varying values of G_{mc} and G_{se}

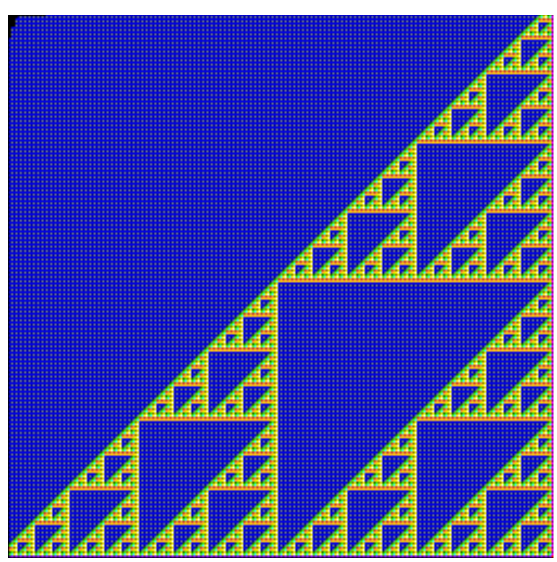

Figure 2: Complete 256 x 256 render of sierpinski2x2.tiles at $\tau = 1.97674$

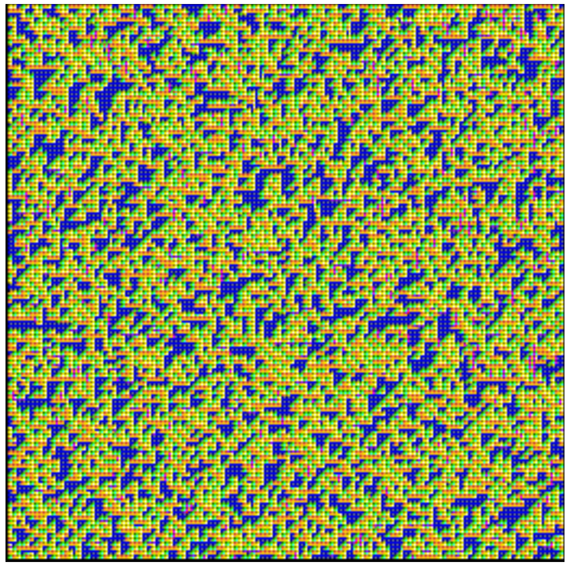

Figure 3: Complete 256 x 256 render of sierpinski2x2.tiles at $\tau = 1$ and after 1.0×10^7 events

Because of proofreading, we are able to damage a system by removing sections of tiles. Once these tiles have been deleted, the resulting structure attempts to fill the hole. In some systems, this does not cause a problem: for example, if a tile is removed along with all tiles that came after it (and all tiles that came after those, and so on), the system simply starts over at that point and continues. However, when tiles are removed but those resulting from the removed tiles remain, the system tries to grow in two different directions, which can occasionally cause problems. In many cases, particularly when τ is close to 2, proofreading allows holes to be filled properly. In more complex systems, small rates of error may occur even when τ is close to 2. If τ is significantly less than 2 (again, certainly if τ is less than 1), a very high rate of error occurs within the hole. [5]

As we have seen, the boundary found at $\tau = 2$ is an important one; being just under or over this boundary can cause the growth of a system to change direction. However, it can be observed that, when a system is self-healing, this boundary is not always accurate. In some cases, having a τ greater than 2 can still result in regrowth in the hole despite the decay of the overall system.

For this study, it is hypothesized that, when regrowing a hole, factors other than the values of G_{mc}, G_{se}, and τ can play a part in the determining whether a system will grow or decay. Early experimentation shows that a small hole (such as a 10 x 10 hole) will, with a τ of just greater than 2, regrow, while a much larger hole will decay under the same circumstances. Therefore, it appears that the size of the hole, along with already-known factors such as G_{mc}, G_{se}, and τ, affects the rate and direction of growth within the hole. Though the term "size" encompasses various other factors (such as area, perimeter, or shape), here we specifically mean that the perimeter, or amount of exposed edges, affects rates, and that rates are in no way influenced by area or shape. That is, for a given τ value (the ratio of G_{mc} and G_{se}), a certain value can be determined that corresponds to the perimeter at which growth changes direction. It is also hypothesized that the strength of bonds within a system could have some sort of effect on the direction of growth, due to the presence of this as a variable in the $k_{r,b}$ equation above.

Experimental

To begin, I downloaded Xgrow, a simulator created for modeling self-assembling tile sets in the 1990's. The simulator comes in the form of several files with thousands of lines of code. Xgrow is intended for use on an X Windows environment, though I used Mac OS X 10.10 (Yosemite) for all experimentation, testing, and data collection. For this reason, it was necessary to use the X11 utility conveniently included with a

Yosemite install. Running the makefile included with Xgrow was initially somewhat problematic, but eventually produced a binary that I was able to use for the remainder of experimentation.

Fresh installations of Xgrow include a large number of test files, with instructions on how to create one's own tile sets. For the purposes of this experiment, it was sufficient to use the AB.tiles and Sierpinski2x2.tiles tile sets included with the Xgrow install.

Xgrow consists of one window, with a display for the loaded tile set and several switches and buttons that control the simulation. Some are fairly self-explanatory, while others require a bit of experimentation to completely understand. "Run/Pause" can be used to pause a simulation, which is useful when users hope to look at the current state of a system or alter the system in some way. The "Cool/Heat" button is useful when cooling or heating a system, which affects the value of G_{se}. Apart from the obvious functions of "Restart" and "Quit", these buttons and their associated functions were essential in carrying out this experiment. While checking systems for errors was not a primary goal, the "Tile/Err" button was occasionally useful in revealing tiles with mismatched edges. Finally, using the right and center buttons on the computer's mouse were crucial; right-clicking allows a user to adjust the values of G_{mc} and G_{se} (and, by extension, τ), while center-clicking and dragging allows a user to break tiles off the assembly.

In order to test my hypotheses, I first ran several tests to ensure that Xgrow was correctly configured and that I properly understood the simulation environment. To do this, I tested several tile sets for the value of τ that would result in a change of direction. I tested each tile set for a variety of τ values (including at extreme values of G_{mc} and G_{se}), documenting each time the whether the rate of growth was positive or negative (whether the system grew or disintegrated). I did not move on to the main experiment until I was satisfied that I was able to use the software accurately.

I then began working on the primary experiment, trying to find a threshold for the perimeter at which the regrowth of a hole would change direction (if such a threshold did, in fact, exist). To do this, I first used AB.tiles, which I selected due to Xgrow's ability to quickly grow the system to fill the 256 x 256 window. For each run of the experiment, I grew AB.tiles under the documented ideal circumstances ($G_{mc} = 13.0$ and $G_{se} = 8.0$ for a τ of 1.625). I then selected various values of G_{mc} and G_{se} that would provide useful data, focusing above τ values equal to 2 (because any τ below 2 was guaranteed to regrow). For each set of values of G_{mc} and G_{se}, I determined the perimeter at which the rate of growth became 0 (or, the point at which growth changed direction). To make this determination, I tried creating holes of various sizes (including various perimeters, areas, and shapes) and then running the simulation and recording the direction of growth along with the hole size. Next, I made minor adjustments, trying to center on the point at which growth changes direction. Once this point was found, I recorded the τ value and the perimeter threshold. After a sufficient amount of data was collected, I plotted values of the perimeter threshold as a function of τ to find the curve at which one could expect the perimeter threshold for a particular τ value to lay. Finally, I tested the same values for G_{mc} and G_{se} on several different tile sets, including sierpinski2x2.tiles.

Results

As expected, results from the first part of the experiment were consistent with previous tests and calculations. For all values of G_{mc} and G_{se} that were used, $\tau = \frac{G_{mc}}{G_{se}} = 2$ was the obvious boundary at which the direction of growth changes for a self-assembling set. While this was no surprise, the testing provided evidence that Xgrow was configured and being used properly. Tests were run for a variety of G_{mc} and G_{se} values (leading to a variety of τ values) and on multiple different tile sets (AB.tiles, sierpinski2x2.tiles, etc.), all giving the same results.

Table 1: Direction of growth for various values of τ

G_{mc}	G_{se}	$\tau\ (= \frac{G_{mc}}{G_{se}})$	result
0	10	0	growth
5	25	0.2	growth
10	25	0.4	growth
10	15	$0.\overline{6}$	growth
15	15	1	growth
30	20	1.5	growth
25	15	$1.\overline{6}$	growth
14	7.2	$1.9\overline{4}$	growth
13	6.6	$1.\overline{96}$	growth
15	7.5	2	decay
13	6.4	2.03125	decay
13	6	$2.1\overline{6}$	decay
35	15	$2.\overline{3}$	decay
15	5	3	decay
30	5	6	decay
10	0	–	decay
20	0	–	decay

The second portion of the experiment gave very interesting and somewhat unexpected results. The first point tested under AB.tiles, when $G_{mc} = 13$ and $G_{se} = 6$ (so $\tau = 2.1\overline{6}$), gave a perimeter boundary of $P = 30$. That is, holes in the system with a perimeter greater than 30 grew larger (tiles fell off), while holes with a perimeter less than 30 grew smaller (tiles were added and the hole filled in). Meanwhile, the system as a whole disintegrated as tiles fell off, regardless of the hole size. Going forward, many additional values of G_{mc} and G_{se} were tested, several with equivalent values of τ, each giving their own value of P. For example, when $G_{mc} = 10$ and $G_{se} = 4.5$ (so $\tau = 2.\overline{2}$), $P = 19$. A table giving selected values of τ with their correlating P values is given in Table 2.

Table 2: *P* threshold values for given values of τ in AB.tiles

$\tau\ (=\frac{G_{mc}}{G_{se}})$	P
2.02899	271
2.03390	164
2.04082	119
2.08955	51
2.09677	40
$\mathbf{2.1\overline{6}}$	30
$\mathbf{2.\overline{18}}$	23
$\mathbf{2.\overline{2}}$	19
2.6	4
3.25	< 4
$\mathbf{4.\overline{3}}$	< 4

It is clear that as τ rises, the value of P shrinks. When $\tau = 2.6$, the boundary P reaches its minimum point (4). When using Xgrow, no smaller perimeter can be achieved, as the area of this hole is 1 square unit. For all $\tau > 2.6$, $P < 4$. Conversely, when the value of τ approaches 2, P becomes very large. Again, values of τ less than 2 were not tested here, as they always result in regrowth of holes. These data suggest some sort of asymptotic behavior near $\tau = 2$. While not a major goal of the experiment, it was observed that no matter what the value of τ, even when $\tau < 1$, AB.tiles never produced errors.

When testing values of G_{mc} and G_{se} for sierpinski2x2.tiles, which has a greater total bond strength b than AB.tiles, it was discovered that the value of the τ boundary for regrowing holes was different than that in the case of AB.tiles (in this case, the value of b was much larger). For example, when $\tau = 2.1\overline{6}$ using AB.tiles, $P = 30$. However, when $\tau = 2.1\overline{6}$ and using sierpinski2x2.tiles with the much larger values of b, $P = 21$. In sierpinski2x2.tiles, using G_{mc} and G_{se} values distant from the ideal conditions ($G_{mc} = 17$ and $G_{se} = 8.6, \tau = 1.9767$) caused proofreading to break down and resulted in large numbers of errors.

Discussion

The data collected were very useful in determining the source of the phenomena explained earlier. Initial data, taken when experimenting with the values of G_{mc} and G_{se}, confirmed that for any system, a system will grow only when the value of τ is less than 2. That is, the system grows only when $G_{mc} < 2G_{se}$. If this is not the case, the system will shrink, eventually disappearing altogether.

Further data explained the behavior of self-healing tile sets and why $\tau = 2$ is not always the perfect boundary at which growth direction changes (and why the value of τ is not always the same). In this experiment, all variables were kept constant, except for G_{mc}, G_{se} (and therefore τ), and P, the perimeter of the hole in the system. After plotting points on a standard XY plane, using τ as an independent variable and the P value as a dependent variable, it is clear that a relationship between the variables does exist. The line obtained from these points shows the boundary at which growth changes direction (points below or to the left of the line indicate growth, while points above or to the right of the line show that the system will decay). The graph obtained for AB.tiles, when b for each tile is relatively small, is given in Figure 4.

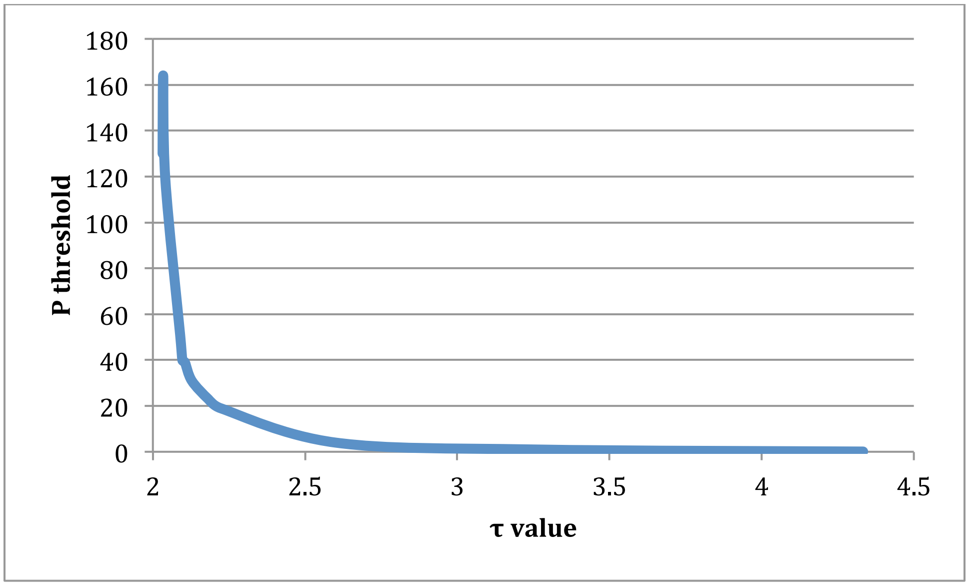

Figure 4: Value of *P* threshold for given τ values for AB.tiles

As expected, the graph has a vertical asymptote at $\tau = 2$ and a horizontal asymptote at $P = 0$. This indicates that, as τ approaches 2 from the right, P goes toward infinity. In other words, when τ gets closer and closer to 2, the perimeter value that causes growth to change direction gets greater and greater. Once the τ value of 2 is reached, there is no value of P large enough to cause a change in direction; the hole will always regrow. The horizontal asymptote indicates that, as τ approaches infinity, P approaches 0. This means that, for very large τ values (certainly anything greater than 2.6), P becomes very small. Since $\tau > 2.6$ always gives $P < 4$, it can be assumed that, in a practical application, $\tau > 2.6$ will always result in decay regardless of the size of P.

The results obtained for sierpinski2x2.tiles, where b for each tile is relatively large, explain that the graph given in Figure 4 does not apply for all tile sets. This was hinted at in the equations $k_f = ke^{-G_{mc}}$ and $k_{r,b} = ke^{-bG_{se}}$, where k_f indicates the growth rate of a system, $k_{r,b}$ indicates the decay rate, and b denotes the total bond strength. Since b is an essential part of the decay rate, it is not a big leap to guess that it affects the decay rate of a hole as well. Indeed, the data suggest that the value of b is an important factor, along with values of G_{mc}, G_{se}, and P, in determining whether a hole will regrow or decay. Based on data collected, higher values of b result in lower P boundary values when τ is kept constant.

From all of the data collected, it is certainly true that the rate of growth and the rate of decay when considering a hole in a self-assembling tile set are both affected by the values of P and b, along with the already-known factors G_{mc}, G_{se}, and τ. When $\tau < 2$, regrowth always occurs, and when $\tau > 2.6$, decay can effectively always be observed. However, when $2 < \tau < 2.6$, and for some b, there exists a value P such that a hole with perimeter greater than P will decay, while holes with perimeters smaller than P will experience regrowth. This value of b is extremely important, as a higher total bond strength will cause the P threshold value to grow smaller. While growth or decay of a system as a whole can be accurately predicted by the value of τ, it is certainly true that this is not always the case inside a hole.

Conclusion

These results are very useful when looking at the rates of growth and decay when regrowing removed tiles. The results are not exactly what one would expect, though certain features of these conclusions, such as the inclusion of b as a factor, are fairly obvious.

Self-assembly can be used in many fields, such as biology (DNA, the lipid bilayer, etc.), mathematics (tiling), and nanotechnology. In any of these cases, tiles can be knocked out of an assembly; depending on the conditions outlined above, this hole may regrow or decay even further. It is worth noting that regrowth should not imply that no mismatches exist in a system (smaller values of τ will produce more errors). While it is no surprise that a system will decay when $\tau > 2$ and a system and hole will regrow when $\tau < 2$, it is interesting to see that holes will still sometimes regrow even if $\tau > 2$ (albeit just slightly greater). Thus, self-assembling systems can decay even while holes in the system can, through self-healing, regrow. These findings can be applied to many different fields where the rate of growth or decay is important.

Further research could potentially yield very interesting results. As we live in a three-dimensional world, many practical applications of these findings would require a conversion to three dimensions. It is hypothesized that, as in the two-dimensional world explored in this experiment, the amount of exposed edges within a hole will affect the positivity or negativity of the growth rate. This means that, while the perimeter P is a crucial factor in two-dimensional systems, surface area of tiles near the hole in a three-dimensional system is likely crucial in this case. Again, finding surface area thresholds for a three-dimensional space is likely to lead to more useful real-life applications.

Another interesting area of study could come from this research; this experiment proves that P and b, in addition to τ, are factors in determining the growth rate inside a self-healing hole. However, more experimentation and calculations in this area could yield some sort of formula in which G_{mc}, G_{se}, and b are used to calculate a value for the P threshold. Such an equation, and a similar equation for a three-dimensional environment, would allow researchers to quickly determine whether a hole will regrow or decay further based on its perimeter.

This experiment was designed to look for factors that affect the rate of growth (or decay, if the rate is negative) in a self-healing system. Based on the results of the experiments outlined above, it is clear that the size of a hole (specifically, its perimeter) is very important and that there exists a threshold P at which growth changes direction. However, the precise thresholds defined above cannot be applied to any given tile set; each tile set will have different P values for each τ due to varying complexity, numbers of tile types, and so on.

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