Turing Reaction-Diffusion -- a World in a Grain of Sand

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Abstract

Turing reaction-diffusion forms the basis for a multi-media, multi-technology approach to capture the mathematical/biological essence of morphogenesis in sculpture. The 2D Kassam algorithm for solving the differential equations defining reaction-diffusion is generalized to 3D. A carefully chosen threshold then generates a compelling isosurface that is polygonalized for 3D printing. Other steps in the process are: 1) Using Fourier filtering to eliminate distracting and poorly reproducible high frequency components, 2) Capping the isosurfaces within the physical printing range while maintaining a solid manifold object for manufacture, 3) Printing the polygon model in plastic and removing support struts, 4) Handcrafting extrapolations to the caps with modeling clay, while preserving tangent plane continuity to the original 3D print, and 5) Finishing aesthetic details by sanding and painting. The resulting sculpture possesses a pleasing visual flow, geometric consistency, tactile appeal, and a "nooks and crannies" element of discovery. On a deeper level, it evokes awe for Turing's proposed mechanism of biological development and diversity.

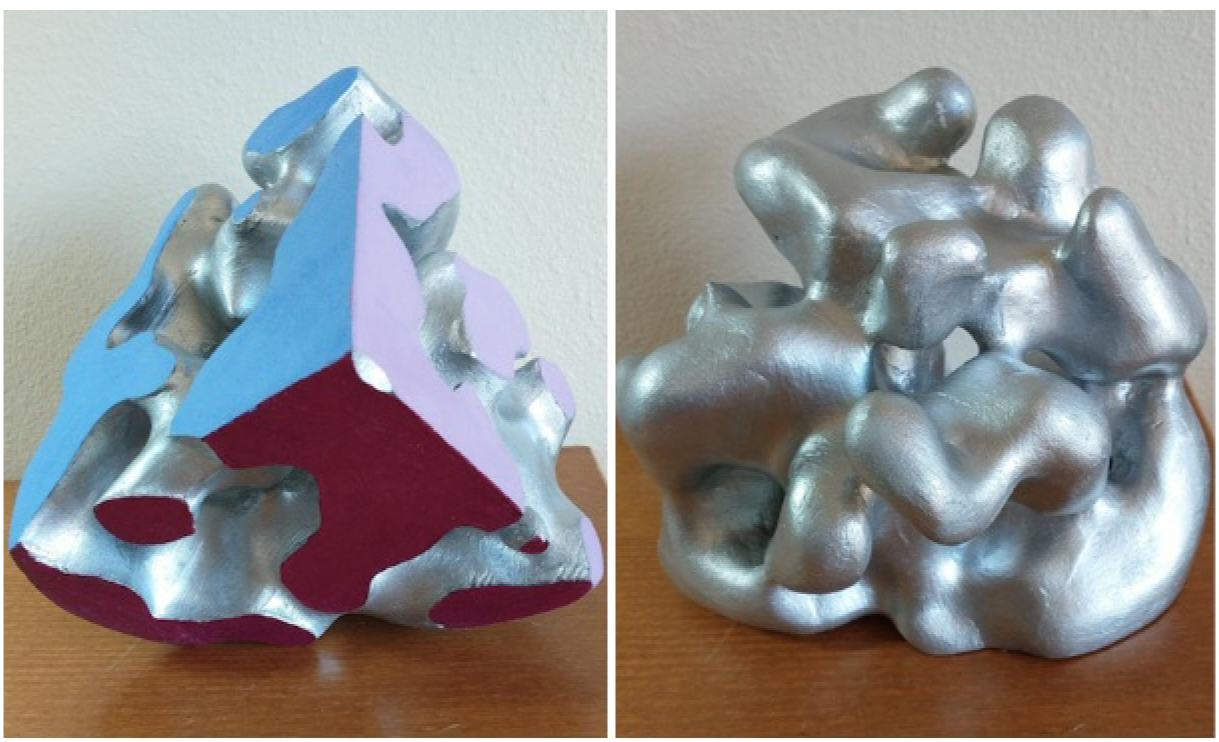

Figure 1: The TuringB reaction-diffusion sculpture: a) view of 2D cuts, and b) full 3D view.

"To see a World in a Grain of Sand
And a Heaven in a Wildflower
Hold Infinity in the palm of your hand
And Eternity in an hour."

-William Blake, *Auguries of Innocence*

Turing’s Other Thesis

The classical (Church) *Turing thesis* asserts that a *Universal Turing Machine* can perform any calculation that is “real-world” computatable. It is one of the most famous concepts in computer science. Many years after this first thesis, Alan Turing posited another, entirely different thesis of note; namely, that morphogenesis was driven by chemical reaction-diffusion. Morphogenesis is the process by which biological cells differentiate during development. In the final publication of his amazingly versatile career [3], Turing asserted that the concentration of chemical reagents drove embryonic cells to develop into more specific varieties, and that this concentration of chemicals resulted from the process known as reaction-diffusion (RD).

As with his first thesis, the thesis on morphogenesis has never been proven. Over the past 70 years, however, increasing anecdotal and scientific studies have buttressed its likely validity. By the early nineties, computers had advanced to the point where some impressive RD patterns could be produced by the computer graphics community. These were 2D, often mapped to 3D surfaces with compelling effects as in Fig. 2a [4]. Simulations have also used the theory to create synthetic digits and limbs [5]. Recent discoveries have shown that epigenetics, i.e. how and when DNA expresses itself, depends on concentrations of the methyl (CH_3) groups in the cells (methylation), though it is not clear that this concentration results from RD [6].

Figure 2: a) 2D RD texture mapped on a 3D surface. b) a 3D RD

In exploring RD patterns we were often struck by the intriguing appeal of the shapes that result, e.g., Fig. 1. In spite of the infinite variety of patterns possible, there was always a consistent esthetic and pleasing flow throughout the pattern. We attempt to capture that essence in sculptures. We created two objects for this paper, one to demonstrate the construction process, called TuringA and another to show the finished sculpture, called TuringB. We describe our approach in the next sections, including a brief overview of the necessary mathematical theory and 3D printing techniques, visualization considerations, and hand-crafted finishing.

Reaction-Diffusion in 3D

Chemical RD is governed by mathematical equations that determine how a mixture of two reagents change concentrations as they 1) react and 2) diffuse within each other. (The computation is a classic cellular automata, finite difference technique). Solutions at a given point in time for high resolutions can be very slow to compute. Kassam [2] improved computational speed by transforming the 2D problem to the Fourier domain and solving it in terms of frequencies, then transforming back to the spatial domain. We took their method and generalized it to 3D. (RD itself was first generalized to 3D images in [1], Fig. 2b). It is straightforward in theory to lift the RD equations to 3D, but as the noted American philosopher, Yogi Berra, once said, “In theory, theory and practice are the same. In practice, they are not.” Implementation of Kassam in 3D required new data structures, convergence tolerances, starting parameters, time step sizes, and many other algorithmic details which required a great deal of thoughtful development, and trial and error. Lomas [7] examines many of these issues.

Besides the propitious speed increases, which varied from 10 to 100 fold, Kassam’s use of the Fourier domain allowed fine surface details to be filtered out with no extra cost. This was essential for 3D printing since small details could spoil the print, leading to unusable results such as dangling threads and tears in the surface. It was a nice piece of serendipity. It didn’t change much in the overall appearance of the sculpture; it simply eliminated some sharp points and small, isolated “islands.”

RD evolves over time. In the beginning of the simulation, the minute variations in concentration showed up as an extremely complex object. By the end, the concentrations had often localized into a few prosaic regions. Somewhere between the extremes one finds the more interesting states that we used. Finding the right moment in time to sample RD was one of the aesthetic tasks.

In theory RD is computed as if the chemicals were in an infinite vat, since boundaries complicate the solution. In practice, of course, 3D printing necessitates boundaries. We implemented our theory with given boundary slices in MATLAB. Besides the necessary mathematical functions to do the RD/Fourier/numerical computations, MATLAB had functions to automatically output polygons which approximated the isosurface and could be used for display.

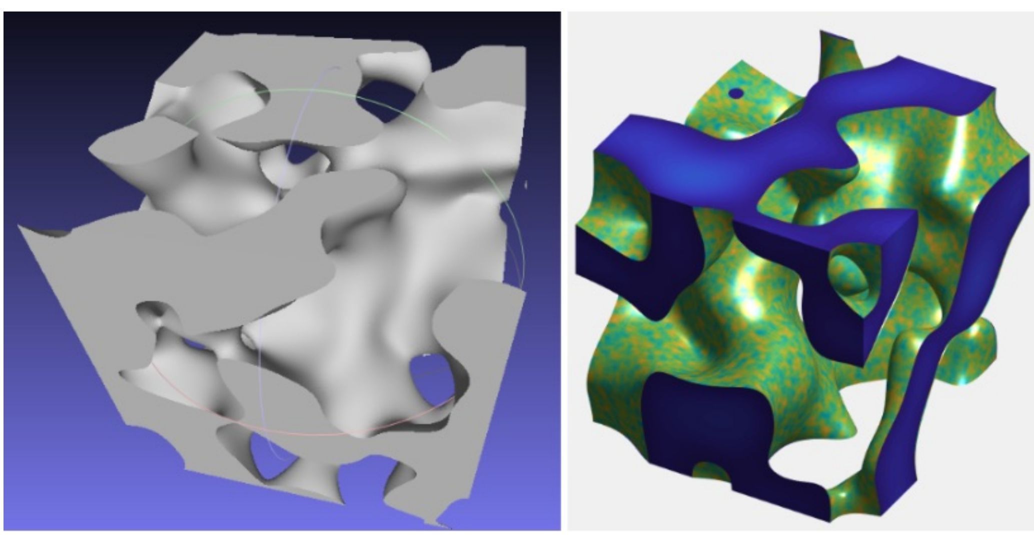

Figure 3: Different views of TuringB model a) Gouraud shaded, b) texture mapped and color coded.

Fig. 3 shows the polygon model with boundaries as output by MATLAB. We found the flat print boundaries themselves to have a charm of their own, and we colored them blue (Fig. 3b). Two-D intersection surfaces are common in morphogenesis e.g. animal hide patterns such as the Holstein cows (Fig. 2a). Computation on a 3D torus is a future option to avoid boundaries altogether.

Visualizing the 3D solution

The concentration of reagents in a solution is a function of the three dimensions of volume, like temperature in a room, or humidity in the atmosphere. Visualizing 3D functions has been an important topic for scientists and computer graphics researchers for decades. Two prominent methods are to visualize it as if the concentrations were a colored gas with opacity, which is higher in regions where the gas is more concentrated, the so-called *volume rendering*. The second is to view contours, or isosurfaces, of the function where all values are equal concentrations, e.g. using a technique known as marching cubes. Fig. 2b shows a volume rendered RD function from [1]. Whereas Fig. 3 is an isosurface rendering of our RD function. Iso-surface rendering is typically achieved by creating small approximating polygons on the surface. Such techniques are mature and readily available, as in MATLAB. The iso-surface rendering offers a convenient segue to 3D printing. The same MATLAB polygons used for rendering can also be used to generate the 3D prints. This is the pathway we took.

As an interesting aside, the polygonalized isosurface offers some attractive rendering options per se. Figure 3b was texture mapped and then lit with a light source. In Fig. 4 the surface was colored based on its curvature. Negative Gaussian curvature is warm colored while positive curvature is cool. The visualization shows that the surface is mostly saddle-like and also that it minimizes the variation of curvature. We speculate that the minimization is one reason the object feels like it has an overall consistency; one senses the harmony.

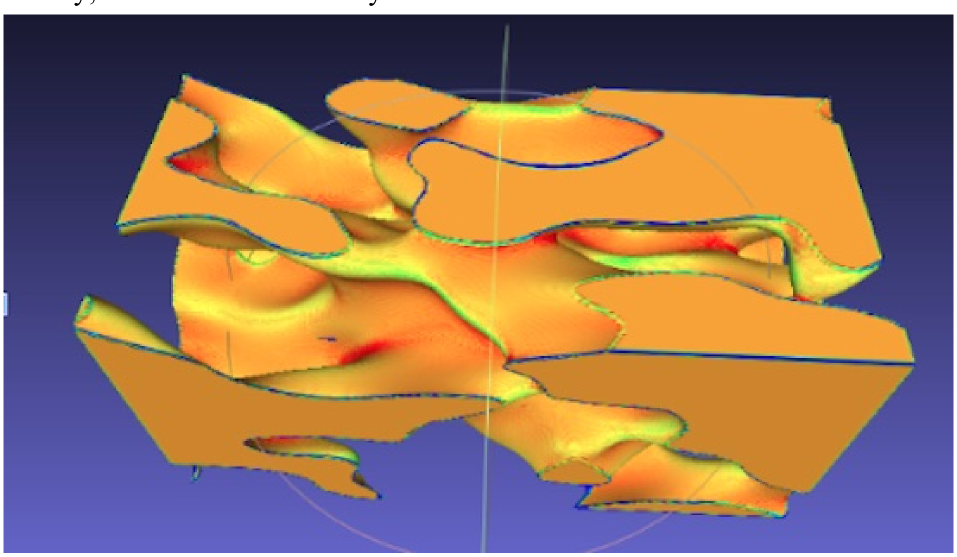

Figure 4: TuringB stretched and rendered according to Gaussian curvature.

The Devil's in the 3D Printing!

Although MATLAB ostensibly gave us the needed polygons for rendering as well as for 3D printing "automatically", as anyone familiar with 3D printing knows, the work is far from complete. We ran the polygon model through the modeling software Blender to check for back facing polys, small gaps, non-manifold and folded over polys etc. It's an exercise that all 3D makerspace acolytes know well. Fortunately, Blender has an array of tools to handle these issues. Additionally, we had to find isolated "islands" and eliminate them manually, as well as size the object and check that the surface could be properly supported with struts without generating too many of them. Those very hard plastic supports have to be removed eventually, and sanded clean. It can be a tedious job given the many intricacies of our Turing sculptures, so the fewer the better. We discovered the size of the prints affects not just the print time (144 hours for a one foot squared object), but more importantly, the likelihood that something will fail and the print won't complete. 3D printers still have substantial room to improve on the engineering front. We managed to complete one 8" cubed piece in only 44 hours.

We used a Lulzbot TAZ 6 3D printer. Watching the sculptures grow slowly from their base mesmerized, and made it all worthwhile. Even cutting out the struts with a Swiss army knife while only partially avoiding being nicked by their sharp ends created satisfaction as the shapes of the objects began to emerge. The white plastic in Fig. 5a is the 3D print for TuringA; the terracotta part is the clay..

Modeling Clay and Final Touches

We had two guiding principles for rounding off the flat sides of a 3D print: 1) The clay extension should maintain tangency to the curved surfaces of the 3D print, and 2) The surfaces should stay consistent with the aesthetic feel of the 3D print, mainly by minimizing the maximum curvature, and repeated eyeballing.

The modeling became a purely artistic effort. It used an air-dried terracotta clay, which had all the tactile/visual joys of pottery or any other sculpture form. Often the 3D print would strongly suggest the shape, other times the clay itself would reveal interesting directions. Sometimes the clay was chiseled off, thrown into the wastebasket and restarted. Fig 5b shows TuringA after sanding, but before painting.

In TuringB we chose to leave three sides flat. As mentioned above, the 2D RD of the boundaries was also interesting. In 3D the flow and turbulence of the object suggested a liquid metal. After some experimentation we decided that a silver tone seemed to belong. The light metal brought out the highlights, and effectively showed off the internal contours. On the other hand, the terracotta of TuringA suggests an organic finish, perhaps a flesh-toned theme? Something yet to be determined.

Figure 5: TuringA sculpture a) clay being added, b) while sanding.

Conclusion

The finished TuringB was invited to be part of a show at the Boulder Canyon Gallery, Boulder, CO. It was exhibited from Feb. 4 until Mar 28. See Fig. 6. It was displayed on a raised plexiglas pedestal over a mirror so that all the colored 2D sides could be viewed along with the 3D sculptured sides. Gallery visitors were encouraged to handle the object, and explore it by touch. In one case, a blind woman examined it for an extended period as Turing's thesis was explained to her. As she returned the sculpture she said, "It's like holding the beginnings of life in my hands." She perfectly captured the original motivation for doing RD sculptures. In the creation process, however, more pleasure was discovered in the intrinsic harmony, intricacy, and flow of the RD objects.

Figure 6: TuringB sculpture on exhibit, mounted on plexiglass over a mirror.

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