Exotic shapes in chemistry and biology

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To his dying day, Jacques Bernoulli was in love with a curve. He was so enamored of the logarithmic spiral that he asked that it be engraved on his tombstone with the inscription *"Eadem mutata resurgo"* ("Though changed, I arise again the same").

The regeneration he had in mind was purely mathematical. For example, the involute of a log spiral is itself a log spiral; though changed by involution, the curve arises again, reborn.[1] Bernoulli's spiral was an optimistic epitaph, a mystic symbol of life and rebirth.

In more recent times, scientists have discovered that certain natural spirals recycle through life, death, and rebirth. These are spiral waves, propagating patterns of activity found in various biological and chemical media. Figure 1 is a life-size snapshot of the Belousov-Zhabotinsky medium, a dish of chemical oxidation-reduction reactions involving a richly colored dye. Visible patterning arises because the reactions are coupled in space by molecular diffusion.[2,3] The light blue spiral is a region of oxidized dye. The spiral wave front advances like a grass fire, oxidizing its neighbors in front and thereby turning them blue. The visual effect is striking: the spiral seems to rotate, turning several times per minute like the spray from a lawn sprinkler. Meanwhile, its passage through the orange medium leaves a burned-out, refractory region in its wake. Gradually, the exhausted region recovers, its color fading back from blue to orange. Thus renewed, the region is again susceptible to the abrupt oxidizing transition, soon to be triggered by the next inner turn of the blue spiral as it encroaches.

The large-scale spiral pattern and the small-scale cycle of quiescence, excitation, and refractoriness are not peculiar to this nonliving chemical reagent. Closely analogous patterns of activity arise in nerve and brain tissue as well as in heart muscle.[4] In the heart, these high-frequency rotating waves can be lethal, usurping control of the heartbeat from the normal pacemaker.[5]

Since heart muscle and brain tissue are both three-dimensional, it may be unfair to regard the wave-conducting medium as a two-dimensional film. What, then, are the three-dimensional analogs of flat spiral

Figure 1. Colored waves of chemical activity move like expanding mirror-image spirals in a thin film of the Belousov-Zhabotinsky reagent. (Photographed in the laboratory of Arthur T. Winfree by F. Goro for *Scientific American*.[2])

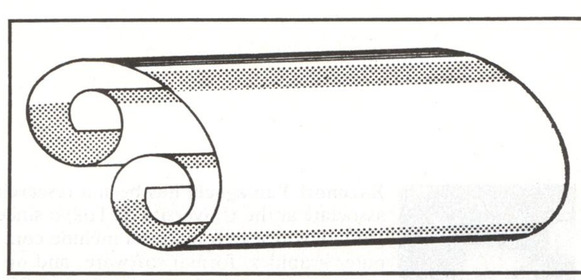

Figure 2. This drawing of a mirror-symmetric pair of scrolls represents the simple basic anatomy of waves in excitable media, but it becomes topologically intricate because the scroll axes close in rings, which may be diversely knotted and linked.

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waves? Here the Belousov-Zhabotinsky reagent is a helpful model system, serving much as a chemical analog computer. Waves shaped like scrolls (Figure 2) have been observed in thick layers of the reagent.[6] In still deeper layers the scrolls close on themselves, forming "scroll rings."[3,7]

We are using computer graphics to help visualize scroll rings.[8,9] The simplest type, shown in Figure 3, is a surface of revolution obtained by transporting a spiral around a circular hoop. The spirals all collide and terminate at a cusp point on the figure's axle, i.e., its symmetry axis. (They are made to terminate because in highly excitable media, colliding waves cannot interpenetrate—just as when grass fires collide neither can continue through the other's ashes.) As time goes by, the waves continue to expand, invading virgin territory and annihilating one another in head-on collisions. The fully evolved wave field is shown in Figure 4.

These pictures had been anticipated before computer graphics, thanks to their high symmetry. But visualizing more complex scroll rings was significantly harder. For instance, what does a *twisted* scroll ring look like? This 3-D wave is characterized by circular transport of a spiral as before, but now we gently twist the spiral in its plane through one full turn as it orbits the axle. Figure 5

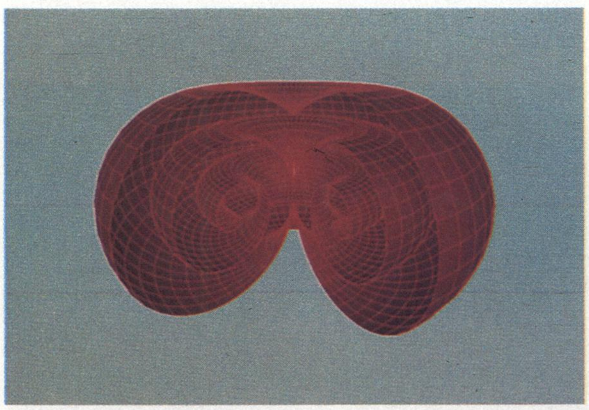

Figure 3. Computerized caricature of a scroll ring wave with a wide sector removed to make the insides visible. The wave has two parts. The inner part resembles a disk with its edge curled into a scroll around an invisible horizontal ring (like a Frisbee or a mushroom cap—see Figure 5 top). The outer part is a closed "bag" formed by the collision of spirals with their diametrically opposite counterparts. Any planar cross section including the axle would resemble Figure 1, but with fewer turns of the spiral and therefore fewer concentric bags.

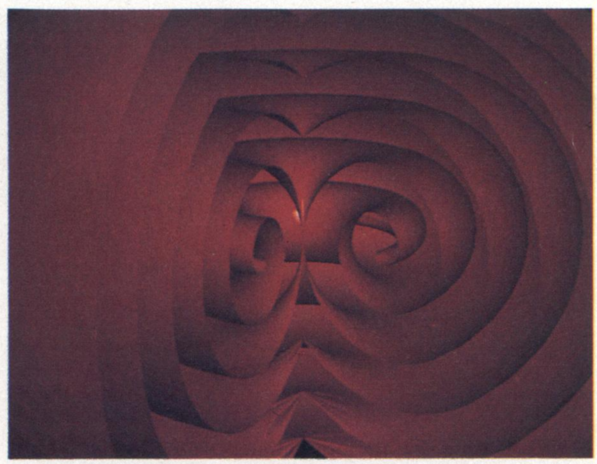

Figure 4. Figure 3 is elaborated by adding more turns to the spiral cross section, thus adding more concentric bags.

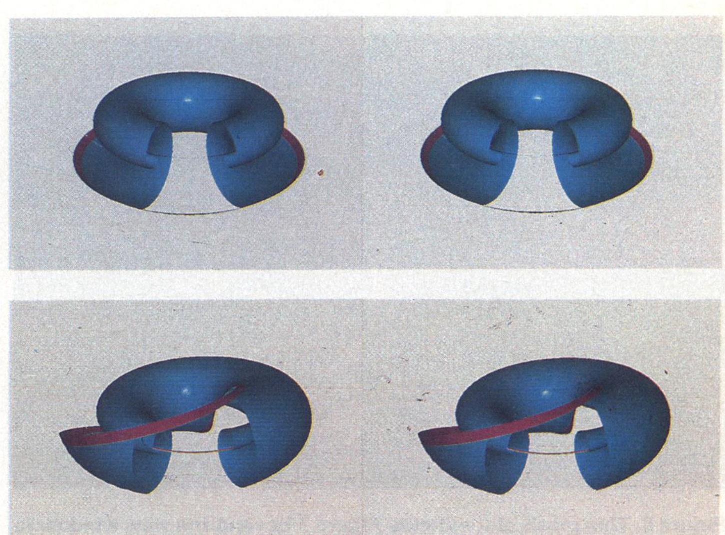

Figure 5. Top: A stereo pair to be viewed with eyes straight ahead, as though looking to infinity. This one corresponds to Figures 3 and 4 but develops the (untwisted) scroll wave from the fine red source only as far as the wide red band. Bottom: Same as above but the spiral is allowed to twist through 360 degrees as it is revolved around the axle. Its development, analogous to Figures 3 and 4, is shown in Figure 7. The white spots are reflections computed from a "sun" assigned to coordinates near the viewer's head. Those who cannot see the pairs in stereo should try looking at them with a paper stereo viewer or a Viewmaster.

presents a stereo pair of the untwisted scroll ring (top) and the twisted scroll ring (bottom). In each, the spirals start from the fine red ring, continuing out to a standard distance substantially less than the ring's radius, so the spirals have no chance to collide. The wide red band is the outer border of the truncated scroll wave. It is not easy to see how this wave pattern should be extended to fill space; one of our early attempts by hand resulted in the embarrassing Escher-like contradiction of Figure 6.

The almost-correct picture is shown in Figure 7, sectored open as in Figure 3 by coloring "invisible" all the cells in the foreground wedge. In Figure 7, as in a parking garage, we can move from one tier to the next by circulating around the axle and never leaving the surface. Accordingly, the wave never ends or closes without edge. Strictly speaking, Figure 7 is a fraud because there is no physically realistic analog of the finite-volume Figure 3; this wave must be continued to infinity (Figure 8, analogous to Figure 4) because there is no way to end it without creating an artifactual edge. In Figure 7 that edge was artfully hidden in the invisible sector.

As it turns out, the screw surface at the axle of this more accurate construction is also ruled out by constraints deriving from physical chemistry. But this region can be removed, as in coring an apple, to be replaced by a physically acceptable screwlike wave front. Letting the waves from each appropriately collide and mutually annihilate allows a realistic pattern of chemical activity to be constructed (Figure 9). The two wave fronts emerging from their distinct source lines can be treated as separate objects (colored red and green). But they fit together exactly, and neither is viable alone. This pair of linked screws is the second member in a periodic table of viable scroll waves (the solitary untwisted scroll ring being the

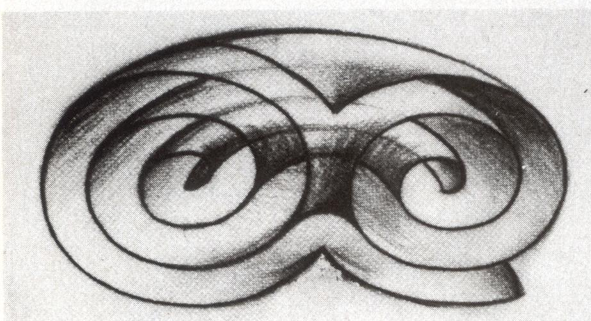

Figure 6. An early attempt (January 1982) to visualize a twisted scroll ring by hand drawing. It is difficult now to imagine such a blunder, but it was nevertheless perpetrated with great care and patience. Without numerical algorithms for realistic construction, comparable faux pas are still difficult to distinguish from chemically viable wave fronts—particularly in the case of topologically more exotic organizing centers.

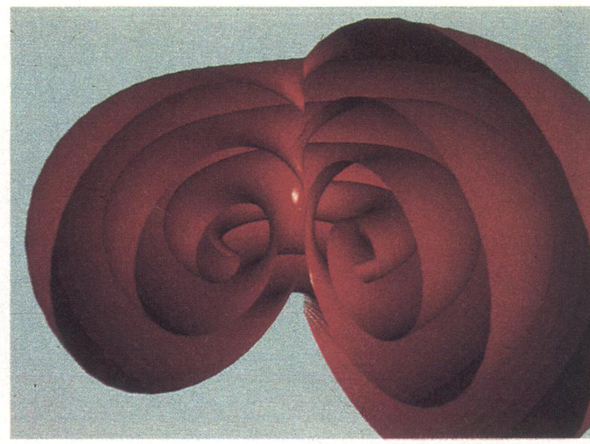

Figure 7. This construction of the twisted scroll ring corresponds to Figures 3 and 4 for the untwisted one. It extends Figure 5 (bottom) well beyond the point of wave collisions at the axle. Strictly speaking, this wave front must be continued to infinity so that it will not have to end somewhere along a nonphysical edge. To make the construction practical, the edge was placed in the invisible sector.

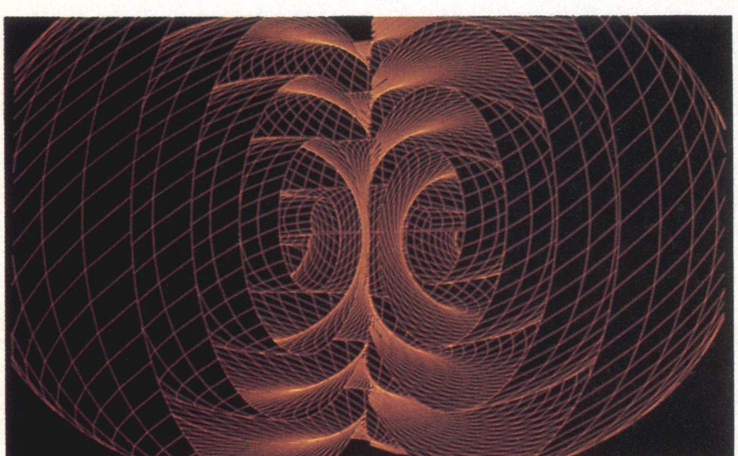

Figure 8. This mesh plot extends Figure 7 beyond the view window to represent an infinitely developed twisted scroll wave.

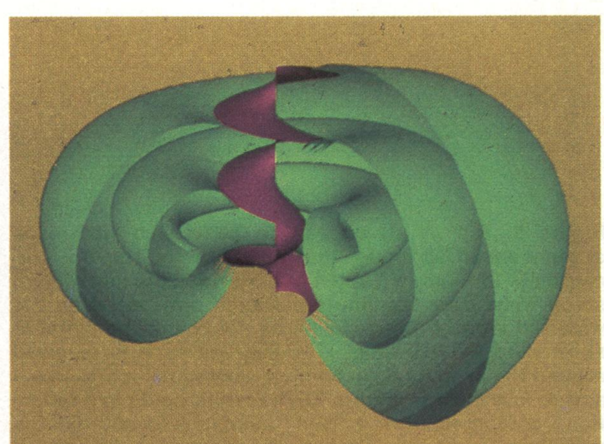

Figure 9. Surgery on the wave front of Figure 7 removes its nonphysical axis where waves seemed to converge to a screwlike collision and replaces it with a surface composed of spiral waves emerging from a physically familiar screw axis. Waves from the two sources collide and mutually annihilate where purple joins green.

first), each topologically distinct, and each more difficult to visualize than its predecessor.[8]

We are using computer graphics to become familiar with these shapes in anticipation of recognizing them in the laboratory.[8,9] It is necessary to depict linked and knotted scroll rings and the loci of mutual annihilation where the spiral waves they emit eventually collide. The main difficulty at present is to compute this collision locus, where the construction of each spiral should be terminated. We would appreciate hearing from anyone with ideas to offer.

To plot these structures, we use a Fortran program called Grafic, adapted to a Cray 1 computer.[9] Input to Grafic can consist of any number of logical meshes, each defining a surface by associating an (x,y,z) coordinate triplet with each node in the rectangular mesh.

Most hidden-surface-removal programs require surface definition by polygons. This presents the user with the difficulty of fitting the polygons together, often compelling him to define each node several times. We found it more convenient with these complex geometries to define each node only once on a logical mesh. We imagine that we start with a rectangular wire grid, then we distort it into any desired shape by specifying the x, y, and z coordinates of the intersections of the wires. After we define the viewpoint and the coordinates of the light sources, Grafic removes the hidden surfaces and plots the image as shaded, colored surfaces in perspective (e.g., Figures 5 and 7). Grafic can also produce mesh plots with shading (Figures 3, 9, and 10) or without shading (Figure 8) between the lines.

The color of each cell of this mesh can be independently defined. To produce a cutaway (Figures 3, 4 and 5) or a window into the interior of the object (Figures 8 and 10), we simply define the color of selected cells to be "invisible."

Grafic is fast enough to economically produce movies showing the evolution of these forms with time, or we can rotate the objects and cause the cutaways to move with the viewpoint so that observers can examine 3-D spiral waves from all angles. (In fact, with Figures 7-9, physical rotation of the viewpoint around the vertical axle is exactly equivalent to time evolution at a fixed viewpoint, sparing the Cray 1 the labor of recomputing the coordinate mesh for each frame.)

These images are useful not only for describing to others the behavior of the waves but also for clarifying their peculiar topology in our own minds. The realistic graphical presentation is valuable also in helping to pinpoint errors in the underlying calculation. The human eye instantly picks out irregularities in the surface—irregularities that would be difficult or impossible to detect by scanning long lists of coordinates.

Acknowledgments

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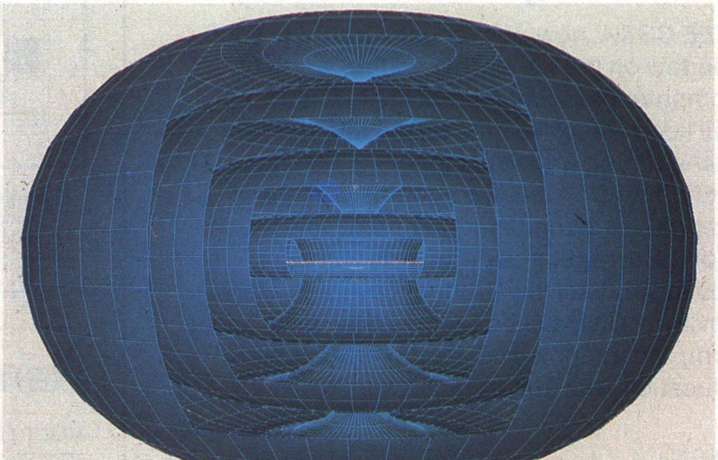

Figure 10. The wave front of Figures 3 and 4 at a stage in its development when two concentric "bags" of wave front have separated from the interior source and are radiating away into an as yet undisturbed medium. Painting rectangular areas of the mesh "invisible" exposes the interior to view. The outer bags are actually parts of a single logical mesh composed only of coordinates for rotated flat spirals, but cells are painted invisible beyond alternating interpenetrations of distinct spirals. As a result, the visible surface resembles wave fronts that have mutually annihilated and separated into disjoint bags.