Caltech computer scientists embed computation in a DNA crystal to create microscopic patterns

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In a demonstration that holds promise for future advances in nanotechnology, California Institute of Technology computer scientists have succeeded in building a DNA crystal that computes as it grows. As the computation proceeds, it creates a triangular fractal pattern in the DNA crystal.
This is the first time that a computation has been embedded in the growth of any crystal, and the first time that computation has been used to create a complex microscopic pattern. And, the researchers say, it is one step in the dream of nanoscientists to master construction techniques at the molecular level.

Reporting in the December issue of the journal Public Library of Science (PLoS) Biology, Caltech assistant professor Erik Winfree and his colleagues show that DNA "tiles" can be programmed to assemble themselves into a crystal bearing a pattern of progressively smaller "triangles within triangles," known as a Sierpinski triangle. This fractal pattern is more complex than patterns found in natural crystals because it never repeats. Natural crystals, by contrast, all bear repeating patterns like those commonly found in the tiling of a bathroom floor. And, because each DNA tile is a tiny knot of DNA with just 150 base pairs (an entire human genome has some 3 billion), the resulting Sierpinski triangles are microscopic. The Winfree team reports growing micron-size DNA crystals (about a hundredth the width of a human hair) that contain numerous Sierpinski triangles.

A key feature of the Caltech team's approach is that the DNA tiles assemble into a crystal spontaneously. Comprising a knot of four DNA strands, each DNA tile has four loose ends known as "sticky ends." These sticky ends are what binds one DNA tile to another. A sticky end with a particular DNA sequence can be thought of as a special type of glue, one that only binds to a sticky end with a complementary DNA sequence, a special "anti-glue". For their experiments, the authors just mixed the DNA tiles into salt water and let the sticky ends do the work, self-assembling the tiles into a Sierpinski triangle. In nanotechnology this "hands off" approach to manufacturing is a desirable property, and a common theme.

The novel aspect of the research is the translation of an algorithm--the basic method underlying a computer program--into the process of crystal growth. A well-known algorithm for drawing a Sierpinski triangle starts with a sequence of 0s and 1s. It redraws the sequence over and over again, filling up successive rows on a piece of paper, each time performing binary addition on adjacent digits.

The result is a Sierpinski triangle built out of 0s and 1s. To embed this algorithm in crystal growth, the scientists represented written rows of binary "0s" and "1s" as rows of DNA tiles in the crystal--some tiles stood for 0, and others for 1. To emulate addition, the sticky ends were designed to ensure that whenever a free tile stuck to tiles already in the crystal, it represented the sum of the tiles it was sticking to.

The process was not without error, however. Sometimes DNA tiles stuck in the wrong place, computing the wrong sum, and destroying the pattern. The largest perfect Sierpinski triangle that grew contained only about 200 DNA tiles. But it is the first time any such thing has been done and the researchers believe they can reduce errors in the future.

In fact the work is the first experimental demonstration of a theoretical

concept that Winfree has been developing since 1995--his proposal that any algorithm can be embedded in the growth of a crystal. This concept, according to Winfree's coauthor and Caltech research fellow Paul W. K. Rothemund, has inspired an entirely new research field, "algorithmic self-assembly," in which scientists study the implications of embedding computation into crystal growth.

"A growing group of researchers has proposed a series of ever more complicated computations and patterns for these crystals, but until now it was unclear that even the most basic of computations and patterns could be achieved experimentally," Rothemund says.

Whether larger, more complicated computations and patterns can be created depends on whether Winfree's team can reduce the errors. Whether the crystals will be useful in nanotechnology may depend on whether the patterns can be turned into electronic devices and circuits, a possibility being explored at other universities including Duke and Purdue.

Nanotechnology applications aside, the authors contend that the most important implication of their work may be a better understanding of how computation shapes the physical world around us. "If algorithmic concepts can be successfully adapted to the molecular context," the authors write, "the algorithm would join energy and entropy as essential concepts for understanding how physical processes create order."

Winfree is an assistant professor of computation and neural systems and computer science; Rothemund is a senior research fellow in computer science and computation and neural systems. The third author is Nick Papadakis, a former staff member in computer science.

Source: California Institute of Technology