Chemical waves used to solve math problem

Researchers at West Virginia University, Morgantown, have developed an innovative technique for using chemical reactions to solve one type of mathematical problem. They set up a system of chemical waves in a labyrinth and then employ time-lapse images to construct a vector field that can be used to determine the shortest path between any two points.

The work was carried out by visiting scientist Oliver Steinbock, graduate student Ágota Tóth, and chemistry professor Kenneth Showalter [Science, 267, 868 (1995)].

Typically, such a problem is solved mathematically by doing iterative searches in which every point in the labyrinth is traced back to some target point until the shortest path is found. The complexity of this class of problem grows exponentially with the size of the maze.

But with the new technique, a chemical wave prepared with the Belousov-Zhabotinsky (BZ) reaction “gives you the optimal path from every single point in the grid back to a target point,” says Showalter. The BZ reaction—the cerium-ion-catalyzed oxidation of malonic acid by acidified bromate—is an oscillatory reaction that produces chemical waves and other types of dynamic patterns.

Showalter believes that when the chemical-wave technique is used, the complexity of the optimal-path problem does not increase exponentially, but only in direct proportion to the optimal path length. “It’s a parallel approach for determining what normally would be done in an iterative manner,” he says.

The technique is reminiscent of a method developed by Leonard M. Adleman of the department of computer science and the Institute for Molecular Medicine & Technology at the University of Southern California. Adleman showed that DNA ligation reactions can provide a massively parallel solution to a computationally difficult class of mathematical problems [Science, 266, 1021 (1994)].

Potential applications of the chemical-wave technique are still somewhat speculative. However, says Showalter, “When we were working on this, I had a vision in my mind of a gigantic Army warehouse with a robot that needs to deliver a package to a loading dock. If the warehouse were big enough and complex enough, this would be a complicated problem. One could conceivably use this type of algorithm to provide the robot with a map of the optimal path to the loading dock from any point in the warehouse.”

It is not necessary to do a chemical experiment to solve such a problem. “The chemical system provides a nice way to explore all the possibilities of this type of behavior,” Showalter notes, but the experiment can also be simulated with a computational algorithm. In fact, the concept of determining optimal paths in this manner was first reported at a 1991 conference on artificial neural networks.

In addition, says Showalter, “Anyone who has ever studied chemical waves kind of knew this—it’s almost obvious that a chemical wave can give you the shortest path. So in that sense our technique builds on the work of everyone who has looked at chemical waves.”

But the West Virginia University group is the first to explicitly demonstrate their use to do mathematical computations. “We’ve taken the concept a step further,” he says.

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