

"particles," whether muskrats or molecules, move at random from position to position.

The model's importance stems from the fact that researchers can express many different physical processes as random-walk problems. "The random motion of particles is at the root of much physics, chemistry and biology," says physicist and team member H. Eugene Stanley of Boston University.

The novel random-walk variation developed at Boston University arose out of a curriculum project designed to introduce concepts of randomness to high-school students. Going beyond the familiar, well-studied problem of depicting the territory covered by a single "walker" randomly wandering from square to square on a grid, project manager Paul Trunfio decided to look at the patterns formed by a swarm of random walkers, all starting simultaneously on the same square, as they independently explored the grid.

Trunfio's computer-generated patterns were sufficiently interesting to prompt further investigation. "We realized ... that this might be an unsolved problem in random walks," Stanley says. "We spent two or three months looking at computer images trying to discover the laws that seemed to govern the behavior we saw."

The computer experiments revealed that the set of visited sites initially has a relatively smooth boundary. But after the territory reaches a certain size, this edge grows increasingly jagged.

Graduate student Hernan Larralde, aided by Shlomo Havlin and George H. Weiss of the National Institutes of Health in Bethesda, Md., then worked out a precise, mathematical solution of the problem in one, two and three dimensions. "At first sight, it looks like a trivial problem to solve," Stanley says. "It was in fact a very difficult mathematical problem."

The analysis unexpectedly revealed that this random-walk process goes through three distinct time regimes representing characteristic but different rates and patterns of growth. "We were surprised by the fact that a relatively simple question about random walks could be so rich," Stanley says. A paper detailing the findings appears in the Jan. 30 NATURE.

"The work of Larralde [and his co-workers] opens up a host of further possibilities — of using interacting walkers, of working in fractal spaces ... and so on," Michael F. Shlesinger of the Office of Naval Research in Arlington, Va., comments in the same issue of NATURE. "These would find applications in fields as diverse as physics and ecology."

"What's nice about this particular problem is that it's sufficiently simple that you can get some feeling for the collective behavior of large numbers of particles," Weiss notes.

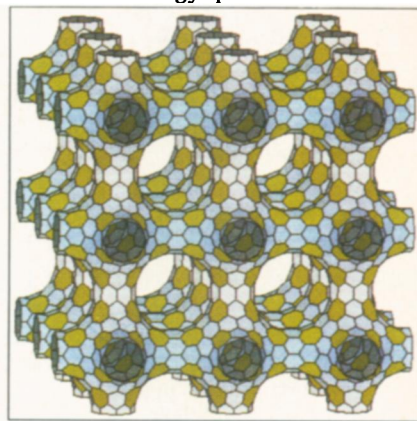
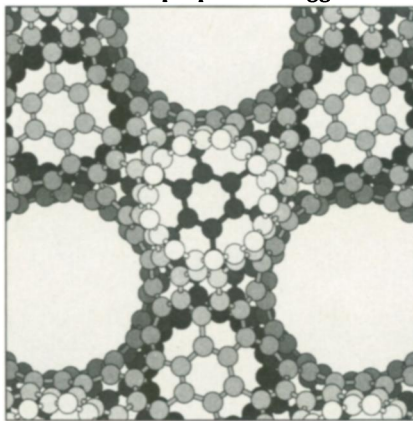
— I. Peterson

Theorists design new-look fullerenes

Add some five-sided rings of carbon to a graphite sheet — with its honeycomb arrangement of carbon atoms — and the sheet curves around to form a buckyball or one of its rounded fullerene cousins.

But if that sheet contained seven-sided carbon rings instead of five-sided ones, an entirely different sort of fullerene would result, two independent groups of theoretical physicists report. These new theoretical molecules would be more stable than a buckyball, and they seem quite light and strong, David Vanderbilt at Rutgers University in Piscataway, N.J., and a colleague conclude in the Jan. 27 PHYSICAL REVIEW LETTERS.

Such useful properties suggest that



These computer images show how seven-sided rings (yellow) give this fullerene its saddle shape (right), and in this sliced open molecule, how atoms are arranged (left).

scientists should start looking for fragments of these molecules in the soot generated during fullerene production, says Veit Elser, whose group at Cornell University studied a theoretical molecule containing 216 carbon atoms.

Vanderbilt and Jerry Tersoff at the IBM Thomas J. Watson Research Center in Yorktown Heights, N.Y., call their new 168-carbon molecule buckygyim because of its repeating, jungle-gym-like structure. Using a computer program, they constructed the buckygyim by substituting seven-sided rings of carbon where fullerenes typically have five-sided rings: Six-sided rings surround each seven-sided ring, and each six-sided ring is surrounded by alternating six- and seven-sided rings.

"If you use this [substitution] pattern, [the molecule] does close in on itself, but in a complex way," Tersoff says. A fullerene's 12 pentagons make the carbon sheet bend inward. But septagons cause the sheet to curl in along one axis and outward along the perpendicular axis, so parts of these sheets resemble saddles. Instead of joining to form a ball, the saddle-like segments form a network of short tubes. Molecules join and

become repeating units in a lattice arrangement. The arrangement is tetrahedral, like the structure of diamond, and leads to a structure that looks nothing like a buckyball's, he adds.

"It's sort of a lacy network, with all this empty space," says Tersoff. "Yet even though it is mostly vacuum, it's still macroscopically rigid." Thus, the teams expect a material made with these molecules to be quite strong, but lightweight. Also, these molecules seem more stable than buckyballs. The seven-sided rings allow carbons to bond with one another with less strain than do pentagons, note both research groups. Vanderbilt and Tersoff calculate that the buckygyim needs about one-sixth the energy per atom that the

buckyball needs to form.

Working with Michael Teter at Corning Inc., in Corning, N.Y., Elser and his group decided to add extra hexagons as well as replace the pentagons with septagons, thereby making it easier for repeating molecules to link up with less strain. In their report in the Jan. 23 NATURE, they call the substance schwarzite. They also studied theoretical molecules with eight-carbon rings.

"The big question is the feasibility of synthesizing these things," says Elser. "We're in the same position that the buckyball people were in five or six years ago." Both groups suspect, however, that parts of these molecules may form during the production of fullerenes. Slow-growing sheets curl inward to make buckyballs, while the fastest-growing sheets of carbon may take on these saddle curves, Elser adds.

To help chemists recognize these new molecules when they see them, Vanderbilt and Tersoff plan to calculate buckygyim's electronic structure and vibration modes, characteristics that would signal the existence of saddle-shaped carbon sheets.

— E. Pennisi

Vanderbilt and Tersoff/Phys. Rev. Lett.

Steve Townsend and Thomas Lenosky/Cornell