The Ties that Bind

Mathematicians unraveling the secrets of the humble knot find it is a scientific jack-of-all-trades.

BY P. J. SKERRETT

Boy Scouts fumbling their way through a big square knot don't imagine it exists. Nor do surgeons tying off a tiny stitch on a blood vessel. Even old salts whipping up a Round Turn Spilled-Hitch Bowline are unlikely to suspect they're also exploring a once-obscure but increasingly important branch of mathematics. Lurking inside the crisscross pattern that forms a knot is a complex theory that has puzzled and challenged mathematicians for more than 100 years.

Thanks to several unexpected connections, knot theory is now emerging as a powerful tool for solving a broad array of practical problems. It explains how tightly coiled DNA manages to replicate inside cells. And it's helping to define the very structure of space. Knot theory is aiding the search for effective antibacterial and anticancer drugs, and it may make computer networks more reliable and efficient. A segment from the videotape "Not Knot," a computer-animated tour of advanced knot theory, even makes a cameo appearance in the Grateful Dead's psychedelic concert light show.

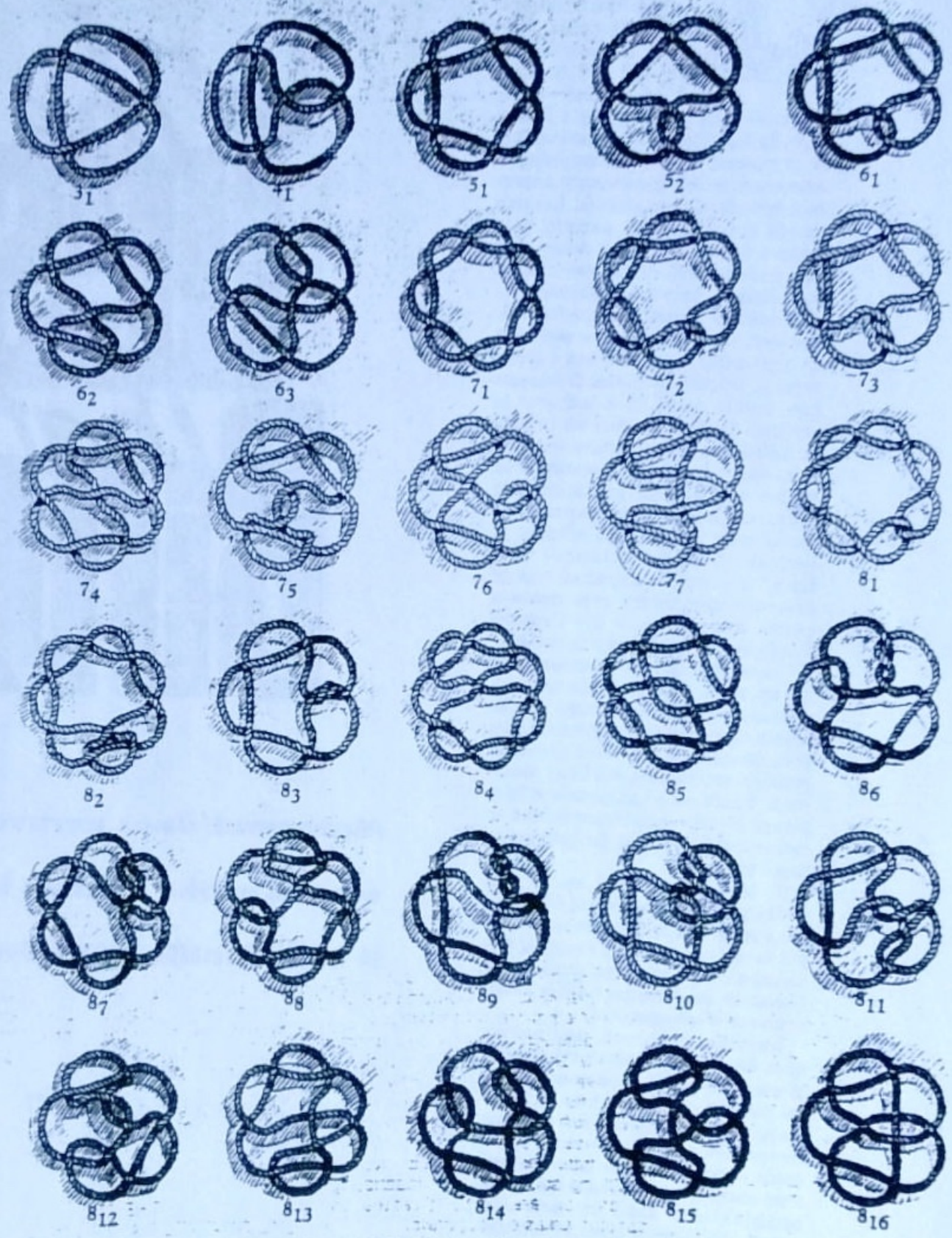
These applications represent just the tip of the "knot-berg." As more scientists struggle to understand this intricate theory and knot theorists turn their attention to real-world problems, practical applications will likely mushroom. That's not a bad turnabout for a branch of mathematics once derided as recreational doodling for terminally bored topologists.

"It is so satisfying to see all this mathematics that we've had sitting on the shelf for 25 or 50 years now being put to use in a stunning variety of disciplines," says mathematician Alvin Thaler at the National Science Foundation in Washington, D.C.

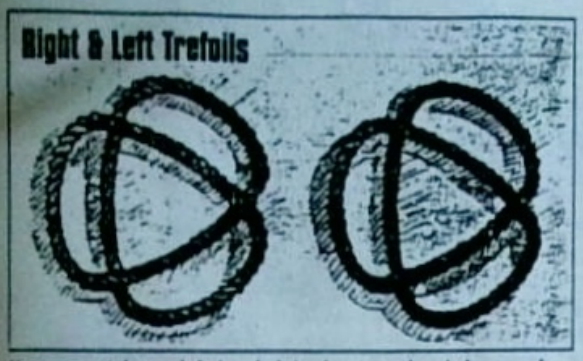
Weavers, fishermen, and sailors have depended on knots for thousands of years; mountain climbers and surgical patients stake their lives on them. Knots appear in artwork and religious ceremonies around the world. Hundreds of different knots have evolved, from the simple overhand to the showy combinations used by macrame artists. The *theory* of knots, by comparison, is a relative newcomer, originating in the 1860s as a perfectly practical offshoot of chemistry.

Dissatisfied with the then-current theory of atoms as hard spheres held together by mysterious forces, William

The Periodic Table of Knots



The number of crossings helps classify knots, much as the atomic number does for elements. In each example above, the larger number represents crossings, while the subscript tells which knot it is in that series. For example, the top right knot, 6_1, is the first knot of three with six crossings. This table contains all possible knots from three up to seven crossings; it has 16 of 21 knots with eight crossings.



Knots are right- or left-handed. In chemistry, handedness makes otherwise-identical compounds behave differently.

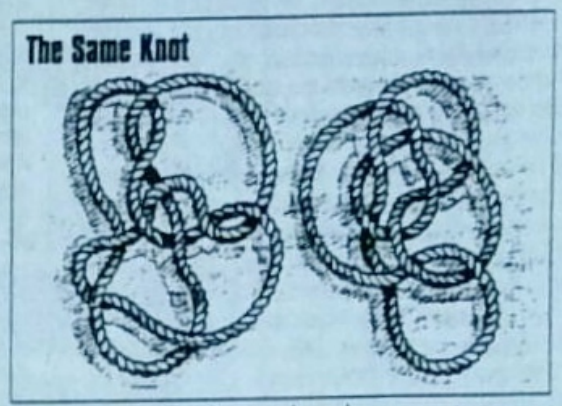
Thomson (who became Lord Kelvin) guessed that atoms might be "knotted vortices in the ether." He imagined these vortices, or elongated whirlpools, bonding together by forming tiny knots. Scottish chemist Peter Tait started cataloging knots and ultimately created a crude periodic table, classifying them by the number of times their strands crossed. Tait and assorted colleagues spent years on this project, and the mathematical relationships they discovered gave birth to a new field.

In the real world of neckties and bakery boxes, knots are simple devices for securing a rope to itself or to something else. In the writings of the scientist-futurist Buckminster Fuller, knots physically store information by capturing (or tracing) the trajectory of two rope-holding hands. Mathematicians, as is their habit, see knots more formally: one-dimensional curves sitting in three-dimensional space that begin and end at the same point and never intersect themselves. That means that linked rings (in fact, any rings), such as those in the Olympic insignia, are knots. It also means the bows we tie on our shoes, or the hopelessly snarled ball of fishing line in the bottom of the boat, aren't really knots.

"If a knotted string has loose ends, it's really not a knot, since you can always slide a free end around and eventually, if you have the time and patience, get back to a nice untangled line," explains De Witt Sumners, a mathematician with Florida State University. To make a knot that would satisfy Sumners and other mathematicians, take an electrical extension cord—or string of pearls if you're feeling extravagant—tie a simple overhand knot, then plug or clasp the free ends together.

Given the no-free-ends rule, the simplest knot is a circle, sometimes called the "unknot" or trivial knot. A trefoil has three crossings of the rope, pearls, or extension cord. The trefoil comes in two "flavors," right-handed and left-handed (see illustration above left). No amount of twisting or sliding can transform one into the other. Only one knot has four crossings, the familiar square knot and its mirror image, the granny knot. From there, the number of knots in a group grows exponentially—there are seven knots with seven crossings, 21 with eight crossings, 49 with nine crossings. The most complete table to date contains 12,965 knots with thirteen or fewer crossings, not counting mirror images.

Mathematicians, following their natural instincts to ferret out patterns that occur in nature, look for some common rules that will let them label a knot, determine whether something is really knotted, or tell whether two dissimilar-looking knots are in reality the same or different. Trivial problems? Think again. It took almost 100 years to prove that two different-looking knots with ten crossings listed in Tait's periodic table were, in fact, the same (see illustration below). This difficulty arises because a single knot can be twisted and rearranged into what looks like different shapes, yet by the rules of topology it remains the same as long as it isn't cut. (Topology, sometimes called rubber-sheet geometry, cares little for point-to-point congruence. To a topologist, a doughnut with a hole in the middle and a coffee cup with a handle are equivalent. That's because a clay doughnut can be stretched into a cup shape, with the hole providing the cup's handle.)

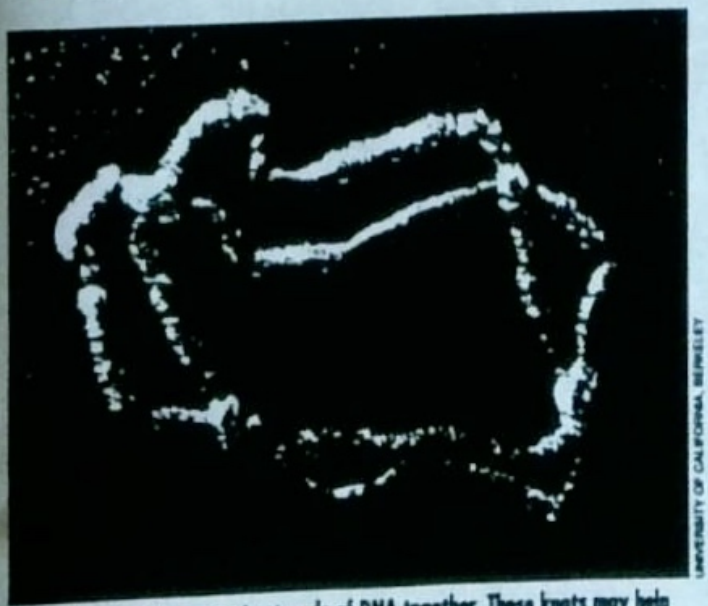


Categorizing can be tricky; it took nearly a century to prove these two different-looking knots are the same.

For several years, mathematicians searched for a universal number or formula that could uniquely define different knots (see "Unraveling Knot Theory"). A breakthrough came in 1984. New Zealand-born mathematician Vaughn Jones discovered a powerful method for labeling knots. Much to everyone's surprise, his startling new approach shared equations with quantum physics and statistical mechanics, the study of systems with a massive number of components.

"The discovery that Jones made linking statistical mechanics and knot invariants [formulas that describe knots] immediately got people wondering how close this relationship was, and where else it might lead," says mathematician Louis Kauffman at the University of Illinois at Chicago. Kauffman is widely credited with exploring this connection and stimulating others to investigate the link between knot theory and the physical sciences. By the time Jones was awarded a Fields Medal—mathematics' equivalent of a Nobel Prize—for his work in 1990, knot theory had become a vital tool in biology, and its applications were rippling through physics, chemistry, and engineering.

Perhaps knot theory's most dazzling, or at least its most practical, application to date is in molecular biolo-



UNIVERSITY OF CALIFORNIA, BERKELEY

Knots in nature: Enzymes tie strands of DNA together. These knots may help tell proteins when, where, and how to act on genetic information.

gy. The DNA inside cells, it turns out, naturally kinks up into knots, loops, and links. These pose serious problems for the enzymes that copy DNA or translate its genetic information, because they only work on flat, untwisted sections. On the other hand, knots and kinks may provide crucial topological stop-and-go signals for these enzymes.

"Knot theory is really the next chapter of the DNA story," now that DNA's structure and chemistry are fairly well understood, suggests mathematician Avner Friedman at the University of Minnesota. DNA, or deoxyribonucleic acid, is an extraordinarily long ladder-shaped molecule that carries the entire genetic code for making and operating a bacterium, a beech tree, or a baby.

Actually, *long* is an understatement. If a muscle cell's nucleus were the size of a basketball, then the DNA packed inside would be as thin as a fisherman's monofilament line and stretch across Lake Michigan and halfway back, or about 125 miles. Cramming that much DNA into a tiny space requires some regular method of compression, and living organisms have adopted supercoiling. This is what happens when you repeatedly twist the ends of a rubber band in opposite directions. Cells also wrap sections of DNA around tiny globular proteins. In addition to making DNA more compact, this wrapping also knots it up, just as wrapping a perfectly untangled garden hose around a circular storage rim causes kinks and twists to form in the hose still lying on the grass.

Biologists have discovered several proteins whose job in life is twisting, knotting, and unknotting DNA. Called topoisomerases, these enzymes act like molecular fingers that tie and untie strands of genetic material. Knot theory has been invaluable in helping unravel the mechanism by which topoisomerases work. It's impossible to watch them in action inside a cell or in a test tube. But when you know the DNA's starting configuration and what it looks like after a topoisomerase does its job (see photo), then basic knot theory "lets you deduce the enzyme's reaction mechanism," says De Witt Sumners of Florida State.

Gyrase, a poetically named topoisomerase, helps twist the DNA double helix into a supercoil. Another class untwists supercoiled DNA, opening the way for yet other enzymes to read or copy the genetic message stored in a particular stretch of the molecule. Still other topoisomerases knot and unknot DNA by snipping open a section of double helix, sliding a nearby section through the break, and resealing the cut. University of California, Berkeley, biologist Nicholas Cozzarelli calls this "incorporealizing the DNA"—making it act for an instant as if it had no body and, like a ghost, could pass through solid DNA strands.

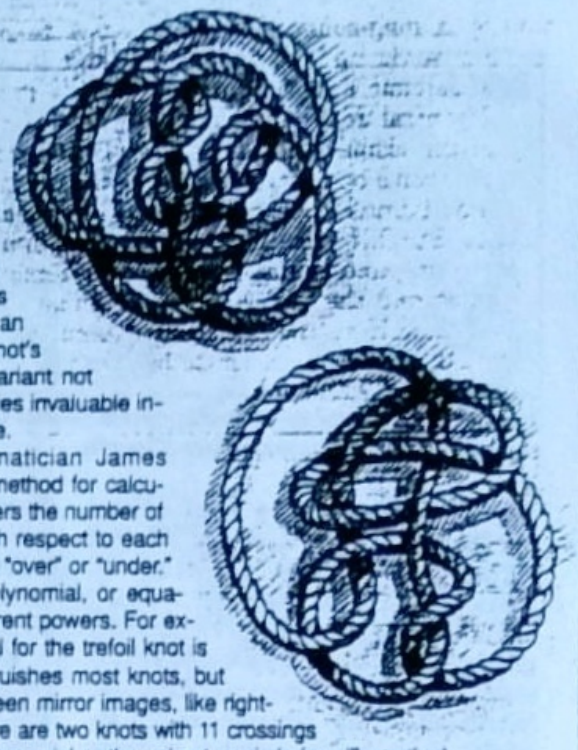
Computer simulations carried out at the Courant Institute of Mathematical Sciences in New York show that small pieces of DNA probably coil up and form simple knots like the two-ringed figure eight even in the absence of any proteins. This writhing, slithering, and twisting—all precisely defined mathematical terms—may create knots or bulges that act as road maps for proteins. "We used to think DNA was just this boring chain of chemicals that sits there and waits for proteins to come along and act on it," says the Courant Institute's Tamar Schlick. "We're learning that all this coiling may actually determine when, where, and how proteins attach to it and act on it."

This new picture of DNA has led to the discovery of powerful drugs that stop bacteria from multiplying inside our bodies and kill cancer cells before they divide out of control. Basically, these new drugs turn a cell's unknotting enzymes against its own DNA. Ciprofloxacin, one of the most effective and widely prescribed antibacterial drugs, allows one kind of topoisomerase in the invading bacteria to untwist DNA and snip it open. But then it blocks the enzyme from resealing these breaks. When the bacterial cells divide, they split into daughter cells with deadly, nonfunctioning DNA. And since the drug doesn't target human topoisomerases, only the bacterial cells are affected. Several anticancer drugs use essentially the same strategy, acting only on cells that divide rapidly, such as tumor cells.

Biology isn't the only field enriched by knot theory. Physicists are using it

[*Continued on page 120*]

UNRAVELING KNOT THEORY



The quintessential problem for knot theorists is finding a unique number or formula that identifies knots known and unknown. This number, which must stay the same no matter how much the knot is twisted or rearranged, is called an invariant. It acts a little like a knot's Social Security number. An invariant not only identifies a knot, it also carries invaluable information about its core structure.

In 1928, American mathematician James Alexander devised an intricate method for calculating a knot's invariant. It considers the number of crossings, their arrangement with respect to each other, and whether a crossing is "over" or "under." Alexander's method yields a polynomial, or equation with variables raised to different powers. For example, the Alexander polynomial for the trefoil knot is $t^2 - t + 1$. This polynomial distinguishes most knots, but not all. It can't discriminate between mirror images, like right- and left-handed trefoils. And there are two knots with 11 crossings that have the same Alexander polynomial as the unknot, or circle (see illustration).

Vaughn Jones at the University of California, Berkeley, has added an extra piece of information to the invariant—the "direction" of two crossing strands. To determine this, begin at an arbitrary point on the knot and paint small arrows all the way around. Using simple rules, knot crossings are labeled as positive or negative, depending on how the arrows point at each crossing. This directionality lets the Jones polynomial tell mirror images apart. For the right-handed trefoil, it's equal to $t^1 + t^3 - t^4$; the left-handed trefoil is $t^{-1} + t^{-3} - t^{-4}$. While more powerful, the Jones polynomial also takes far longer to compute. A fast computer might take an hour to spit out the Jones polynomial for a knot with two dozen crossings. Since 1984, a host of new, faster-to-compute polynomials has appeared.

Polynomials aren't knot theorists' only concern. Last year, three groups of mathematicians determined how to calculate the so-called Gordian number. Named after the mythical knot that Alexander the Great untied with a single slash of his sword, the Gordian number represents the least number of steps required to turn a knot into a circle. These steps involve momentarily cutting one strand, allowing another to move through the opening, and then resealing. "The concept is very intuitive, but it's also a bear to compute," says one of the discoverers, mathematician William Menasco of the University of Buffalo in New York. His new approach uses an interesting number called the braid index. Every knot, no matter how complex, can be rearranged into several braided loops that resemble a coiled lanat. The number of coils equals the braid index.—*P. J. S.*

The ties that bind

[Continued from page 119]

to develop a long-sought theory of gravity that works on both the galactic and subatomic scales. Einstein's theory of general relativity explains gravity in the visible world—the attraction between a boulder and Earth, or how stars influence the movement of planets. But his equations don't work at the tiny, unseen distances between atoms and the basic building blocks of matter. Here, the mathematics of quantum mechanics must be used to explain particle interactions.

A team of scientists thinks that knot theory may help tie general relativity and quantum mechanics into a unified theory of quantum gravity. Their work also gives new meaning to the term "fabric of space." In 1988, physicists Carlo Rovelli and Lee Smolin noticed that a new translation of Einstein's equations by physicist Abhay Ashtekar bore an uncanny resemblance to equations from knot theory. Rovelli suggested melding Ashtekar's equations with different knot polynomials—equations that describe various knots. The combination clicked, especially for the class of knots called links, open circles connected to each other.

These hybrid knot equations appear to explain gravity at all distances. They also point to a physical model of space that could resemble The Weave, something Rovelli built using hundreds of key rings, each attached to several neighboring rings. "I emptied stores of key rings," he says, laughing. If Rovelli and his associates are right, space looks like three-dimensional chain mail. Each link represents a single loop of space, measuring ten to the minus 33 centimeters across. That's so small that if a loop were enlarged to the size of the period at the end of this sentence, a single atom would be ten times larger than the entire Milky Way. The extraordinarily small size of these loops ensures that space appears solid even at the atomic level, just as a woven cotton sheet looks solid to us from a distance.

The loop model even describes gravity graphically. When two bodies approach each other, they may increase the number of links in space, or the loops may link up with a greater number of neighbors, says Rovelli.

Chemistry also has its knot theorists. In 1989, French chemists synthesized the first knotted compound ever made, a 124-atom molecule shaped like a trefoil. More knotted molecules are in the works. Chemist David Walba of the University of Colorado uses a Mobius strip molecule—a circle with one or more half twists—made from carbon and oxygen as the starting point for pretzel-shaped trefoils, square knots, and more complex chemical arrangements. Why bother? Partly because of the challenge, explains Walba. "Buckyballs were first made just because of their cool geometry. Now they're appearing in all sorts of useful applications. By tackling targets that are impossible to make, we develop new synthetic pathways and elements."

Knots also share the property of chirality, or handedness, with many natural and artificial compounds. A square knot and a granny knot can't be superimposed unless you lift them off the plane. (Like your hands—the only way to match opposite thumbs and fingers is to lift them into the air and place them palm to palm.) Handedness plays a crucial role in chemical activity. Right- and left-handed thalidomide, for example, share identical chemical formulas and structures. But left-handed thalidomide

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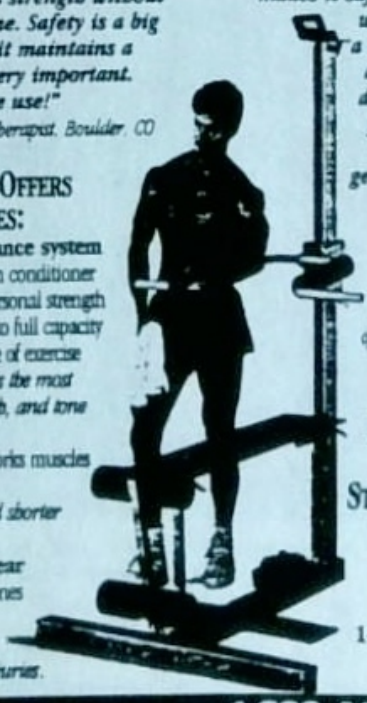
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acts as a powerful tranquilizer while its right-handed twin severely disrupts fetal development. This sinister difference wasn't discovered until long after pregnant women who took thalidomide in the 1950s bore children with severe birth defects. Elements of knot theory used to distinguish mirror-image knots may someday help chemists do the same with newly synthesized molecules, says mathematician Kenneth Millett at the University of California, Santa Barbara.

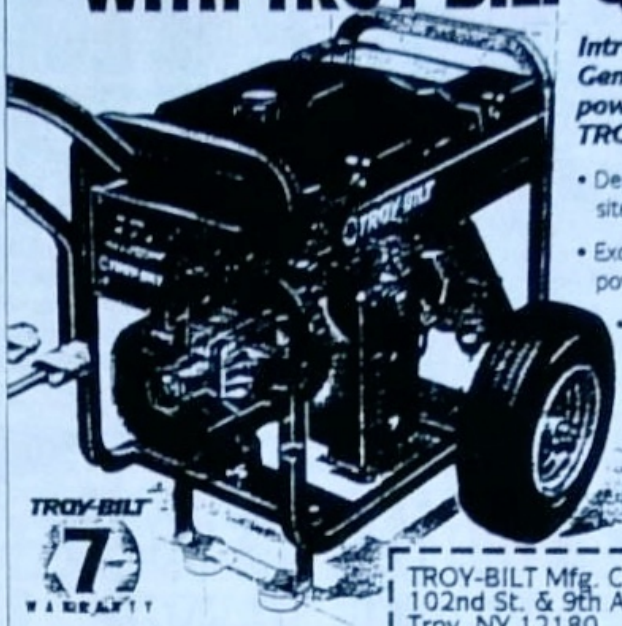
Even computer science is benefiting from a dash of knot theory. Until recently, programmers found it nearly impossible to predict how fast, or even *if*, a computer could solve a particularly complex problem. U.C., Berkeley, mathematician and Fields Medal-winner Steve Smale borrowed a page from braid theory, one of knot theory's close cousins, to devise a solution. Essentially, he found that the more "if-then" statements a program requires, the more tangled its braids, and the longer the computations must run.

Computer-network reliability may be the next target, says Lorenzo Traldi, a mathematician at Lafayette College in Easton, Pa. Like knots, networks contain segments that are directly linked together and others that aren't. Knot theory should be able to analyze the relationships between linked and unlinked segments and help determine which are most prone to failure.

Even as it is applied to an ever-expanding number of problems, knot theory is evolving at a fairly rapid clip. This is partly due to the field's reinvigoration by Vaughn Jones and those he has inspired. It is also due to mathematical tools imported from the very fields where knot theory is now being applied. The new polynomials and elegant solutions for knot, braid, and tangle problems that are emerging may eventually be put to work in as-yet-undreamed applications.

That's not to imply that knot theorists always work with one eye on practical problems. In fact, perhaps the bulk of current knot-theory research is being performed without any application in mind. John Sullivan and his associates at the University of Minnesota's Geometry Center, for example, want to know what happens when you distribute a negative charge evenly around a computer-drawn knot. "I can't imagine what practical use this might have," he says. "But mathematicians have great faith that if you find something that exhibits really interesting patterns, it will eventually have some application." SS

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