Why Is The Helix Such A Popular Shape? Perhaps Because They Are Nature's Space Savers

Science Daily (Mar. 2, 2005) — PHILADELPHIA – Something about nature loves a helix, the ubiquitous spiral shape taken on by DNA and many other molecules found in the cells of living creatures. The shape is so useful that, while researching the means of creating self-assembling artificial helices, physicists at the University of Pennsylvania believe that they have come across a plausible mathematical reason for why the helical shape is so common. Their findings appear in the Feb. 18 issue of the journal Science.

The classic answer is that helices are helical because the shape is dictated by bonds between molecules. But that only answers how a helix is formed and not why they are that shape," said Randall Kamien, a professor in Penn's Department of Astronomy and Physics. "It turns out that a helix, essentially, is a great way to bunch up a very long molecule, such as DNA, in a crowded place, such as a cell."

In the dense environment of the cell, long molecular chains frequently adopt ordered helical conformations. Not only does this enable information to be tightly packed, as in DNA, but it also forms a surface that allows molecules, such as the machines that enable DNA transcription and repair, to grapple on to it at regular intervals.

To picture how space matters to the formation of helices, Kamien and graduate student Yehuda Snir envisioned the system as a flexible, unbreakable tube immersed in a mixture of hard spheres, analogous to a molecule in a very crowded cell. As they saw it, the space occupied by the tube is space that could be otherwise occupied by the spheres. They find that the best shape for the short flexible tube – the conformation that takes the least amount of energy and takes up the least space – is that of a helix with a geometry close to that found in natural helices.

"It would seem that the success of the helix as a shape in biological molecules is a case of nature working the best it can with the constraints at hand," Kamien said. "The spiral shape of DNA is dictated by the space available in a cell much like the way the shape of a spiral staircase is dictated by the size of an apartment."

Adapted from materials provided by University Of Pennsylvania.

Why do proteins coil up into spirals? A new answer to this question, which could aid the effort to identify the genetically determined shapes and functions of human proteins, was published in the 20 July 2000 issue of the journal <u>Nature</u>. "We have discovered a simple explanation, based solely on principles of geometry, for the protein's preference for the

helix as a major component of its overall structure," said **Jayanth Banavar**, professor of <u>physics</u> at Penn State and a member of the team of U.S. and Italian research physicists that made the discovery. The finding is expected to be useful in such wide-ranging research areas as structural genomics, pharmaceuticals, protein engineering, and materials science.

"We applied mathematical ideas about optimal shapes of strings with maximum thickness to proteins, which are string-like in that they have an amino-acid backbone that curls and bends itself into a number of characteristic shapes, including the helix," Banavar said.

Proteins are the product of genes and also the structural stuff of cells and tissues. Like any tool, each protein's shape plays a large role in determining its function. Banavar and his colleagues asked in mathematical language what shape would lead to certain known properties of proteins. This approach is different from the intensive ongoing effort in biochemical research to understand what shape a protein is most likely to take based on each chemical bond that can form within its backbone's distinctive sequence of amino acids. "Many different amino-acid sequences fold into the same or similar structures, which suggests that the structure may be of more fundamental importance than the amino-acid sequences," Banavar said. "Our work yields a simple and logical way of looking at protein shapes independent of complex biochemical interactions."

"A fascinating question to think about is why proteins take on certain basic shapes in their folded states," said **Amos Maritan**, professor of physics at the <u>International School</u> for Advanced Studies in Italy (SISSA) and a member of the research team.

As a simple example of this approach, the researchers asked a series of mathematical questions about the optimal working shape of proteins, including the maximum space around each amino acid in the proteins' folded form, or "native state," and their ability to form that compact shape rapidly. For each calculation, the answer turned out to be a spiraling helix.

A protein's backbone needs to be compact in order to squeeze out water molecules from its central region. The backbone also needs to have enough room for its atomic components to fit along its winding path with a little extra space for movement. When the researchers calculated the shape that would result in just the right compromise between absolute compactness and maximum wiggle room, the result was a helix.

"The main result of this calculation is that the natural consequence of these two constraints alone is a helix with an equal amount of room both along the pitch axis of the helix and in the plane perpendicular to it--a pitch-to-diameter ratio very close to the helices we find in natural proteins," said **Cristian Micheletti**, a postdoctoral researcher at SISSA and a member of the research team.

"Half a century ago **Linus Pauling** showed with an extremely beautiful theoretical calculation that to get a repeating pattern along the protein's backbone with strong covalent bonds along the sequence and as many weaker hydrogen bonds as possible, that pattern would have to be a helix with a certain pitch-to-radius ratio determined by the chemistry of the bonds," said **Antonio Trovato**, a graduate student at SISSA and a member of the team. Experiments have confirmed this particular helix occurs naturally in proteins.

"Now we have shown it is possible to strip away all the chemistry and still get the same result by asking the even more elementary question of what is the shape of a string that allows the maximum breathing room for the protein's amino acids while still being compact," Banavar explained.

The researchers also investigated the protein's ability to compact itself rapidly and reproducibly into its working native-state shape after initially being formed or being temporarily loosened by various forces. "Our calculations indicate that the dynamics required for the rapid folding of a denatured protein--or other biologically viable polymer--into its native-state structure also favor the formation of helical motifs," said Maritan. "This is a simple consequence of the local contacts present in a helix and has been observed experimentally as well." Banavar added, "A simple analogy is the packing of clothes into a suitcase, which entails the bending and curling of the clothes into lower-dimensional units. The helix and other component shapes in a protein are indeed such lower-dimensional units."

The researchers also showed how a protein's characteristic shape can be used to predict how it might naturally form. They asked how the chemical bonds could form rapidly to transform a protein's loose unfolded structure into its compact folded structure held together by all of the fully formed chemical bonds. "This question is of great interest from an experimental and an engineering point of view," Maritan said.

The researchers compared several natural protein structures to decoy structures they created with compactness similar to the natural proteins but with no secondary motifs like helices. They then calculated mathematically the number of ways each structure could be taken apart halfway; that is, until only about 50 percent of the bonds remained intact. They found that the naturally occurring structures had many more of these half-formed configurations than did the artificial structures without any secondary motifs. "It is faster for a large crowd to enter a stadium through lots of doorways than through just a few doorways," Cristian Micheletti explained.

"There seems to be a principle by which nature selects those structures that have as many transitional entryway structures as possible. In other words, secondary motifs like helices seem to give proteins many more options for snapping themselves together, so the folding process should be able to proceed more rapidly," said **Flavio Seno** of the <u>University of Padova</u>, Italy, and a member of the research team. He added, "Moreover, we found certain contacts that seem to appear again and again in these entryway structures, and those are precisely the ones that experimenters have found form early and are critical for the successful folding of a protein."

This direct comparison with experimental results indicates the team's approach could provide further insights into the protein-folding process.

SPIRL understand universal features of the protein-folding process using simple principles is complementary to the biochemical approach of developing a tightly focused and detailed understanding of the structure of proteins. "There may be some value to looking at the same thing in different ways," Micheletti commented.

"The development of an easier way to reliably predict what shape a protein folds into from a knowledge of the sequence of its amino acids would lead to a renaissance in the field of human genomics and our work may help to advance this effort," Banavar said. "We also would like to understand what the fundamental shapes are in nature and whether there is some really simple principle behind nature's selection of these shapes."

SPIRAL

a plane curve traced by a point circling about the center but at increasing distances from the center

in mathematics, a spiral is a curve which emanates from a central point, getting progressively farther away as it revolves around the point.

A spiral is a curve in the plane or in the space, which runs around a centre.

If you draw a circle with x=cos(t) and y=sin(t) and pull it evenly in z-direction, you get a spatial spiral called cylindrical spiral or helix.

Ammonites, antlers of wild sheep, Archimedes' water spiral, area of high or low pressure, arrangement of the sunflower cores, @, bimetal thermometer, bishop staff, Brittany sign, circles of a seaeagle, climbs, clockwise rotating lactic acid, clouds of smoke, coil, coil spring, corkscrew, creepers (plants), curl, depression in meteorology, disc of Festós, double filament of the bulb, double helix of the DNA, double spiral, electron rays in the magnetic longitudinal field, electrons in cyclotron, Exner spiral, finger mark, fir cone, glider ascending, groove of a record, head of the music instrument violin, heating wire inside a hotplate, heat spiral, herb spiral, inflation spiral, intestine of a tadpole, knowledge spiral, licorice snail, life spiral, Lorenz attractor, minaret at Samarra (Iraq), music instrument horn, pendulum body of the Galilei pendulum, relief strip of the Trajan's column at Rome or the Bernward column at Hildesheim, poppy snail, road of a cone mountain, role (wire, thread, cable, hose, tape measure, paper, bandage), screw threads, simple pendulum with friction, snake in resting position, snake of Aesculapius, snail of the interior ear, scrolls, screw alga, snail-shell, spider net, spiral exercise book, spiral nebula, spiral staircase (e.g. the two spiral stairs in the glass dome of the Reichstag in Berlin), Spirallala ;-), Spirelli noodles, Spirills (e.g. Cholera bacillus), springs of a mattress, suction trunk (lower jaw) of the cabbage white butterfly, tail of the sea-horse, taps of conifers, tongue and tail of the chamaeleon, traces on CD or DVD, treble clef, tusks of giants, viruses, volute, watch spring and balance spring of mechanical clocks, whirlpool, whirlwind.

The Double Helix

Quick, what do you get when you double a helix? The answer, as everyone knows, is a Nobel Prize. Exactly fifty years ago this month, on April 25, 1953, the molecular biologists James D. Watson and Francis H. C. Crick published their pivotal paper in *Nature* in which they described the geometric shape of DNA, the molecule of life. The molecule was, they said, in the form of a double helix - two helices that spiral around each other, connected by molecular bonds, to resemble nothing more than a rope ladder that has been repeatedly twisted along its length. Their Nobel Prizewinning discovery opened the door to a new understanding of life in general and genetics in particular, setting humanity on a path that in many quite literal ways would change life forever.

Watson and Crick with their model of DNA (1953), alongside a modern illustration of the now famous molecule

"This structure has novel features which are of considerable biological interest," they wrote. Well, duh. You're telling me it does. But does the structure have any mathematical interest? More generally, never mind the double helix, does the single helix offer the mathematician much of interest?

Given the neat way the two intertwined helices in DNA function in terms of genetic reproduction, you might think that the helix had important mathematical properties. But as far as I am aware, there's relatively little to catch the mathematician's attention.

The equation of the helix is quite unremarkable. In terms of a single parameter t, the equation is

 $x = a \cos t$, $y = a \sin t$, z = b t

This is simply a circular locus in the xy-plane subjected to constant growth in the z-direction.

A deeper characterization of a helix is that it is the unique curve in 3-space for which the ratio of curvature to torsion is a constant, a result known as Lancret's Theorem.

Helices are common in the world around us. Various sea creatures have helical shells, like the ones shown here

Helical shaped shells

and climbing vines wind around supports to trace out a helix.

In the technological world of our own making, spiral staircases, corkscrews, drills, bedsprings, and telephone handset chords are helix-shaped.

A spiral staircase: where the helix leads to a higher things

The popular Slinky toy, pictured below, shows that the helix is capable of providing amusement for even the most non mathematical among us.

The popular Slinky toy

And what kind of a world would it be without the binding capacity the helix provides in the form of various kinds of screws and bolts.

Making a bolt for it: the helix in everyday use

One of the most ingenious uses of a helix was due to the ancient Greek mathematician Archimedes, who was born in Syracuse around 287 BC. Among his many inventions was an elegant device for pumping water uphill for irrigation purposes. Known nowadays as the Archimedes screw, it comprised a long, helix-shaped wooden screw encased in a wooden cylinder, like this:

The Archimedes screw

By turning the screw, the water is forced up the tube. The same device was also used to pump water out of the bilges of ships.

But when you look at each of these useful applications, you see that there is no deep mathematics involved. The reason the helix is so useful is that it is the shape you get when you trace out a circle at the same time as you move at a constant rate in the direction perpendicular to the plane of the circle. In other words, the usefulness of the helix comes down to that of the circle.

So where does that leave mathematicians as biologists celebrate the fiftieth anniversary of the discovery that the helix was fundamental to life? Well, if what you are looking for is a mathematical explanation of why nature chose a double helix for DNA, the answer is: on the sidelines. On this occasion, the mathematics of the structure simply does not appear to be significant.

On the other hand, that does not mean that Crick and Watson did not need mathematics to make their discovery. Quite the contrary. Crick's own work on the x-ray defraction pattern of a helix was a significant step in solving the structure of DNA, which involved significant applications of mathematics (Fourier transforms, Bessel functions, etc.). Based on these theoretical calculations, Watson quickly recognized the helical nature of DNA when he saw one of Rosalind Franklin's x-ray diffraction patterns. In particular, Watson and Crick looked for parameters that came from the discrete nature of the DNA helices.

Now, in the scientific advances that followed Crick and Watson's breakthrough, in particular the cracking of the DNA code, mathematics was much more to the fore. But that is another story. In the meantime, I hope I speak for all mathematicians when I wish the double-helix a very happy fiftieth birthday.

A spiral is a curve that winds itself round a certain point. 1 While not being a circle, the radius will vary along the angle.

In mathematics, a **spiral** is a curve which emanates from a central point, getting progressively farther away as it revolves around the point.

VORTEX

A **vortex** (pl. *vortices*) is a spinning, often turbulent, flow of fluid. Any spiral motion with closed streamlines is vortex flow. The motion of the fluid swirling rapidly around a center is called a vortex. The speed and rate of rotation of the fluid are greatest at the center, and decrease progressively with distance from the center

A vortex can be seen in the spiraling motion of air or liquid around a center of rotation. Circular current of water of conflicting tides form vortex shapes. Turbulent flow makes many vortices. A good example of a vortex is the atmospheric phenomenon of a whirlwind or a tornado or dust devil. This whirling air mass mostly takes the form of a helix, column, or spiral. Tornadoes develop from severe thunderstorms, usually spawned from squall lines and supercell thunderstorms, though they sometimes happen as a result of a hurricane.

In atmospheric physics, a *mesovortex* is on the scale of a few miles (smaller than a hurricane but larger than a tornado). ^[2] On a much smaller scale, a vortex is usually formed as water goes down a drain, as in a sink or a toilet. This occurs in water as the revolving mass forms a whirlpool. This whirlpool is caused by water flowing out of a small opening in the bottom of a basin or reservoir. This swirling flow structure within a region of fluid flow opens downward from the water surface.

When fluid is drawn down a plug-hole, one can observe the phenomenon of a **free vortex**. The tangential velocity v varies inversely as the distance r from the center of rotation, so the angular momentum, rv, is constant; the vorticity is zero everywhere (except for a singularity at the center-line) and the circulation about a contour containing r=0 has the same value everywhere. The free surface (if present) dips sharply (as r^{-2}) as the center line is approached.