Abstractions

LAST AUTHOR

We have long known that a protein's amino-acid sequence dictates its three-dimensional structure, but the structures of most proteins remain unknown. In most cases, the correct structure exists when the molecule is in its lowest energy state. But finding that state is a huge challenge because of the large number of possible conformations. On page 259, David Baker, at the University of Washington in Seattle, and his colleagues describe a computational approach to refining protein structure models that provides highly accurate predictions. Baker explains how thousands of home computers made this work possible.

What part did the home computers play?

Predicting protein structures requires a vast amount of processing power. A couple of years ago, we started a distributed computing network called Rosetta@home. This takes advantage of any spare processing power available in the computers of volunteers while they are online. About 160,000 people are now signed up worldwide, although probably only about 20,000 are online at any given time. Their contribution allows us to do things that we simply couldn't do using our in-house computing resources alone. Rosetta@home is equivalent to a reasonably sized supercomputer, or about 62.7 teraflops.

What else contributed to this work?

A community-wide experiment called CASP (critical assessment of techniques for protein structure prediction) that tests how well current structure-prediction methods work. It has the flavour of a competition because everyone wants to see how well their method stacks up. I met co-author Randy Read, from the University of Cambridge, UK, at the CASP7 meeting in Pacific Grove, California. One of our predictions on a solved-but-unpublished structure was highly accurate. While at the meeting, Randy used our prediction and a program he had written named Phaser, and solved the X-ray crystal structure of the protein.

What is your paper's take-home message?

That you can combine conventional experimental methods such as X-ray crystallography with current protein-prediction methods and solve structures. And that there are cases in which a protein's three-dimensional shape can be accurately predicted using only its amino-acid sequence.

What is your favourite aspect of the project?

It's been fun explaining to people how their computer time is being used and the possible implications of the project — for example, in helping to develop HIV vaccines, anti-malarial agents and gene therapy. ■

MAKING THE PAPER

Philippe Zarka

Satellite findings show that Saturn's rotation is affected by solar wind.

It is difficult to measure the rotation rate of gas-giant planets, because we cannot see landmarks on their surfaces by which to track a full turn. In the early 1980s, Saturn's rotation period was estimated to be 10 hours, 39 minutes and 24 seconds — but with a 7-second uncertainty. This has vexed astronomers like Philippe Zarka of the Paris Observatory in Meudon, France, ever since, and the expectation was that data from new spacecrafts would resolve the issue.

What researchers needed most were long-term measurements of the radio waves emitted by Saturn —thought to relate to the planet's internal magnetic field — that are used as a proxy for the planet's interior speed. But when in 1999 a group of Zarka's colleagues used radio measurements recorded by the Ulysses spacecraft (which was launched in 1990 to orbit the Sun), they got surprisingly variable results: Saturn's radio-rotation period varied by about 1% during a period of just a few months.

"That is a huge variation," says Zarka. "On Earth, that would be 15 minutes per rotation." He thought that this variation could be explained by either internal factors altering the planet's magnetic field or internal or external factors confounding the radiowave source in the magnetic field.

Drawing on his experience and intuition, Zarka wondered whether the solar wind — the weak stream of charged particles from the Sun that interacts with planetary magnetic fields — might account for the variable rotation measures. He knew that Saturn's radio emissions vary with the solar wind and that the solar wind speed at Saturn has a 'sawtooth' pattern of sudden increases followed by slow decreases.

In 2005, Zarka and his graduate student Baptiste Cecconi published a theoretical paper predicting that radio waves could mimic the 'sawtooth' pattern. But the variation remained, which seemed counter-intuitive to a community expecting the variability to average out over many rotation cycles. "Many people did not believe it," says Zarka, agreeing that it's strange to think that external phenomena, such as the solar wind blowing, could affect a planet's rotational clock. The group would need data to support their theory.

"Astronomers have to be opportunists," says Zarka — they need to know when to quit digging into existing data and when to capitalize on new missions. "The difficulty is seizing the right time to plug into an older problem."

The Cassini spacecraft, which reached Saturn in 2004, provided an opportunity. Zarka and his colleagues adopted Cassini team member David Southwood's technique of superimposing measurements in order to compare them, and used this method to look at Saturn's magnetic field. Measurements are available only for two or three rotations a month, when Cassini is closest to Saturn, but by 2007 the researchers had three years' worth of Cassini data.

They found a prominent oscillation that occurred over 25-day periods. The 25-day timing has particular significance — it's the rotation period of the Sun as seen from Saturn, or the time it takes the solar wind to make a full turn in the Solar system (see page 265).

Zarka and his co-authors feel confident that the solar wind causes variations in Saturn's radio clock. Next, they plan to use Cassini's imaging abilities: "If we can simultaneously measure the motion of the radio source and the period of rotation of Saturn, we can subtract the two to deduce the real rotation period," says Zarka. If they succeed, this will validate their 2005 explanation of the phenomenon. ■

FROM THE BLOGOSPHERE

Who was the first scientist? The Science Writers' forum on Nature Network extends the topic, which was previously debated at the Royal Institution (http://tinyurl.com/2ba6ft). At the debate, reports forum moderator Brian Clegg, "Lewis Wolpert championed Archimedes, I stood up for Roger Bacon, and Frank James spoke for James Clerk Maxwell. Archimedes won, with Bacon a close second." According to Clegg, the reasoning was that "Archimedes was the first to use maths in science, Bacon the first to emphasize the importance of experimental verification, maths and the communication of results, and Maxwell because the word 'scientist' wasn't invented until his time." Although the question is arbitrary, Clegg invites nominations, with a reason, for the person you think of as the first scientist.

So far, these include Galileo, Eve, 'Uncle Quentin' — a character from a children's book series — and the unnamed man, woman or ape who first worked out how to make fire. Post your suggestions at the Network forum and receive a copy of Nurture, our authors' magazine. ■

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