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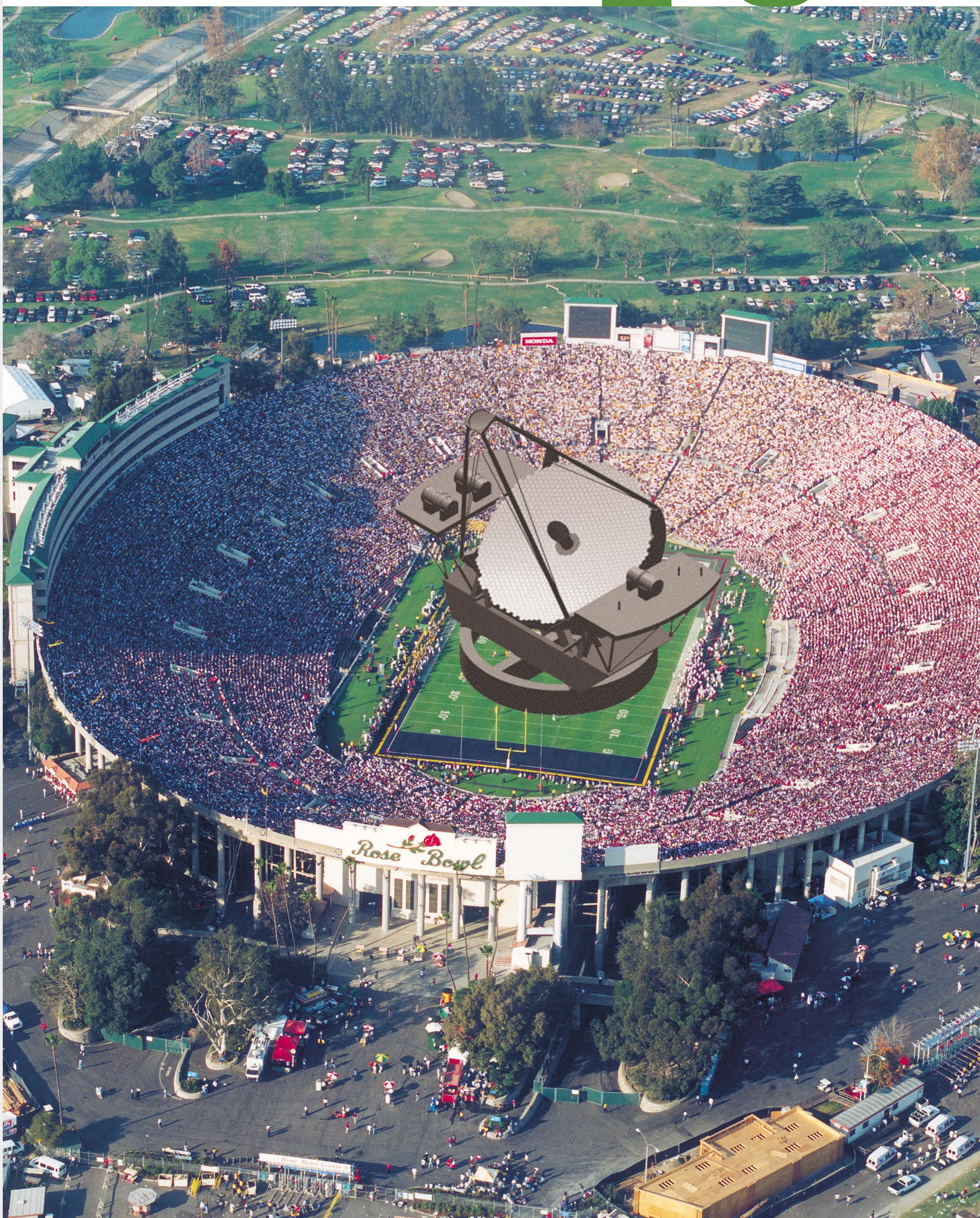

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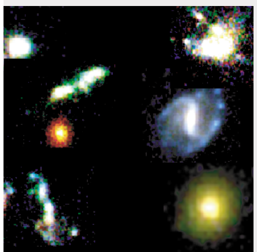

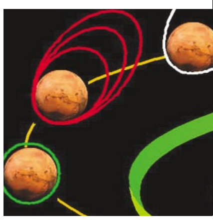

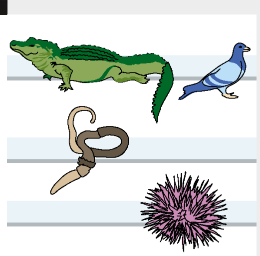

On the cover: The proposed California Extremely Large Telescope (CELT), if placed inside Pasadena's world-famous Rose Bowl, would fit quite neatly astride the 50-yard line. Actually, the telescope, with its 30-meter mirror, will more likely sit on a remote mountaintop in Hawaii or Chile, rather than in a stadium, cheered on to greater discoveries by 93,000 fans. How such a huge telescope could look back in time and show how galaxies evolved into the universe we see today is explained in an article beginning on page 12.

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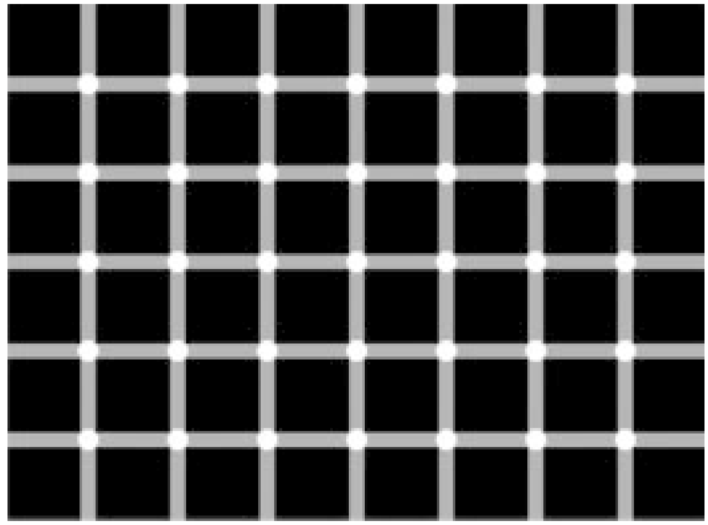
Hot and Cold Running Neutrons

It's really too bad that Superman has X-ray vision. Not that there's anything wrong with that, but if he'd had neutron vision, he'd be able to see a lot more. Neutrons, like X rays, can behave as waves. When you fire a beam of neutrons (or X rays) into a chunk of matter, some of them ripple off the atoms in the sample, and the angles at which the waves are strongest tell you how those atoms are arranged. But X rays interact with electrons, so that the more electrons an atom has, the easier it is to see. Because neutrons interact with atomic nuclei, all kinds of atoms are visible, even hydrogen. Neutrons can even find out what the atoms are doing. If the wave sets up a vibration in the sample, the neutron's frequency will drop by the amount of energy lost and the neutron will slow down. Or the wave can cancel out an existing vibration, punting the neutron to a higher frequency and speeding it up. (These collisions are called "inelastic," as opposed to "elastic" ones in which no energy is exchanged. And they don't have to be single-atom collisions—some of the vibrations are ensemble affairs.) So you need a device that not only tells you where the neutron went but how long it took to get there. Such machines have been around for about 50 years, says Professor of Materials Science Brent Fultz, but the catch is that you need a lot of neutrons—a "bright source," in the lingo—to make them work well. Otherwise it's like trying to read the fine print in a phone book by flashlight. The Spallation Neutron Source (SNS), now under construction at the Department of Energy's Oak Ridge National Laboratory in Tennessee, will be the brightest neutron source in the world by a factor of 10, and Fultz is principal investigator of a team building an instrument to take full advantage of it.

This instrument, called

Right: The SNS's physical plant, drawn in on an aerial photo of the construction site. The hydrogen ions are made in the front-end building, and shoot down the linear accelerator, or linac, en route to the accumulator ring and eventually the mercury target.



How many black dots do you see in the white circles? In fact, there aren't any. In this optical illusion, the black dots appear and vanish in a manner correlated with their fellows in both space and time. The phenomenon spans about four unit cells (a unit cell is a crystal's basic repeating structure) and has a frequency of roughly four cycles per second. ARCS will measure correlated vibrations and spins on similar scales in real crystals.

ARCS (short for **A** high-**R**esolution direct geometry **C**hopper **S**pectrometer, whose complete, vowel-impaired acronym would have been utterly unpronounceable) is one of five instruments slated to be on line when the SNS opens for business in 2006. The Department of Energy will spend $15 million on ARCS—a modest sum compared to the entire project's $1.4 billion price tag. As an instrument at a national facility, ARCS will be open for use by all comers, but Fultz and therefore Caltech in general will get a guaranteed time allotment. Eventually, the SNS will host 18 instruments to be built over a 10-year period, and will make the United States the world leader in neutron science—a distinction we'd lost to Europe over the past couple of decades.

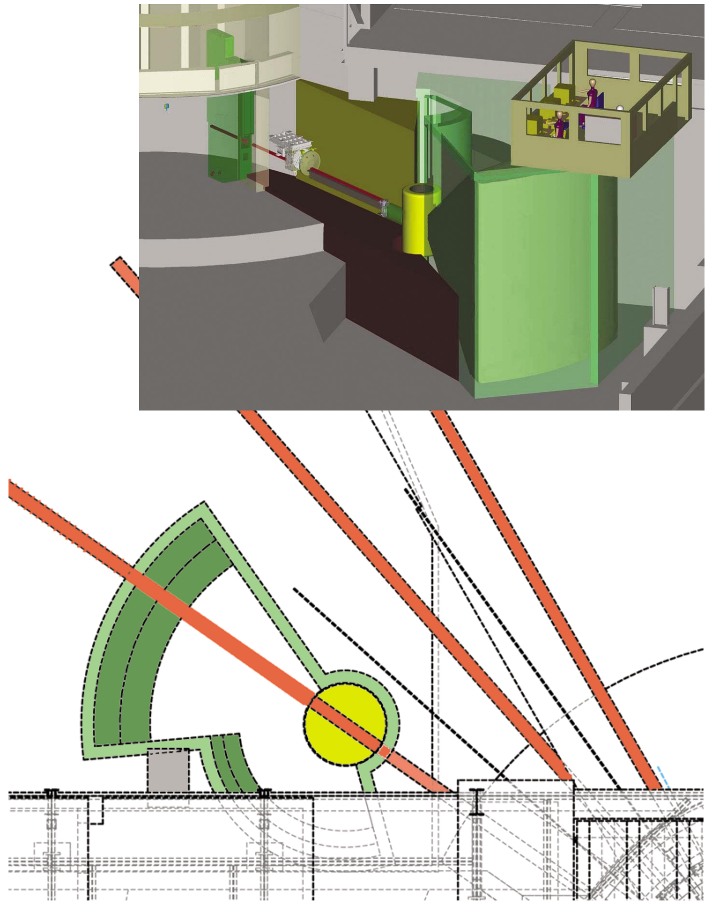
The SNS will be a busy place indeed. Neutrons have no electric charge so they don't ionize the samples they penetrate, and because they can "see" hydrogen atoms, you can use them to study the structures of proteins, DNA, and whatnot. And each neutron is a tiny magnet, so it interacts with magnetizable materials. Thus everybody from basic biologists to drug designers to the folks who develop ever-smaller hard drives for your computer will be standing in line, not to mention the chemists looking to create better catalysts or develop new materials with made-to-order properties. And since the neutron's speed determines the frequency of its associated wave, you can tune the neutron beam to the energy range of your choice.

ARCS looks for inelastic collisions ranging in energy from a few millielectron volts (meV) to 500 meV, which are quite gentle and require very slow neutrons. They're called thermal neutrons in the trade, as room temperature is equivalent to about 25 meV. This range is particularly intriguing as it includes phonons, or quanta of vibrational energy that have been linked to high-temperature superconductivity; magnons, which are magnetic spin waves that move through a material like wind through a wheat field and may lead to a theory of quantum magnetism; and a host of other vibrational modes.

These vibrations contribute a degree of randomness, or entropy, to a material, and that's what Fultz is interested in. The atoms in a crystal sit in preferred positions, like the marbles in their wells in a game of Chinese checkers. As the vibrational energy increases, the atoms stray farther and farther out of position. This disorder creates vibrational entropy. But entropy has many faces. As the "game" heats up, the red and blue balls intermingle and gaps open up between them, increasing the configurational entropy. At some point, the atoms have become so thoroughly rearranged that the crystal takes on a brand-new form—a so-called phase transition. Even the "board" itself can change—perhaps morphing from a triangular grid into a square one, as in Western checkers. But a few years ago, Fultz discovered that vibrational entropy alone could cause phase transitions, even if the crystal also had a lot of conformational entropy. "I'm pretty proud of that," says Fultz. "It's not every day that you find a new type of entropy that's important in thermodynamics." So Fultz and his grad students are using neutron scattering to find precisely where the entropy in various phase transitions comes from.

The SNS is Big Science. The system starts out with hydrogen atoms that have been given an extra electron each so that they have a negative charge. These get fired down a 300-meter-long particle accelerator that revs them up to energies of 1 billion electron-volts, the equivalent of 1 megawatt of electricity and six times Caltech's entire power consumption. At the far end of a quarter-mile of plumbing—the same length as a drag strip!—they shoot through a micron-thick carbon foil that strips off their electrons, leaving naked protons that are dumped into a storage ring the diameter of a Wal-Mart parking lot. Sixty times a second, or roughly once every 1,200 orbits, a kicker magnet flings the ring's entire contents out in a pulse less than a millionth of a second long. This slug of screaming-hot protons slams into 5.6 liters (76 kilograms) of mercury, banging some of its neutrons loose in a process called spallation. (In the outside world, "spallation" means to knock flakes or slabs off a larger body, such as when you chip concrete with a hammer.) Mercury was chosen because it has a bucketful of neutrons—120 per nucleus, on average—and because, being a liquid, it can be pumped through the hot zone. It takes 1,500 liters of mercury cycling continuously through a cooling system to handle the punishment. So

ARCS has been assigned beam line 18, the leftmost of the three shown in red in the plan view. The neutron detector fills a three-story, high-vacuum chamber (light green); for comparison, note the size of the control room in the 3-D view. The detector (olive), built in two sections to accommodate a concrete pillar (gray), wraps 60° vertically and 160° horizontally around the sample chamber (yellow).



you get a boatload of neutrons, which is good, but they're almost as hot as the protons, which is bad. In order to cool them a million- or billionfold, to the point where they're actually usable, they pass through a "moderator," which is a bath full of either water or liquid hydrogen, depending on how cold you want them, en route to the experimental stations.

The neutrons come flying out in all directions, so the 18 experimental stations are arranged around the mercury target like the spokes of a wagon wheel. Each experiment therefore has a pie-slice-shaped piece of real estate in which to set up shop, which leads to some design challenges, says Fultz. You can either build a small detector close to the source, or a big one farther away. The ARCS team opted for the close-in approach for maximum neutron intensity. Once the neutrons hit the sample, they again scatter to all points of the compass; thus the detector has to surround the sample as completely as possible. Wedging a big detector into the pointy end of the space is further complicated by an unhandily placed concrete pillar that supports an overhead crane and, incidentally, the roof. The details of the design are still being worked out, Fultz says, as some things depend on what the neighbors on the adjoining beam line decide to do—the exact boundaries between the instrument spaces are negotiable—and on what other chopper spectrometers wind up being built. "If they build another one that's optimized for magnetic studies, we'll optimize for vibrational studies, for example, and this governs where we put our detectors."

Even after passing through the moderator, the neutrons still have an assortment of speeds, which is where the Fermi chopper comes in. The chopper is a rapidly spinning cylinder pierced by a slit through which the incoming neutrons pass. The rate at which the cylinder rotates governs the speed of the neutrons that make it through, and the moment when the slit is in alignment (i.e., open) sets the reference time that allows you to measure whether the inelastic collision has sped the neutron up or slowed it down. The chopper, the helium-3-filled detector tubes (which can tell where the neutron has hit to within a few square centimeters), and the rest of the hardware are not too far beyond off-the-shelf technology.

Argonne National Laboratory's Doug Abernathy, the instrument scientist and project manager, is responsible for putting it all together and will be on-site to supervise construction.

Meanwhile, Fultz will be overseeing the design of the software that runs the hardware, collects the time-of-flight and position data from the detectors, and calculates each neutron's momentum in order to measure the sample's vibrational and magnetic energies. In typical Caltech fashion, this means assembling a multidisciplinary team—for example, Oscar Bruno, professor of applied and computational mathematics, has been working on more efficient methods for tracing scattered neutrons through the sample. "Software development has historically been neglected in the neutron-spectroscopy community, which means that people haven't been able to extract all the science that's available in the data," says Fultz. "Each run gives about half a gigabyte of data—not big by high-energy physics standards, but still modestly large. And this is where Caltech can really make a contribution, by developing not only a software package for this instrument but also standards and procedures the entire community can use." Caltech's Center for Advanced Computing Research (CACR) has considerable expertise in this area, so Fultz is collaborating with software integrator Michael Aivazis, a member of the professional staff at CACR.

Compatibility issues run rampant, says Aivazis. The package will contain many disparate pieces of code contributed "typically by scientists whose main focus

PICTURE CREDITS: 4 – SNS; 6 – Doug Abernathy

is to solve a particular problem. They generally produce code that contains the right science done very well but that is very hard to extract from its context." Aivazis has created a software framework, or environment, in which the assorted bits of code can coexist. Called Pyre for PYthon Research Environment (Python being the language it was written in), it "grabs pieces of code written in Fortran, C, C++, and what have you, and produces a veneer, if you will, that gives you access to how they do physics without your having to be a software engineer. You don't need the specialized knowledge that went into producing the code in order to use it successfully in your application." Pyre also reduces the risk that innocent changes in one person's code may produce astonishing results in the other's. Aivazis will be in charge of setting standards for how data is handled and exchanged between the codes, and making sure that all the pieces play well with one another.

But in the long run, says Fultz, Caltech's biggest contribution may be in opening new avenues of research. "In the past, these instruments have been treated as a piece of hardware—you come in with your sample and you get a result. We're trying to make a deeper connection with theory in order to design better experiments. There's a lot of science involved in figuring out how to write the software, so we'll be doing extensive prototyping work on other machines before ARCS is running. ARCS won't miss many neutrons, and we want to be sure we take full advantage of our capabilities. That's what I find most rewarding—the voyage of discovery to learn what the machine can do." □—*DS*