Los Alamos Science and Technology Magazine | July 2016

1663

Neutron life expectancy

Tundra in turmoil

Quantum computer at Los Alamos

Fusion on the cheap

GOING WHERE THE GAS IS GREENER

Los Alamos
NATIONAL LABORATORY
EST. 1943

A masterpiece of Renaissance architecture and a major attraction for tourists visiting Tuscany, the dome of the Santa Maria del Fiore cathedral in Florence is showing its age. Wide cracks along the *Last Judgment* frescoes that cover its interior hint at greater damage inside its walls. But with the help of Los Alamos imaging technology and subatomic particles raining down from the sky, preservationists will soon have the guidance they need to safely pursue future restoration activity. See "Can Free Particles Save a Priceless Treasure?" on page 4.

1663

LOS ALAMOS SCIENCE AND TECHNOLOGY MAGAZINE

About the Cover:

Fossil fuels ultimately owe their energy content to photosynthesis that took place millions or more years ago. When we burn these fuels, we effectively reverse the photosynthesis that produced them: the carbon dioxide absorbed over the eons by the organisms that formed these fuels is returned to the atmosphere in the geologic blink of an eye. And while electricity can be effectively generated by renewable sources, most transportation systems—planes, trains, ships, and automobiles—depend on chemical fuels. Biofuels are a promising option because fuel crops absorb carbon dioxide as they grow. Then when they are burned, they release the carbon dioxide they previously absorbed. Los Alamos scientists are developing the chemistry to unlock the energy stored in plants cheaply and efficiently—and in a way that can scale up to cover the transportation needs of our society.

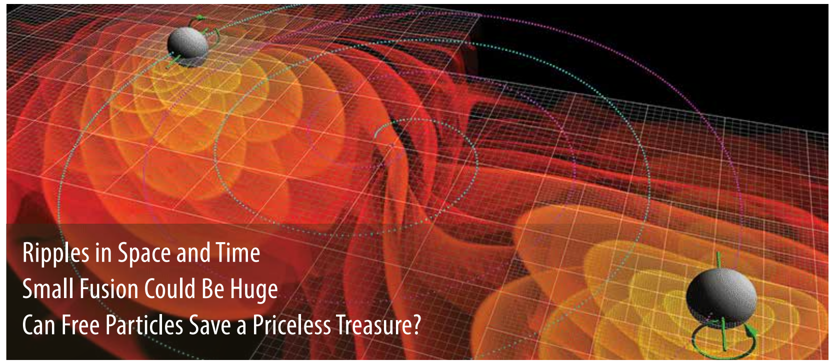
About Our Name:

During World War II, all that the outside world knew of Los Alamos and its top-secret laboratory was the mailing address—P. O. Box 1663, Santa Fe, New Mexico. That box number, still part of our address, symbolizes our historic role in the nation's service.

About the LDRD Logo:

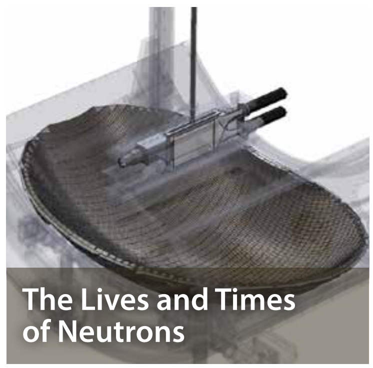
Laboratory Directed Research and Development (LDRD) is a competitive, internal program by which Los Alamos National Laboratory is authorized by Congress to invest in research and development that is both highly innovative and vital to our national interests. Whenever *1663* reports on research that received support from LDRD, this logo appears at the end of the article.

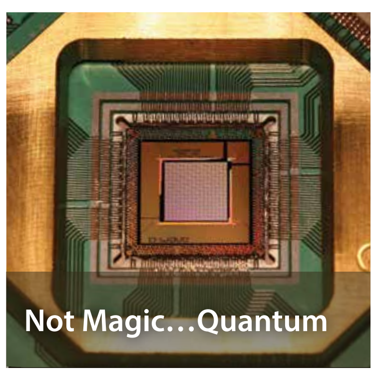
Spotlights

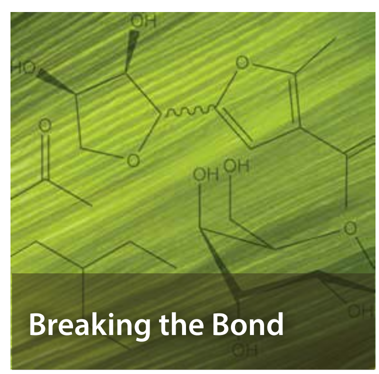


CREDIT: C. Henze/NASA

Features







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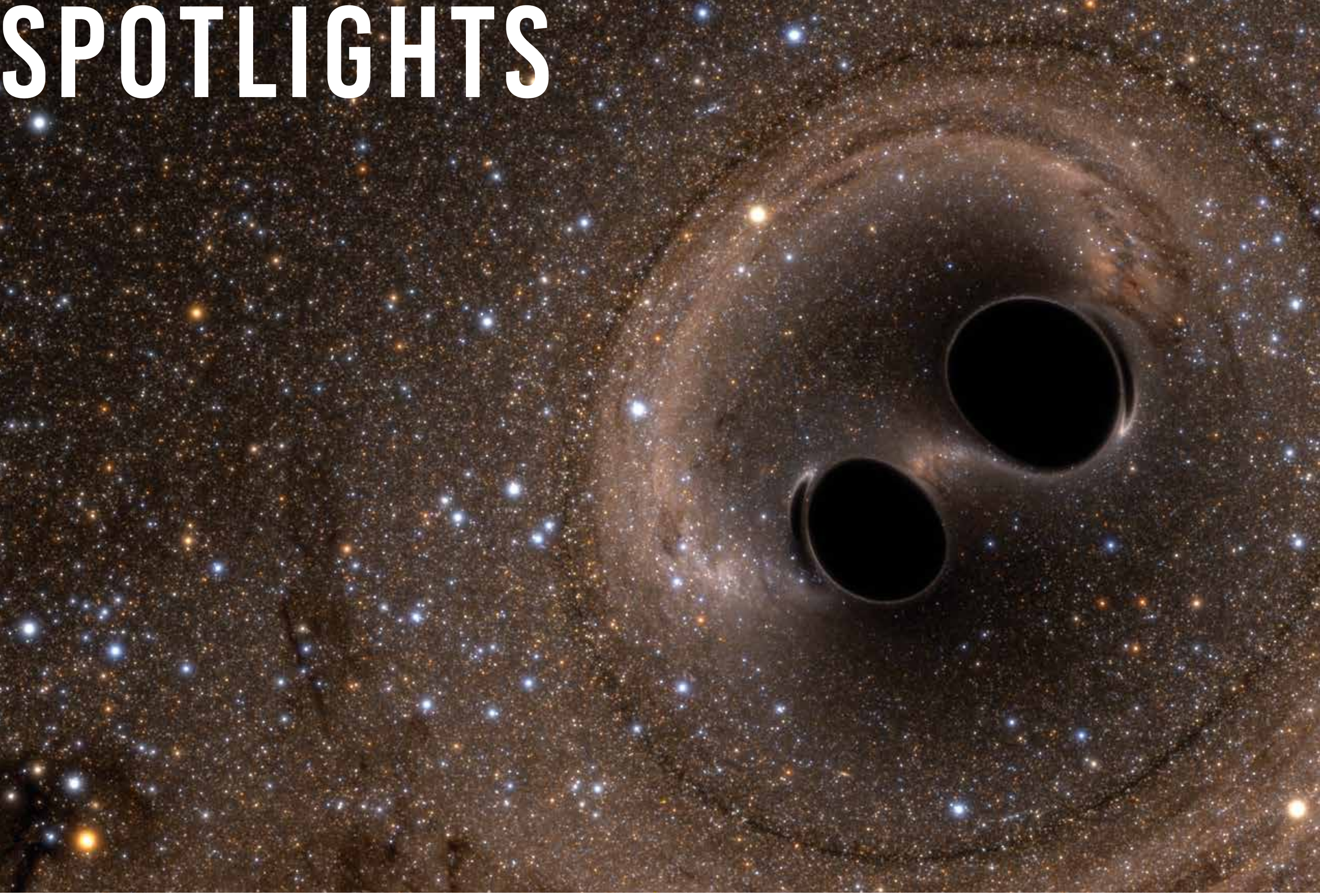


Ripples in Space and Time

WHEN THE DISCOVERY OF GRAVITATIONAL WAVES from a cosmic black-hole collision was announced earlier this year, the scientific community was absolutely abuzz. Not only was it a tremendous achievement for the Laser Interferometer Gravitational-wave Observatory (LIGO)—first approved 26 years ago and under construction or operating with no confirmed detections until now—but it was also the first-ever direct measurement of gravitational waves, whose existence Einstein predicted with his theory of spacetime exactly 100 years ago.

The discovery also confirmed a Los Alamos prediction from 2010: based on the population statistics of objects capable of producing detectable gravitational waves, the most likely event for discovery would be the merger of two black holes. Because of the extreme gravity of black holes, their collision dramatically distorts the fabric of the universe, producing ripples in spacetime that, upon reaching Earth, minutely alter the distance traveled by each four-kilometer-long laser beam in LIGO's ultrasensitive interferometers. Making such a delicate observation is groundbreaking to be sure, but Los Alamos astrophysicist Chris Fryer says it's only the beginning.

"The detection LIGO announced is actually one of three strong signals currently in their rumor mill," Fryer says. "We may soon begin to obtain detections in quantities that allow us to do new kinds of studies on the prevalence of such mergers in the galaxy." Indeed, Fryer and his collaborators recently calculated the distribution of black hole masses likely to be found in binary systems that could produce observable merger events. They based these calculations on the types of stars that form black holes when they go supernova and the force with which the black holes are propelled by their violent birth. All three potential detections to date conform to his mass predictions.

Yet much of the excitement of gravitational-wave astronomy may not center upon black holes at all. Another highly compact object with extreme gravity, also formed when massive stars go supernova, is known as a neutron star and can merge with either black holes or with other neutron stars. Such neutron-star-on-neutron-star mergers are the main focus of Fryer's research. They allow him to examine the rich physics at work in extreme environments inaccessible to Earth-bound laboratories—physics that may be responsible for the very existence of certain natural elements found on Earth.

Middleweight metals like iron, the 26th element, are made by nuclear fusion of lighter elements inside stars. But making much heavier metals like platinum or gold (numbers 78 and 79, respectively) requires higher-energy processes that combine explosive conditions with an abundance of neutrons. Astrophysicists have long reasoned that supernova explosions could be the source of those processes, but supernova simulations have difficulty reproducing robust signatures in the element-abundance data. Instead, they show that precious metals and other heavy elements are unlikely to emerge in significant quantities.

In a binary black-hole system, the black holes spiral inward and eventually merge into one, emitting gravitational waves in the process. Observations of this process were reported for the first time earlier this year.
CREDIT: Simulating eXtreme Spacetimes (SXS) project

However, according to recent computer simulations, those elements would be ejected en masse during neutron-star mergers. New research even suggests that a nearby neutron-star merger that took place shortly before the formation of our solar system may have gifted our future planet with a modest excess of these valuable elements. Then the two neutron stars combined into a single black hole that has since wandered away across the galaxy.

Fryer believes there is much to learn from neutron-star mergers and their gravitational-wave emissions in terms of the evolving population of black holes, production of heavy metals, and extreme physics. He is currently working to identify observable events that would sharpen human understanding of the unobservable structure and dynamics of neutron-star interiors. He is also preparing to use merger statistics, as they roll in, to help resolve a longstanding ambiguity concerning the cutoff mass above which stars are destined to become black holes instead of neutron stars. His recent publications lay the groundwork for these advances.

But beyond pure science, Fryer's research is a matter of national security. In addition to neutron-star collisions likely being the ultimate supplier of key national-security materials, including uranium, their explosive nuclear dynamics are applicable to nuclear-weapons research. And many of the Los Alamos scientists who work with Fryer on astrophysical problems subsequently join him and others on essential national-security computations as well. LDRD

— Craig Tyler

Small Fusion Could Be Huge

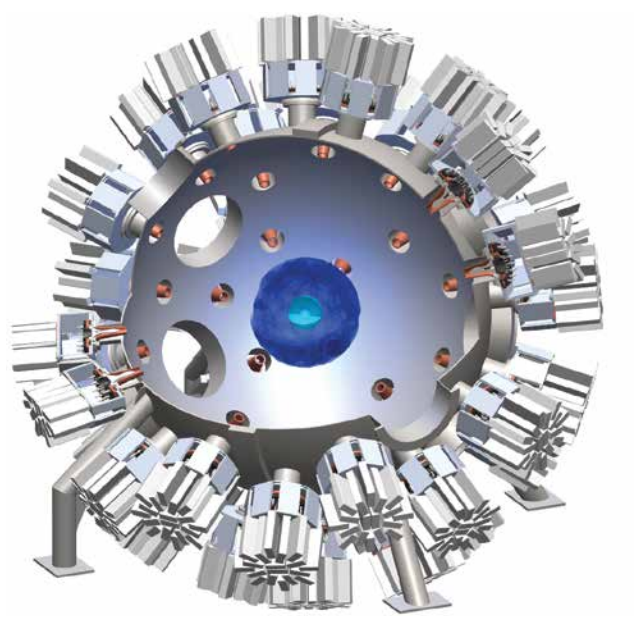
COMMERCIAL POWER FROM NUCLEAR FUSION is 30 years away. We know this because the fusion-energy research community has been saying so for 50 years.

If fusion energy ultimately works, its benefit to humankind is virtually impossible to overstate. The nuclear energy release is about four million times greater than the chemical energy released by burning coal, oil, or natural gas, and for that reason it requires very little fuel. Sixty kilograms of fusion fuel—which one strong person could physically carry into the power plant—would power a city of a million for a year. It would take 400,000 metric tons of coal to do the same. On top of that, the fusion reaction produces no carbon emissions, nor any other pollutant.

The reaction works by joining, or fusing, nuclei of hydrogen-2 (or deuterium) and hydrogen-3 (tritium) together to make helium-4 (a harmless and useful gas) plus a neutron, which then interacts with lithium in a way that "breeds" tritium for subsequent fusion reactions. The inputs, deuterium and lithium, are both present in seawater in quantities that would last millions of years at least.

The world's grandest fusion project to date is an international collaboration called ITER that comprises a massive reactor under construction in France. Once finished, it will be an experimental platform for demonstrating a sustained fusion reaction that generates more power than it consumes, similar to what goes on at the core of the sun. It was originally scheduled to come online this year at a cost of $12 billion, but its director-general recently stated that it would not be finished before 2025—and for no less than $20 billion—producing a net energy gain no earlier than 2035. The U.S. share alone is now expected to grow from $1.1 billion to closer to $5 billion. And that's just for a fusion *experiment*—the precursor to an actual power plant.

While ITER is a major step toward proving the feasibility of fusion, many scientists and energy-policy experts believe it is important to



Cutaway view of an imploding plasma liner (blue), formed by 60 inward-directed plasma jets, as it engages a magnetized plasma fuel target. (Plasma is hot, ionized gas.)
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work in parallel on other aspects of fusion power. In addition to the U.S. Department of Energy's earlier commitment to ITER, its Advanced Research Projects Agency-Energy (ARPA-E) last year announced nine research grants "to create… new, lower-cost pathways to fusion power and to enable more rapid progress in fusion research and development." The largest of these grants, awarded jointly to Los Alamos National Laboratory and HyperV Technologies Corp., comes in at about one thousandth the projected cost of the U.S. contribution to ITER.

The project leader, Los Alamos physicist Scott Hsu, explains that their work is one embodiment of an approach called magneto-inertial fusion (MIF), which combines the benefits of two large-scale fusion paradigms, magnetic confinement and inertial confinement. ITER, for instance, is a magnetic-confinement device, using ultra-powerful magnetic fields to contain the 150-million-degree plasma undergoing nuclear fusion. (Such high temperatures are necessary for fusion because only at high temperatures can positively charged atomic nuclei slam into each other with sufficient speed to overcome their mutual electrical repulsion and fuse into larger nuclei.) By contrast, the National Ignition Facility at Lawrence Livermore National Laboratory in California is an inertial-confinement device, using inward-directed lasers to implode a nuclear-fuel pellet.

In an exploratory experiment of Hsu's approach to MIF, 60 electromagnetic plasma guns, designed and built by HyperV and mounted all around a spherical vacuum chamber, simultaneously fire supersonic jets of plasma. (A full-scale reactor would employ hundreds of plasma guns.) The jets converge at the center of the chamber for the purpose of compressing another plasma of laser-magnetized nuclear fuel, injected moments earlier.

Such plasma-jet driven MIF builds upon success obtained recently at Sandia National Laboratories. There, researchers obtained conditions suitable for fusion by compressing a solid liner surrounding the hot, magnetized fuel. However, the Sandia experiment was not designed for the repetitive pulsing required for fusion energy, as each compression, or "shot," severely damages the liner and other components. Hsu's plasma-jet compression is designed to overcome this by effectively constructing a plasma liner, instead of a solid one, that's reestablished with each shot.

"We will be able to fire one shot every second, continuously restoring fusion conditions without damaging the hardware," says Hsu. In theory, that could be sufficient to achieve ignition—the all-important and maddeningly elusive state of getting significantly more power out than what is put in. Initial simulations suggest that, in principle, the fusion energy output could be quite large, possibly reaching up to 30 times the energy supplied to the plasma jets. Of course, actually achieving such a large gain, or really any gain at all, will not be so straightforward.

"Remember, the closer you come to ignition, the more unforeseen problems arise," says Hsu. "The history of fusion-energy research has shown that time and time again." With each snag encountered, studied, and overcome along the way, he plans to progressively improve simulations of the system's performance for ever-more realistic predictions. "But if we do achieve ignition, then our technology should scale well for commercial power applications. In fact, that's one of the key reasons for taking this approach."

—Craig Tyler


Cathedral of Santa Maria del Fiore in Florence, Italy

Can Free Particles Save a Priceless Treasure?

SADNESS COULD HAVE OVERWHELMED LOS ALAMOS particle physicist Elena Guardincerri last summer when she saw the ever-expanding cracks threatening the dome of the Cathedral of Santa Maria del Fiore (better known as the Duomo), a Renaissance icon in Florence, Italy. Engineered by famed master builder Filippo Brunelleschi, it was completed in 1436, and the secrets of what hidden supports or unidentified vulnerabilities might lie behind its walls have been lost to the ages. But Guardincerri was in Florence on a mission to aid restoration: to meet with the president of the Opera del Duomo, the corporation that has managed the cathedral since its construction, and present an innovative imaging solution sourced from the cosmos with which to peer inside.

Though widely renowned for his skill at solving engineering problems, Brunelleschi was considered foolish by some for abandoning flying buttresses and other conventional supports in favor of his own unorthodox ideas for constructing the dome. He deliberately left no drawings behind, and his design still poses a few riddles: Does the double-shell dome have an inner support system of iron chains inside the masonry, as alluded to in historical documents? Is the inner wall made of rubble masonry as well as bricks? Such information is essential as architects and engineers enhance their models of the dome and decide how to protect this world treasure from further damage—or outright collapse.

Instead of metal detectors, x-rays, or ultrasonic inspection, Guardincerri's team will use cosmic-ray muon trackers to create vivid images of hidden reinforcement elements inside the dome's masonry and exam-

ine the cracks deep inside the dome's 2.25-meter-thick inner wall. The award-winning technology pairs detectors with high-tech software to construct images from high-energy particles called muons created in collisions between cosmic rays from space and molecules in the earth's upper atmosphere. Most of the time, these muons rain down on us, pass through our bodies, and penetrate deep into the earth unnoticed. And from them, preservationists will get 3D-like images of the structural details they have sought for decades. The images will help them understand, for example, what keeps the 37,000-ton dome from toppling any time there's earthquake activity.

After Guardincerri presented the results of her team's feasibility study and obtained approval to build customized muon trackers for the dome, the Italian native entered the majestic Florence cathedral for the first time in her life. Architects showed her where she will eventually begin the search for iron reinforcements that other methods have failed to locate.

"This will be a great stage to show the world how well muon imaging works," she said.

Muon-imaging technology was originally invented in the 1950s. At that time, it didn't track muon scattering, but rather muon transmission and attenuation through objects. Archaeologists have exploited this method to search for hidden chambers inside the Egyptian pyramids. Los Alamos later invented the muon multiple-scattering technique, and following the September 11, 2001, terrorist attacks, its threat reduction team and commercial partner Decision Sciences Corporation developed muon-scattering tomography to expose smuggled nuclear material in ship cargo containers, vehicles, and rail cars—even when the material is shielded from conventional screening systems, such as x-rays. The Lab has found its muon-scattering tomography to be effective for arms treaty verification and nuclear reactor imaging as well, with Japan planning to use the technology to peek inside its tsunami-ravaged Fukushima Daiichi nuclear reactor.

In Florence, however, the Lab's existing muon trackers won't do because they weigh 800 pounds each, and it seems wise to presume that the dome shouldn't be subjected to that much additional weight. So the Los Alamos physicists and their collaborators are creating lightweight muon trackers that can be shipped to Italy, disassembled for transport up spiral staircases and through narrow passageways, and reassembled in different locations for measurements.

One muon tracker will be suspended inside the cathedral near Giorgio Vasari's *Last Judgment* fresco; another will be placed between the dome's two shells, in a walkway closed to the public. With the structure flanked on both sides by detectors, the team can collect multiple scattering angles from the muons striking denser objects hidden inside the overall structure; these scattering events are used to create a computer image. To obtain sufficient resolution, Guardincerri's team must measure the muons entering and exiting the structure for at least two weeks.

While making a critical contribution to stabilizing and preserving the Florence cathedral, the Los Alamos team will unveil the first application of muon tomography to infrastructure monitoring. Once miniaturized, the muon trackers could become inspection tools for imaging thick archaeological artifacts, assessing the structural stability of dams and bridges, diagnosing damage in pipes, and generally seeing through all manner of hard-to-access structures and systems of value to civilization.

— Diana Del Mauro


RIP
A FREE
NEUTRON
BORN JULY 15, 2016
DIED 10 MINUTES LATER

THE LIVES & TIMES *of* NEUTRONS

Most neutrons inside atoms are stable. But get one on its own, and it will disintegrate in about ten minutes.

There are only three subatomic particles that make up everyday objects, and one of them is unstable. The neutron, while stable enough when found inside an atom's nucleus alongside protons, disintegrates after about ten minutes on its own. But therein lies the rub—*about* ten minutes—because the neutron has been surprisingly reluctant to give up the exact number.

Radioactive decay, such as the one that enacts the death of a neutron, happens as a function of chance, making it impossible to know how long any particular neutron will live. However, scientists can characterize the half-life for a population of neutrons—how long it takes for half the neutrons to decay—and, in principle, do so with great precision. Experimental physicists have worked diligently to that end, broadly succeeding and improving the precision of neutron half-life measurements by more than a factor of ten in recent decades. But they have hit a snag. Increasingly high-tech measurements, with ever-smaller uncertainties, are converging to not one but *two* different answers.

Some experiments gather neutrons and count how many remain after an elapsed time. Other experiments count the particles left behind when neutrons decay. Both are expertly done, but their results do not jibe with one another, leaving two possibilities. Either the experiments are wrong somehow or the neutron itself is more complex than anyone thought. At Los Alamos National Laboratory, a bold new variation on the neutron-counting experiment aims to resolve this dilemma.

Ubiquitous but elusive

James Chadwick, credited for the 1932 discovery of the neutron, and Ernest Rutherford, Chadwick's mentor who was himself renowned for discovering the atomic nucleus, initially conceived of the neutron not so much as a distinct subatomic particle, but rather as a close arrangement of electron and proton: the negative particle hovering near and canceling out the positive one. This turned out to be wrong; the neutron is its own entity. But the conception of the neutron as a proton-electron blend was still valid in a sense, because when neutrons decay, two of the three particles that emerge are in fact proton and electron. (The third is the antiparticle to the uncharged and almost massless neutrino.)

This neutron-disintegration process, known as beta decay, also occurs in neutron-rich isotopes of various elements. An energetic electron and antineutrino speed out of the nucleus, and a proton remains in the former neutron's place. The resulting atom, now with one more positive charge in its nucleus, advances one position up the periodic table. That's if the atom is in some sense overloaded with neutrons to begin with. Conversely, if an atom is "satisfied" with its relative number of protons and neutrons, then its neutrons apparently never decay. For example, the isotope iron-58, with 26 protons and 32 neutrons, appears perfectly stable. But iron-59, with 26 protons and 33 neutrons, undergoes beta decay. Moreover, how long neutrons survive inside a nucleus before decaying similarly depends on the nucleus in question. Iron-59 has a half-life of more than six weeks, while iron-63, with four more neutrons, lasts only six seconds. But for a free neutron, unattached to any atom, it's always about ten minutes.

Officially, the neutron half-life is quoted at 611.0 ± 1.0 seconds. This level of precision is not atypical among particle-physics lifetimes, but it is far from the best. The lifetime of the muon, for example—a difficult-to-detect, heavier cousin to the electron that can only exist for a millionth of a second—is known to within a trillionth of a second. And most of the other lifetimes known with comparable precision to that of the neutron apply to particles that are never observed in nature and can only be made to appear for a miniscule fraction of a second in the laboratory.

BEAM AND BOTTLE EXPERIMENTS ARE STRIKINGLY INCOMPATIBLE WITH ONE ANOTHER, DIFFERING BY NEARLY SIX SECONDS.

Yet even the comparatively lumbering one-second precision for the neutron lifetime may be overstated because of the pronounced discrepancy between the two major categories of neutron-lifetime experiment. Each produces self-consistent results to within about one second as advertised, but measurements from experiments in one category are strikingly incompatible with those from the other, differing by nearly six seconds—and this for the lifetime of a particle that children learn about in middle school, one of only three that comprise all the objects in the world.

Of beams and bottles

In one type of experiment, a beam of neutrons is launched through an arrangement of electric and magnetic fields that separate out the positively charged protons produced when neutrons undergo beta decay. The remaining neutrons, being uncharged, continue on, but protons accumulate and are subsequently diverted into a detector. Both the capturing and the detection of charged protons are less error-prone than comparable processes for uncharged neutrons.

In theory, one can simply compare the proton count with the number of neutrons in the beam to obtain the information needed to calculate the neutron lifetime. Figuring out how many neutrons were in the beam to begin with is trickier than counting the protons, but experimenters have devised a clever way to circumvent that problem. They use a lithium-based neutron detector for which the detection rate is known to depend upon the neutrons' speeds in exactly the same way that the number of neutrons passing through the proton-collection segment of the beam does. In this way, the uncertainty in the number of neutrons that go undetected by the lithium detector cancels out of the math entirely.

The upshot is this: beam experiments ought to calculate the neutron half-life quite reliably. An average of beam-experiment measurements over the last 25 years or so gives a neutron half-life of 615.5 ± 1.5 seconds.

So-called bottle experiments disagree. In a bottle experiment, neutrons are confined in a container. Then, after waiting for different amounts of time, they are counted to see how many neutrons remain. But unlike working with charged protons, both confining and counting are difficult with neutrons. Because of their lack of electrical charge with which to interact with other particles, neutrons are generally able to penetrate into (or even through) solid matter, including the walls of the bottle and the detector material.

Here again, as with counting neutrons in beam experiments, experimenters have devised a workable solution: they chill the neutrons down to ultracold temperatures. Then, instead of zipping about at rapid particle-physics speeds and plunging into the walls of the bottle, the neutrons drift about very slowly, gingerly bouncing off its walls. Some neutrons might get out, but their loss rate can be adjusted—for example, by varying the temperature—and then extrapolated to a loss-free condition. Detector losses can be accounted for in a similar fashion, and 25 years of bottle experiments average out to 609.7 ± 0.4 seconds for the neutron half-life.

Bigger, better bottle

At Los Alamos, working with neutrons is practically a way of life. The work is never easy, and Los Alamos scientists have learned how to live with that. To resolve the measurement discrepancy between beams and bottles, someone has to get in there and ferret out any possible source of systematic uncertainty. In a bottle experiment, for example, any neutron that escapes without being properly accounted for in the calculations will make experimenters think it decayed, causing them to underestimate the neutron survival rate. Any misunderstanding of the sensitivity of the neutron detector will similarly skew the results.

"I think a lot of us in the physics community secretly trust the beam results, and we've been expecting to uncover a flaw in the design of previous bottle experiments," says Susan Seestrom. Seestrom is a Los Alamos physicist who came out of retirement specifically to search for that flaw. She had been promoted up the chain to manage the experimental physics directorate during her official Los Alamos career and ultimately chose to both retire and un-retire to get back to doing the science that most inspires her—solving one of the world's great experimental-physics mysteries.

"The only way to find out why beam and bottle experiments disagree with one another so systematically," says Seestrom, "is to adjust or improve upon one of them and then see if the changes make a difference." Together with Los Alamos colleagues, postdoctoral scientists, students, and external collaborators (at Indiana University, North Carolina State University, Tennessee Technological University, and elsewhere), Seestrom is working to improve a special kind of magnetic bottle for neutrons. While uncharged, neutrons are faintly magnetic, and because magnetic walls have different confinement properties than material walls, that difference could help scientists identify the source of the measurement discrepancy.

The magnetic walls are constructed from about 6000 powerful permanent magnets, each 1-inch square by 2 inches long, glued together in a pattern of rotating orientations to make what's called a Halbach array. It is designed to produce a consistent magnetic field—20,000 times stronger than the earth's magnetic field—everywhere along the bottle's surface. At the bottom of the array is a trapdoor through which ultracold neutrons enter to start the experiment.

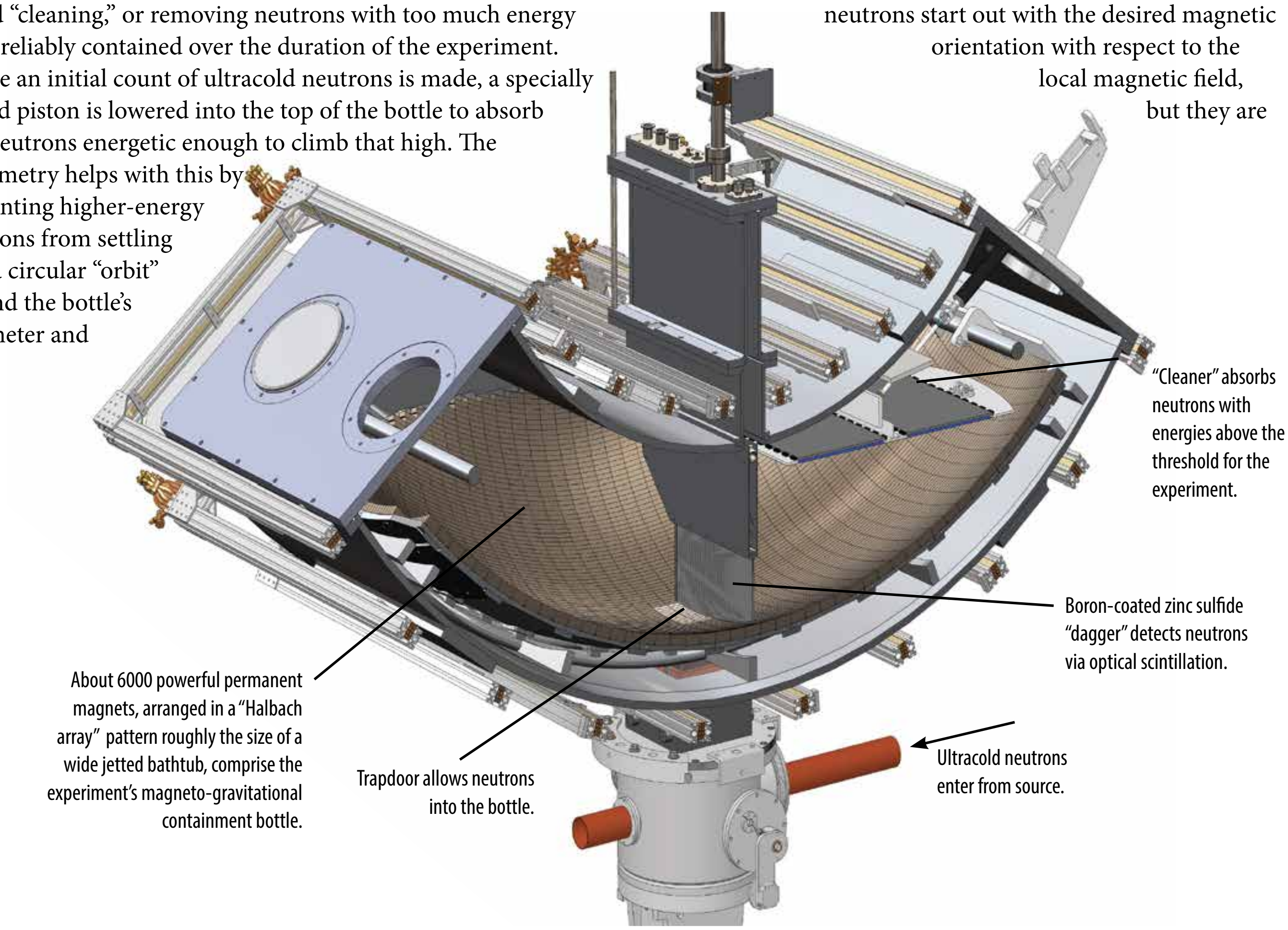
The magnetic bottle doesn't look much like a bottle, however; it looks more like a broad, slightly lopsided, metallic bathtub. Its top is open, both to allow instrumentation to be lowered in and because gravity is sufficient to keep the ultracold (that is, ultralow energy) neutrons from climbing out. Its bottom (magnetic) surface is somewhat asymmetrical, shaped like an egg sliced in half along its length, to help with a process called "cleaning," or removing neutrons with too much energy to be reliably contained over the duration of the experiment. Before an initial count of ultracold neutrons is made, a specially coated piston is lowered into the top of the bottle to absorb any neutrons energetic enough to climb that high. The asymmetry helps with this by preventing higher-energy neutrons from settling into a circular "orbit" around the bottle's perimeter and thereby escaping the cleaning process.

The whole setup, designed at Los Alamos, is undeniably a marvel of science and engineering. But Steven Clayton, one of Seestrom's colleagues on the project, notes that its improvements over conventional bottle experiments come with a cost.

"I'm confident that magnetic containment is the way to go because it's impossible to know the exact surface properties of even the smoothest of physical walls," says Clayton. "But switching to magnetic walls doesn't simply eliminate the uncertainties of physical walls the way you would want it to. It replaces them with different uncertainties that we have to understand and control."

In particular, magnetic containment only works if the neutrons' internal magnetism is pointing the right direction. Otherwise, the magnetic field would pull them into the bottle's walls, making it appear that they had been lost to beta decay, rather than reflect them back into the bottle's interior. The neutrons start out with the desired magnetic orientation with respect to the local magnetic field, but they are

It's the most highly instrumented neutron-lifetime experiment ever done.



The Los Alamos magnetic-bottle experiment is poised to resolve the present ambiguity in the measured half-life of the neutron. Unlike previous bottle-type experiments, it combines magnetic neutron containment (instead of solid walls), a comparatively large volume (for better data statistics), an asymmetric shape (to drive out unwanted high-energy neutrons), real-time visual neutron detection inside the primary container (to minimize detection uncertainties), and blinded data processing (to eliminate human bias).

vulnerable to reversals in magnetic orientation if they move through either a steep gradient or a gap in the surrounding magnetic field. Detailed calculations show that gradients steep enough to affect the experiment shouldn't pose a problem, and an additional applied magnetic field ought to eliminate any gaps. Clayton will need to perform a comprehensive magnetic-field mapping inside the bottle to be certain, but indications to date suggest that magnetic reversals are unlikely to affect the results.

After running down such sources of uncertainty, all that remains is to count the neutrons. Comparing two measurements—one soon after filling the bottle and another more than two half-lives later—reveals the timescale for beta decay and, therefore, the lifetime of the neutron.

Boron-battered blade

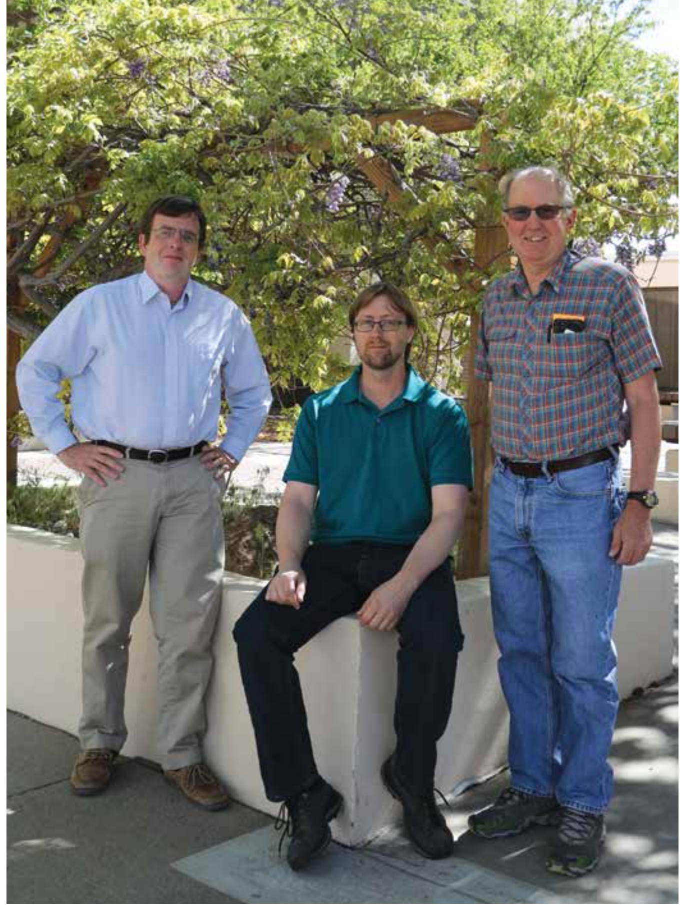
"Even the easy stuff—like *counting*—is unbelievably difficult when it comes to experimental physics at a precision below 0.1 percent," says Chris Morris, a Los Alamos nuclear physicist. Initially, the plan was to open the trapdoor at the bottom of the bottle and let the neutrons drain out to be counted. It may sound simple, but just as walls and magnetic fields come with their own complications, so too does draining the neutrons.

"If how long the neutrons have been in the bottle affects the way they're sloshing around when the trapdoor is opened, we'll get biased counts and biased results," Morris explains. "So we came up with a better way. And after that, we came up with an even better way."

First, Morris and the team developed a different mechanism for counting neutrons without draining them from the bottle, making their counts directly inside the bottle instead. They created a rigid "dagger" coated on both sides with the isotope vanadium-51. (The term refers to the retractable daggerboard some sailboats employ as a keel for stability.) When lowered into the bottle, the dagger would absorb neutrons, thereby converting its vanadium-51 into vanadium-52, which is radioactive with a 3.7-minute half-life. Then all the scientists had to do was count the subsequent vanadium decays with radiation detectors—and of course work out the backgrounds and efficiencies of those detectors. The problem was, how many 3.7-minute time periods could they afford to wait?

"It worked, and we got good data, but it was taking too long," recalls Morris. "We only get so much time with the ultracold neutron source, and increasing the precision of our results means conducting experiments in rapid succession for better counting statistics and better understanding of systematic errors. We couldn't very well do that if we had to wait around for all the vanadium to decay each time."

Help ultimately came from the Lab's chemistry division, where researchers had independently developed a technique for depositing a nanometer-scale coating of a different neutron absorber, boron-10, onto a zinc-sulfide surface. When a neutron strikes boron-10, an alpha particle (helium nucleus) is emitted, causing the zinc sulfide—a scintillator material used



Left to right: Andy Saunders, Steven Clayton, and Chris Morris, with upwards of ten thousand trillion trillion neutrons in each of their bodies. Fortunately, these neutrons are not free, but rather locked up inside atomic nuclei and therefore, by and large, in no danger of decaying.

by experimental physicists for about 100 years—to glow. This happens instantly, so there's no half-life to wait out. And it happens visually, so a specialized camera focused on the dagger, even from some distance away, could track all the neutron impacts in real time. Because of this, there would no longer be any ambiguity about whether the neutrons were sloshing around differently from one measurement to the next. Such effects could be directly observed and mathematically taken into account.

Matter Particle Life Expectancy

As far as anyone knows, the proton and electron could be perfectly stable, never undergoing radioactive decay. At the very least, they are extremely long-lived, with minimum known lifetimes enormously in excess of the 14-billion-year age of the universe. Among the three primary matter particles, only the neutron is unstable. Had the primordial neutrons produced in the big bang not found their way to safety inside atomic nuclei before a few of their half-lives had expired, no elements beyond hydrogen would have been produced. As Los Alamos's Susan Seestrom says, while gesturing at trees, buildings, and other people, "none of this would be here."

There's still much work to be done to optimize the system—the ideal size and shape of the dagger, the ideal camera setup, some lingering aspects of the higher-energy neutron cleaning process, and so on. But it is now clear that the experiment will work to measure the neutron half-life without the same uncertainties present in previous bottle experiments.

"Our prototype worked the first time," proclaims a visibly incredulous Clayton. "This is the most highly instrumented neutron-lifetime experiment ever done, and we're actually ahead of ourselves."

The expectations game

The researchers aim to iron out the details of the experiment and obtain results in two phases. Over the next year, they intend to obtain a neutron half-life measurement with 1-second uncertainty. This will put them on par with the best existing measurements and in the range of obtaining data that could affect scientists' understanding of particle physics overall. Then in the following years, they expect to further develop techniques to drive those uncertainties down to 0.2 seconds, at which point they will be able to advance human understanding of physics and, to some extent, help explain what went on at the birth of our universe.

When the universe was just a few seconds old and still very hot, particle interactions produced equal numbers of protons and neutrons, which could merge into nuclei of various isotopes of hydrogen, helium, and lithium. As the universe expanded and cooled, neutrons began to decay, and protons became relatively more numerous. But exactly how much more numerous? That depends on the neutron lifetime and strongly affects how much of each nucleus was able to form. Observational measurements of these abundances in the universe today provide a sensitive probe of the dynamics of the big bang—currently limited by our knowledge of the neutron lifetime.

"Grand though they may sound, and as important as they are, advancing particle physics and the big bang theory with better-precision measurements may not ultimately be the primary prize of this work," says collaboration spokesperson Andy Saunders. "They might even be considered a sort of consolation prize." Many leading physicists are expecting the results to defy previous bottle-type experiments, helping to point out where those experiments went wrong and thereby bringing bottle measurements in line, so to speak, with beam-experiment measurements. This would be success: resolving a longstanding physics dilemma. But the alternative, not resolving the dilemma, might in some sense be even better.

IN EXPERIMENTAL PHYSICS, EVEN THE EASY STUFF—LIKE *COUNTING*—CAN BE UNBELIEVABLY DIFFICULT.

If the Los Alamos experiment supports other bottle experiments and continues to defy beam experiments, it could suggest new and unexpected physics. After all, bottle experiments count the number of neutrons remaining, while beam experiments count the number of protons created by neutrons undergoing beta decay. If neutrons decay or otherwise disappear by some other process, in addition to beta decay, that would explain why the beam experiments come up with longer neutron lifetimes: they're only counting one of the ways neutrons die. In other words, it could mean that both kinds of experiments are correct, but only bottle experiments measure the neutron's overall lifetime. Beam experiments measure its beta-decay lifetime.

Thus, if the bottle-beam discrepancy holds up, it would mean the discovery of an entirely new physical process. A discovery like that doesn't come along every day, and there's no telling what future scientific and technological advances it might ultimately generate. So what's it going to be, spokesperson Saunders? Do your preliminary results point toward resolving the bottle-beam dilemma, or do they point to something potentially bigger?

"We don't have results to share using the boron dagger system yet, and those will be the ones to watch," Saunders says. "But our previous-generation experiment with the vanadium dagger yielded a neutron half-life of 609.5 ± 2.9 seconds, smack-dab in the middle of the nonmagnetic bottle-experiment range. Even with the fairly large uncertainty, that's distinctly outside of the beam-experiment range.

"Now, we didn't pursue tighter uncertainties with this result because we had already moved on to the boron-blade detector," Saunders continues. "But if it holds up, it will either imply a flaw in the beam experiments or the discovery of new physics." New physics from a particle we've known since 1932—either that, or the experiment will lay to rest a major unresolved issue in physics, as planned. LDRD

—Craig Tyler

More **neutron science** at Los Alamos

- **Groundbreaking neutron-beam measurement of plutonium**
  http://www.lanl.gov/discover/publications/1663/2015-october/a-community-of-electrons.php
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  http://www.lanl.gov/science/NSS/issue1_2012/story4.shtml
- **Neutron research on biological cells**
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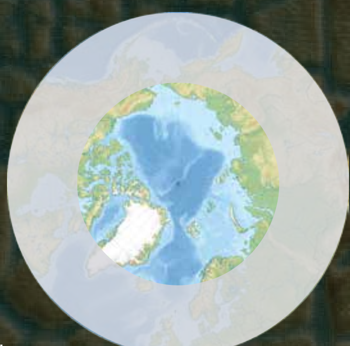
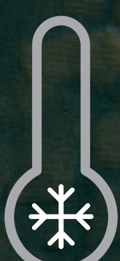
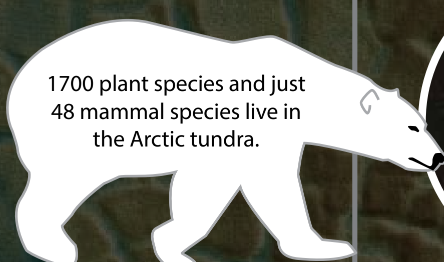
About four million people in eight different countries live in the Arctic: the United States, Canada, Greenland (Denmark), Iceland, Norway, Sweden, Finland, and Russia.



The Arctic tundra is one of the driest regions on Earth, with less than 10 inches of precipitation per year in most locations—less than the desert states of the American Southwest.

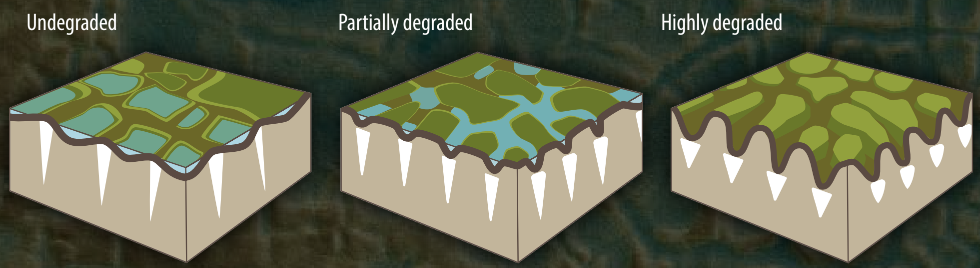


There is considerable variability in the Arctic climate, with winter temperatures occasionally dropping below -50°C (-58°F) and summer highs sometimes exceeding 30°C (86°F).



The oceans are 30% more acidic than they were when Mozart began composing at age four in 1760.

The Arctic ocean is acidifying twice as fast as other oceans.

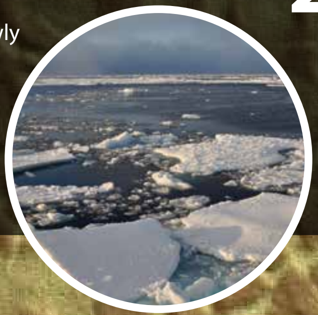


Arctic warming is causing drastic changes to the tundra topography. (Left) In the undegraded state, low-centered, water-inundated polygons are surrounded by higher ridges that form above ice wedges. (Center) As ice wedges melt, the land above them collapses into troughs filled with water from the polygon ponds. (Right) In advanced degradation, the troughs become connected, forming a drainage network surrounding high-centered polygons.

Arctic air temperature has increased by 5°C over the last 100 years.

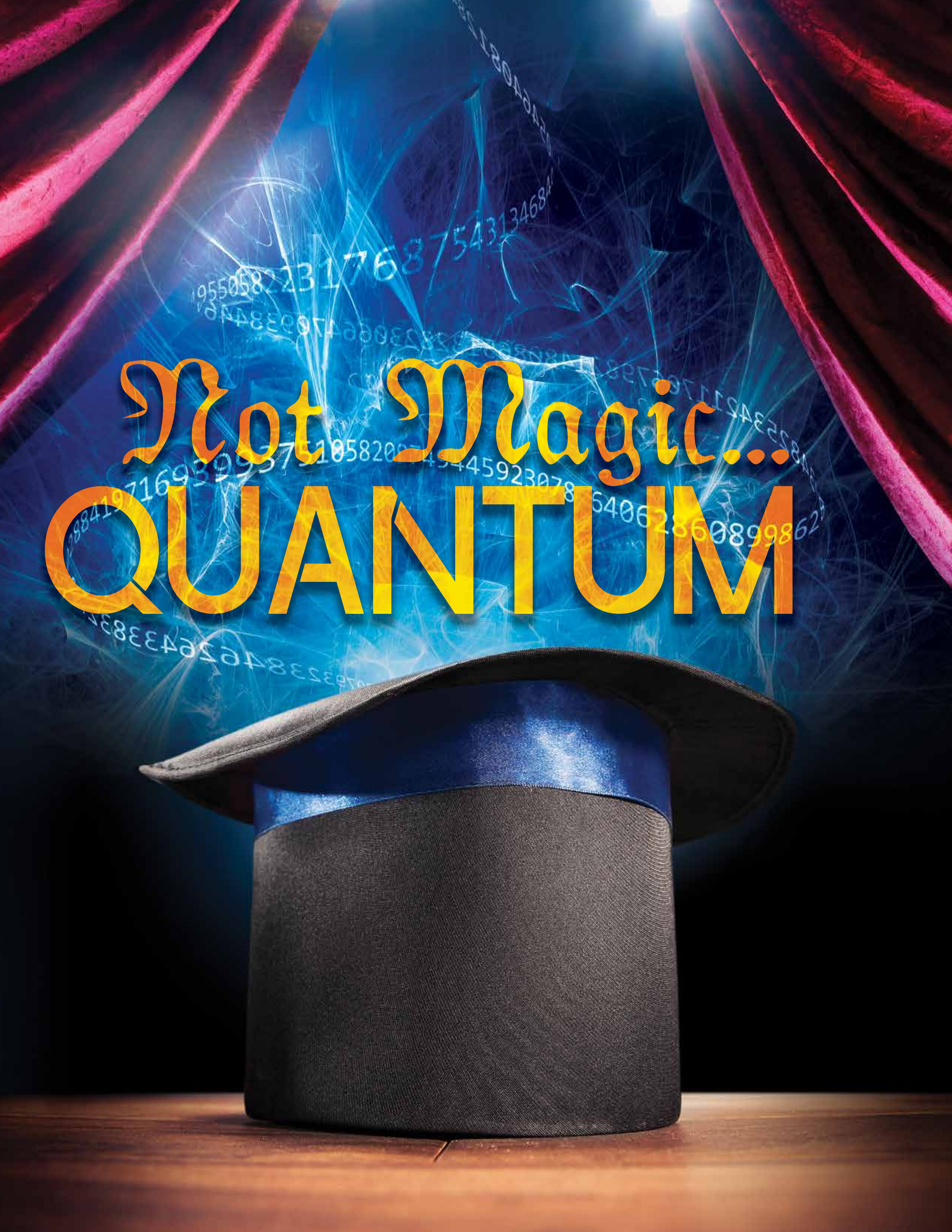
Thawing permafrost is exposing a huge quantity of biomass, mostly dead plants, that has been frozen for eons. The decomposition of this biomass by microorganisms releases carbon into the atmosphere, further compounding warming and accelerating thaw.

The melting of Arctic ice can contribute to rising sea levels and increased heat absorption by newly exposed soil, rock, and seawater.



Low-centered polygons

High-centered polygons


Not Magic...
QUANTUM

A nascent commercial quantum computer has arrived at Los Alamos. It could solve certain problems with such astonishing speed that it would be like pulling answers out of a hat.

A famous physicist once said, "If you think you understand quantum mechanics, you don't understand quantum mechanics." That physicist was Richard Feynman—Los Alamos alumnus, wisecracker, and Nobel laureate—describing a mind-bending subfield of physics wherein the rules of classical mechanics seem to vanish in a puff of smoke.

During Feynman's years at Los Alamos, the fledgling laboratory's "computers" were mostly women, many the wives of scientists, who sat at desks for eight hours a day, computing by hand the complex calculations required by the Manhattan Project. Shortly thereafter, the top-secret ENIAC (Electronic Numerical Integrator And Computer)—located in Pennsylvania and regarded as the first general-purpose electronic computer—helped post-war Los Alamos scientists to refine nuclear weapons and to explore other weapons technologies. Soon Los Alamos officials recognized the need for on-site leading-edge computing technologies. The first and second MANIAC computers (Mathematical Analyzer, Numerical Integrator, And Computer) were built in-house during the 1950s and 60s. In the 1970s supercomputers came on the scene and the Laboratory was first to purchase Cray, Connection Machine, and IBM supercomputers. At present, the Laboratory is installing its latest Cray supercomputer, a classical-computing beast dubbed Trinity, which once installed will be one of the most advanced computers in the world. But last month the newest addition to the Lab's family of futuristic computers arrived, and it's a horse of a different color: a quantum computer with potentially extraordinary capabilities that are just beginning to be explored.

Quantum computers have long been on the horizon as conventional computing technologies have raced toward their physical limits. (Moore's Law, an observation that the number of transistors that can fit onto a computer chip doubles every two years, is nearing its expiration date as certain features approach the size of atoms.) And to be certain, general-purpose quantum computers remain on the horizon. However, with the acquisition of this highly specialized quantum computer, Los Alamos, in partnership with Lawrence Livermore and Sandia National Laboratories, is helping to blaze the trail into beyond-Moore's Law computing technology. This new machine could be a game changer for simulation and computing tools that support the Laboratory's mission of stockpile stewardship without nuclear testing. It may also enable a slew of broader national security and computer science applications. But it will undoubtedly draw a community of top creative thinkers in computational physics, computer science, and numerical methods to Los Alamos—reaffirming the Lab's reputation as a computing technology pioneer.

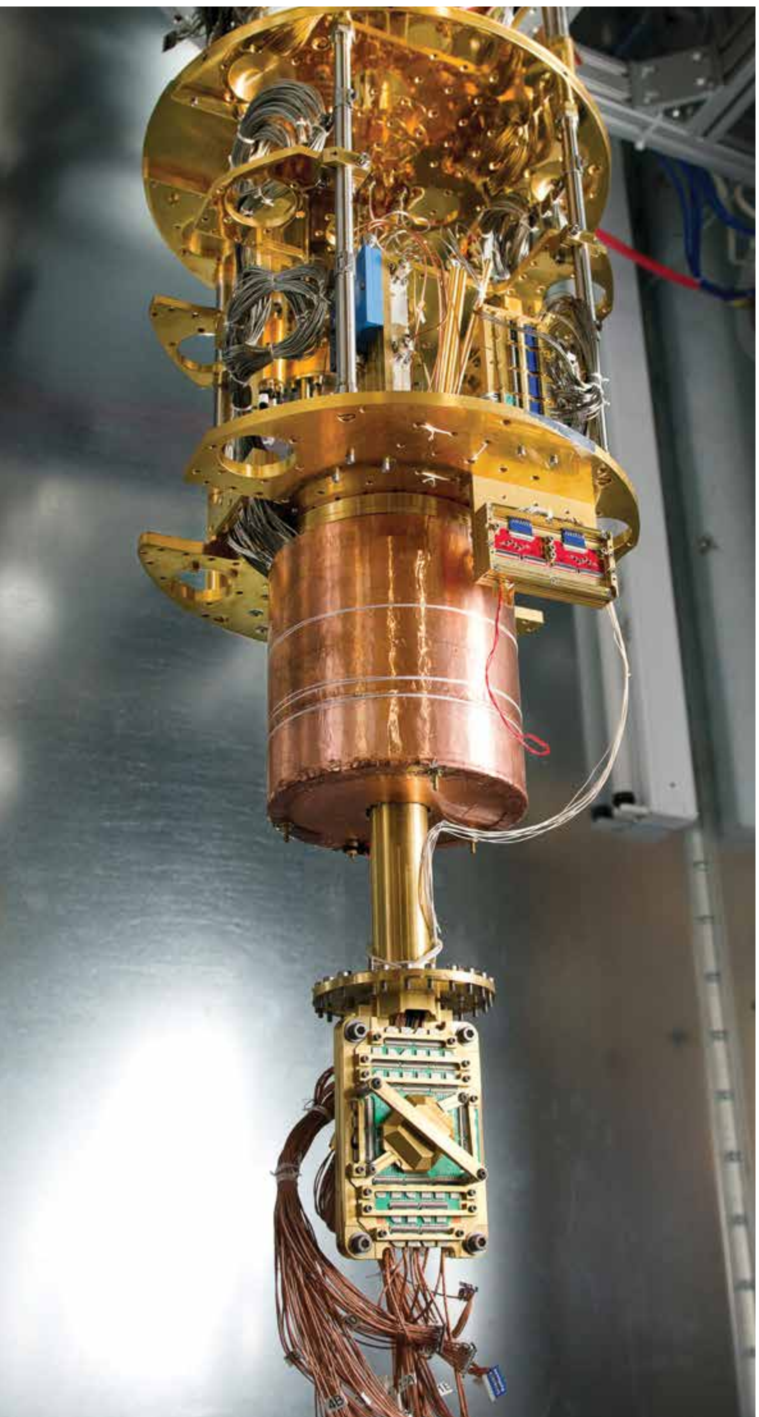
Weird science

Albert Einstein famously rejected parts of the theory of quantum mechanics. His skepticism is understandable. The theory, after all, said that a single subatomic particle could occupy multiple places at the same time. A particle could move from one location to another without traversing the space between. And multiple particles that had previously interacted and then separated by vast distances, could somehow "know" what each other was up to. It didn't seem to align with what scientists thought they knew.

Einstein's friend and contemporary, Niels Bohr, argued in favor of the theory and embraced its peculiarities, declaring, "Everything we call real is made of things we cannot call real." Einstein and Bohr publically hashed it out over the years in a series of collegial debates that delved deep into the philosophy of nature itself. Bohr's view prevailed and science has since borne it out. Even though Einstein was never fully satisfied by it, quantum mechanics is now generally accepted as the fundamental way of the world.

One of the hard-to-get-your-head-around concepts at the heart of quantum mechanics is called superposition. Simplistically, superposition is the idea that something can be in multiple states at the same time. A single electron can have both up and down spin, a single photon can travel both this path and that one, and, conceptually, a luckless cat in a box can be both dead and alive. Until you check, that is. Once the electron's spin is measured, or the photon is tracked, or the box lid is lifted, the system goes classical and assumes either one state or the other.

The lifting of the lid causes decoherence—another oddity of the quantum world. For a system to exist in a state of superposition it must not interact with its environment at all, including observers or scientific instruments. The loss of any



information from the system to the environment—the lid being lifted and the condition of the cat becoming known—causes the system to decohere. This is why a taxi driver can't choose the fastest route to the airport by taking them all at once—the car, the road, the driver, the very atoms in the air, everything in the macroscopic world interacts in innumerable ways. Everything we can touch or see or record, by virtue of being touched or seen or recorded, decoheres, and therefore appears classical, not quantum.

Particles that interact with one another enter into a strange relationship with one another. This relationship, known as entanglement, is preserved as long as the two particles remain sheltered from the rest of the environment, lest their entanglement decohere. For example, if two electrons were

Einstein wasn't entirely convinced, but quantum mechanics is now accepted as the way the world is.

entangled in such a way that they must necessarily spin in the same direction—but are initially in a superposition of both possible directions—then the instant one of them assumes a firm spin orientation (due to a measurement, perhaps), the other assumes the same orientation as well. Derisively branded by Einstein as "spooky action at a distance," this phenomenon holds even if the two electrons have moved thousands of light years apart.

Superposition, decoherence, and entanglement are head-scratchers to be sure. But that doesn't make them any less real. If these weird principles of science can be harnessed somehow, then it might become possible to really blow some curtains back.

Wiring the weirdness

A classical computer uses bits as units of information. The term "bit" comes from "binary digit," which illustrates its two-state nature—it must always be in one of two states, which is denoted by a 1 or a 0. The two states can be just about any binary set—open and closed, on and off, up and down, positive and negative—and the state of the bit describes the state of some part of the physical device.

A quantum computer, on the other hand, relies on quantum bits or "qubits" as units of information. A qubit

Top: The D-Wave 2X is a big black box with a 150-square-foot footprint (including the adjoining controls cabinet). It is essentially a walk-in freezer that is highly shielded from outside interference, creating a specialized environment for the world's first commercial quantum processor. The environment around the chip has a magnetic field 50,000 times weaker than Earth's ambient magnetic field, a pressure 10 billion times lower than Earth's atmospheric pressure, and a temperature hundreds of times colder than interstellar space. Bottom: An array of 16 layers of shielding and filters (removed to show the device inside), serve to drastically reduce the temperature of, and interference with, the quantum processor (visible at bottom behind a diagonal gold bar).

All photos courtesy of D-Wave Systems, Inc.

can also be just about any two-state thing, like the spin of an electron or a photon, that avoids decoherence and therefore acts in a quantum way. The power of a quantum computer comes from the superposition of its qubits—they are all in both states at the same time. So, while a system of three classical bits can assume any of eight different configurations (000, 001, 010, 100, 101, 110, 011, 111), it can only try one at a time. But a system of three qubits can try all eight configurations at once. For problems with large numbers of possible answers, a quantum computer would be ideal because a qubit processor could evaluate all possibilities at once and present the correct answer in an instant. So a quantum cab driver could indeed try every route to the airport at once to find the fastest one.

It follows to ask, then: To build a quantum processor, how can individual electrons or photons be completely, utterly isolated from the environment in such a way as to maintain their quantum state but also be wired up to an interface so that macroscopic, human operators can use the computer?

They can't.

Yet.

That's what quantum computer developers are working on. The current state of the art for general-purpose quantum computers is less than 10 qubits—housed in isolation, not wired to an interface—in various laboratories around the world. And that in itself is a pretty big deal.

About 500 qubits can test, simultaneously, more possibilities than there are atoms in the visible universe. For a very specific kind of quantum computer, called a quantum *annealing* computer, the current state of the art is over 1000 qubits, housed in an extremely cold chamber, inside a big black box. And this is what recently rolled off the truck at Los Alamos.

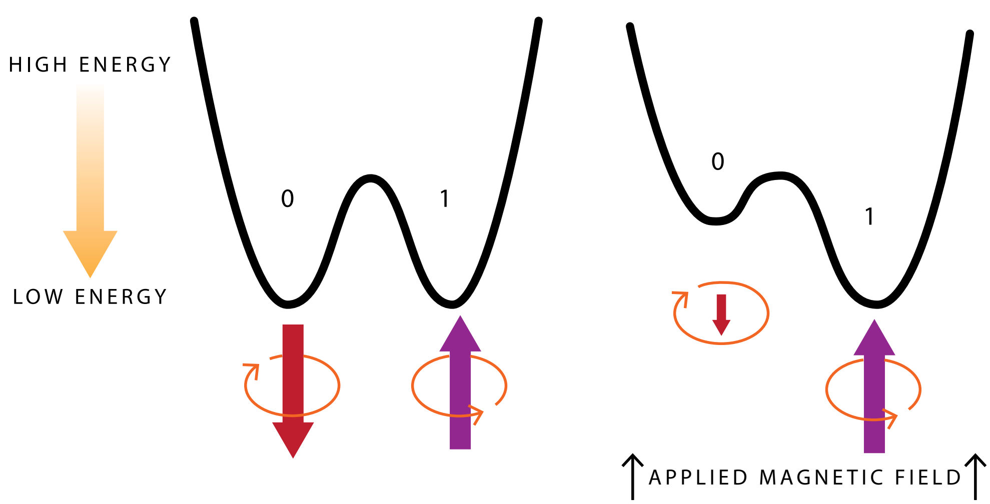
Qubits and pieces

The computer is made by the Canadian company D-Wave Systems and is its third-generation quantum annealer, called the 2X. How did D-Wave build a qubit-based processor when qubits are so hard to handle? Well, it had two good tricks up its sleeve. The first was focusing only on annealing, rather than trying to build a general-purpose processor. The second trick involved the qubits themselves.

Annealing is a term that refers to something going from a highly disorderd state to a less disordered state. In metallurgy, annealing is used to make metal stronger through high heating followed by slow cooling. The atoms in the metal gain energy from the heat, and then as they cool, they settle in to a less disordered, very low-energy configuration. In computing, annealing refers to solving a problem by finding the minimum energy state. What a quantum annealing computer is good for is optimization problems, which aim to find the best, or least-disordered, lowest-energy solution from a large range of possible solutions. A useful example is the traveling salesman problem: If a traveling salesman must visit all the cities in his territory and wind up back where he started, what is the best route and method of transportation to minimize time and cost? Should he travel by car, train, plane, or bus? Should he travel in a zigzag, radial, or random pattern? Is there any road or airport construction to consider? And what about fuel prices? Optimization problems are among the kinds of problems that conventional computers struggle with. So D-Wave chose to focus on building a processor that specializes in them.

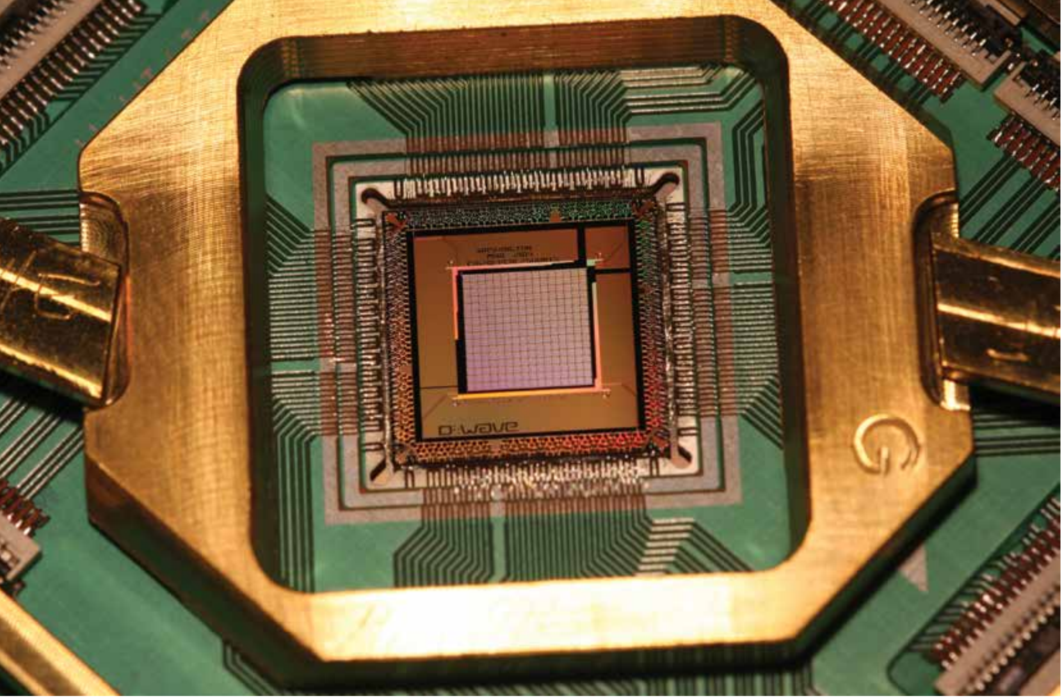
The second thing that D-Wave did differently involved its choice of qubit. Decoherence is one of the biggest hurdles to building a quantum computer—a qubit is a qubit only as long

FIVE HUNDRED QUBITS CAN TEST MORE POSSIBILITIES IN THE BLINK OF AN EYE THAN THERE ARE ATOMS IN THE VISIBLE UNIVERSE.



Biasing qubits is a part of building the energy landscape for an optimization problem, which is how the quantum annealer is programmed. (Left) An energy diagram with a double-well potential illustrates two possible states of one qubit (red and purple arrows). There is equal probability of the qubit ending up in either well, with the low point on the left corresponding to the 0 state and the low point on the right corresponding to the 1 state. (Right) If a bias is applied to the qubit, in the form of an external magnetic field, the probabilities are no longer equal. The qubit is now more likely to end up in the lower-energy well on the right and take the 1 state.

All images adapted with permission from D-Wave Systems, Inc.



The quantum annealing computer's 1152-qubit processor, named Washington (its predecessors were the 128-qubit Rainier and the 500-qubit Vesuvius), is smaller than a wristwatch and can evaluate more possibilities, simultaneously, than there are atoms in the visible universe.

as it doesn't decohere. And how can you manage decoherence if your qubit is a single photon? It turns out a qubit needn't be so small. A macroscopic qubit is the key, and rather than a cat in a box it turned out to be a squid in a freezer.

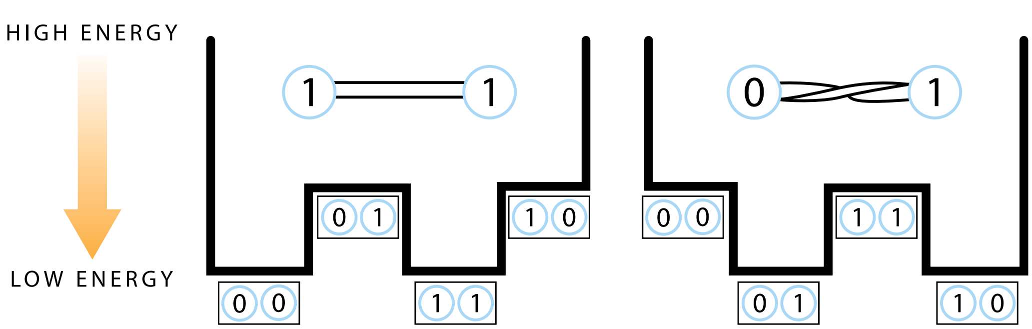
Superconducting quantum interference devices, or SQUIDs, have been used in a wide variety of applications that depend on measuring very small magnetic fluctuations. From portable medical imaging devices to earthquake prediction to gravitational-wave detection, ultrasensitive SQUIDs have been the key to some major scientific breakthroughs, in addition to quantum computing. In the D-Wave 2X, SQUIDs create small magnetic fields that encode all the processor's 1s and 0s.

A temperature several hundred times lower than the temperature of interstellar space is required for proper function of the SQUIDs. At this temperature, the metal niobium, a superconductor, begins to exhibit distinct quantum mechanical effects on a much larger scale than is ordinarily possible, making it an ideal material for the quantum processor. The SQUIDs in a 2X are long, skinny, niobium wire loops arranged in groups of eight on a grid. At normal temperatures each loop can run an electric current in either a clockwise or counter-clockwise direction, which creates either an "up" or "down" magnetic field. But when the temperature plunges to a frigid 10 millikelvins, the SQUIDs become superconducting, and quantum mechanical effects turn on. The electric current runs in both directions simultaneously, and the SQUIDs become qubits.

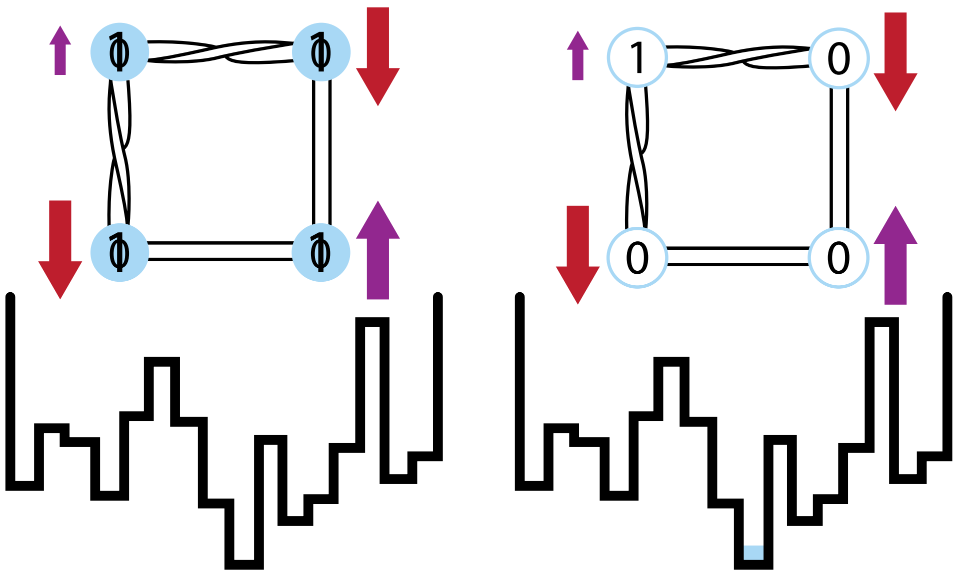
The annealer reports to a classical computer on the outside of the big black box so the user can see the result. The unique environment surrounding the chip, which requires not just extremely low temperature but also extremely low pressure and magnetic field, is maintained with a series of 16 filters and shields. But underneath all that, the business end of the processor is unexpectedly small—about the size of a thumbnail. And the big black box isn't actually full of insulation or banks of electronics—it's mostly empty. It's only that big so that a person can fit comfortably inside to perform occasional mundane maintenance or processor modification.

Solving an optimization problem with the 2X isn't remotely like making a spreadsheet on a conventional computer. "You wouldn't want to use it to balance your checkbook," explains John Sarrao, the Laboratory's Associate Director of Theory, Simulation and Computation. "If you need to get an exact answer, then any beyond-Moore's-Law technology is going to be a poor choice. But if quick and close is good, then D-Wave is the one." That's because it doesn't necessarily give a precise *right* answer, it gives a *very good* answer. And with repeated query, the confidence in that answer grows.

The question has to be framed as an energy minimization problem, so that the answer will exist in the low spots of an energy landscape. Imagine a golf course with hills and dips and occasional holes, and the goal is to get a ball into the hole whose bottom sits closest to the center of the earth. A classical computer has to drop a few balls and hope that one rolls into one of the deeper holes. With the 2X, the balls can explore all the holes at once and can even burrow underground from one hole to a deeper hole, as long as those holes aren't too far apart



Couplers are used to entangle qubits together, helping build the energy landscape for the optimization problem being considered by the quantum annealer. (Left) To entangle two qubits so that they take the same state, the coupler reduces the energy of those states relative to the alternatives. (Right) Qubits can also be entangled so that they necessarily have opposite states from one another. In this case the coupler reduces the energy of the mismatched states compared to the matched ones.



An energy landscape emerges when many qubits are biased and entangled in a variety of ways. (Left) Biases can raise or lower the possibility of a qubit taking a particular state (red and purple arrows), and entanglement links the states of multiple qubits together as either "same" (straight bars) or "opposite" (twisted bars). (Right) Once the problem is posed by building the energy landscape, the anneal is performed and the qubits slowly settle in to their minimum-energy, classical states of either 0 or 1, revealing the lowest-energy location in the energy landscape (blue spot).

(this action is called tunneling and is yet another curiosity of quantum mechanics).

Each question demands its own custom golf course, which the scientist using the machine must construct through biasing and entangling the qubits. This is basically how the quantum computer is programmed. Biases are achieved with magnetic fields applied to individual qubits, and entanglement is done with devices called couplers, which are superconducting loops. The couplers work by lowering the energy of the preferred state in comparison to the alternative, increasing the likelihood that the qubit will take the preferred state. The scientist chooses a whole set of "same" and "opposite" couplings between the qubits to build a unique energy landscape, for which the

> **SQUIDs have been key to major breakthroughs before, like portable medical imaging, earthquake prediction, and gravitational-wave detection.**

annealing process finds the lowest energy required to form those relationships. The more complicated the landscape, the more likely quantum annealing is to find an answer more accurate answer than conventional optimization would provide.

The control circuitry for creating the energy landscape—for standardizing the qubits, creating interactions between qubits, turning quantum effects on and off, and reading out the final answer—take up most of the processor chip and most of the user's time. While the computation itself is lightning quick, setting up the problem takes a lot of time and that's where initial research will be focused. Right now it takes many hours of planning to run a millisecond experiment, but the more the scientists work with it, the better they'll get at the planning, and the more use the machine will get.

D-Wave of the future

Los Alamos and other entities with D-Wave systems in residence (the Los Alamos machine is the third D-Wave machine to be sited outside D-Wave headquarters) aren't customers so much as they are collaborators. No one really knows everything the machine can do, and the best way to find out is to get it into the hands of a bunch of scientists.

"It's an investment in learning," says Mark Anderson of the Weapons Physics Directorate who spearheaded the effort to bring a D-Wave 2X to Los Alamos. "We are building a community of scientists who want to explore the capabilities and applications of quantum-annealing technology." There is already a short queue of users at Los Alamos, who have been running experiments on a 2X machine at D-Wave headquarters in Canada. But now that there is one here, the line, and the excitement, is growing.

In 1982, in the keynote lecture of a theoretical physics conference, Feynman spoke about the possibilities of quantum computing. "Nature isn't classical, dammit," he said in his concluding remarks, "and if you want to make a simulation of nature, you'd better make it quantum mechanical, and by golly it's a wonderful problem, because it doesn't look so easy."

And he was right.

—*Eleanor Hutterer*

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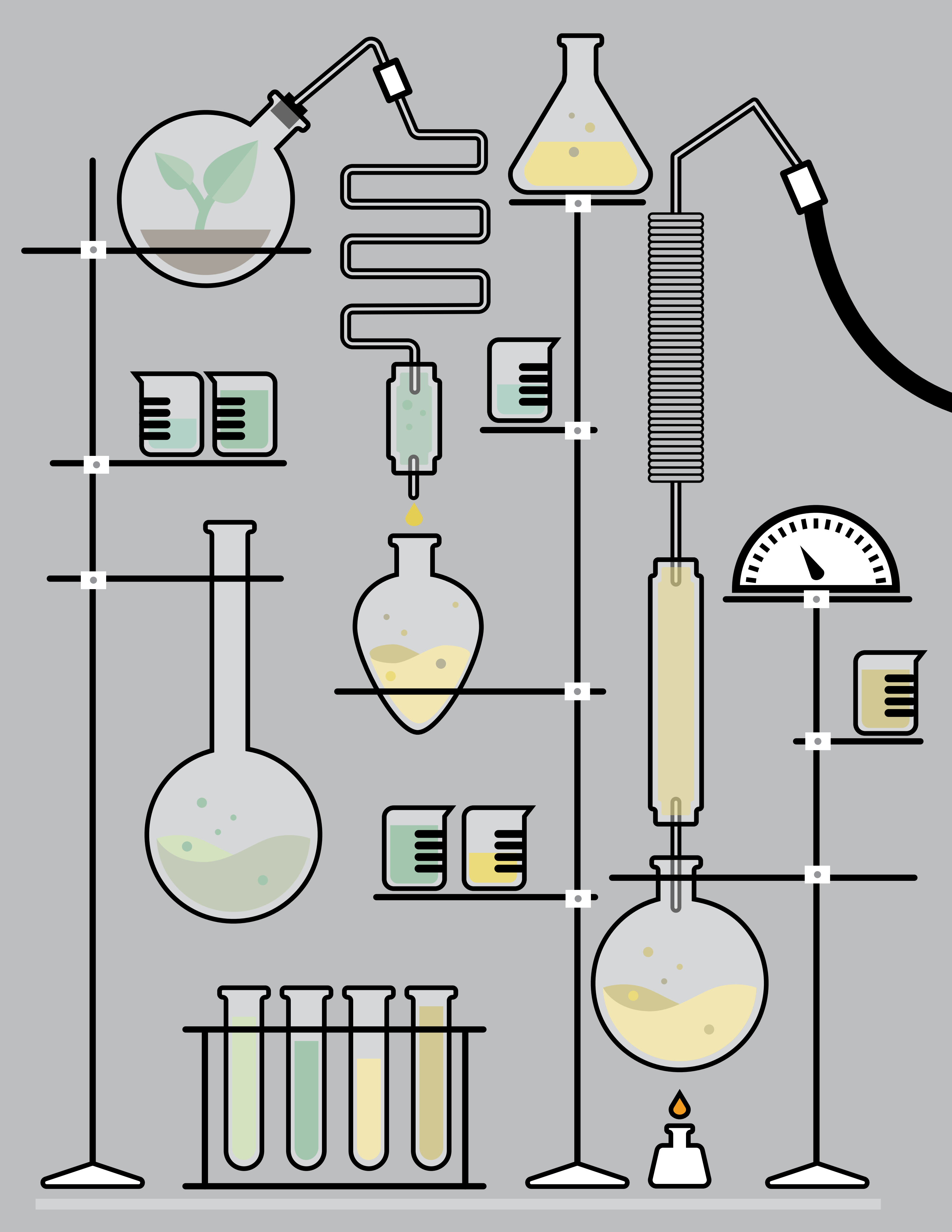
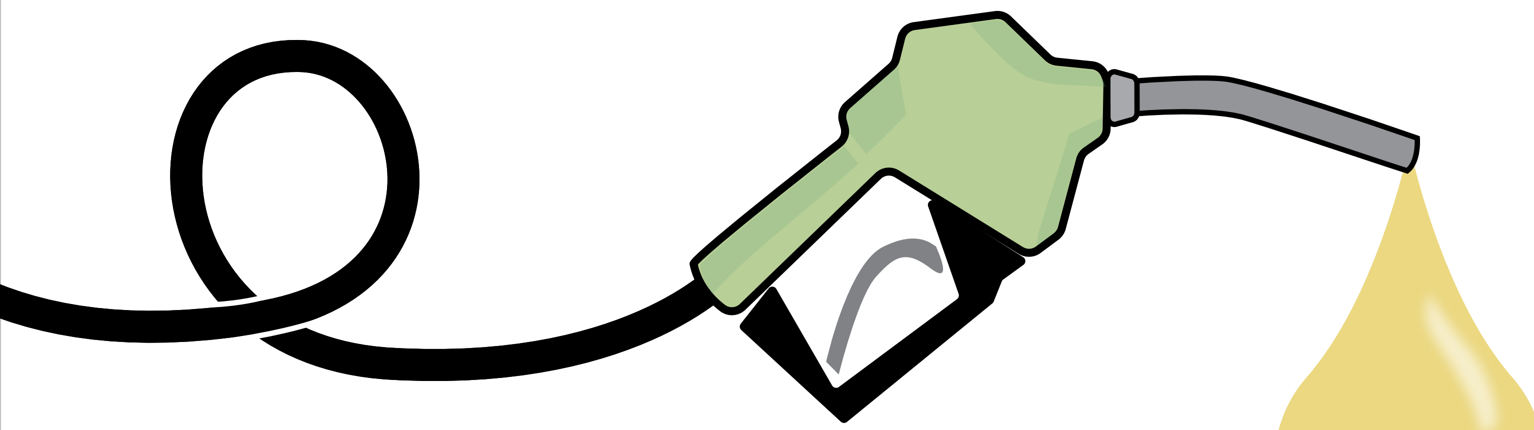


BREAKING THE BOND

CAN CHEMISTRY HELP UNBIND US FROM FOSSIL FUELS?



When crude oil is pumped out of the ground, it contains atoms from plants and animals that lived millions of years ago. Mother Nature gave those organisms nearly the same ingredients she gives plants and animals today. The difference is that microbes, heat, pressure, and Father Time have done all the work to dismantle the complex living things into simpler molecules that are now used to produce energy. To make similar fuels directly from plant matter today, scientists—including some at Los Alamos—have developed multiple approaches to do the dismantling themselves.

The simple molecules in crude oil are mostly long chains of carbon and hydrogen atoms aptly called hydrocarbons. Hydrocarbons are suitable for making fuel because they are energy dense, meaning that a small volume can produce a large amount of energy. Fossil fuels, such as oil, coal, and natural gas, are found all over the world, and although they require refining after extraction, this processing is fairly straightforward and is now well established, making the fuel relatively inexpensive to buy.

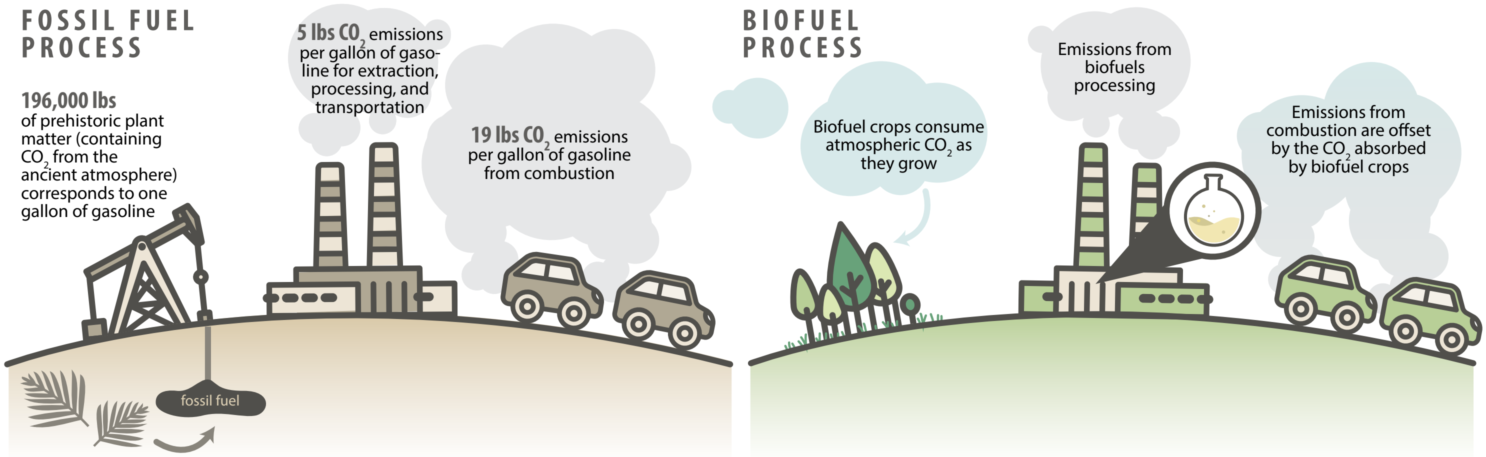
Until recent decades, however, multiple impacts of fossil fuels were largely ignored. First, there is damage to the environment: releasing previously buried carbon into the atmosphere dramatically alters the climate, with grave consequences for life on Earth. Second, importing oil from foreign countries can be unreliable; this concern has been voiced since the early 1900s and has prompted efforts to secure energy from domestic sources instead. And finally, reliance on fossil fuels is unsustainable because the supply is finite and someday it will simply run out.

All of these factors have pushed scientists to pursue alternative energy sources, such as wind and sun. Slowly but surely, these alternatives are replacing fossil fuels in our electricity supply, but when it comes to cars, trucks, and airplanes, fossil fuels are still at the forefront. Electric and hybrid cars are available, but because trillions of dollars are currently invested in fossil-fuel-specific vehicles and infrastructure, finding liquid fuels that can be dropped directly into this system will create the most immediate improvement. Biofuels have long been touted as a potential solution. However, biofuel production is challenged both by the ability to grow enough plants (biomass) that are not otherwise needed as food and by the ability to efficiently process that biomass into a fuel that is competitively priced, energy dense, and versatile enough to be used for various types of vehicles and conditions.

Scientists at Los Alamos are tackling this challenge from many angles—from increasing the growth of plants and algae to developing strategies to convert biomass into fuel and other useful chemicals. This latter task, converting biomass, is significant because harvesting hydrocarbons from contemporary plants is not as easy as it is from fossilized ones, and once harvested, they are not anything like crude oil. Fortunately, a handful of Los Alamos chemists have been studying the process and are closing in on a strategy to condense millions of years of fossilization into a few chemical reactions—thus removing Father Time from the equation completely.

Taking the bio out of biofuels

Chemist Andrew Sutton came to Los Alamos as a postdoctoral fellow to work on hydrogen storage for energy research. But when his mentor, Lab chemist John Gordon, began to investigate biomass conversion as a new direction for energy improvements, Sutton—now a staff scientist—became engaged as well. Their goal: to use chemistry to construct gasoline-like hydrocarbons from plant sugars. This approach deviates from traditional, long-standing biological methods of using microbes to convert plant sugars into alcohol fuels.



Biofuels are desirable as alternatives to fossil fuels because instead of releasing previously buried carbon into the atmosphere, the carbon dioxide released comes from plants that actively removed it from the atmosphere during their growth. The downsides to biofuels are mostly associated with the energy and resources required to grow the plants and process the fuel. Chemical conversion of plant sugars to third- and fourth-generation hydrocarbon biofuels has the potential to significantly reduce this energy input and cut greenhouse gas emissions by 80 percent compared to fossil fuels. *SOURCES: Jeffrey Dukes in Climate Change, Union of Concerned Scientists*

Alcohol-based fuels such as ethanol were used in many of the first car engines. In 1925, Henry Ford was quoted in *The New York Times* as saying, “There is fuel in every bit of vegetable matter that can be fermented. There’s enough alcohol in one year’s yield of an acre of potatoes to drive the machinery necessary to cultivate the fields for a hundred years.”

Today, ethanol fuel—a so-called first-generation biofuel—is made from sugars found in corn and sugarcane. Plant biomass is mostly made of sugars, which are rings of five or six carbon atoms connected to many oxygen atoms. Multiple sugars linked together make carbohydrates, which provide fuels for living creatures large and small. Humans and other animals convert them into energy, water, and carbon dioxide, while some microbes, such as yeast and bacteria, use a fermentation process to convert them into carbon dioxide and an alcohol, such as ethanol.

The carbohydrates in corn kernels and cane sugars are easy to access for fuel production. However, corn and sugar are food crops that will increase in price if a portion of the supply is also being used to power cars. To address this, researchers have been improving ethanol production from other, less valuable plant parts such as non-edible leaves and stalks, or from non-food plants such as grasses. This production, however, is more difficult because leaves, stalks, and grasses have evolved to be strong and stable, and their sugars are trapped in a complex molecular structure. The carbohydrate building blocks are locked together within a polymer called cellulose, which is then wrapped up with another polymer called lignin.

Through a lot of hard work, scientists have been successful in deconstructing this lignocellulose into its carbohydrate building blocks so that microbes can ferment them into ethanol fuel. Unfortunately, this second-generation fuel, dubbed cellulosic ethanol, is still not a complete replacement for traditional gasoline because the fermentation process releases carbon dioxide, which both increases the overall carbon footprint of ethanol as a fuel, and decreases its energy density.

“Ethanol’s benefits are limited,” says Pete Silks, a chemist at Los Alamos who has worked on biomass conversion for many years. “It is corrosive, and it is not as energy dense as gasoline. Also, it freezes at low temperatures so it can’t be used as aviation fuel.” Furthermore, because most people don’t drive ethanol-ready vehicles, the only way to have widely useable biofuels in the near term is to create gasoline and diesel, instead of ethanol, from plants.

But how? The current process of making ethanol relies on microorganisms that convert five-carbon sugars into two-carbon ethanol. Gasoline and diesel fuels are made of hydrocarbons that have many more carbon atoms, fewer oxygen atoms, and fewer double bonds. So, unless someone discovers a new organism that digests sugar directly into gasoline, scientists are challenged to remove oxygen atoms, break double bonds, and extend carbon chains—as would naturally happen during the eons-long fossilization process—in the confines of a chemistry lab.

The language of fuel

Traditional petroleum-based fuels are made of a mixture of different types of hydrocarbon molecules, and getting the right mixture is critical. Gasoline, for instance, can contain molecules that range from 5 to 13 carbon atoms in length. Diesel hydrocarbons range from 10 to 25 and jet fuel from 9 to 13. Some of the molecules contain double bonds between carbon atoms, while others don’t. Some contain rings of carbon, while others are linear. And although carbon and hydrogen are the dominant elements in fuels, there are sometimes a few oxygen molecules present as well.

To improve their fuel-development research, Sutton and his Los Alamos colleagues have been able to fine-tune their approach by collaborating closely with fuel engineers—despite it seeming, at first anyway, that they were speaking entirely different languages! For example, chemists often think about which atoms are connected to what, so to them, the term “octane” describes an eight-carbon molecule with many hydrogen atoms. However, fuel engineers tend to focus on the properties of a molecule; in that context, octane is an indicator of performance. High-octane fuel might contain a large number of eight-carbon molecules, but to a fuel engineer, it generally conjures up discussion of how much the fuel-air mixture can be compressed without causing engine damage.

Through this collaboration, the Los Alamos chemists began to map fuel-related characteristics—viscosity, flash point, and volatility—to various types of molecules available from biomass, such as those with a carbon atom double bonded to an oxygen atom (ketones) and those containing carbon rings (cycloalkanes). Their most recent paper describes many of these relationships, including how the length of a carbon chain affects the density of a fuel and what happens to the boiling point if there are any double bonds within the molecule. This analysis has helped the scientists realize, for instance, that they did not actually have to remove all the oxygen atoms from the sugars, as they had previously thought. Instead they should be strategic about which types of oxygen-containing molecules to retain and where they should be located.

> **WE ARE CONDENSING MILLIONS OF YEARS OF FOSSILIZATION INTO A FEW CHEMICAL REACTIONS.**

Coaxing carbons to cooperate

In a cellulosic ethanol production line, the fuel conversion happens toward the end. Biofuel crops must first be grown, harvested, and preprocessed to break apart the lignocellulose structure. Some methods use extreme temperatures and pressures to unlock the structure and release the chemical building blocks. Another method of processing essentially cooks the biomass in water, acid, and cellulose-breaking enzymes. The result is a brown, mucky-looking liquid called hydrolysate that contains mostly glucose and xylose sugars. The hydrolysate sugars can then be fed to microbes that will convert them into fuel.

This is where Sutton and his colleagues step in. Instead of sending the hydrolysate to a bioreactor for microbes to ferment into ethanol, their chemistry-based approach uses regular, off-the-shelf chemicals under mild conditions to create hydrocarbon fuels.

In order to convert five- and six-carbon sugars into gasoline, the chemists must first add carbon atoms to make longer carbon chains that more closely resemble fuel hydrocarbons. This reaction uses a catalyst (a molecule that can speed up the reaction without itself getting used up) to take a six-carbon sugar and a simple three-carbon molecule, such as acetone, to make a nine-carbon molecule. Other variations can create a range of 8 to 16 carbon atoms.

After elongating the carbon chain, the Los Alamos scientists break apart the rings and remove some of the oxygen atoms. They had to experiment with various ways of opening the ring first, because removing the oxygen first would make the ring more stable and therefore harder to break. For this, they developed a novel protocol that uses acid, hydrogen gas, and palladium as a catalyst to successfully transform the molecules while keeping energy input at a minimum.

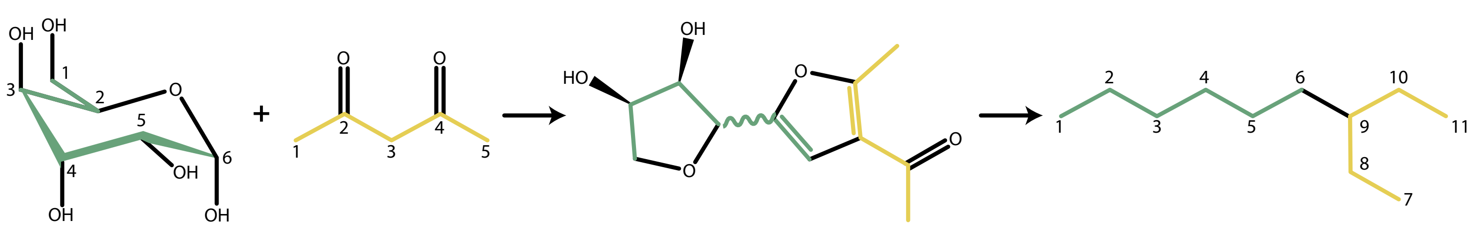
The team has refined these protocols using various starting materials, including sugar, a sugar derivative called 5-hydroxymethylfurfural, and a potato. Then they tried their methods on hydrolysate and were able to demonstrate feasibility for an industrial production environment.

Once these basic steps had been mastered, Sutton and his colleagues began to experiment with various ways of improving the sugar-to-fuel conversion to make it even more efficient and less expensive. These modifications are critical for making biofuels cost-competitive.

The big time

Global transportation infrastructure is designed for fossil fuels, and traditional gasoline is currently much less expensive than biofuels. Every approach to biofuel production is faced with this reality, pushing scientists to examine each step of the process to find improvements. Some of the comparatively high costs and high emissions of biofuel production lie in the growing, harvesting, and preprocessing of biomass. However, in looking at their conversion protocol, Sutton and his team were able to identify a number of additional changes they could make that may further help.

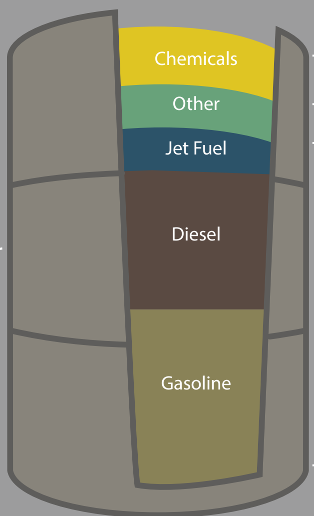
"By keeping temperatures relatively low and pressures close to normal, we can do these reactions in distributed facilities. In other words, we don't have to transport all the biomass to large biorefineries," says Sutton. Transporting such biomass—which is heavy because it is full of water—not only adds cost but also increases its carbon footprint.



6-carbon glucose — 5-carbon acetylacetone — 11-carbon intermediate — 11-carbon linear hydrocarbon for fuel

An example of chemical conversion wherein a six-carbon glucose molecule is combined with a five-carbon acetylacetone molecule. The final product is an 11-carbon hydrocarbon fuel molecule, similar to those found in crude oil, color coded above to indicate where its carbon atoms originated. (As is customary in organic chemistry, each vertex or endpoint not otherwise labeled is assumed to be a carbon atom, plus any hydrogen atoms needed to occupy the carbon bonding sites not already specified in the drawing.)

CATALYZING A NEW ECONOMY



Three-quarters of the volume of U.S. crude oil is used to make fuel, with revenues totaling $935 billion. A mere 16 percent goes toward chemicals for consumer products yet still generates comparable revenues of $812 billion. Such petrochemicals are everywhere—they are used to make solvents, plastics, waxes, detergents, pharmaceuticals, and even artificial flavors. When it comes to making competitively priced biofuels, researchers would like to offset the biofuel production cost by supplying comparably profitable bio-derived chemicals in place of the petroleum ones.

Los Alamos chemists Pavel Dub and John Gordon spent the last few years studying how molecular catalysts work, and what they've learned could greatly improve the prospects for creating commodity chemicals from biomass. In 2001, the Nobel Prize in Chemistry was jointly awarded to three chemists, including Ryoji Noyori, who discovered a very efficient molecular catalyst for adding hydrogen atoms (hydrogenation) to molecules that contain carbon-oxygen double bonds. The catalyst contains a metal center bound to several different molecules called ligands. In this particular type of catalyst, one of the ligands contains a nitrogen atom bonded to a hydrogen atom. The efficacy of this catalyst is linked to the N-H group; it was believed that this N-H functionality facilitates the reaction by transferring a hydrogen atom.

Recent work by Dub and Gordon challenges this idea, suggesting instead that the ligand really facilitates the catalytic reaction by holding the hydrogen atom in a strong hydrogen bond interaction rather than transferring it.

"The strength of this hydrogen bonding interaction, or its absence, determines whether or not the N-H functionality is even necessary," says Gordon. Through this work, he and Dub discovered a new class of catalysts without the N-H functionality, the activity of which is comparable to Noyori-type catalysts.

How will this help create greener shampoos and plastics? Most of the biomass-derived chemicals that could be made into commodity items include carbon-oxygen double bonds that need to be hydrogenated. This hydrogenation could be done using the new catalysts in small amounts, under mild conditions, at low cost, and with operational simplicity, which raises the possibility that the new catalysts could be used on a petrochemical scale. Since scientists are looking for all possible routes to replace the entire barrel of crude oil with plant matter, this discovery could truly be a catalyst for change.

Troy Semelsberger (left) and Andrew Sutton stand alongside the continuous flow reactor developed by their team. This high-throughput environment stands to improve biofuels production by enabling more efficient chemical conversion of biomass into hydrocarbon fuels.

The team also determined that the catalyst palladium, which costs about $30 per gram, could be replaced with a type of nickel that only costs $0.08 per gram. And to address the large costs incurred separating catalysts and reagents from reactants at various steps of the process, Sutton's team found ways to streamline everything by changing some of the chemicals used—such as eliminating corrosive acids—so the separations would no longer be necessary.

A less expensive conversion process is definitely a step in the right direction, but another problem is scaling; in order to produce billions of gallons of fuel, scientists need to demonstrate how to convert biomass on a very large scale. To tackle this, Sutton and his team enlisted the help of Los Alamos engineers Bill Kubic and Troy Semelsberger to create a continuous flow reactor in which the chemical conversion could take place in a high-throughput environment more conducive to producing large amounts of fuel at a time. The flow reactor also allows the chemicals to be in constant contact with the catalysts, thus increasing efficiency.

Altogether, these improvements are advancing next-generation bio-gasoline, biodiesel, and bio-aviation fuel. Although Sutton doesn't expect cars to be running on 100 percent biofuel anytime soon, he knows it won't be long before they are using a blended combination of fuels—ethanol, bio-gasoline, and regular petrol. Making more hydrocarbon fuels from biomass would not only be good for the planet, but would also allow existing infrastructure to be used and not go to waste—meaning people could go green without having to buy a new car. And that means leaving more of Father Time's legacy untouched, which would surely make Mother Nature proud.

—Rebecca McDonald

More **biofuels research** at Los Alamos

- **Advances in algal biofuels research**
  http://www.lanl.gov/discover/publications/1663/issues-archive/january2012.pdf
- **Genomics for identifying candidate fuels**
  http://www.lanl.gov/discover/news-stories-archive/2016/February/acids-from-algae.php
- **Improving photosynthesis to increase yield for fuels and food**
  http://www.lanl.gov/discover/news-release-archive/2015/December/12.03-frontiers-in-science.php

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Ice-wedge polygons and an eroding shoreline at Cape Halkett on the Beaufort Sea coast of Alaska. Ponds sit in low-centered polygons, which are formed by subsurface ice wedges pushing the topsoil up to form ridges. When the ice wedges melt, the ridges on top of them collapse into troughs, which then drain the water from the polygon ponds and form dry, high-centered polygons surrounded by lower trough-ponds. Troughs then connect and form a drainage network, removing much of the water and permanently altering the ecosystem. Coastal erosion is also a chronic and widespread problem, posing threats to important defense and energy infrastructure, natural shoreline habitats, and nearby Native American communities. For more about Arctic climate change, see "Turmoil at the Top of the World" on page 12.

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