PHYSICS TODAY
July 2021 • volume 74, number 7
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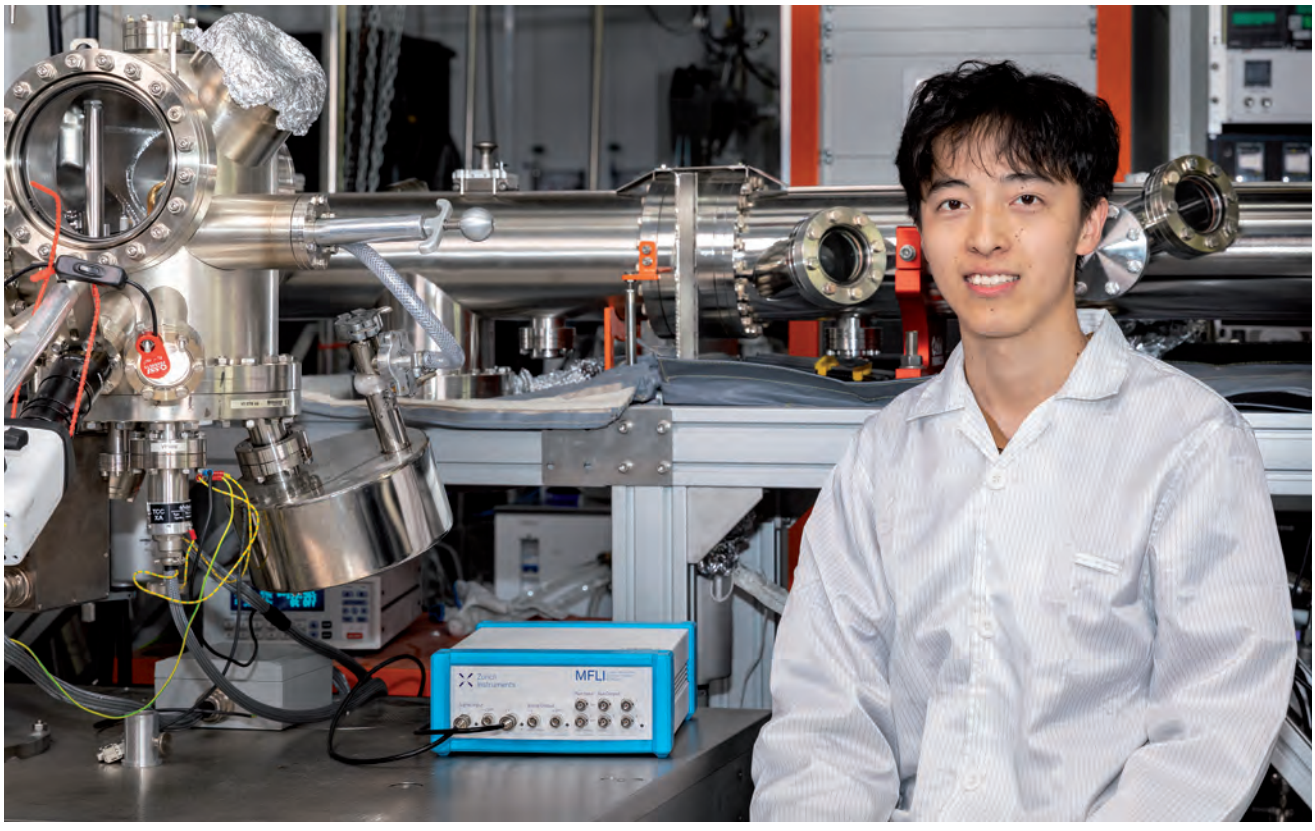
Making mining green

Macroscopic entanglement

Uranium prospecting in Russia

Lead's thick neutron skin



Yumeng Yang, Spin InfoTech Lab, ShanghaiTech University

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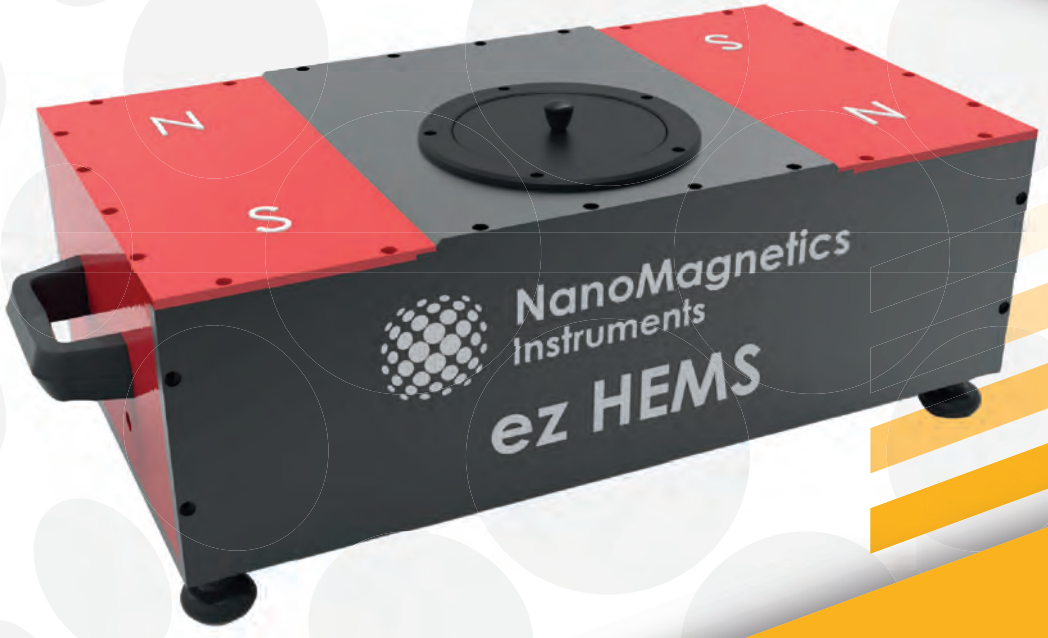

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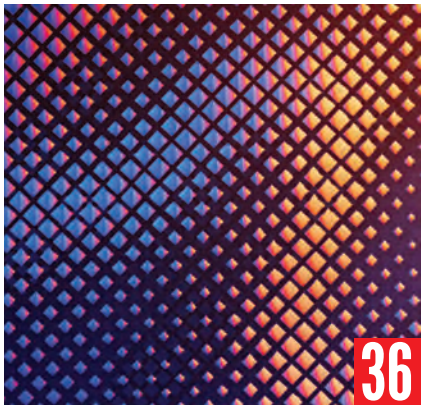

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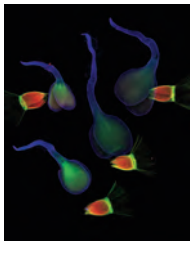
FEATURES



ON THE COVER: This x-ray fluorescence image shows chemical elements in live seedlings of the nickel hyperaccumulator plant *Berkheya coddii*. Calcium appears in red, nickel in green, and potassium in blue. Hyperaccumulators extract nickel, cobalt, and other metals from certain soils and incorporate them into their biomass. To find out how the Advanced Research Projects Agency–Energy is exploring the plants' potential to sustainably mine metals that are critical to clean-energy technologies, turn to the story on **page 24**. (Image courtesy of Antony van der Ent/University of Queensland.)

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DEPARTMENT OF ENERGY

Army microreactors

The Department of Defense is developing small nuclear reactors that can be airlifted to army bases in conflict zones. The National Academies of Sciences, Engineering, and Medicine and a nuclear nonproliferation advocacy organization have raised concerns over the program's necessity and safety.

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DENNIS WISE/UW

Women in biophysics

Among US physics PhD recipients, women are about twice as likely to do a dissertation in biophysics as men. PHYSICS TODAY's Toni Feder reports on how the field's welcoming environment, multidisciplinarity, and critical mass of women help explain the numbers.

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Press and citations

Journal editors select which of their articles to promote with additional editorial coverage and other means. A new statistical analysis of a sample of papers from *Physical Review Letters* shows that those promotional efforts are correlated with more citations.

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Terraforming Mars

Charles Day

"Thank God for Terraforming Mars!" my friend Kate told me recently. Her gratitude was directed not at the ambitious goal of making Mars human habitable but at the board game that she and I play with our respective spouses. During the pandemic, when we couldn't get together in person, we figured out a way to keep playing via Zoom. The game kept our morale buoyant.

Released in 2016 to prompt acclaim, Terraforming Mars is a game of card drafting, tableau building, and resource management. Players assume the roles of corporations whose investments and actions enable them to vie for supremacy while they work to raise the temperature and oxygen level of the Martian atmosphere and lay down cities, greeneries, and oceans on the Martian surface.

Having played the game many times, I became intrigued: How close is it to the real science of terraforming? And did that science make its way into the game, which was designed by Jacob Fryxelius?

The term "terraforming" was introduced by Jack Williamson in the short story "Collision Orbit," which appeared in the July 1942 issue of *Astounding Science-Fiction*. Scientific papers about terraforming tend to cite as the field's origin Carl Sagan's 1961 review of the atmosphere, surface, and possible biology of Venus.[1] Having concluded that the planet is likely devoid of life, Sagan went on to explore the prospect of making it habitable.

The surface of Venus is hostile to life in part because the thick carbon dioxide–rich atmosphere traps so much outgoing heat that the mean temperature is 471 °C. Sagan proposed reducing the greenhouse effect by seeding the cooler heights of the Venusian atmosphere with photosynthetic bacteria that would convert carbon dioxide into formaldehyde (CH_2O). If the bacteria sank to lower, hotter altitudes, the CH_2O in their bodies would be oxidized to carbon.

In 1965 NASA's *Mariner 4* mission to Mars confirmed that the planet's atmosphere is mostly CO_2 and that it's too thin to exert a strong greenhouse effect. The mean temperature of the Martian surface is −63 °C. Schemes to terraform Mars have tended to propose ways to boost the greenhouse effect by releasing sequestered CO_2.

Prospects seemed good at first. If Mars's polar caps were made mostly of solid CO_2, melting them would release huge, maybe planet-altering amounts of the gas. Sprinkling black dust to raise the caps' albedo was one option. But it turned out that the polar caps are made mostly of water ice. Reducing carbonate regolith or rock became the next best option.

When I searched for research on terraforming Mars, I discovered that most of the highly cited papers were from the 1980s and early 1990s. Perhaps not uncoincidentally, 1992 saw the publication of Kim Stanley Robinson's *Red Mars*, the first of three novels about humans' centuries-long project to terraform Mars. Some of the ideas in the scientific literature made it into Robinson's Mars trilogy and into Fryxelius's board game.

Among the most influential papers of that heyday was Martyn Fogg's "Terraforming: A review for environmentalists."[2] I asked Fogg via email why scientific interest in terraforming Mars had waned. He acknowledged that the broader topic of planetary engineering was, and is, on the fringe. What sustained it briefly, he told me, was the chance conjunction of a small number of keen personalities, like Sagan, who were also capable scholars. "People's interests have moved on, including mine."

In a 2018 paper, Bruce Jakosky and Christopher Edwards marshalled data from four 21st-century spacecraft that orbit Mars to conduct an inventory of all the sources of CO_2 available for terraforming Mars.[3] The pair concluded that there isn't enough. If Mars is to be made habitable, new technologies will be needed.

In his 1993 paper, Fogg advocated using terraforming Mars as an educational tool. It remains an excellent idea. To dispel the notion that terraforming is far-fetched, he demonstrated that human builders, farmers, and miners already displace more of Earth's crust than do the natural processes of erosion and weathering. Humans are already emitting more greenhouse gases than natural processes do. The amount of energy from the Sun, he calculated, is more than enough to power terraforming schemes whose feasibility is readily evaluated with an attractively interdisciplinary mix of biology, chemistry, geology, and physics.

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1. C. Sagan, *Science* **133**, 849 (1961).
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3. B. M. Jakosky, C. S. Edwards, *Nat. Astron.* **2**, 634 (2018).

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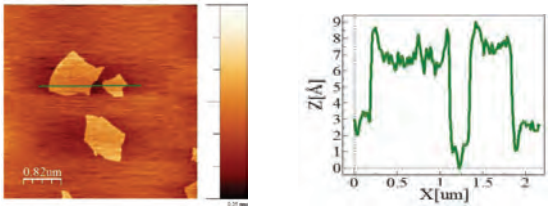

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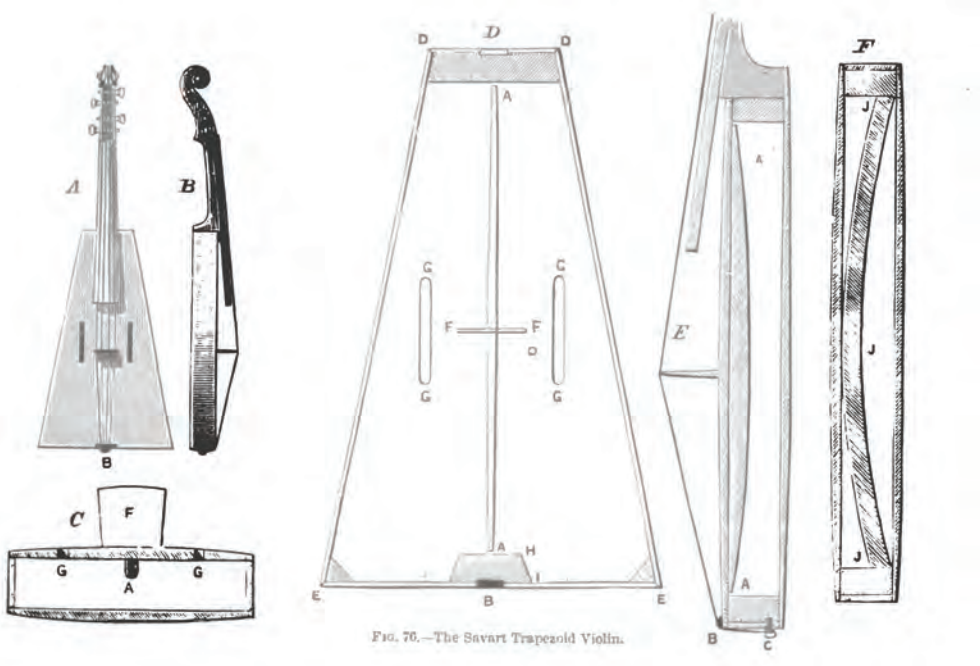
More accounts of mingling art and science

Toni Feder's excellent story "Mingling art and science opens minds" (PHYSICS TODAY, April 2021, page 24) is of special interest to me as someone who has had both a career in physics and a second career in art. Feder describes many instances where an artifact of science or of art inspires work in the other's field, and she also talks of improving dialog between those fields. But I would have liked to see stronger emphasis on the motive that drives many, if not most, scientists and artists—namely, the joy of discovery.

I was an undergraduate teacher and grant-supported physicist at Williams College for 32 years, then a sculptor for 21 years (for some examples, see www.fieldingbrown.com). The nexus between those two careers was the satisfaction I received when I actually found or did something new. When I was doing physics, that might be from a trifling bit of experimental technique or, more broadly, something publishable. When doing sculpture, it was from completing a new piece and finding it artistically pleasing.

When asked about the Nobel Prize in an interview for the BBC show *Horizon*, Richard Feynman replied, "I've already got the prize. The prize is the pleasure of finding the thing out, the kick in the discovery, the observation that other people use it [my work]—those are the real things."[1,2] So I find myself in good company regarding the joy of discovery: It must be an important part of the "mingling" of art and science.



TRAPEZOIDAL VIOLIN by Félix Savart. (Adapted from E. Heron-Allen, *Violin-Making, As It Was and Is*, E. Howe, 1914, p. 117.)

References

1. R. Feynman, *The Pleasure of Finding Things Out: The Best Short Works of Richard B. Feynman*, J. Robbins, ed., Perseus Books (1999), p. 12.
2. A. Lightman, *Probable Impossibilities: Musings on Beginnings and Endings*, Pantheon Books (2021), p. 77.

Fielding Brown
Westwood, Massachusetts

In her article "Mingling art and science opens minds" (PHYSICS TODAY, April 2021, page 24), Toni Feder mentions many interesting intersections between visual art and science. In 1819 physicist Félix Savart (1791–1841) said, "The efforts of scientists and those of artists are going to unite to bring to perfection an art that, for so long, has been limited to blind routine."[1]

Savart is best known to physicists through the Biot–Savart law in electromagnetism. He is, however, also known for studying the acoustics of violins.[2] His friendship with luthier Jean-Baptiste Vuillaume (1798–1875) provided Savart with opportunities to investigate instruments made by Antonio Stradivari (ca. 1644–1737). Savart started asking how we could understand the performance of a violin from the plates before they are assembled.[3] He even made a trapezoidal violin (see the sketches above) whose acoustics proved that the instrument's characteristic shape serves only aesthetic purposes. For him the art is about the violin.

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Julian Ting
(juhilian@gmail.com)
De-Font Institute for Advanced Studies
Taichung, Taiwan

Physicists' real-world contributions

Rajan Menon's letter "Nobels neglect fluid dynamics" (PHYSICS TODAY, January 2021, page 10) correctly points out how the importance of physicists' real-world contributions have been undervalued in the physics community. Many physicists apparently have the misunderstanding that finding elementary forces among particles solves the world's problems. The reality is far from it.

Since Isaac Newton's time, it's been well known that the three-body system cannot be solved analytically, and numerical approaches can lead to chaos. The real world consists of infinitely many–body systems whose temporal evolution is intrinsically unsolvable. Even for the simplest hydrodynamics systems, the Navier–Stokes equation, which is only an approximate model, is not solvable. Plasmas are much more rich in their time evolution, and a large number of fundamental discoveries in that area have not been properly appreciated in the physics community. Some unexpected discoveries in nonlinear continuous media certainly deserve higher valuation in terms of their real-world contributions; conspicuous examples include the applications of optical solitons in high-speed transcontinental communications and the influence that self-organization of plasma turbulence has had on fusion confinement.

So far the only reliable universal law of physics in nonlinearly interacting many-body systems remains the second law of thermodynamics, which states that the entropy of an isolated system will not spontaneously decrease. That law's unique stature simply shows that a real physical system is unpredictable, so any new discoveries that go against the entropy law for at least a limited period of time deserve more attention. For example, in quasi-two-dimensional hydrodynamics systems, such as planetary atmospheres, a quantity called the enstrophy (the squared vorticity) is conserved in addition to the total energy, and the entropy can be defined with regard to either the uncertainty in the energy spectrum or the uncertainty in the enstrophy spectrum. The maximum-entropy state of enstrophy can lead to ordered structure in the energy spectrum and to nontrivial states such as zonal flows observed on the Jovian surface.

Akira Hasegawa
(a.hasegawa@solitoncomm.com)
Osaka University
Suita, Japan

Tales in tech transfer

I was pleased to see Toni Feder's piece in the February 2021 issue of PHYSICS TODAY on technology transfer (page 24). I have held tech transfer positions in industry and academia for more than 20 years. Tech transfer has been a very satisfying career for me. Moreover, it is a field that is particularly well suited to my background as an experimental physicist.

When speaking to physics students about my career, I like to tell the story of my time as a member of a team that included experienced engineers. We were fortunate enough to be inundated with projects across a broad spectrum of technologies. Although I was self-conscious about my lack of deep technical knowledge compared with my colleagues with traditional engineering backgrounds, I was very pleased to hear the way our boss would describe our team: "When we have a silicon invention, we give it to our silicon expert. When we have a photonics invention, we give it to our photonics expert. And when we don't have any expertise in an invention, we give it to our physicist."

I have found that the strong fundamentals and "outside the box" problem solving that I developed in my physics training have enabled me to come "up to speed" quickly across a broad range of inventions that run the gamut from nerve-regeneration devices to pollutant-capture technologies to high-performance concrete compositions and beyond. That flexibility is a vital skill for a tech transfer professional.

David Zimmerman
(dzimmer3@stevens.edu)
Stevens Institute of Technology
Hoboken, New Jersey

Correction

May 2021, page 27—The building in the photo is erroneously identified as Cambridge University's Cavendish Laboratory. In fact, in Ernest Rutherford's day, the photographed building housed the department of engineering's Electrical Laboratory, which was later subsumed into the department of physical chemistry. Today the building houses the department of history and philosophy of science and the Whipple Museum of the History of Science. Below is the actual entrance to the Cavendish. (Photo by R. T. Phillips.) PT

Lead-208 nuclei have thick skins

A precise measurement of the nucleons' radial extent constrains models of dense nuclear matter.

In studies of nuclear structure, lead-208 is special. It has a whopping 44 more neutrons than protons, but unlike most other neutron-rich isotopes, it's stable and doubly magic—both its proton and neutron numbers, 82 and 126 respectively, correspond to full nuclear energy shells. Each nucleon type thus forms a sphere of nearly constant density.

The radius R_p of the proton distribution in an atomic nucleus is straightforward to measure using electron scattering. But because neutrons lack electric charge, an atom's neutron-distribution radius R_n is much trickier to probe. Models indicate that the extra neutrons in ^{208}Pb extend beyond R_p, and the difference between the two radii—the neutron-skin thickness—depends on just how hard the extra neutrons push back against being crammed in tightly among the protons.

The Lead Radius Experiment (PREX) at the Thomas Jefferson National Accelerator Facility in Newport News, Virginia, was designed to directly measure the neutron-skin thickness of ^{208}Pb. The collaboration's first analysis,[1] published in 2012, found $R_n - R_p = 0.33\ ^{+0.16}_{-0.18}$ fm. That result was twice the 0.15–0.18 fm range that was generally expected. But the measurement's large error bars left room for doubt.

Now the researchers have reduced the measurement uncertainty by more than half. The new result, $R_n - R_p = 0.283 \pm 0.071$ fm, corroborates the researchers' initial finding of a thick neutron skin and challenges existing models of neutron-rich matter.[2]

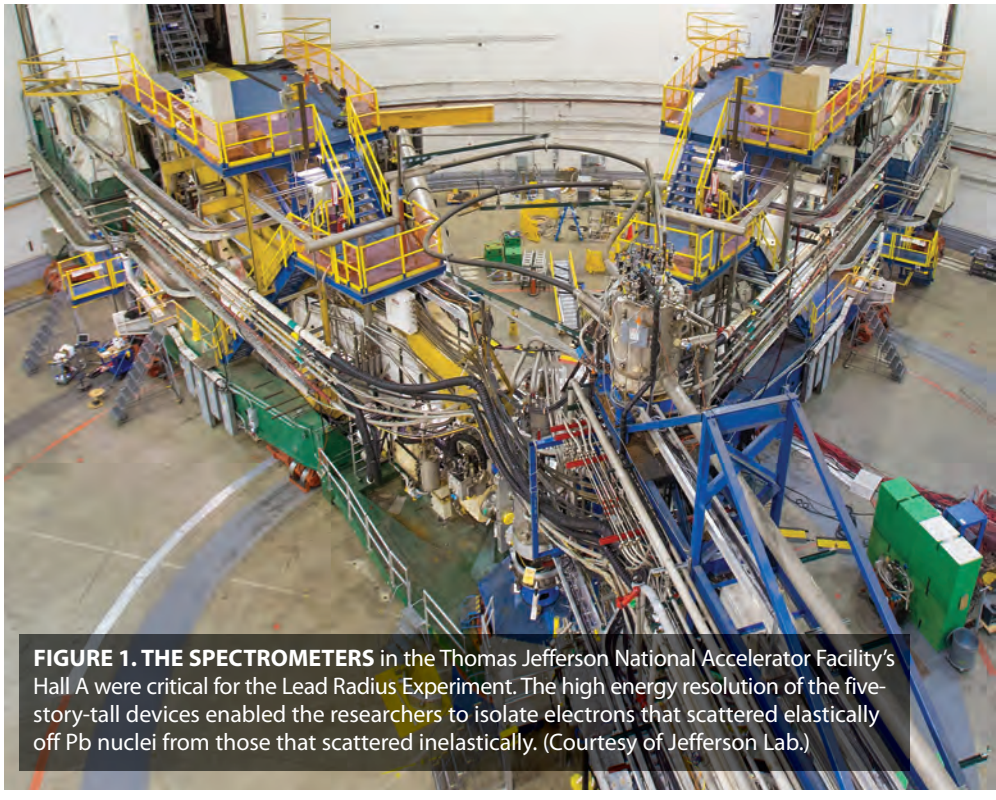

FIGURE 1. THE SPECTROMETERS in the Thomas Jefferson National Accelerator Facility's Hall A were critical for the Lead Radius Experiment. The high energy resolution of the five-story-tall devices enabled the researchers to isolate electrons that scattered elastically off Pb nuclei from those that scattered inelastically. (Courtesy of Jefferson Lab.)

Skewed scattering

Studying the distribution of neutrons in a nucleus requires a probe that is sensitive to the neutral particles. Earlier experiments used hadrons, such as pions and protons, that interact with neutrons through the same strong force that holds nuclei together. But those scattering events typically involved multiple interactions between the probe and the target, and the resulting neutron-skin values were therefore highly model dependent.

PREX's measurements rely on the weak force's contribution to electron–nucleus scattering. The upside of using electrons is that their interactions with nuclei are easier to interpret because they don't interact through the strong nuclear force. And weak scattering off nuclei is dominated by neutron contributions because, compared with the proton, the neutron couples to the weak force an order of magnitude more strongly.

The challenge, however, is that electrons scatter off nuclei primarily through their electromagnetic interaction with protons. At the energies relevant for probing nuclear structure, electromagnetic-scattering cross sections are about 10^{12} times as large as weak-scattering ones.

To disentangle neutron-dominated weak scattering from the proton-dominated electromagnetic contribution, PREX took advantage of an asymmetry in weak scattering that doesn't affect electromagnetic scattering. When an electron scatters elastically off a neutron by exchanging a weak-force-mediating Z^0 boson, the exchange depends on chirality. All other things being equal, right-handed electrons—those whose spins are aligned with their direction of motion—scatter off Pb nuclei more often than left-handed ones whose spins are antialigned. Data collection therefore entailed flipping the polarization of an incident electron beam and measuring the slight difference in the number of scattered electrons over millions of cycles.

PREX conducted both of its runs in Jefferson Lab's Hall A, shown in figure 1. The facility's high-resolution spectrometer was critical for isolating the elastically scattered 1 GeV electrons, which leave the nucleus in its ground state, from inelastically scattered ones that excite it. In the PREX setup, the energy difference can be as small as 3 MeV. A magnetic field in the spectrometer sorts the electrons by energy, and that tiny energy difference man-

ifests as a spatial separation of about 5 cm at the top of the five-story-tall device.

The first PREX run in 2010 was successful enough to yield a measurement, but it also uncovered some unexpected experimental challenges. The researchers discovered, for example, that over the course of a few days, the incident electron beam degraded the Pb target. Although the soft metal was cooled to 20 K, it still melted and deformed under the beam's bombardment. Small nonuniformities in the target thickness vary the scattering rate, and over the course of the experiment they eventually generated enough noise to swamp the tiny weak-scattering signal.

The PREX researchers found that they could significantly reduce the sensitivity to target-thickness variations by synchronizing the scattering-rate measurements with the back-and-forth motion of the beam as it sampled different areas on the target. That technique was used for their second run in 2019, and they made extra targets so each one could be switched out as soon as it showed signs of degradation. Those improvements proved crucial for gathering enough data, plotted in figure 2, to precisely measure R_n.

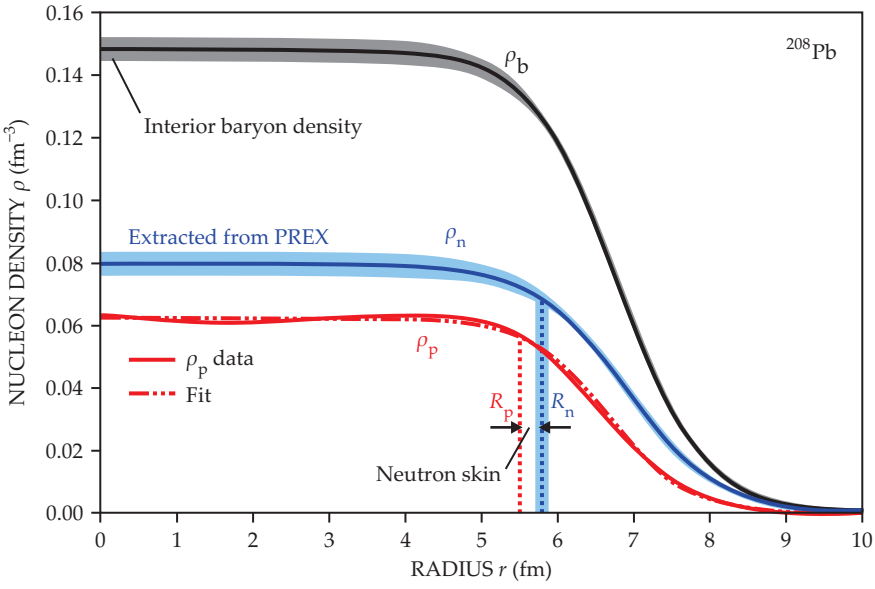

FIGURE 2. A LEAD-208 NUCLEUS has nearly constant interior densities of protons (ρ_p) and neutrons (ρ_n). The nuclide has 44 more neutrons than protons, and because the additional neutrons push back against being squeezed in with the protons, the neutron distribution extends beyond that of the proton one. The difference between the two radial extents is the neutron-skin thickness. Its measured value of $R_n - R_p = 0.283 \pm 0.071$ fm is larger than the 0.15–0.18 fm that most researchers expected. (Adapted from ref. 2.)

Ad astra

The size of the neutron sphere in ^{208}Pb is set by a balance between surface tension, which favors a compact configuration, and symmetry pressure, an outward push caused by having more neutrons than protons. The competition between those forces is captured in the nuclear equation of state, which relates the density of nuclear matter to the outward pressure it generates.

Physicists studying atomic nuclei aren't the only ones interested in pinning down the equation of state for neutron-rich matter. "That's the holy grail of nuclear astrophysics," says Krishna Kumar, a professor at the University of Massachusetts Amherst and a member of the PREX collaboration. The equation is also important for describing neutron stars because the same symmetry pressure that determines R_n in a nucleus also supports the stars against collapse. (For more about the connection, see the article by Jorge Piekarewicz and Farrukh Fattoyev, PHYSICS TODAY, July 2019, page 30.)

Atomic nuclei have core nucleon densities around 0.15 fm^{-3}, whereas neutron stars can reach several times that density; they constitute the densest stable matter in the universe. Theoretical descriptions of neutron-rich matter connect the disparately sized systems by predicting how symmetry pressure changes with density. Although the descriptions are consistent with all well-understood observables, they accommodate a range of neutron-skin thicknesses and neutron star properties.

The new PREX result further constrains theoretical models, and "there are relatively few models that would be comfortable describing a 0.28-femtometer neutron skin with all the other data they have," says Kent Paschke, a professor at the University of Virginia and a member of the PREX collaboration. Such a thick neutron skin would indicate a strong symmetry pressure, so a neutron star of a given mass would be larger and less dense than many predictions.[3] It also suggests that neutron stars might contain a higher fraction of protons than previously thought, which could trigger an enhanced cooling process at smaller-than-expected stellar masses.

NASA's Neutron Star Interior Composition Explorer (NICER), an x-ray spectrometer mounted on the International Space Station, is measuring the masses and radii of the dense structures.[4] So far, the NICER data are consistent with a ^{208}Pb neutron-skin thickness of up to about 0.31 fm, although they would also have been consistent with a thinner skin in the predicted range. Together, the NICER and PREX data sets rule out a handful of models.

Gravitational-wave data throw a wrench in the machinery. Observations by the LIGO (Laser Interferometer Gravitational-Wave Observatory) and Virgo collaborations of a merging binary neutron star system yielded a measurement of the stars' tidal deformability, a parameter that describes how much each one could be stretched by the other's gravitational pull.[5] That measurement points to a decidedly smaller neutron-skin thickness that would lie more than one standard deviation below the PREX measurement.

The disagreement, though, doesn't cast doubt on PREX's measurement of the neutron-skin thickness. "The power of our technique is the cleanliness of the interpretation and the fact that we are statistics limited," says Kumar. Detection of a few more neutron star mergers would help clarify whether the discrepancy is real. If it is, "then you start to question all kinds of assumptions about how you go from neutron-skin to neutron star observables," says Paschke.

Existing theories suggest that the properties of dense nuclear matter can

be extrapolated from the average density of about 0.1 fm^{-3} found in ^{208}Pb to the 0.3–0.6 fm^{-3} of neutron stars, but the situation might not be so straightforward. For example, the material could undergo a phase transition. Superfluid and superconducting phases are thought to exist inside neutron stars, but the phases' dynamics are poorly understood. Some researchers have speculated that the environment could support a fluid of deconfined quarks or even host hyperons, which are baryons that contain the usually unstable strange quark.

Tighter constraint

A more precise measurement of the neutron-skin thickness would help clarify the connection between atomic nuclei and neutron stars, but PREX has reached its limit. There's no way PREX could get an entire year of run time at Jefferson Lab, which is what it would need to appreciably improve its measurement precision. A new dedicated facility in Germany, the Mainz Radius Experiment (MREX), is its planned successor. In addition to enjoying longer run times, MREX will be able to capture and isolate elastically scattered electrons at a higher rate using a purpose-built spectrometer.

With its targeted design, MREX is expected to shrink the uncertainty of the ^{208}Pb neutron-skin-thickness measurement by a factor of two. But, according to Paschke, the experiment's start is likely at least five years away. In the meantime, the NICER and LIGO–Virgo collaborations will continue generating data to inform evolving models, and theorists have their work cut out for them.

Christine Middleton

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A microscope for measuring surface acidity

An atomic tug-of-war offers a rare insight into the chemistry of complex environments.

Atoms and molecules, the invisible building blocks of everything around us, quickly become complicated as their size and numbers increase. A molecule of just two atoms can occupy any of a multitude of rotational, vibrational, and electronic quantum states, each with potentially different behavior in a chemical reaction. With lasers and molecular beams, physical chemists can prepare and probe many of those states individually and thus dissect the dynamics of a gas-phase molecular reaction in exquisite detail.

But when a reaction takes place on a solid surface—a common scenario in industrial catalysis, materials science, and geology—it's much more of a black box. Because every atom on a rough, irregular surface is situated a little bit differently, they can have dramatically different reactivities, even to the point of steering the reaction toward different sets of products (see PHYSICS TODAY, September 2018, page 17).

Those chemical distinctions among surface sites are extremely difficult to assess directly. Experiments usually measure only the average reaction output for the whole surface; they can't readily track individual reactant molecules to see where on the surface they reacted. Re-

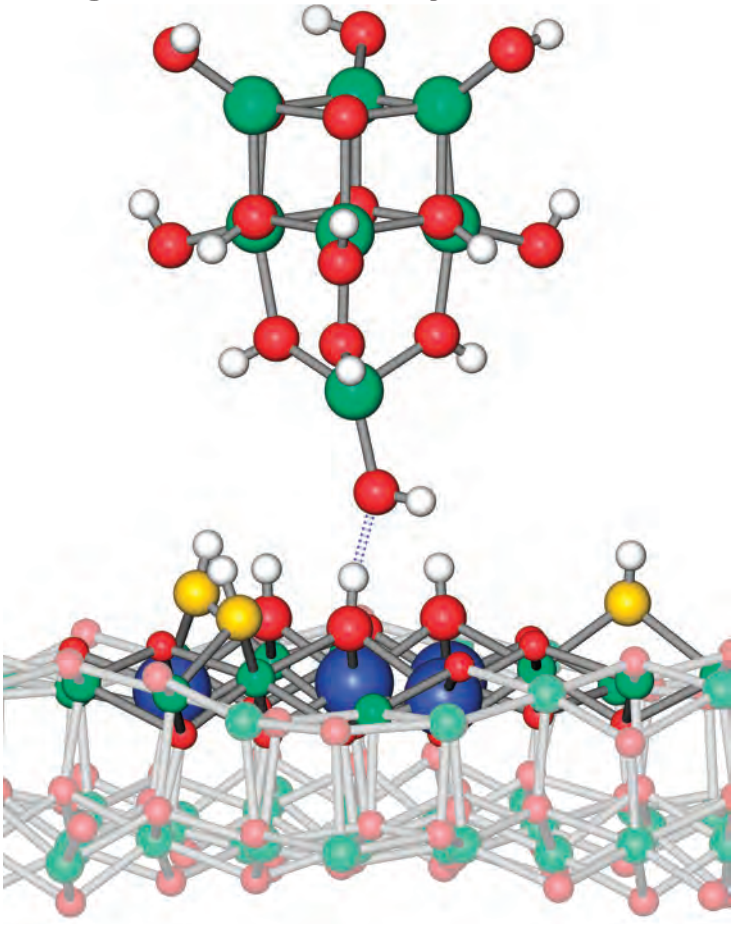

FIGURE 1. ACIDITY MICROSCOPE. When an atomic force microscope tip made of hydroxylated indium oxide descends toward a surface of the same material, the oxygen atom at the end of the tip feels an attractive force (dotted line) to a hydrogen atom on the surface below it. The force is related to the surface site's acidity: how readily it releases its H atom in a chemical reaction. Indium atoms are shown in green and blue, O atoms from adsorbed water in yellow, other O atoms in red, and H atoms in white. (Adapted from ref. 1.)

searchers are therefore limited in their ability to rationally design new solid catalysts, counteract corrosion on metal surfaces, and understand the weathering of rocks and minerals.

Now the Technical University of Vienna's Ulrike Diebold, her postdoc Margareta Wagner, and their colleagues have adapted an atomic force microscope (AFM) to map a surface chemical property—proton affinity, otherwise known as acidity—with atomic resolution.[1]

Acid–base chemistry—the transfer of an H^+ ion from one molecule or surface site to another—is a fundamental feature of many reactions, and surface reactions are no exception. (For just one example, in the catalytic cracking of hydrocarbons, a solid catalyst needs to transfer protons from its surface to fill out the newly severed C–C bonds.) By separately measuring how readily each site attracts and releases protons, the researchers offer an unprecedented look at the sites' respective roles in such a reaction.

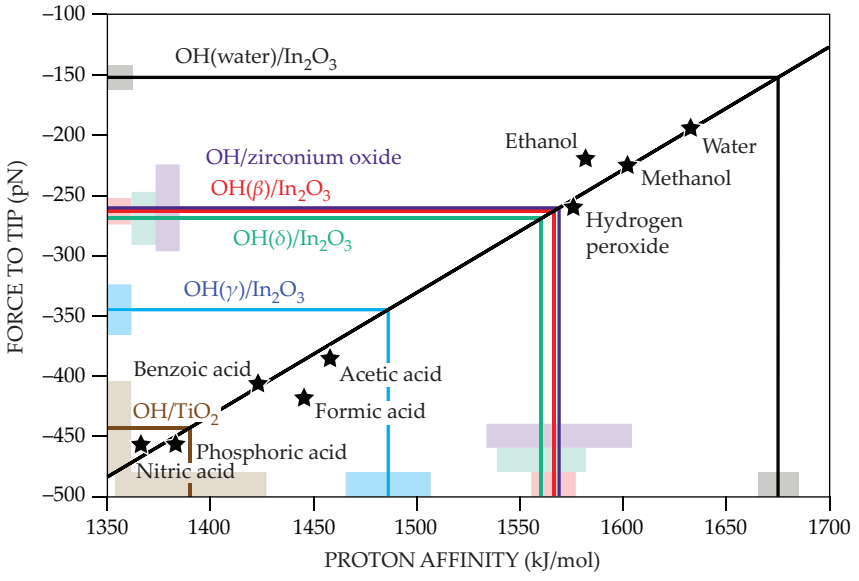

FIGURE 2. THE QUANTITATIVE RELATIONSHIP between proton affinity and atomic-force-microscopy (AFM) forces is derived from a series of density functional theory calculations on molecules of known acidity (black stars). The best-fit calibration line can then be used to convert measured AFM forces to proton affinities for surface sites. So far, proton affinities have been found for three oxygen sites on indium oxide (red, green, and blue), water adsorbed on indium oxide (black), and oxygen sites on zirconium oxide (purple) and titanium dioxide (brown). The shaded blocks represent the surface measurements' error bars. (Adapted from ref. 1.)

Oxygen sites

Like many discoveries, the work grew out of research with a much different initial direction. Diebold, Wagner, and colleagues were studying water adsorption on surfaces of indium oxide. When doped with tin, In_2O_3 has the valuable combination of optical transparency and electrical conductivity, so it's commonly used to make the top electrodes in solar cells and liquid-crystal displays. In its undoped form, it's a transparent semiconductor used in some types of coatings. The Vienna researchers wanted to explore whether or how the material's properties change when H_2O clings to its surface.

Given its simple chemical formula, In_2O_3 has a surprisingly complicated structure. Each O atom is surrounded by four In atoms, but all four of those O–In bonds have different lengths. At a crystal surface, O atoms can occupy four geometrically (and potentially chemically) distinct sites—denoted by α, β, γ, and δ—depending on which of the four bonds is missing. Furthermore, some surface In atoms are surrounded by six O atoms, just as they are in the bulk, and some are surrounded by five.

In previous work, Diebold and colleagues observed[2] that when a molecule of H_2O sticks to the In_2O_3 surface, it breaks apart into OH and H. The OH situates itself atop the oxide surface, with the O atom bridging two of the fivefold-coordinated In atoms and the H protruding upward. The split-off H then binds to a neighboring O atom on the oxide surface, which happens to always be one of the β sites.

The OH from the water molecule pokes higher above the surface than the OH on the β oxide site. "Initially we wanted to know if we could see the height difference with our AFM," says Wagner. "That does not sound very spectacular, I admit." But then they noticed something odd. The forces between the AFM tip and the OH differed markedly for the two types of OH site. For the water OH, the maximum force of attraction felt by the tip was around 150 pN; for the β oxide OH, it reached more than 250 pN.

When the researchers used the AFM tip to nudge the H atoms to different oxide O sites, they found that those sites, too, had their own characteristic attractions to the tip: 270 pN for an OH on a δ site, almost 350 pN for one on a γ site. (The α site proved too difficult to access and wasn't part of their analysis.)

What's more, those values were surprisingly reproducible, even across different experiments that used different AFM tips. "Usually, the chemical makeup of a tip—the atom or atoms at the tip's apex that interact with the surface—is a big unknown in techniques like this, unless you functionalize the tip on purpose," explains Wagner. "And chemically different tips can result in forces that differ by a factor of 2 to 10." The tips appeared to be chemically identical, even though the researchers weren't doing anything special to ensure that they were.

From forces to acidity

To find out what was going on, the experimenters turned to Bernd Meyer, a theorist at Friedrich–Alexander University Erlangen–Nuremberg. With density functional theory, Meyer calculated the forces between the OH groups on the surface and several hypothetical model AFM tips.

The best match to the experimental results came from a model tip, shown in figure 1, made of hydroxylated In_2O_3—the same material as the surface. In retrospect, it made sense: Tip-preparation procedures often end up transferring some material from the surface onto the tip, and the experimenters always prepared their tip over the In_2O_3 surface. "And it turned out to be the perfect tip for these experiments," says Diebold. "Once we realized that, we prepared the tip that way deliberately."

As figure 1 shows, the In_2O_3 tip has an OH group dangling from the end. As the

O atom on the tip approaches a surface-bound H atom, the two experience an attractive force, represented by the dotted line in the figure. The attraction sets up a tug-of-war for the H atom between the tip and the surface.

The tip always loses the battle: The terminal O atom already has one H atom bound to it, so the attraction it feels to a second H is weaker than the chemical bond holding the H to the surface. In fact, the more strongly the H clings to the surface O atom, the more weakly it's attracted to the tip.

To relate the AFM force measurements to conventional notions of acidity, Meyer had the idea to calculate the force between the model tip and the H atoms of a suite of small molecules whose acidities are known. From those calculations, he derived a linear calibration, shown in figure 2, that relates the AFM force to proton affinity—how strongly each molecule holds on to its H atom rather than releasing it as an H^+ ion into the surrounding solution. A more attractive (that is, more negative) force to the AFM tip corresponds to a lower proton affinity and thus a higher acidity: All the molecules with "acid" in their names are clustered in the lower left corner of the figure.

The calibration line makes it possible to convert the measured AFM forces on a surface to proton affinities for each surface site. The water OH site, as plotted in black, is the least acidic site on the In_2O_3 surface; the γ site, as plotted in blue, is the most. Using the same In_2O_3 AFM tips, the researchers have begun extending their measurements to other surfaces, including titanium dioxide (brown) and zirconium oxide (purple).

So far they've studied only regular surfaces with just one or a few types of surface O sites. Eventually, though, they want to look at surfaces with steps, defects, and impurities to see how those features affect surface chemistry. "The next big open challenge," says Diebold, "is to do all the same measurements in liquid water."

Johanna Miller

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Macroscopic systems can be controllably entangled and limitlessly measured

Two oscillating membranes demonstrate correlations forbidden by classical physics.

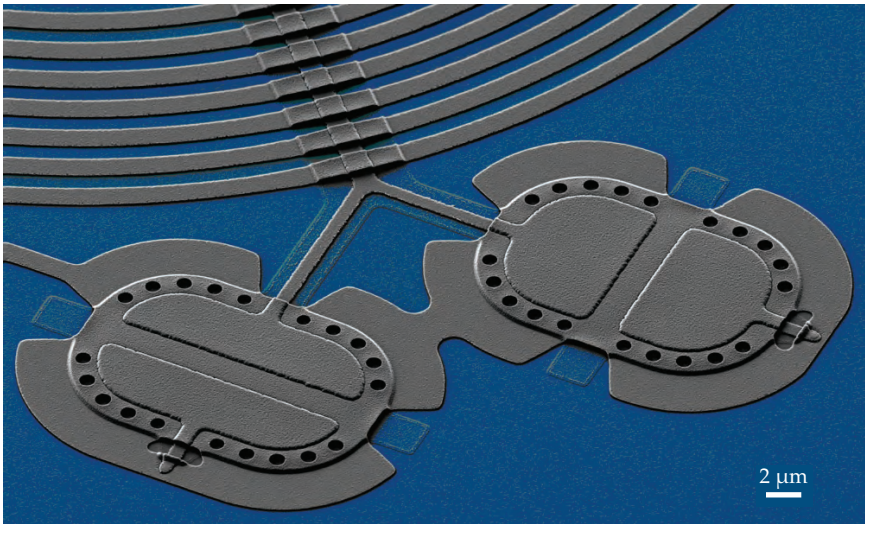

FIGURE 1. ALUMINUM DRUM membranes suspended above a sapphire substrate vibrate in a direction perpendicular to it. Each membrane forms the top plate of a capacitor, while the bottom plate is fixed to the substrate. A spiral inductor links the capacitors to form a microwave cavity. Radiation pressure from microwave pulses that impinge on the cavity drives the two membranes' oscillations to an entangled state. (Image courtesy of Florent Lecocq and Shlomi Kotler/NIST.)

What Albert Einstein skeptically referred to as "spooky action at a distance" has turned out to be one of the most important drivers of quantum technology. That spooky action, or entanglement, describes a phenomenon in which measuring the state of one particle instantaneously generates effects on another particle. The entangled particles' measurable properties are so strongly correlated that the relationship can't, statistically, have happened by chance or be explained by classical physics.

Although quantum effects are most easily observed in tiny objects, quantum mechanics is not limited to the atomic scale. In principle, objects of all sizes should behave according to quantum mechanics. But at the macroscale, quantum effects are all but impossible to detect because of limits of modern measurement tools and the tendency of larger objects to interact with noisy environments.

To bridge the gap between our daily classical experience and our expectation that quantum mechanics is universally valid, experimentalists seek quantum phenomena on larger systems. Pushing the envelope on systems in which quantum effects are observable could eventually reveal whether quantum theory does have a physical boundary.

Two research groups now report direct verification of macroscopic quantum effects that cannot be described by classical physics. In one paper, Shlomi Kotler, now at the Hebrew University of Jerusalem, and his colleagues at NIST in Boulder, Colorado, deterministically generated and directly measured the correlations needed to verify entanglement between separate macroscale mechanical objects.[1] In the other, Laure Mercier de Lépinay and her colleagues at Aalto University in Finland developed a similar system in which they could make quantum measurements that appeared to be at odds with fundamental limits associated with the Heisenberg uncertainty principle.[2]

Both sets of experiments involved pairs of micrometer-scale drumhead membranes that oscillate together in near-perfect synchronization. That scale is large compared with the atomic-scale systems in which quantum effects are usually observed. Besides enlarging quantum theory's observed realm, those effects—and the ability to manipulate and detect them—could also lead to new designs for logic gates and enhanced measurement techniques.

Mechanical revolution

Quantum effects are most readily observable in atoms and subatomic particles. For example, excited atoms can decay by emitting two photons within nanoseconds of each other. When those photons are emitted in opposite directions, conservation of angular momentum requires that their polarizations be correlated. Knowing one's polarization provides irrefutable information about the other's: the two photons are entangled.

Other strategies can be used to entangle physically distant atomic particles. Holding pairs of ions in traps and exciting them to a state from which they emit oppositely polarized photons causes the ions to end up in two different states. If the two photons are detected simultaneously, measuring the emitted light reveals one ion's resulting energy state, which must be opposite to that of the other ion. (See PHYSICS TODAY, November 2007, page 16.)

Entanglement has also been demonstrated in systems with mechanical degrees of freedom. In 2009 NIST researchers demonstrated entanglement in a pair of atomic-scale mechanical oscillators.[3] Pairs of vibrating ions, kicked into motion by a laser beam, behaved like two balls connected by a spring. The pairs vibrated in perfect unison, even when separated in space. That entangled behavior resulted from utilizing the ions' internal spin states.

But what about a much bigger mechanical oscillator, one with trillions of atoms? Experiments that use vibrating micron-scale membranes, fabricated as part of separate cavities and set into motion by microwave- and optical-frequency radiation, have already shown evidence of entanglement.[4,5] Photons scattered off the resonators and captured by detectors or made to interfere with each other match what would be expected if the vibrations were perfectly correlated. But unlike the new work, those experiments were either nondeterministic or they relied on complicated inferences and ad hoc subtraction of noise from amplifiers used as part of the readout.

Different drum

Deterministically producing and directly verifying entanglement in a system that's much larger than atom-scale, without relying on complicated inferences, is a different ballgame. Kotler, working with John Teufel and other colleagues at NIST, fabricated two oblong 10-μm-long aluminum drumhead membranes that were connected via a resonant cavity, as shown in figure 1. Each membrane was effectively a plate in a vibrating capacitor, coupled to a microwave-frequency AC circuit.

Two incident microwave pulses cooled the devices and steered them into synchronized oscillations. The pulses were generated at two different frequencies that inextricably linked the membranes. Had the membranes responded independently to the pulses, one would have heated up and the other would have Doppler cooled. Instead, one membrane's interaction with photons generated by the other's oscillation created entangled motion.

The motion mimicked that of two pendulums swinging with equal amplitude and opposite velocity, depicted in figure 2a. "They're tiny trampolines. Each one can go up and down. The name of the game is to synchronize their motions perfectly," says Kotler. (See the article by Keith Schwab and Michael Roukes, PHYSICS TODAY, July 2005, page 36.)

When another microwave pulse was incident on the oscillating membranes, the reflected light was Doppler shifted in a way that carried information about each membrane's position and momentum. By amplifying the readout signal immediately on its exit from the device, Kotler and his colleagues ensured that the measured signal could be clearly distinguished from noise.

Unsurprisingly, a single measurement of a pulse-driven oscillation did not show any clear connection between the two membranes. But by repeating the experiment 10 000 times and charting the evolution of the membranes' movements, the researchers found that the instantaneous positions tracked one another with precision beyond the threshold

permitted by classical physics. That perfect correlation, plotted in figure 2b, is a hallmark of quantum entanglement. "This shows both that these kinds of large mechanical systems can be controllably entangled and measured with high enough precision to directly see the entanglement," says Aashish Clerk of the University of Chicago.

Virtual measurements

Simultaneously measuring the position and momentum of an object should be impossible. According to Heisenberg's uncertainty principle, precisely observing an object's position has a perturbing effect on the object's momentum. That perturbation, called quantum back action, places a limit on how precisely position may continuously be measured. Might that quantum limit be evaded in a mechanical system?

To find out, Mercier de Lépinay and her colleagues also created entangled aluminum membranes. Their approach was to create a single virtual oscillator from two vibrating membranes, housed in separate microwave cavities. The membranes' stable entangled motion was driven collectively by microwave beams. Microwave beams of slightly different frequencies ensured that the oscillating membranes in each cavity moved in a coordinated but not identical way, vibrating in opposite phase to each other.

The motion of the membranes mimicked that of two objects, one with an effective negative mass, each attached to a coiled spring and coupled to a cavity. The coupling between the entangled membranes caused their momenta to change by the same magnitude when the same force was applied to both. However, because of its negative mass, one of the oscillators was displaced in the opposite direction. The result was an effective single harmonic oscillator that was delocalized from the component oscillators and whose position and momentum commuted with one another.[6]

By treating the membranes as a single virtual entity, the researchers could make direct observations of the entangled system without destroying its state. The uncertainty associated with each membrane canceled out, or was hidden in the part of the system that wasn't directly observed—the momenta of the individual membranes. "The uncertainty principle holds for one degree of freedom, and it is a law of nature. We can bypass it in a multimode system," says Mika Sillanpää, also of Aalto University.

Observing the single virtual oscillator allowed for complete measurement of its position while ensuring that quantum back action did not disturb the system's overall state or destroy its entanglement. "This is the first experiment to realize this kind of physics using only mechanical degrees of freedom," says Clerk.

Future tech

The Aalto team's virtual system is what's known as a quantum mechanics–free subsystem. It provides a possible path toward measuring extremely weak classical forces that act on the system, while circumventing the measurement limits imposed by quantum mechanics. The measurement technique could be applied to develop sensors that exceed the abilities of their classical counterparts.

The NIST team's pulse-driven entangled system could be further developed into an information-processing system, with each membrane pair serving as a qubit. Doing so would require ensuring that a measurement clearly stands out above the noise. For two membrane pairs, applying a multistep logic protocol in which one step depends on the outcome of the previous step would demonstrate that each logic gate measures above the system's noise and advances to the next step in a useful manner, according to Kotler. Eventually, combining multiple membrane pairs linked by wires could lead to a quantum processor based on entanglement.

Compared with atomic devices, the vibrating membrane platform can be easily manufactured and manipulated. It provides a tool for exploring the limits of quantum phenomena and creating useful devices at the macroscale.

Rachel Berkowitz

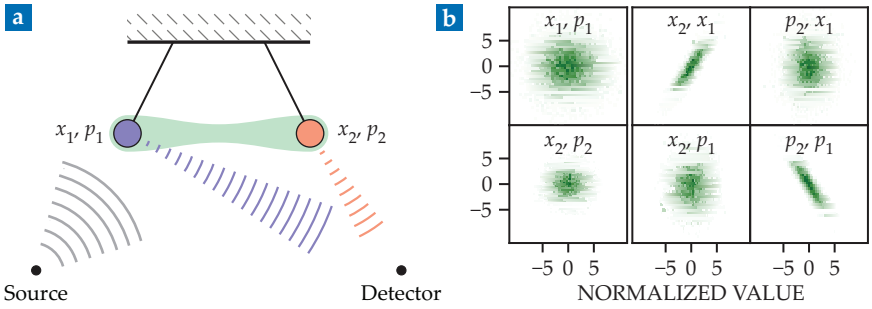

FIGURE 2. MECHANICAL OSCILLATORS in an entangled state, like the ones shown in figure 1, mimic the motion of two pendulums. **(a)** Microwave radiation, Doppler-shifted as it reflects off the pendulums, carries information about each oscillator's position (x_1 and x_2) and momentum (p_1 and p_2) and verifies the entangled state (green shaded region). **(b)** Full tomography directly shows the entangled state of macroscopic mechanical objects. A 10 000-repetition experiment that sets the membranes into entangled motion reveals the membranes' strongly correlated positions (x_1, x_2) and anticorrelated momenta (p_1, p_2). Each membrane's individual state (x, p) is consistent with a Gaussian distribution having large variance, which indicates that energy has been added to the system. Variables are normalized so that the ground state of each membrane has variance ½. (Adapted from ref. 1.)

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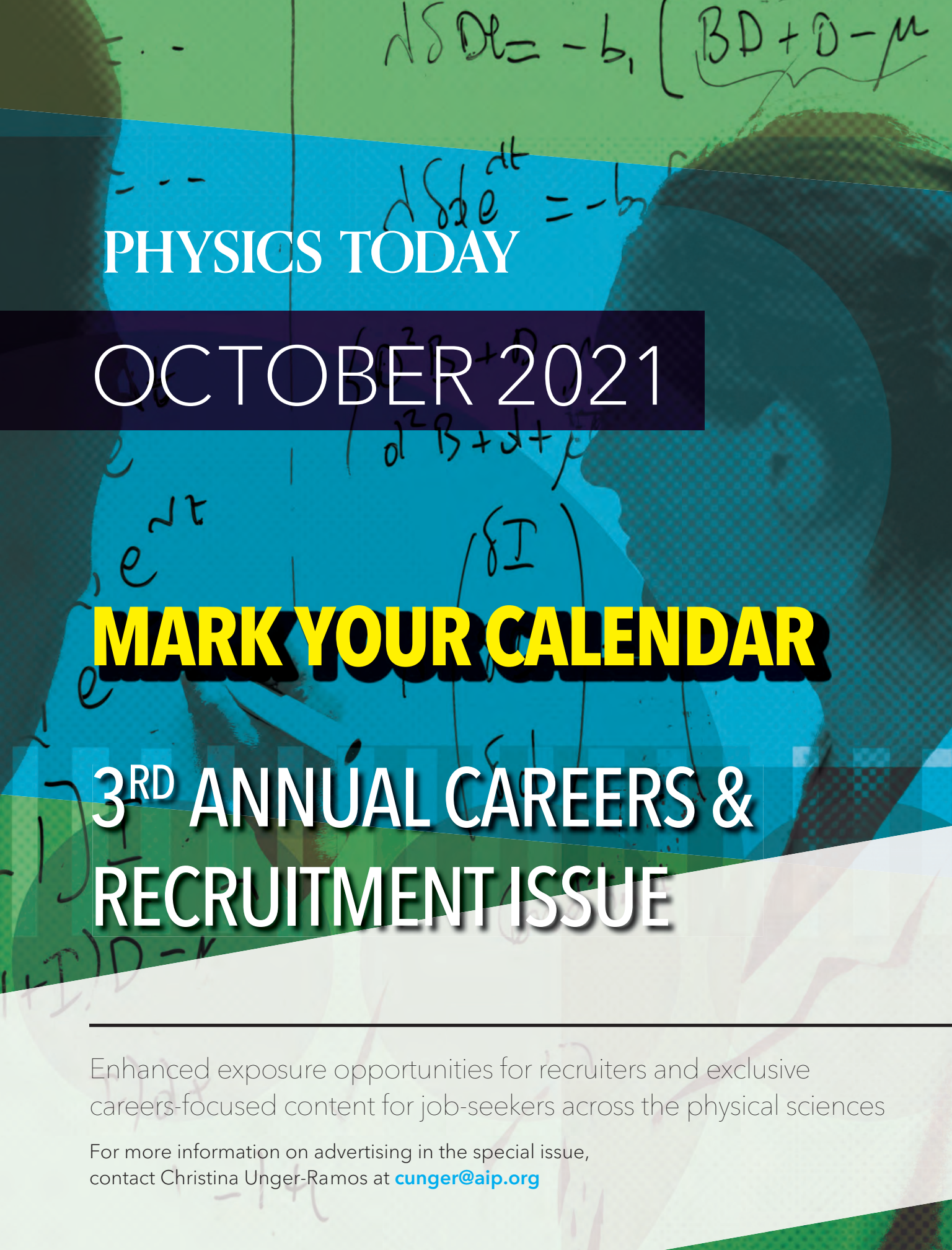

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Universities ramp up efforts to improve faculty gender balance and work climate in STEM

Small actions can cumulatively lead to big advances.

Calls for increased gender balance and diversity in academia are intensifying in many parts of the world. At the national government level, for example, the US NSF has since 2001 funded competitive initiatives in STEM (science, technology, engineering, and mathematics). And starting next year, the European Commission is amping up its push by requiring grant proposals to include plans related to gender equality.

Other high-level initiatives offer funding to institutions to improve their gender balance or, like the UK's Athena SWAN program, bestow recognition to academic departments that are doing well in recruiting and retaining female faculty members. Increasingly, universities are taking on the challenge themselves.

"Despite its very best intentions, the academy is not a perfect meritocracy," Cornelis Storm, a professor of theoretical biophysics at the Eindhoven University of Technology in the Netherlands, wrote in *Europhysics News* in 2019. "For decades, appointment and promotion committees have based their decision making on noisy, biased measurements and the results are the staff compositions we see today." With about 13% female full professors in 2017, Eindhoven had the smallest representation of any Dutch university. It stepped up its efforts in 2019 with what became a sensationalized sprint to hire female researchers; by late 2020 the proportion was nearly 20%.

Also in 2019 Chalmers University of Technology in Gothenburg, Sweden, launched its ambitious Gender Initiative for Excellence, known as Genie. The aim is to boost representation of women faculty to 40% at all levels and across all the university's 13 academic departments in 10 years. Women currently make up about 17% of full professors university-wide.

But Genie and the other initiatives are not only about numbers: "The most important aspect is to create a work environment that lets the women in the system, and all faculty, thrive," says Genie leader Pernilla Wittung-Stafshede, a professor of biology and biological engineering at Chalmers. The motivation for Genie, she says, is to enhance excellence in research, education, and innovation. "For future success and maintaining Chalmers's top reputation, we cannot miss out on 50% of the available talent in society."

LISA TUNE

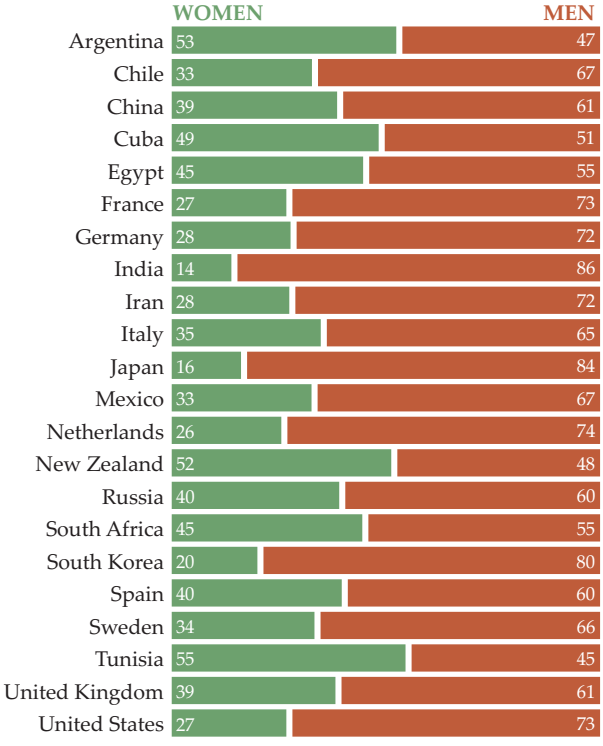
THEATER SKETCHES are one tool employed at the University of Michigan to advance equitable educational and professional practices. This scene is from a 2019 workshop for academic leadership teams that focused on creating work climates resistant to sexual harassment. Eamann Al-Azem (standing) portrays a professor working with her therapist to process Islamophobic incidents and sexual harassment that she and her students have experienced. The role play is followed by guided audience discussion. This and other professional development events are organized and run by the university's Center for Research on Learning and Teaching.

Out of the bottle

Genie grew out of an internal call for the Chalmers community to come up with transformative proposals. Genie won 300 million Swedish krona (about $36 million) over 10 years; two other proposals, in artificial intelligence and project-based teaching pedagogy, received similar awards. Genie's annual funding is about 0.75% of the university's budget.

Genie has three main goals: increase the proportion of female faculty; remove structural and cultural barriers that hamper women's careers; and create a diverse, inclusive working environment that is "supportive of excellence in research and teaching," according to the project's white paper.

Paul Walton, a chemistry professor at the University of York in the UK, has been involved in gender-equity issues in academia for two decades and serves as an adviser to Genie. "It has set itself ambitious goals to rebalance faculty," he says. "Part of its solution is to throw money at the problem. The program also has thought, expertise, and strategy." Genie bears watching from the rest of the world, he adds. "Gender inequality is a problem at all universities."



PERCENTAGES OF FEMALE and male researchers in STEM fields for a sampling of countries. Data are from UNESCO and are from 2017 or the latest year available. The US figures, from 2019, are from the US Census Bureau. (Data compiled by Madison Brewer.)

Walton was instrumental in his department's receiving the first Athena SWAN Gold award, in 2007. To achieve that recognition, the department began successfully responding to its own gender-equity problems. One of the department's "greatest triumphs," he says, was in 2015 when it eliminated the median gender pay gap for professors. (See PHYSICS TODAY, November 2017, page 24.)

Improving gender equality requires raising awareness and then changing behavior, Walton says. Studies by social scientists show that a diverse workforce is associated with improved outcomes. For example, he says, companies with gender-balanced boards perform better. "And strong evidence is emerging that equity is correlated with better academic performance measures." (See the box below.)

Now in its third year, Genie crafts guidelines for recruiting, helps departments implement equity-promoting activities, and proffers advice to the university, departments, and individuals. It has also broadened the university's survey of researchers; one finding across all fields is that females are less likely than males to picture themselves now or in the future as "a successful researcher in academia." Genie also analyzed data on time to promotion, pay, and other metrics. It found, for example, that the mean pay gap is shrinking, from men earning 11.1% more than women in 2018 to 9.1% in 2021.

Other Genie activities and actions to date include funding visiting female scientists, awarding funds to individuals for gender-equity activities, and giving each department 2 million Swedish krona over five years for such activities. Proposals have been funded, for example, to start summer schools, update course curricula, create a department family room, and investigate differences in the aging of vehicle batteries when the main driver was female versus male. Each department has its own culture and needs, says Wittung-Stafshede. "We at Genie can suggest ideas and provide advice, but the departments need to come up with activities and do their own work."

The Genie crew is setting up a group with representatives from each department to liaise with each other and Genie. Wittung-Stafshede is working with the university's senior management to count participants' time toward a percentage of their salary. "There is no silver bullet for building equity," says Genie project coordinator Maria Saline, whose background is in biophysics. "You have to do a lot of small things—mentorship, networking, making people aware, . . ."

Before the disruptions caused by COVID-19, the university organized a workshop on leadership and gender equality. Several PhD students from each department met in one- or two-day sessions over several months. Filippa Lundin, a physics graduate student who works on batteries, participated in the workshop. "One of the eye-openers was learning to observe and notice instances of unconscious bias," she says. Imagine switching the men and women in a scenario, she suggests. "If it seems ridiculous, something is wrong. That is a tool you can use to check for biases."

Chalmers physics chair Thomas Nilsson is planning a similar workshop for PhD students and their advisers in his department, for which he is applying for Genie funding. "I'm not 100% sure we are succeeding in changing the culture yet," he says, but the department members are talking about diversity and inclusion and about biases in hiring and judging merits. "We have to do this, even if it's slow," he says. "The environment in physics is hypercompetitive and masculine. There are lots of men who don't like that either." (See "Why does biophysics attract a disproportionate number of women?," PHYSICS TODAY online, 7 June 2021.)

Perhaps Genie's boldest move so far was to hire five women on short notice. Every second year, the university opens a search for excellent researchers in any field. In 2018 more than 1000 people applied for 10 positions. The top-ranked candidates were a mix of men and women. But when Wittung-Stafshede

Further reading

The articles listed below are part of a growing body of work showing that a diverse workforce and a welcoming climate in academia and other research sectors lead to better performance and improved conditions for everyone.

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CHALMERS UNIVERSITY OF TECHNOLOGY

PERNILLA WITTUNG-STAFSHEDE spearheads the Gender Initiative for Excellence, or Genie, at Sweden's Chalmers University of Technology.

and her Genie colleagues saw the caliber of the women who were ranked second, they decided to cover the cost of five additional positions for five years and to contribute to startup funds. One of those women is an assistant professor in the physics department.

The target of 40% female representation by 2028 is ambitious, especially given that the university is not growing. And, says Wittung-Stafshede, Genie cannot pay for enough new hires. "We need to use our funding to create movement and initiate change. The university will have to spend other money as well to reach our goals."

Genie is giving carrots to departments, says Julie Gold, a professor in the physics department and chair of Chalmers's faculty appointment and promotion committee. People hear "money" and "female" and say, "Let's go for it." Now, two and a half years into the initiative, the attitude is starting to change, she says. "It is no longer just money. Deans and recruitment committee members are starting to couple diverse environments with excellence. I think Genie has something to do with that."

Global efforts

One of the most successful US gender-equality programs is at the University of Michigan. The program goes back to 2001 and the first round of NSF ADVANCE awards, which were established to increase the representation of women in academic STEM careers. When the external funding expired, the university continued the program and later expanded it to include all faculty. The program supports recruitment and retention, an inclusive work climate, leadership training, and more. Over time, the percentage of women on the faculty has increased. In natural sciences, for example, the percentage of women faculty at all ranks grew from 12% in 2003 to 28% in 2018.

Introduced in 2012, Michigan's mentoring approach is notable for its strength. New assistant professors in participating university units meet monthly with a team of mentors. "It can feel intimidating," says Isis Settles, associate director of the university's ADVANCE program and a professor of psychology and Afro-American and African studies. "But the formality is outweighed by the insider information they get, and the program is highly rated by new faculty."

Michigan astronomy professor Ted Bergin has long been involved in the university's ADVANCE program. To change the culture, he says, "you need full professors, particularly white men, to play a role, to stick out their necks and be active in this space—working toward equity." One challenge is that tenured professors are bosses, Bergin says. "If someone wants to resist things, what leverage do you have? Culture change in this environment requires time, effort, and buy-in from the department members."

In Japan, which has among the world's lowest representation of women in STEM fields (see the chart on page 21), efforts toward gender balance are spotty. But recently the Okinawa Institute of Science and Technology (OIST) got a boost: On 19 May a New York–based foundation launched the Rita R. Colwell Impact Fund for the Advancement of Women in Science. The $50 000 fund will be used for outreach activities to attract local Okinawa schoolgirls to STEM fields and to foster gender equality and diversity at OIST. "We want to do small things that have impact," says OIST provost Mary Collins. "We should try to plug gaps." Covering childcare when faculty members travel is an example, she says.

Myriad measures

At the University of Groningen in the Netherlands, the faculty of science and engineering increased the proportion of female full professors from 4% in 2002 to 19% in 2019. Condensed-matter experimentalist Petra Rudolf became the first full physics professor in 2003—and was one of only three in the country at the time. "I got a lot of visibility and used it to push women's issues along with my science issues," she says.

The university initiated the Rosalind Franklin Fellowships in 2003, through which it has hired 130 female faculty members across the sciences and engineering. "There is no question that there are enough highly qualified female candidates," she says. "It's just a matter of getting them and then helping them along in their careers." The climate has completely changed, she says. "We have lots of very good women. And now when we have a job opening and not enough women apply, everyone worries. That is wonderful to see."

In terms of recruiting female scientists, Groningen and other places have found success by tweaking both their advertisements and their approaches to interviewing. In general, wide calls are better than narrow ones, says Rudolf. For example, it's better to advertise for "an ambitious scientist who can contribute to our research" than for a laser physicist. "The more criteria you list, the fewer women apply." In the interview process, Rudolf adds, potential bias is mitigated when each committee member individually ranks candidates before discussing them with others. York's chemistry department goes further, says Walton: It

now invites trained observers to keep an eye out for bias during interviews.

When female physicists arrive at Groningen from other countries, Rudolf helps them navigate the Dutch research and funding landscape; for new arrivals in other fields, she taps colleagues. Rudolf has helped in practical ways, too, by finding tax advisers, nannies, and real estate agents. She is especially proud of Groningen's commitment to making offers to faculty spouses who are also in academia. "That is unusual in Europe," she says.

Eindhoven's Storm says the university had reached the point where it had to do something drastic. And the only thing that could guarantee increasing the proportion of women was to hire more of them. The Eindhoven sprint as originally cast opened jobs exclusively to women for six months, with men eligible after that. A lawsuit claiming discrimination forced the university to loosen the rules: For the duration of the five-year initiative, the delay in considering men applies to 30–50% of positions, depending on each department's current female-to-male ratio.

At the start, the dean collected names of top female scientists from every staff member, says Storm. "It didn't matter if they were on the market or didn't fit a profile for a subdiscipline. The dean looked for good people. We got people who ordinarily would not have applied." The university also padded startup packages and arranged mentors for women hired under the program. Offering startup packages is new and "has a major impact," says Storm. "We are becoming a better department, and that makes us more attractive to anyone who comes knocking."

Since Eindhoven began its efforts in 2019, it has hired 65 female faculty members: 6 are full professors, 3 are associate professors, and 56 are assistant professors. Internal promotions also contributed to increasing the proportion of females to 20% of the university's 170 full professors.

One of the new female hires at Eindhoven is Janne-Mieke Meijer, who studies self-organization of colloidal particles. People want to be recognized for their capabilities, she says, so women don't want to be hired based on their gender. "But I decided not to let that stop me. The further I got in my career, the fewer women I saw. So although I am ambivalent about discriminating against men, we need to do this now, and hopefully it will later sustain itself."

Culture change is hard work

Whether top-down or bottom-up, university initiatives require buy-in from both the administration and faculty members. The approaches that universities and individual departments take vary in scale, detail, and degree of success; they overlap but are also tailored to specific contexts. Often a single person or a small group is the driving force behind efforts to improve gender balance.

Among the widely shared challenges is initial resistance. Another is dual hires. In the US, available and affordable childcare can be a major obstacle to hiring female faculty members; in Sweden, childcare is not a problem, but accommodating dual-academic couples is. But the biggest challenge, says Walton, "is stamina. It's hard work, and you need committed people for a long time."

Toni Feder

ARPA–E explores paths to emissions-free metal making

The agency is seeking advice from industry and academia on how to make mining, smelting, and remediation less polluting and more energy efficient.

AUSTRALIAN metals mining wastes (top) and the metal hyperaccumulator plants *Alyssum murale* and *Berkheya coddii* (bottom). The former plant can take up 1–3% of its weight in nickel. It has demonstrated yields of up to 400 kg of nickel per hectare annually, worth around $7000 at current prices, excluding processing and production costs. (Images adapted from A. van der Ent, A. Parbhakar-Fox, P. D. Erskine, *Sci. Total Environ*. **758**, 143673, 2021.)

When it comes to making steel greener, "only the laws of physics limit our imagination," says Christina Chang of the Advanced Research Projects Agency–Energy (ARPA–E). Chang leads the agency's Steel Made via Emissions-Less Technologies (SMELT) program as an ARPA–E fellow. During her two-year tenure, she will guide program creation, agency strategy, and outreach. Steelmaking currently accounts for about 7% of the world's carbon dioxide emissions, and demand for steel is expected to double by 2050 as low-income countries' economies grow, according to the International Energy Agency.

Founded in 2009, ARPA–E is a tiny, imaginative office within the Department of Energy. SMELT is one part of a three-pronged thrust by ARPA–E to green up processes involved in producing steel and nonferrous metals, from the mine through to the finished products. Another program seeks ways to make use of the vast volumes of wastes that accumulate from mining operations around the globe—and reduce the amounts generated in the future. The agency is also exploring the feasibility of deploying plants that suck up from soils elements such as cobalt, nickel, and rare earths. Despite being essential ingredients in electric vehicles, batteries, and wind turbines, the US has little or no domestic production of them. (See PHYSICS TODAY, February 2021, page 20.)

Steelmaking

The first step in steelmaking is separating iron ore into oxygen and iron metal, which produces CO_2 through both the reduction process and the fossil-fuel burning necessary to create high heat. An ARPA–E solicitation for ideas to clean up that process closed on 14 June. The agency is looking to replace the centuries-old blast furnace with greener technology that can work at the scale of 2 gigatons of steel production annually. It may or may not follow up with a request for research proposals to fund.

Among the many proposed technologies are electrodeposition, reduction using hydrogen in place of carbon, and renewable biomass that would replace the coke—purified coal—in the blast furnace. In a presentation at ARPA–E's annual summit meeting in May, Chang focused on electrodeposition, also known as electrowinning, in which a current of electrons replaces carbon monoxide as the reductant. To be emissions free, the electricity would come from renewable sources.

Boston Metal, an MIT spinoff backed by the Bill Gates–founded Breakthrough Energy Ventures, is developing a high-temperature iron-electrowinning process. A 12-member consortium known as SIDERWIN, headed by ArcelorMittal, the world's largest steelmaker, has been working since 2017 to scale up a low-temperature electrowinning process. That effort is funded by the European Union's Horizon 2020 R&D program (see PHYSICS TODAY, March 2014, page 26).

The low-temperature process, which proceeds at around 110 °C, occurs in an aqueous alkaline electrolyte and is analogous to water electrolysis. Boston Metal's process, which is carried out at 1600 °C in a molten oxide electrolyte, is more similar to aluminum smelting, which takes place at about 960 °C. The iron that forms on the cathode in SIDERWIN's cells is periodically removed as a 1-cm-thick plate; Boston Metal's process taps batches of molten iron from the bottom of the cells. Neither technology has been commercialized yet in volume steel production.

Chang says electrowinning currently is too costly and can't achieve the volumes necessary to compete with traditional steelmaking. One possible way to increase output is by using slurry electrodes—particles suspended in the electrolyte—to replace two-dimensional electrodes. That would greatly increase the surface area available for iron deposition.

MIT metallurgist Antoine Allanore worked on the SIDERWIN collaboration and later codeveloped a chromium–iron anode that's used in Boston Metal's process. He says scaling up the electrowinning processes could be done by building more and bigger electrolytic cells. The overall footprint might not exceed that of a conventional integrated steel plant and its blast furnaces and cok-

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MINE TAILINGS killed 270 people near Brumadinho, Brazil, in 2019, when the dam confining them burst. The total of the world's mining wastes could fill Lake Erie.

ing ovens. Allanore says other alternative iron-making processes have drawbacks. Hydrogen, for example, is difficult to store and transport, and it would be needed in very large quantities, while biomass would be competing with agriculture, forestry, and bioenergy for a finite amount of arable land.

Other potential methods to reduce steelmaking's energy use include inductive heating and the direct transfer of molten iron into furnaces where alloying into steel takes place. Today, iron from blast furnaces is solidified before it is reheated in basic oxygen furnaces. Making furnaces more efficient would also reduce energy use.

Downstream parts of the steelmaking process, such as hot rolling of slabs into sheet steel and fabrication of sheet into products, are ripe for energy-efficiency improvements, Chang says.

Ultimately, steelmaking might be transformed from its current multiple-vessel process of heating and reheating into one that resembles 3D printing. "It's totally possible that there's a black-box technology where you dump in rocks at the top and out comes a steel can, and it breathes out oxygen" instead of CO_2, says Chang.

Phytomining

ARPA–E fellow Elizabeth Troein, a biogeochemist, is pitching so-called hyperaccumulating plants as a domestic source of energy-critical metals that would reduce the need for carbon-intensive hard-rock mining. More than 500 species of such plants accumulate nickel in concentrations greater than 1000 μg/g of dry weight, far above the 50–100 μg/g that's toxic to most plants. Those same plants also accumulate cobalt, to an extent, and in some cases rare-earth metals.

Most grow in the 2–3% of Earth's land surface that has serpentine soils, which are nutrient poor and have high concentrations of heavy metals. About 60% of those soils are arable, says Rufus Chaney, a retired Department of Agriculture scientist whose research focused on what he calls phytomining—cultivating crops of hyperaccumulators for their mineral content. Large areas of serpentine soils occur in the Asia-Pacific region and in the Middle East; in the US they are mostly centered in northern California and Oregon.

Cobalt is increasingly in focus because of its scarcity, its price, and the rapidly rising demand for its use in lithium-ion batteries (see PHYSICS TODAY, May 2021, page 20). Most of the world's cobalt is mined in the Democratic Republic of the Congo, where social and political instability is high. Troein says that planting hyperaccumulators in a field the size of Rhode Island (2700 km^2) could satisfy the current 10 000-ton-per-year US demand for cobalt until the land is depleted in 10 years or so. There are at least 16 000 km^2 in the US with the type of surface rock (ultramafic) that weathers to produce serpentine soils, she says.

Farming an area of those soils equivalent to the size of Maryland and Delaware (30 000 km^2) could produce sufficient cobalt to meet global demand for a decade, Troein says. A second type of metal-rich soil more widely found in the US might also support cobalt accumulators, she adds.

Antony van der Ent, who studies the biopathways of trace elements at the University of Queensland in Australia, offers a somewhat different take. Little R&D has gone into cobalt phytomining to date, he says, and while there is potential, the emphasis should be in central Africa, where large areas with cobalt-enriched soils and mine waste exist. Cobalt hyperaccumulators are native to that area, and they could also be suitable for semiarid and Mediterranean climates.

Van der Ent says that any nickel hyperaccumulator plant will take up some cobalt, but only in appreciable amounts when the nickel content in the soil is very low. The two metals will compete for uptake, and in typical serpentine soils, where the nickel content is 10 times as great as the cobalt content, the plants will accumulate very little cobalt. Chaney says bioengineering could convert one of those species into a cobalt hyperaccumulator that ignores nickel.

Chaney, for whom the 2-meter-tall nickel hyperaccumulating plant *Phyllanthus rufuschaneyi* is named, says the mining potential of a particular plant can't be determined until it has been grown as a crop with appropriate fertilizers and soil pH. Several species of hyperaccumulators are not tall plants, making their harvesting difficult and their value low. The hyperaccumulators can be burned and the metals separated from the ash. Alternatively, they can be pressed and the metals extracted from the liquid. Because hyperaccumulators extract the metal of interest from the soil or ore matrix, purifying the metal is much less expensive than conventional refining, he says.

Nickel phytomining is underway in Albania and Indonesia, Chaney says, but it has yet to become commercial in the US. After working with the Department of Agriculture under a cooperative R&D agreement that ended in 2002, the US company Viridian tested two nickel hyperaccumulator species at a site in Oregon. In 2005 the state declared the plants to be noxious weeds after some had been found on nearby lands. The researchers could have avoided the problem if they

had harvested the plant before its seeds ripened, Chaney says, adding that the incident effectively brought an end to real-world experiments that used hyperaccumulators in the US.

Mine tailings

"The scale of mining is almost incomprehensible, even before the [carbon-free] energy transition," says Douglas Wicks, an ARPA–E program director. The volume of wastes, or tailings, produced in the world each year is 50 gigatons. Sometimes the piles can lead to disasters, as occurred in 2019, when a tailings dam at an iron mine near Brumadinho, Brazil, burst, killing 270 people (see photo, page 25).

The minerals needed for humanity's transition to green energy produce some of the largest volumes of wastes on a per-ton basis: Each ton of cobalt, for example, produces 1000 tons of tailings. With demand for the minerals expected to skyrocket, "we're now on course to leave a trillion tons of waste for the next generation," Wicks says.

Many mines are "laser focused" on a single metal and leave behind others that they could extract, which would lessen the need to dig up more Earth, says Wicks. When nickel is mined, cobalt, manganese, aluminum, and iron are often left behind in the tailings. Processes could be developed to mine the minerals that are present in lower concentrations, he notes, perhaps through electrochemistry that exploits the different potentials of the metals to fractionate each out from solution. Once all the mineral value has been exhausted, the remaining wastes could be used as building materials. That's what's done with steelmaking slag.

The wastes could also serve as sinks for CO_2. Were CO_2 reactions properly integrated into nickel mining, the activity could go from a carbon-emitting process to a carbon-negative one, Wicks says. Olivine rock, in which nickel deposits are found, will absorb up to 63% of its weight in CO_2 under the right conditions, he says. In an ore that is 0.25% nickel, 400 tons of rock will be left behind for every ton of nickel recovered. That rock has the potential to chemically sequester 250 tons of CO_2 per ton of nickel liberated, compared with the 14–20 tons of CO_2 that is currently generated to produce a ton of nickel.

ARPA–E wants industry, academia, inventors, and entrepreneurs to propose new mining processes that require less land, water, and power. "Clean mining is key to a sustainable energy transition," Wicks says.

Greeshma Gadikota, who directs the Sustainable Energy and Resource Recovery Group at Cornell University, says her research aims to accelerate the time in which chemical reactions such as rock weathering take place from hundreds and thousands of years to as little as hours. Some of those reactions lock up CO_2 in stable carbonates.

"We've started to learn more about how we can engineer the reactions to gain control and how we can start to implement them in industrial processes," Gadikota says. "We are working out the thermodynamic feasibilities and the kinetic limitations. Can we understand the factors that make the reactions go slower or faster, and how expensive will it be to do that? How can we leverage the increasingly low costs of renewable electricity to tune these reactions?"

David Kramer PT

SOVIET

The V. G. Khlopin Radium Institute in Saint Petersburg, Russia, with plaques commemorating Vitaly Khlopin (left) and Vladimir Vernadsky (right). (Image by Svglass/Dreamstime.)

URANIUM BOOSTERS

ROBYNNE MELLOR

Robynne Mellor is a historian of science and the cofounder of Sunmount Consulting, a historical research company based in Santa Fe, New Mexico. She received her PhD in environmental history in 2018 from Georgetown University, where she wrote her dissertation on the global history of uranium mining.

In the Soviet Union, private entrepreneurship was largely forbidden, and scientists were in charge of prospecting for radioactive minerals. Their work in the early 20th century laid the basis for the Soviet nuclear project.

Contrary to popular belief, the tale of the Soviet nuclear bomb began not with atomic spies like Klaus Fuchs and David Greenglass, who penetrated the Manhattan Project during World War II, but with a little-known radium mine in Central Asia discovered at the end of the 19th century. In those days, that edge of the Russian Empire was much like the American Southwest: a vast borderland where Russian entrepreneurs hoped to strike it rich by finding sources of precious metals, such as gold, silver, and copper.

In 1899 one of those mineral hunters, V. A. Spechev, located what he thought might be a promising copper mine at Tiuia-Muiun on the border of the Fergana Valley in present-day Kyrgyzstan. Hoping to find the moneymaking reddish-brown metal, he extracted a rock sample for testing, but it turned out that the sample (see figure 1) did not contain rich stores of copper. With his dreams of wealth dashed, Spechev soon let go of his connection to the find.

Over the next five years, though, Spechev's sample gradually found its way into the hands of scientists at the St Petersburg Mining Institute, and they determined that it contained uranium. It then caught the eye of Khristofor Antunovich, a businessman and mining engineer. What attracted him to the sample was not the uranium itself but the radium that could be refined from it. That rare element was a

decay product of uranium that Marie Curie and Pierre Curie had discovered in 1898. Mania for radium soon spread across Europe, and Antunovich saw a chance to strike it rich. In 1908 his company began mining operations at Tiuia-Muiun. It was Russia's first radioactive-minerals mine.[1]

Under the czarist regime, entrepreneurs willing to invest private capital, engineers who developed technology, and scientists interested in experimenting with minerals informally cooperated in discovering and developing mines like Tiuia-Muiun. But when the Bolsheviks, led by Vladimir Lenin, seized power in 1917, they suppressed private enterprise. Gone were prospectors like Spechev, who hunted for wealth, and investors like Antunovich, who took a chance on a deposit in the name of profit. Moreover, the young nation was internationally isolated, which stifled the possibility for economic and consumer stimuli that drove mining in other nations. That shift hampered radioactive-mineral prospecting and production for decades.

Nevertheless, it did not disappear entirely. Although the Bolsheviks rejected capitalism, they were keen to support applied science. In part, their reasoning was pragmatic. They hoped that the products of applied science would help build their new state. It was also in line with their ideology, as the Soviet interpretation of Marxist theory emphasized applied science. Scientists reliant on the state thus stepped in to replace the earlier generation of independent prospectors and entrepreneurs who had driven the search for radioactive minerals.

Yet government support for applied science proved to be a mixed blessing for proponents of radiogeology, geochemistry, and mineralogy. Although it opened up new avenues of funding, it also meant that Soviet scientists, including Vladimir Vernadsky and his pupils Alexander Fersman and Vitaly Khlopin, had to lobby the government for funding and prospect for minerals on top of their usual research program. Not only were they faced with the task of studying radioactive minerals, but they also had to create demand for those materials and engineer their supply. It was a Gordian knot: They needed more minerals for further research but needed to do further research to locate more minerals. Eventually they also had to contend with Joseph Stalin's purges and the Great Terror.

Vernadsky, Fersman, and Khlopin made modest progress in the face of those obstacles, but not enough to keep pace with other countries that were producing radioactive minerals. On the eve of the German invasion in June 1941, the Soviets had no significant infrastructure for extracting uranium ore, nor had they located any promising deposits of uranium. Although they made some headway on the uranium problem during the late stages of World War II, the Soviets ultimately entered the Cold War well behind the US in terms of prospecting for and extracting the radioactive element.

Radium under the Bolsheviks

A famous geochemist, mineralogist, and radiogeologist, Vernadsky was a towering figure in Russian and Soviet science during the first half of the 20th century. Minerals and the processes of Earth fascinated him, and he was a relentless spokesman for the significance of the emerging field of radiogeology.[2] During

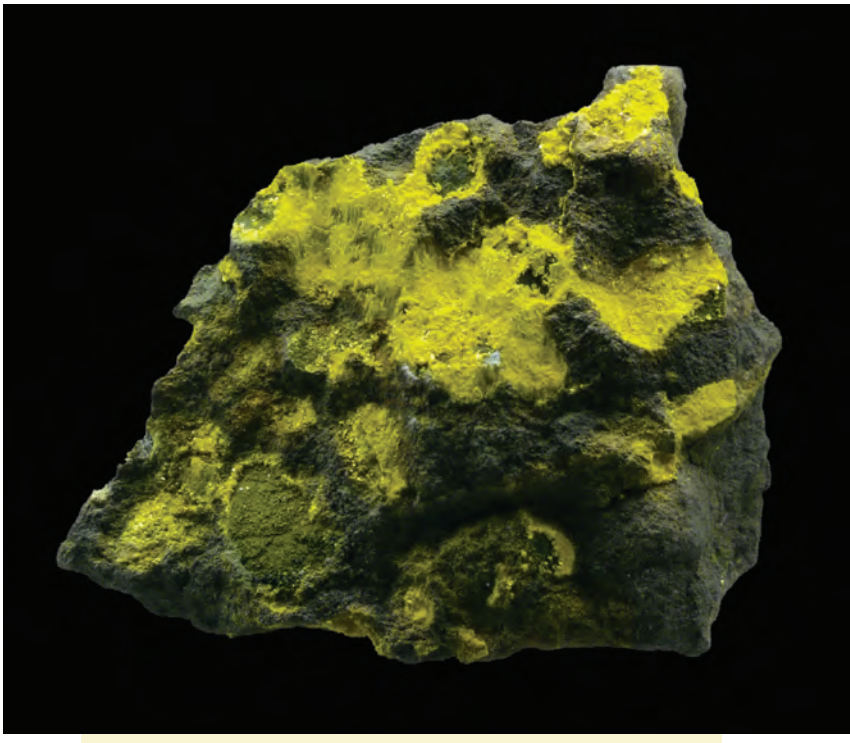

FIGURE 1. A TYUYAMUNITE SAMPLE. The radioactive uranium-containing mineral was discovered by V. A. Spechev at the Tiuia-Muiun mine in present-day Kyrgyzstan. (Image by Rob Lavinsky, iRocks.com/CC BY-SA 3.0, adapted by Donna Padian.)

World War I, in 1915, he started the Commission for the Study of Natural Productive Forces (KEPS), in part to mobilize science for the war effort. Designed with an eye toward mineral exploration and prospecting, KEPS attracted the attention of the Bolshevik government that emerged after the 1917 revolution. Unlike the czarist regime, under which science focused largely on theory, the Bolsheviks foregrounded science's practical applications and supported lines of scientific inquiry that could lead to economic and technological advances. They quickly began funding KEPS, and in 1918 Fersman, a trailblazing geochemist, was named chairman of the commission's radium division.

Fersman had set out to study mineralogy as a student in 1901 but, finding it painfully boring, changed his field to chemistry. He went to Moscow in 1903, started training under Vernadsky, and quickly became one of Vernadsky's favorite pupils (see figure 2). Fersman had a sharp scientific mind and a prolific pen. In the first half of the 20th century, he became another tireless advocate for radioactive-mineral research. Under Fersman, KEPS's radium division continued to work on mineral exploration during the tumult of the Russian Civil War, which lasted until 1921. But the searches that Vernadsky and Fersman carried out during that time did not produce any radioactive-mineral findings of practical significance. Tiuia-Muiun remained the only worthwhile radioactive-mineral deposit then known to exist in the fledgling Soviet Union.

Ironically, the domestic turmoil of the civil war allowed Soviet radium research to flourish because it gave scientists unprecedented access to radioactive materials. Before World War I, Russian scientists had little to no opportunity to study uranium

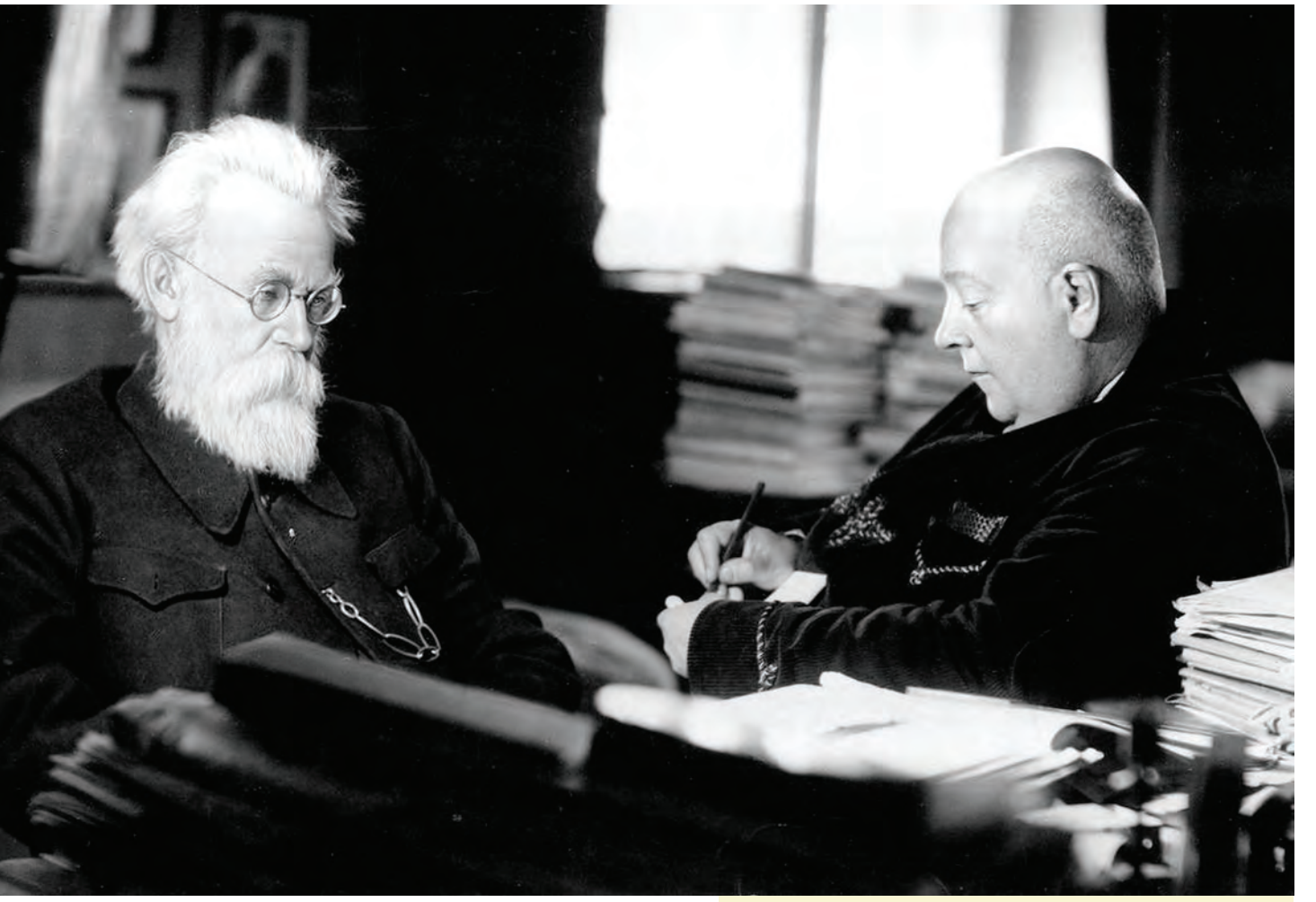

FIGURE 2. VLADIMIR VERNADSKY (left) with Alexander Fersman (right), pictured in 1940. (Image from Album/Alamy Stock Photo.)

and radium mined at Tiuia-Muiun because it was shipped outside the country's borders for processing and sale. In the postwar period, however, Western governments took a hostile stance toward the new Bolshevik leadership. Moreover, the war devastated the German economy, which was once the market for Russian ores. Furthermore, the commercial class to which Antunovich belonged—the one that had sent uranium ore abroad—largely disappeared after the Bolsheviks targeted its members as bourgeois enemies of the people. Thus Tiuia-Muiun's ore became available to scientists, who had government support to study it.

It was not long before the increased state funding began to pay off. By the end of 1921, radiochemistry pioneer Khlopin managed to successfully isolate radium from the uranium that had been abandoned in Petrograd—as Saint Petersburg was renamed in 1914—during the war years. Only 31 years old at the time, Khlopin had worked with Vernadsky since 1915 and had years of experience with radioactive products. He was one of the few radiochemistry specialists in the Soviet Union. Perhaps spurred by Khlopin's breakthrough, the Bolshevik government authorized the founding of the State Radium Institute (now the V. G. Khlopin Radium Institute) in January 1922, with Vernadsky as director and Khlopin as his deputy.

Yet the new government also brought added responsibilities and pressures for scientists. In the Soviet Union's state-run economy, most forms of private entrepreneurship were banned. That meant scientists had to take up the task of hunting for promising deposits of radioactive minerals. And because of the Soviet Union's isolation, they had to do so without the help of foreign investment and technology or international markets. Efforts at finding radioactive-mineral deposits became focused solely within the Soviet scientific community.

In 1923, after the Radium Institute and the Soviet state deemed it favorable for commercial exploitation, production at Tiuia-Muiun resumed (see figure 3). Yet the amount of radium extracted from it remained small. Tiuia-Muiun's ore was low-to-medium grade, containing 0.14–4.52% uranium oxide. Because the ratio of radium to uranium in nature is typically 1:3 000 000, the mine produced merely 1 gram of radium for every 250–300 tons of uranium ore mined. From 1923 to 1936, miners extracted 5000 tons of ore from Tiuia-Muiun—about 17–20 grams of radium.

Tiuia-Muiun did not remain the only radium mine in the Soviet Union for long. The state geological institution, the Geological Committee, continued to look for other radioactive deposits by analyzing rock samples that amateur and professional geologists had collected over the years. In 1925 the committee members found a highly radioactive sample in a museum's rock collection. Tracing that sample back to its origin, they located the Taboshar deposit (now Istiklol) in 1927 in what is now northern Tajikistan. Taboshar remained the richest-known source of uranium in the Soviet Union for decades, but like Tiuia-Muiun, its ore was low grade. Thus radium remained extraordinarily difficult and expensive to extract at both Soviet deposits. With little economic incentive to

continue production, the Taboshar mine was shut down in 1929. Only Tiuia-Muiun continued operating, producing small amounts of ore.[3]

Radioactive minerals under Stalin

Vernadsky was instrumental in keeping alive the moribund efforts to find raw radioactive materials. After a stay in France, where he toyed with the idea of permanently emigrating from the Soviet Union, he returned to his native land in the late 1920s and continued to look for radium. Although he made a few discoveries that excited scientists, the authorities did not deem them worthy of expensive full-scale extraction operations because the finds were low grade and contained radium that was difficult to process. The chief reason for their exploitation remained purely scientific study, which was a hard sell to a government focused on applied science and its economic benefits.

Nevertheless, scientific study of those deposits continued, albeit extremely slowly. Operations at Tiuia-Muiun tapered off in the late 1920s, no new mines began operation in the 1930s, and in 1936 Tiuia-Muiun shut down entirely after miners hit groundwater. The only exception was at the Ukhta oil field in the north-central Komi Republic, where oil drilling uncovered salt water that contained radium (see figure 4). Because its connection to oil production made costs manageable, Ukhta became the Soviet Union's main source of the radioactive element.

But a dearth of radioactive-mineral discoveries and a lack of funds to exploit the few that were found frustrated ambitions among mineralogists, geologists, and physicists in the 1930s. Inadequate knowledge and scarce material for experimental work stymied Vernadsky and his colleagues. Additionally, a practical application that would justify radium's extraction cost continued to elude its promoters.

Graver problems threatened the scientific community. Following Lenin's death in 1924, a protracted power struggle among the Soviet elite broke out, from which Stalin emerged triumphant in 1927. The scientific world quickly felt the effects of his rule. Between 1927 and 1931, the Academy of Sciences of the Soviet Union faced restructuring, an influx of party loyalists, and an expunging of czarist-era scientists. Further purges followed, reaching their apex with the Great Terror of the late 1930s. Experimental work, which a lack of material already constrained, was further impeded when one of its chief patrons in the government, Sergo Ordzhonikidze, killed himself in 1937. Following his death, mass arrests eviscerated his commissariat, which had supported nuclear research.

FIGURE 3. ALEXANDER FERSMAN (center, on tracks, with hat) at the Tiuia-Muiun mine in 1928. (Image from the Academy of Sciences of the Soviet Union/Wikimedia Commons/Public Domain.)

From radium to uranium

As Soviet scientists coped with a wretched domestic situation in the 1930s, trouble began to flare up abroad. In the dying days of summer 1939, World War II began in Europe when Germany invaded Poland. The war initially was disastrous for the worldwide radium market, as it closed off international trade and di-

Fortunately for Vernadsky, he and his field of study escaped the worst, but some young scientists with whom he worked were arrested. Deeply disturbed by those arrests, Vernadsky distanced himself from his students in an effort to protect them from the purges. His detachment inhibited intellectual exchange and undoubtedly also hampered efforts at raw-materials prospecting.[4]

FIGURE 4. LOCATIONS WHERE radioactive minerals were extracted in the former Soviet Union (depicted in its pre-1945 borders). (Image from *Soviet Russia Today*/Wikimedia Commons/Public Domain, adapted by Donna Padian.)

verted resources to wartime economies. Exchange in the radioactive element effectively ground to a halt. But the conflict subsequently introduced new opportunities when several of the warring parties turned their attention to the military application of nuclear fission. Uranium, once the waste product of radium production, now became the primary material that those interested in radioactive minerals sought.

Otto Hahn, Lise Meitner, and Fritz Straßmann discovered fission in 1938, and many physicists around the world quickly realized that it could be weaponized. In the US, Albert Einstein and Leo Szilard sounded the alarm about the military application of fission in an August 1939 letter to President Franklin Roosevelt. The letter, which eventually sparked the Manhattan Project, warned that Nazi Germany had access to uranium and might build an atomic weapon. Yet there was no contemporary equivalent to the Einstein–Szilard letter in the Soviet Union.

Two major reasons were behind the Soviet Union's delayed response to the discovery of fission. The first was geopolitical. Unlike the US, the Soviet Union did not officially consider Germany to be a threat because the two countries had recently signed the Molotov–Ribbentrop Pact, a nonaggression agreement. Second, the Soviet scientific community, including Vernadsky, did not view research into possible applications of nuclear fission as a short-term priority. He and other Soviet scientists instead saw such work as a long-term goal, and even then, not all believed that the main benefit would be its military application.[5]

Vernadsky, however, still believed research into nuclear physics and radioactive minerals was important. With the discovery of nuclear fission, he could finally make a strong case about the practical applications and economic benefit of such work. Seizing the opportunity, Vernadsky, with the help of Khlopin and Fersman, began writing appeals to the Academy of Sciences and high-level government officials in 1940. They highlighted the specter of German and US dominance in the field of nuclear technology and presciently emphasized the importance of studying radioactive minerals so that the Soviet Union would be ready if applications of nuclear fission were discovered.[6]

Along with making recommendations as to how to encourage work on atomic energy, the troika of scientists made a case for stockpiling raw materials needed for that research. To that end, they outlined uranium prospecting plans in the Fergana Valley and Central Asia. Although the plans were ambitious, the choice to limit prospecting solely to that area was practical and risk-averse—and thus indicative of the scientists' precarious and difficult situation. Unfortunately for Soviet nuclear prospects, difficult-to-extract and low-grade ores speckled the region.

The Commission on the Uranium Problem

In 1940 World War II had not yet reached Soviet soil. Although work on nuclear research had increased, it did not have priority over other scientific questions. The same was true for the quest for uranium that accompanied it. Nevertheless, the Academy of Sciences recognized that such work could be important in the long term, and in an effort to coordinate work on all aspects of nuclear research and uranium prospecting, it established the Commission on the Uranium Problem. Vernadsky, then 77, declined to head the commission because of his age, so Khlopin was put in charge (see figure 5).

Khlopin, Fersman, Vernadsky, and the commission's chemists and geologists devoted considerable attention to locating uranium deposits, but many obstacles stood in their way. The biggest problem was their inauspicious prospects. Almost all known Soviet uranium deposits were in the Fergana region, dotted across what is now Kyrgyzstan, Uzbekistan, and Tajikistan, and they mostly contained low-grade and scattered ores that were expensive to extract. The Soviet radioactive-mineral industry had yet to break free from the region Spechev discovered four decades earlier.

Beyond the absence of rich sources of uranium, the Uranium Commission also lacked funding. It cost an enormous amount to extract low-grade ores: 500 rubles to produce 1 ton

of uranium. That was 10 times as expensive as it was to extract any other metal. To justify that cost to the Soviet state, which was still interested largely in applied research, Khlopin and the commission sought yet again to find a use for the ore outside of pure science.

Yet they again faced a paradoxical situation. To produce enough uranium for experimentation, they needed to find a practical application for the ore, but to find that application, the commission needed more uranium for research. Their roles as both prospectors and experimental researchers hamstrung them. Vernadsky and his colleagues had little choice but to work with what they had—a meager 1.5 tons of uranium by the end of 1940—and to expedite research into a practical application as best they could.

Lack of organization also dogged uranium prospecting efforts. Different groups across the Soviet Union worked on studying and producing uranium, but they barely communicated with one another. To address the problem, the Uranium Commission in fall 1940 created a subcommission, with Fersman as its head, to direct all raw-materials activity. It succeeded in bringing organization to the effort, but Fersman and its members made only minor progress prospecting for uranium. Bureaucratic setbacks persistently hindered efforts. Moreover, the government continued to show little interest in pursuing known uranium deposits like those at the Taboshar mine. Although the mine began producing ore in 1934, its status was officially downgraded in 1941 in what Vernadsky called "unintentional sabotage" of uranium work. As late as 18 June 1941, Vernadsky lamented in his diary that uranium remained a niche scientific concern in the Soviet Union.[7]

Uranium and World War II

Four days later, on 22 June, a disruption far greater than onerous bureaucracy interrupted Soviet uranium mining endeavors when Germany invaded the Soviet Union. As the Germans marched across Soviet soil, the military situation was far too desperate for Soviet scientists to spare any thoughts for seemingly inconsequential long-term goals like nuclear fission and uranium prospecting. The Academy of Sciences resolved to dedicate all its resources to the war effort, the work of the Uranium Commission came to a standstill, and most scientists halted work on the uranium problem.

About a year later, based on warnings from a physicist on the home front and intelligence from agents in the West, the Soviets began to consider the military application of nuclear fission. In late 1942 the Battle of Stalingrad waned and relieved pressure on Soviet forces. That shift, along with the acquired intelligence, prompted Stalin to pursue the bomb project seriously in the fall of 1942, and work on the task began.[8] But lack of access to uranium was still a serious constraint. To address the problem, the uranium search was put under the direction of the wartime State Defense Committee, a state organ of extraordinary power with Stalin at its helm. The committee ordered the reopening of the Taboshar mine and conducted a large-scale search for the element in 1943 and 1944. But there were no new discoveries, and the Soviet Union continued to face uranium shortages.

Later in 1944, a new force stepped in to shore up production: the Soviet secret police, or NKVD. Its leader, the infamously brutal Lavrentiy Beria, successfully argued that those in charge of the uranium search had been ineffective in locating the coveted element. As a result, the State Defense Committee granted the NKVD control of all existing uranium mines. Under Beria, the NKVD ran the Soviet gulag system. It forced prisoners in its labor camps to work in uranium mines and mills that formerly employed ordinary workers.[9]

FIGURE 5. VITALY KHLOPIN, in an undated portrait. (Image from Album/Alamy Stock Photo.)

Yet the NKVD's harsh tactics could not force Earth to reveal rich stores of uranium. In spring 1945, as the war with Germany drew to a close, the NKVD counted only 430 tons of available ore—much less than the US had on hand at that time. As the contours of the Cold War came into focus, the Soviets' uranium stores were dismal.

Foreign windfall

Lack of access to uranium stalled the progress of the Soviet bomb program in the first few years after the war, but not for long. At the end of World War II, the Soviet Union extended its sphere of influence into Eastern and Central Europe and obtained a windfall of uranium from substantial deposits located in Czechoslovakia and the Soviet occupation zone of Germany. The influx of uranium fueled the Soviet nuclear bomb project. But even though those deposits eased Soviet uranium scarcity, they were not ideal because their location on the front lines of the Cold War in Europe made them strategically vulnerable. Moreover, by the 1950s, signs of unrest in those client

states made Soviet dependence on their uranium even more problematic.[10]

Vernadsky was not a part of the wartime uranium search effort. Without him, the project lacked its chief raw-materials authority and booster. He died in January 1945. Fersman, his staunch ally in the uranium crusade, was nearly 20 years younger than Vernadsky, but he was already exhausted. He died only four months after his mentor, in May 1945, at age 61. Khlopin's life and work had also depleted him. He worked on the Soviet bomb project for five years until his death at 60 in 1950.

For decades the three scientists drove the search for radioactive minerals. Their task was herculean, the stresses were enormous, and their achievements were often limited. But the scientists had successfully kept the industry and the study of radioactive minerals alive for years, thereby ensuring that a foundation of knowledge and expertise existed when the Soviets began to pursue the bomb during World War II. Nevertheless, the Soviet decision to place scientists in charge of prospecting not only took an immense toll on the scientists themselves but also put the Soviet Union at a strategic disadvantage during the early Cold War.

The Soviet Union did not find what Vernadsky called for—a rich, secure source of domestic uranium—until the 1963 discovery of an extensive deposit in the Transbaikal region of Siberia. Industrial exploitation of that deposit commenced when the Priargunsky mines began operating in 1968, and only with that uranium source would the Soviet Union reach nuclear weapons parity with the US in the 1970s.

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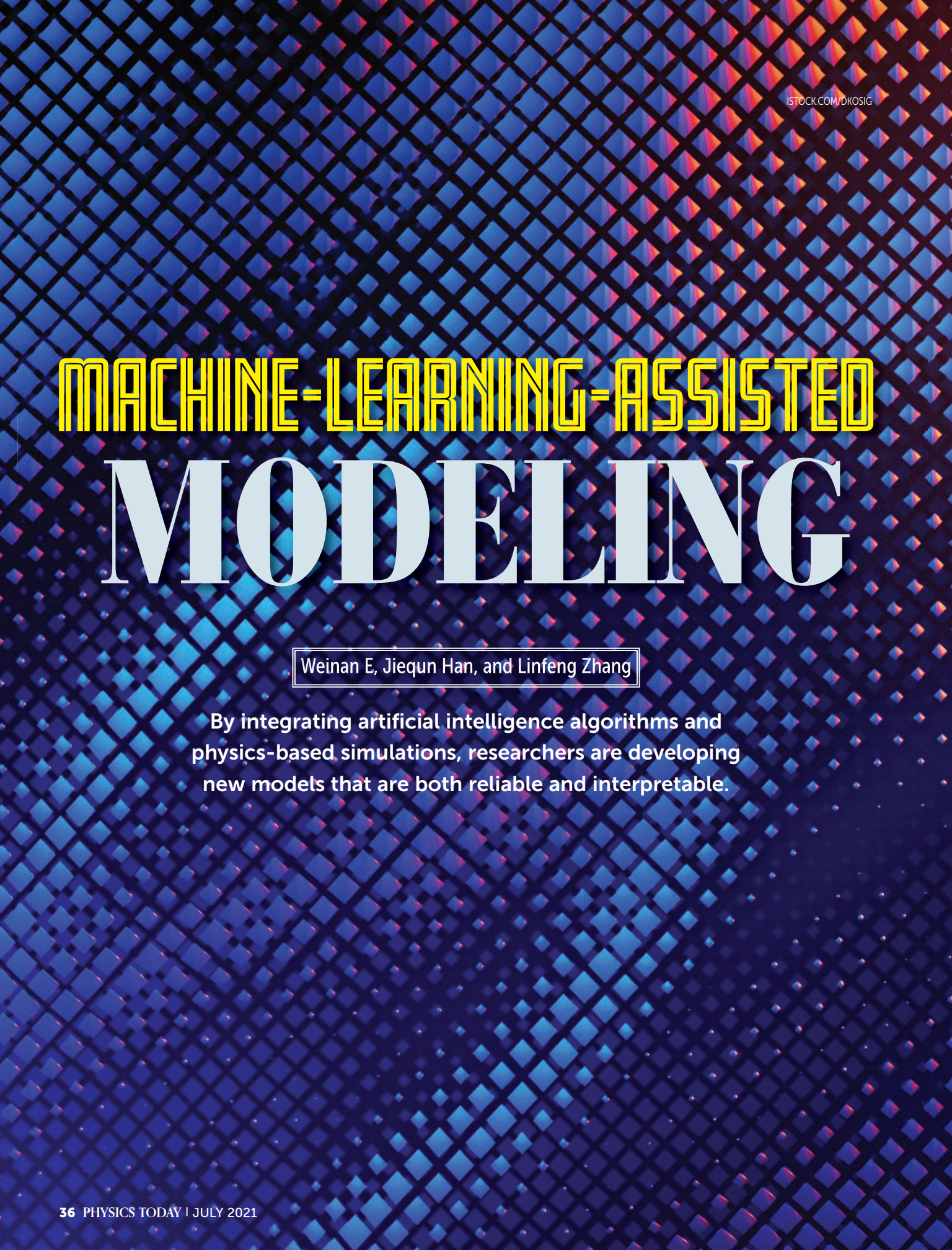

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MACHINE-LEARNING-ASSISTED MODELING

Weinan E, Jiequn Han, and Linfeng Zhang

By integrating artificial intelligence algorithms and physics-based simulations, researchers are developing new models that are both reliable and interpretable.

Weinan E is a mathematics professor and **Jiequn Han** is a mathematics instructor in the department of mathematics and the program in applied and computational mathematics at Princeton University in New Jersey. **Linfeng Zhang** is a researcher at the Bejing Institute of Big Data Research in China.



To understand problems in biology, chemistry, engineering, and materials science from first principles, one can start, as Paul Dirac advocated, with quantum mechanics.[1] Scientific advances made since the early 20th century attest to that view. But solving practical problems from a quantum mechanical perspective using the Schrödinger equation, for example, is a highly nontrivial matter because of its various complexities. To overcome the mathematical difficulties, researchers have proceeded along three lines of inquiry: looking for simplified models, finding approximate solutions using numerical algorithms, and developing multiscale models.

Each of those approaches has advantages and disadvantages. Simplified models—a constant theme in physics—capture the essence of a problem or describe some phenomenon to a satisfactory accuracy. Ideally, simplified models should have the following properties: They should express fundamental principles, such as conservation laws; obey physical constraints, such as symmetries and frame indifference; be as universally applicable as possible; be physically meaningful or interpretable; and require few externally supplied parameters.

One particularly successful simplified model is Euler's set of equations for gas dynamics. They accurately model dense gases under general conditions and are less complex than their quantum equivalents. For ideal gases, the only parameter required is the gas constant. For complex gases, one needs the entire equation of state, which is a function of only two variables. Other success stories include the Navier–Stokes equations for viscous fluids, linear elasticity equations for small deformations of solids, and Landau's model of phase transitions.

Unfortunately, not every effort to develop simplified models has been as successful. A good example is the work of extending Euler's equations to rarified gases.[2] Since the mid 20th century, researchers have made numerous efforts to develop Euler-like models for the dynamics of gases whose molecular mean free path exceeds the system's relevant length scale. But so far none of those models has been widely accepted.

For systems in which analytical solutions are rare or unobtainable, one has to resort to numerical algorithms. Many such algorithms, including finite difference, finite element, and spectral methods, solve the partial differential equations that arise in physics. The widespread availability of the algorithms has changed the way scientific and engineering applications are performed. Numerical computation now influences how researchers study fluid and solid mechanics and, to a lesser extent, atmospheric science, combustion, materials science, and various other disciplines.

Algorithms are now more or less sufficient for studying low-dimensional problems. But such studies quickly become much more difficult as the dimensionality, or the effective degrees of freedom, increases beyond three. The issue that lies at the core of many difficult problems is the curse of dimensionality: As the dimensionality grows, the complexity, or computational cost, grows exponentially.

One idea to overcome modeling difficulties that can't be ameliorated with simplified models or numeral algorithms is multiscale modeling.[3] The approach simulates the behavior of macroscale systems by using reliable models at a range of smaller scales instead of relying on ad hoc macroscale models. It uses the results of the microscale model on much smaller spatial and temporal domains to predict the macroscale quantities of interest. That general philosophy is valid for a range of scientific disciplines. But the success of multiscale modeling has been less spectacular than what was expected 20 years ago. Many factors are to blame, including the inaccuracy in the microscale models, the difficulty associated with moving from one scale to the next, and the lack of adequate data-processing techniques for analyzing the solutions of the microscale models to extract useful macroscale information.

Problems without good models

Although simplified models, numerical algorithms, and multiscale models have limitations, researchers have used them in combination with physical insight and trial-and-error fitting to solve numerous problems. Examples include performing density functional theory calculations, predicting properties of materials and molecules, and using general circulation models to study the climate. However, we still lack good models for many important areas of research, some of which are shown in figure 1.

The exchange-correlation functional, for example, is a crucial component of density functional theory (see the article by Andrew Zangwill, PHYSICS TODAY, July 2015, page 34). Formulated to embody the many-electron wavefunction, the exchange-correlation functional uses simple approximations to determine the energy associated with all exchange and

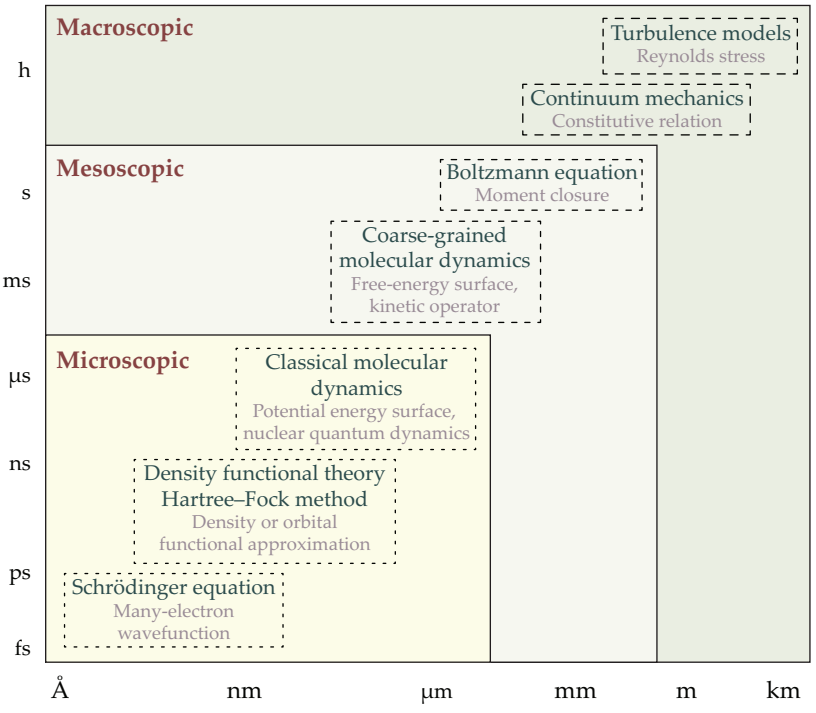

FIGURE 1. REPRESENTATIVE MODELS for various systems (black text) span a range of temporal and spatial scales. By combining their most important theoretical ingredients (gray text) with machine-learning algorithms, researchers are beginning to develop more efficient, reliable, and interpretable physical models. (Image by Weinan E, Jiequn Han, Linfeng Zhang, and Freddie Pagani.)

correlation effects. Systematically developing efficient and accurate exchange-correlation functionals is still a challenging task. Other difficult problems include implementing coarse-grained molecular dynamics (MD) for macromolecules, developing hydrodynamic models for non-Newtonian fluids, modeling moment closure for rarified gases, and accurately representing the potential energy surface (PES) that describes the interaction between the nuclei in the system of an MD model.

The list continues. Fluids can be modeled with the Navier–Stokes equations, but what is the analogue for solids? Besides linear elasticity models, researchers hardly agree on a set of continuum models for solids, and plasticity in solids is even more problematic to simulate. Another example is turbulence models, which have faced challenges ever since the work of Osborne Reynolds in the 19th century. Physical scientists still lack the tools to systematically and robustly simulate turbulent and convective motions.

In all the identified problems, the most essential obstacle is the curse of dimensionality. Without systematic approaches, one has to resort to ad hoc procedures, which are neither efficient nor reliable. Turbulence modeling is an excellent example of the kind of pain one has to endure in order to address practical problems.

However, the problems that are made difficult by the curse of dimensionality may be more tractable because of recent advances in machine learning, which offers an unprecedented capability for approximating functions of many variables.[4,5] (See the article by Sankar Das Sarma, Dong-Ling Deng, and Lu-Ming Duan, PHYSICS TODAY, March 2019, page 48.) As spectacularly successful as machine learning is, it carries a label that is particularly harmful to applications in the physical sciences: It's often described as functioning either as black magic or in a black box. Researchers have made substantial progress in understanding the magic behind machine learning. This article focuses on how practitioners can use machine learning to find new interpretable and truly reliable physical models. See the box on page 40 to learn more about the process that underpins neural-network-based machine learning.

Accomplishing such a task entails meeting a few requirements. First, the model should satisfy the properties listed above for ideal simplified models, although a model with only a few externally supplied parameters isn't necessary. Second, the data set used to construct the model should represent all the practical situations the model is intended for. Fitting some data is relatively straightforward, but it is considerably more difficult to construct reliable, generalizable physical models that are accurate for all practical situations. And third, to reduce the amount of ad hoc, error-prone human intervention, the construction of the model should be automated end to end.

Concurrent machine learning

In standard approaches to supervised machine learning, researchers first provide a labeled data set to an algorithm. Then the machine-learning model interprets individual items of an unlabeled data set to, for example, recognize pedestrians in an image of a busy city street. But when machine learning is used in connection with physical models, data generation and training often become an interactive process in which data are analyzed and labeled on the fly as the model training proceeds. Analogous to multiscale modeling,[3] the standard approach can be called sequential machine learning; and the interactive process, concurrent machine learning.

For physical models derived from machine learning to be reliable, they need to be fed reliable data. The data set should ideally represent all the situations a model is intended for. For example, a reliable model for a molecule's PES should be accurate for all the configurations that the molecule can have. But generating training data typically involves solving the underlying microscale model, which is quite often computationally expensive. Therefore, researchers usually aim to have the smallest possible data set.

To generate such data adaptively and efficiently requires a strategy such as the exploration-examination-labeling-training (EELT) algorithm. Illustrated in figure 2, it requires a macroscale explorer, a criterion to decide whether a given state or configuration should be labeled, a microscale model for labeling, and a machine-learning model for the quantities of interest.[6] The model is a slight modification of the exploration-labeling-training algorithm formulated in reference 6, though similar ideas can be traced back further. Starting without data and only a microscale model, the EELT algorithm proceeds iteratively with the following steps: (1) exploring the state or configuration space; (2) examining which configurations need to be labeled; (3) computing the microscale solutions for the states or configurations

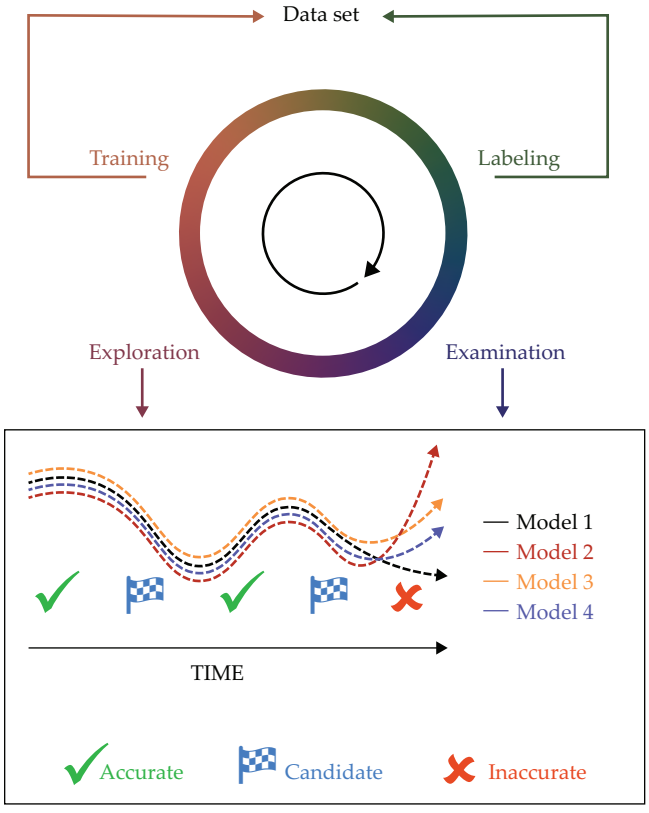

FIGURE 2. THIS SCHEMATIC of the concurrent machine-learning method and the exploration-examination-labeling-training algorithm illustrates one way to improve the modeling of complex physical processes. The algorithm iteratively explores the state or configuration space in a physical system and examines whether the modeled configurations need labeling to identify meaningful information. The box shows an example: Four models produce agreeable results that then begin to diverge as time progresses, which indicates the explored state should be labeled or evaluated using a specific physical model. To obtain labels, the algorithm computes microscale solutions and extracts information. The labels are then placed in a training data set for the model, and the cycle repeats. (Image by Weinan E, Jiequn Han, and Linfeng Zhang.)

that need labeling and placing them in the training data set; and (4) training the machine-learning model.

Molecular modeling

One of the most successful applications of machine learning to scientific modeling is in MD. Researchers study the properties of materials and molecules by using classical Newtonian dynamics to track the nuclei in a system. One critical issue in MD is how to model the PES that describes the interaction between the nuclei. Traditionally, modelers have dealt with the problem in several ways. One approach, *ab initio* MD, was developed in 1985 by Roberto Car and Michele Parrinello[7] and computes the interatomic forces on the fly using models based on first principles, such as density functional theory.[8] Although the approach accurately describes the system under consideration, it's computationally expensive: The maximum system size that one can handle is limited to thousands of atoms. Another approach uses empirical formulas to model a PES. The method is efficient, but guessing the right formula that can model the PES accurately enough is a difficult task, particularly for complicated systems, such as multicomponent alloys. In 2007 Jörg Behler and Parrinello introduced the idea of using neural networks to model the PES.[9] In that new paradigm, a quantum mechanics model generates data that are used to train a neural-network-based PES model.

To construct reliable PES models, one has to impose physical constraints and collect high-quality data. For the first problem, the main physical constraint is symmetry. In other words, the PES should be invariant under translation, rotation, and permutation of atoms of the same chemical species. As can be seen in figure 3a, even a poor man's version of enforcing symmetry[10] can drastically improve the test accuracy. In that version, trans-

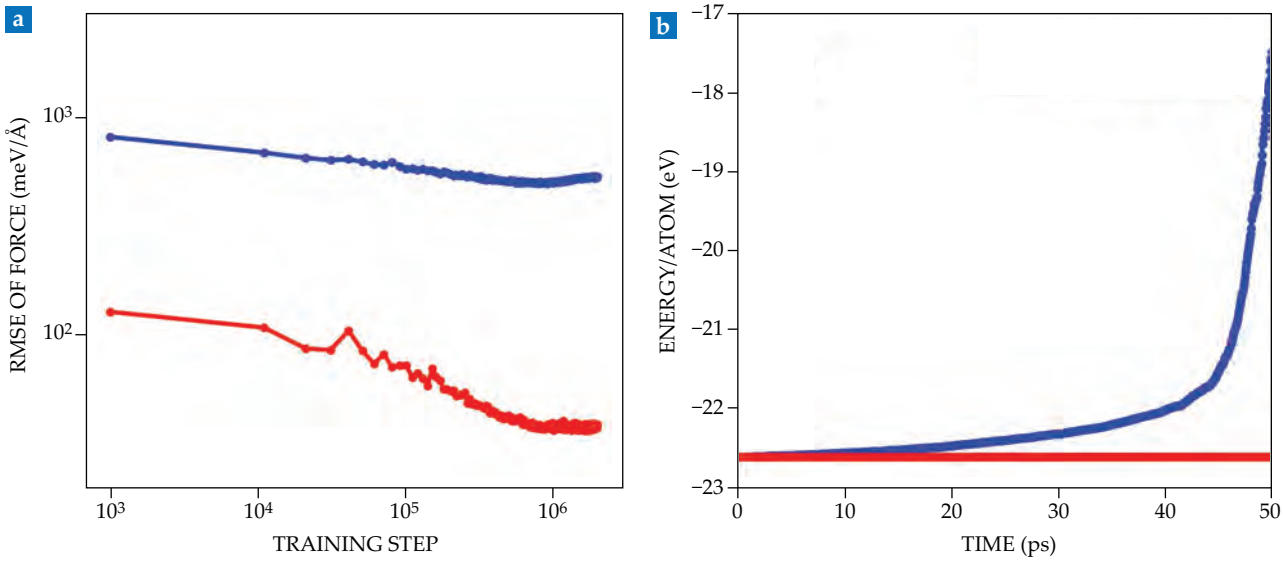

FIGURE 3. MOLECULAR DYNAMICS (MD). A neural-network approach **(a)** that enforces permutational constraints (red) has a lower root-mean-square error (RMSE) and is more accurate than the approach without permutational symmetry (blue).[10] **(b)** Microcanonical MD simulations reveal how the total energy per atom as a function of time erroneously balloons when a limited, nonsmooth symmetry constraint is used for a neural-network (blue) compared with a smooth embedding network (red). (Image by Weinan E, Jiequn Han, and Linfeng Zhang.)

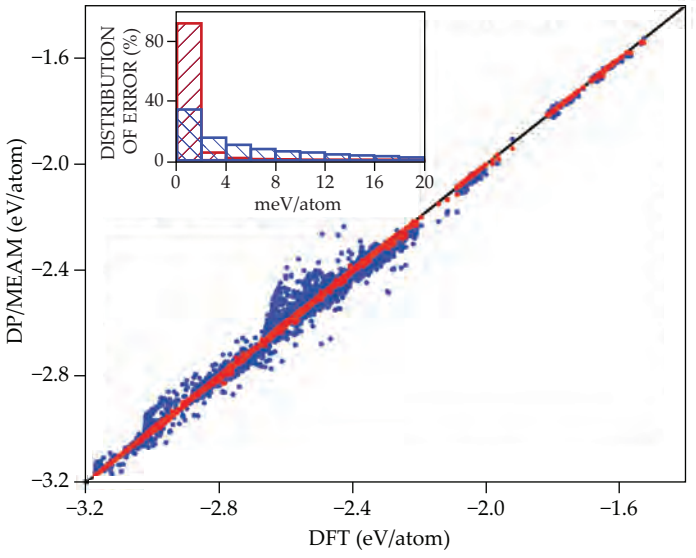

FIGURE 4. COMPARING MODELS. The energies per atom along the interstitial relaxation path of an aluminum–magnesium alloy are predicted by density functional theory (DFT; black line), the deep-potential model (DP; red circles), and an empirical potential-energy model (MEAM; blue circles). The predictions use as inputs 28 different structures identified in the Materials Project database. (Adapted from A. Jain et al., *APL Mater.* **1**, 011002, 2013.) Data points on the diagonal indicate that the prediction agrees exactly with the corresponding DFT results. (Adapted from ref. 14.)

lational and rotational symmetries are enforced by fixing a local coordinate frame, and permutational symmetry is enforced by fixing an ordering of the atoms in the local coordinate frame.

The only problem with the poor man's version is that the order-fixing procedure creates small discontinuities when the ordering of the atoms near a particular atom changes. Although negligible for sampling a canonical ensemble, the discontinuities manifest themselves in a microcanonical, or constant energy, MD simulation, as shown in figure 3b. To construct a smooth PES model that satisfies all the symmetry constraints, practitioners must reconsider how to represent the general form of symmetry-preserving functions. One idea is to have the fitting network in each subnetwork succeed an embedding network that produces a sufficient number of symmetry-preserving functions and that can be optimized via training.[11] In such an approach, the model automatically preserves symmetry. The idea of an embedding network can also be used in other situations in which symmetry is an important issue.

To address the second problem of generating good data, one can make use of the EELT algorithm. At the macroscale level, one samples the temperature–pressure space of thermodynamic variables. For each temperature–pressure value, the canonical ensemble is sampled using the approximate potential available at the current iteration. By adopting that procedure, only a minuscule percentage of the explored configurations need to be labeled. The constructed PES is called the deep-potential model.

Figure 4 shows the accuracy of the deep-potential model generated using the EELT algorithm. From the perspective of a materials scientist, the model achieves uniformly accurate predictions of all the target properties.[12] When combined with the state-of-the-art, high-performance computing platform Summit at Oak Ridge National Laboratory, MD simulations with *ab initio* accuracy are now feasible in systems of up to 100 million atoms. The achievement makes it possible to study more complex phenomena, such as properties and dynamics of defects in materials, that require large-scale simulations[13] with *ab initio* accuracy.

Moment closure in gas dynamics

The Boltzmann equation for the phase space density function of a single particle is particularly well suited for modeling the dynamics of gases. Such a simulation is rather complicated because of the dimensionality of the phase space and the complexity of the collision operator. Dense gases have long been

THE TRIUMPH OF NEURAL-NETWORK-BASED MACHINE LEARNING

Why is neural-network-based machine learning so successful in modeling high-dimensional functions? Although the reason for its success is still the subject of active research, one can get a glimpse through some simple examples.

The one area that has had many successes in handling high-dimensional problems is statistical physics, when Monte Carlo methods are used to compute high-dimensional expectations. If we use a grid-based quadrature rule, such as the trapezoidal rule, to calculate the expectations, the error behaves like $I - I_m \sim m^{-2/d}$. Here, I is the quantity to be calculated, I_m is the approximate value obtained using the quadrature rule, m is the number of function evaluations used, and d is the dimensionality. To reduce the error by a factor of 10, m must be increased by a factor of $10^{d/2}$. The dependence on d is the curse of dimensionality. If a Monte Carlo approach is used instead, then $E(I - I_m)^2 = \text{var}/m$, where var is the variance. Note that the error rate is independent of the dimensionality of the problem, though the variance can be very large in high dimensions. That's why variance reduction is a central theme in Monte Carlo methods.

What about function approximation? To gain some insight, consider the Fourier representation of functions:

$$f^*(\boldsymbol{x}) = \int_{\mathbb{R}^d} a(\boldsymbol{\omega}) e^{i(\boldsymbol{\omega},\boldsymbol{x})} d\boldsymbol{\omega}.$$

Typically this expression is approximated by some grid-based discrete Fourier transform and suffers from the curse of dimensionality. But consider the alternative approach of representing the functions by

$$f^*(\boldsymbol{x}) = \int_{\mathbb{R}^d} a(\boldsymbol{\omega}) e^{i(\boldsymbol{\omega},\boldsymbol{x})} \pi(d\boldsymbol{\omega}) = \mathbb{E}_{\boldsymbol{\omega}\sim\pi}\, a(\boldsymbol{\omega}) e^{i(\boldsymbol{\omega},\boldsymbol{x})},$$

where π is a probability distribution on the Euclidean space $\mathbb{R}^d$. Then the natural approximation becomes

$$f^*(\boldsymbol{x}) \sim \frac{1}{m} \sum_{j=1}^{m} a(\boldsymbol{\omega}_j) e^{i(\boldsymbol{\omega}_j,\boldsymbol{x})},$$

where $\boldsymbol{\omega}_j$ are independent and identically distributed samples of π. That approximation does not suffer from the curse of dimensionality. The right-hand side of the equation immediately above is an example of the neural-network functions with one hidden layer. Activation function σ and independent variable z are defined by $\sigma(z) = e^{iz}$.

modeled accurately using Euler's equations,[2] and since the mid 20th century, many people have tried to develop Euler-like models for rarified gases. But such modeling is difficult because of the non-equilibrium state of rarified gases.

Euler's equations can be viewed as the projection of Boltzmann's equation on the first few moments of the distribution function for the gas particles. Thus one possible way to develop Euler-like models for rarified gases is to generalize the moment-projection scheme by considering projections onto larger sets of moments. To get a closed model, researchers have to address terms that include moments outside of the set of moments in the projection scheme.

That issue is known as the moment-closure problem for gas dynamics. Despite many efforts and much progress over 70 years, it remains unsolved. Attempts to elucidate it are often ad hoc. Another issue is that the equations obtained may violate the second law of thermodynamics, a known issue in the 13-moment model.[2]

To develop reliable and uniformly accurate Euler-like models for dense and rarified gases, researchers can use machine learning to identify not only accurate closure models but also the best set of moments to represent the distribution function. Supervised learning can find accurate closure models in much the same way as learning about a PES, as discussed earlier. Identifying the best set of moments can be solved by using an autoencoder, a well-known dimension-reduction technique in machine learning.

Another problem is that the moment-closure equations, unless corrected, violate the second law of thermodynamics. The problem is subtle and can be fixed in one of two ways. The first addresses the problem by explicitly enforcing an entropy-like condition, which is analogous to Boltzmann's entropy-dissipation inequality. The second way sidesteps the problem by contending that as long as the model is accurate enough, it should not violate the second law of thermodynamics because the original Boltzmann's equation does not. Therefore, our efforts should be spent on making the model uniformly accurate enough under all practical situations. Some promising results that follow the uniformly accurate approach have been obtained,[14] and a related result is shown in figure 5.

The lessons learned from the moment-closure problem might be helpful in addressing other, more complex physical problems. The problem discussed in regards to gas dynamics is representative of the situation when researchers try to obtain turbulence models or hydrodynamic models for non-Newtonian fluids. In those situations, too, the closure problem needs to be addressed, and the second law of thermodynamics must not be violated.

A balancing act

Physicists are used to models based on first principles. Many of them are simple and elegant—they contain only a few parameters that are physically meaningful and measurable—and are widely applicable. Unfortunately, the world is often not so simple: Complexity is inherent to most, if not all, of the practical problems that physicists face. When dealing with complex systems, machine-learning-based models such as the ones discussed in this article may offer the solutions that researchers need.

Even though models that use machine learning are typically clumsier and involve more parameters than the ones based on first principles, they are in some ways not so different from the kinds of models we are used to. The main difference is that some functions used in the models exist in the form of subroutines. In Euler's equations for complex gases, for example, the equation of state is stored as tables or subroutines.

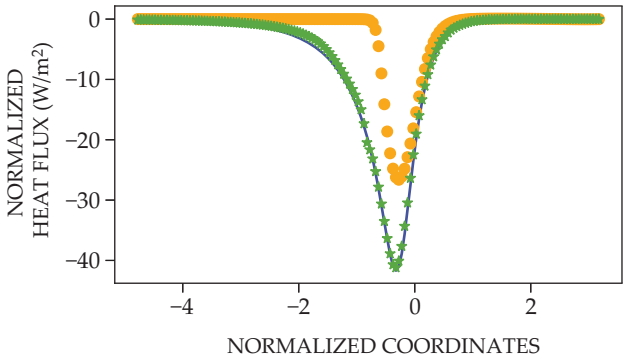

FIGURE 5. HEAT FLUX associated with the structure of normal shock waves with Mach number 5.5 is obtained from the Boltzmann equation (blue line), the Navier-Stokes-Fourier (NSF) equations (orange circles), and a machine-learning-based closure function (green stars). The machine-learning function tracks the Boltzmann equation more closely than the NSF approach. (Figure by Jiequn Han and Zheng Ma.)

In principle, the same procedure and the same set of protocols discussed in this article are also applicable in a purely data-driven context without a microscale model. In that case, the labels would be replaced with experimental results. In fact, one can imagine connecting an experimental setup to some machine-learning model using the EELT algorithm to minimize the experimental effort required for obtaining a reliable model. That promising approach remains relatively unexplored. Similar ideas are also relevant to such situations as data assimilation, in which physics- and data-driven approaches are combined to improve the overall reliability of the models. Researchers have only recently begun those kinds of efforts.

In the short term, more effort should be devoted to using machine-learning-assisted modeling to develop new reliable models for complex physical systems, such as complex fluids, and to perform optimization and control analyses on those systems. In the long term, researchers should study how to use machine learning and innovative modeling in areas such as economics, in which first-principle-based models are hard to develop.

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PT

ASTEROIDS IN THE INNER SOLAR SYSTEM

Sarah Greenstreet

Observations and computer simulations of their orbits and interactions with planets yield insights into the asteroids' dynamic lives.

About 500 meters wide, Bennu orbits our Sun in the Apollo population of near-Earth asteroids. It was visited and photographed by spacecraft *OSIRIS-REx* in December 2018.

NASA/GODDARD/UNIVERSITY OF ARIZONA

Sarah Greenstreet is a senior researcher with the B612 Asteroid Institute in Mill Valley, California, and a research scientist with the Dirac Institute at the University of Washington in Seattle.

People tend to think of the solar system as a static environment, in which the orbits of the planets, asteroids, and comets have remained the same over its lifetime. But although its current architecture has existed for roughly the past 4.5 billion years, the solar system is far from the unvarying environment that we imagine.

The gravitational influence of the planets over small bodies, particularly those in the solar system's inner regions, has modified many asteroid orbits in quite dramatic ways. For example, the interactions can push asteroids from nearly circular orbits in the main asteroid belt between Mars and Jupiter to highly elliptical orbits that cross those of all the terrestrial planets. Eventually, those perturbations can move the asteroids' perihelia—their closest orbital distance from the Sun—to within the star's radius. They are known as Sun-grazing orbits. The asteroids' transformation from main-belt orbiters to Sun grazers can take place in the surprisingly short time scale of a million years. That's less than 0.02% the age of the solar system.

In addition to decreasing the asteroids' perihelia, gravitational interactions can also decrease their aphelia—their farthest orbital distance from the Sun—and push them to increasingly smaller orbits. That movement progressively nudges asteroids onto hard-to-reach orbits that are closer to the Sun than either Earth's orbit or Venus's orbit; the asteroids are known as Atiras and Vatiras, respectively. The orbital evolution of those rare Atira and Vatira asteroids is a reminder that their trajectories can change dramatically over their lifetimes and take them throughout the inner solar system. That evolution can tell us where the asteroids have likely been and where they will likely go as their orbits continue to evolve. More practically, it can tell us where to point our telescopes to find those elusive objects.

From main-belt to Sun-grazing orbits

More than 525 000 numbered asteroids with well-known orbits and in sizes ranging over several orders of magnitude—from hundreds of meters to a thousand kilometers—currently inhabit the main asteroid belt. Several basic parameters describe their orbits around the Sun. The semimajor axis refers to an asteroid's average orbital distance from the Sun. That distance is often measured in astronomical units, with 1 AU defined as the mean Earth–Sun distance. The eccentricity is the asteroid's orbital ellipticity. It equals 0 for a circular orbit and 1 for a parabolic orbit, a trajectory whose energy is the minimum required for an asteroid to become unbound from the Sun and escape the solar system. For all values between those extremes, the orbit is more or less elongated. The inclination refers to the orbit's angular tilt relative to the plane of the solar system in which the planets lie.

Figure 1 shows two commonly used projections of the known main-belt asteroids between Mars and Jupiter. Compared with the roughly circular planetary orbits, main-belt asteroid orbits are more elliptical and are inclined by as much as 30°. The first person to arrange the ever-growing number of discovered asteroids by average distance from the Sun was mathematician and astronomer Daniel Kirkwood. Upon arranging the asteroids that way in 1866, Kirkwood noticed sharp drops, now called Kirkwood gaps, in the number of asteroids located at specific semimajor axes. Few asteroids reside in the Kirkwood gaps, and they span large ranges in eccentricity and inclination.

Kirkwood identified the most obvious gaps in the asteroid population at 2.50, 2.82, 2.95, and 3.27 AU as locations of the 3:1, 5:2, 7:3, and 2:1 orbital resonances, respectively, with Jupiter.[1] An orbital resonance occurs when an asteroid's orbital period is an integer multiple of a planet's. For example, the 2:1 resonance with Jupiter occurs when an asteroid orbits the Sun exactly twice for every orbit of Jupiter. Resonances occur at specific semimajor axes because, as Kepler's third law tells us, the square of an object's orbital period is proportional to the cube of its semimajor axis. Thus, because those resonances occur for specific orbital periods, they are located at the corresponding semimajor axes.

Why are so few asteroids located in the resonances associated with the Kirkwood gaps? The main belt hosts numerous orbital resonances with Mars, Jupiter, and Saturn, and several of them overlap in the gaps. The overlapping resonances cause the orbits of the asteroids in the region to be unstable, and the instability leads to an excitation, or increase, in asteroid eccentricities. The semimajor axis of an asteroid in a resonance cannot itself change, so as the asteroid's orbit evolves, its eccentricity follows a vertical path from low to high values in the plot of eccentricity versus semimajor axis (see figure 1b). Eventually, the eccentricity reaches values larger than the moderate eccentricities seen in the main belt.

As an asteroid's eccentricity increases, its orbit becomes increasingly less circular and more elliptical. The elongation

causes the asteroid's perihelion to decrease and its aphelion to increase, eventually putting the asteroid on a terrestrial planet-crossing orbit. If the orbit becomes so highly elongated that the perihelion drops to within the solar radius, the asteroid reaches a Sun-grazing orbit and incinerates during its next perihelion passage. Over time, the resonant-eccentricity-excitation process has nearly emptied the Kirkwood gaps of asteroids as they are transported from the main belt to the inner solar system.

How long does it take for an asteroid orbit to be altered from main-belt to Sun-grazing? A landmark study performed by Paolo Farinella and colleagues in 1994, when Farinella was a visiting professor at the Nice Observatory in France, found that low-eccentricity asteroids located in a resonance with a planet can evolve onto Sun-grazing orbits in as little as 1 million years.[2] Over the past 4.5 billion years of solar system history, asteroids located along the borders of those resonances have slowly diffused into the resonances and supplied at a steady rate the sunward transportation of asteroids from the main belt.

That slow diffusion most frequently occurs through gravitational close encounters with the planets, which can change an asteroid's semimajor axis. Just as a spacecraft can gain or lose speed by passing closely behind or in front of a planet, so can an asteroid. Because orbital speed is inversely proportional to orbital period and the period squared is proportional to the semimajor axis cubed, an increase in orbital speed causes a decrease in semimajor axis and vice versa. Planetary interactions can thus change the semimajor axis of an asteroid located just outside the border of a resonance enough to move it into the resonance.

Near-Earth asteroids

Not all asteroids in resonances reach Sun-grazing orbits. Once an asteroid's eccentricity increases enough, a gravitational close encounter with a planet can move the asteroid out of the resonance. The interaction leaves the asteroid on a planet-crossing orbit that is no longer on a resonant path to a Sun-grazing orbit. Because orbital periods close to the Sun are quite short, the asteroid experiences frequent planetary close encounters once it reaches terrestrial planet-crossing orbits. Each encounter causes a small change in the asteroid's semimajor axis, and frequent encounters scatter asteroids throughout the inner solar system. The process feeds the population of what are called near-Earth asteroids (NEAs). That population is defined to have perihelia smaller than 1.3 AU.

Traditionally, NEAs are divided into four dynamical subpopulations—Amors, Apollos, Atens, and Atiras—whose orbits are categorized relative to Earth's orbit. Amors follow orbits that are always farther from the Sun than is Earth's. Atiras, by contrast, follow orbits that are always closer to the Sun than is Earth's. Apollos and Atens are both on Earth-crossing orbits. Based on a rare, dynamical subset of orbits found in our simulations of the NEA subpopulations, in 2012 I and my colleagues Brett Gladman and Henry Ngo, then all at the University of British Columbia, proposed the addition of a fifth subpopulation we called the Vatiras.[3] That asteroid class is similar in nature to Atiras, but they follow orbits that keep them closer to the Sun than Venus's orbit—hence their name as a play on Venus and Atira. Figure 2a shows a schematic of sample orbits for each of those five subpopulations.

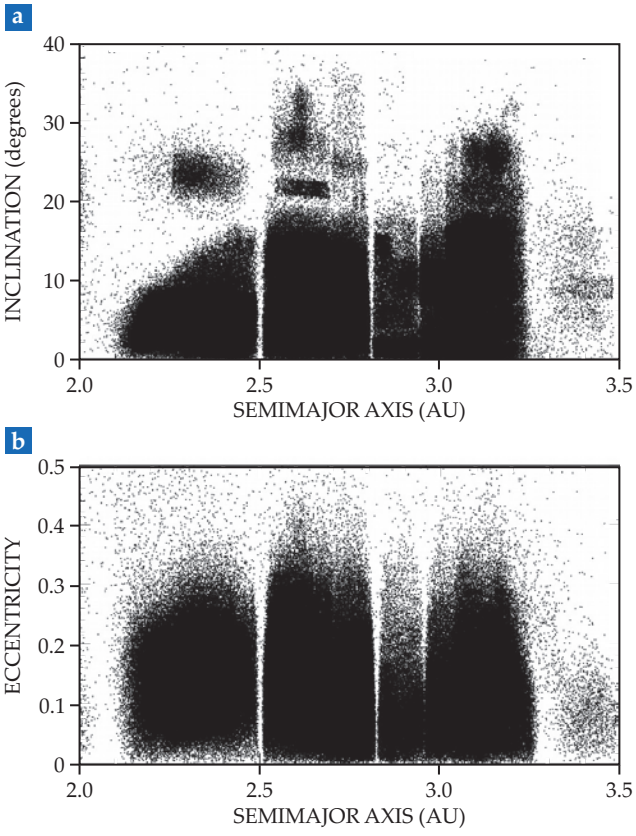

FIGURE 1. ORBITAL DISTRIBUTIONS of the roughly 525 000 asteroids in the main asteroid belt. The data come from the Minor Planet Center Orbit Database, a public list of computed orbits for all known small bodies in the solar system. The semimajor axis measures the average orbital distance from the Sun relative to the Earth–Sun distance (1 AU). **(a)** Inclination measures the angular tilt of the orbit out of the planetary plane. **(b)** Eccentricity measures the orbital ellipticity. Main-belt asteroids sit between the orbits of Mars and Jupiter on moderately elliptical and inclined orbits. So-called Kirkwood gaps can be seen at specific semimajor axes, where orbital resonances exist and the number of asteroids drops sharply. (Image by Sarah Greenstreet.)

Our NEA dynamical model and an updated model produced by the University of Helsinki's Mikael Granvik and colleagues in 2016 independently predict that the Amor, Apollo, Aten, Atira, and Vatira subpopulations contain roughly 39%, 55%, 4%, 1%, and less than 1% of NEAs, respectively, at any given time.[3,4] Together, the Amors and Apollos make up the vast majority (94%) of NEAs. That's partly the result of the much larger volume of near-Earth space they cover. The curves shown in figure 2b mark the boundaries of each subpopulation and follow the perihelia and aphelia of Earth, Venus, and Mercury. For example, while all NEAs must have perihelia that are less than 1.3 AU, Amors must have perihelia that are larger than Earth's aphelion (1.017 AU) to remain farther from the Sun than Earth's orbit is.

Apollos have perihelia that are smaller than Earth's aphelion and semimajor axes that are greater than the semimajor axis of Earth (1 AU). Atens have semimajor axes that are less than 1 AU and aphelia that are larger than Earth's perihelion (0.983 AU).

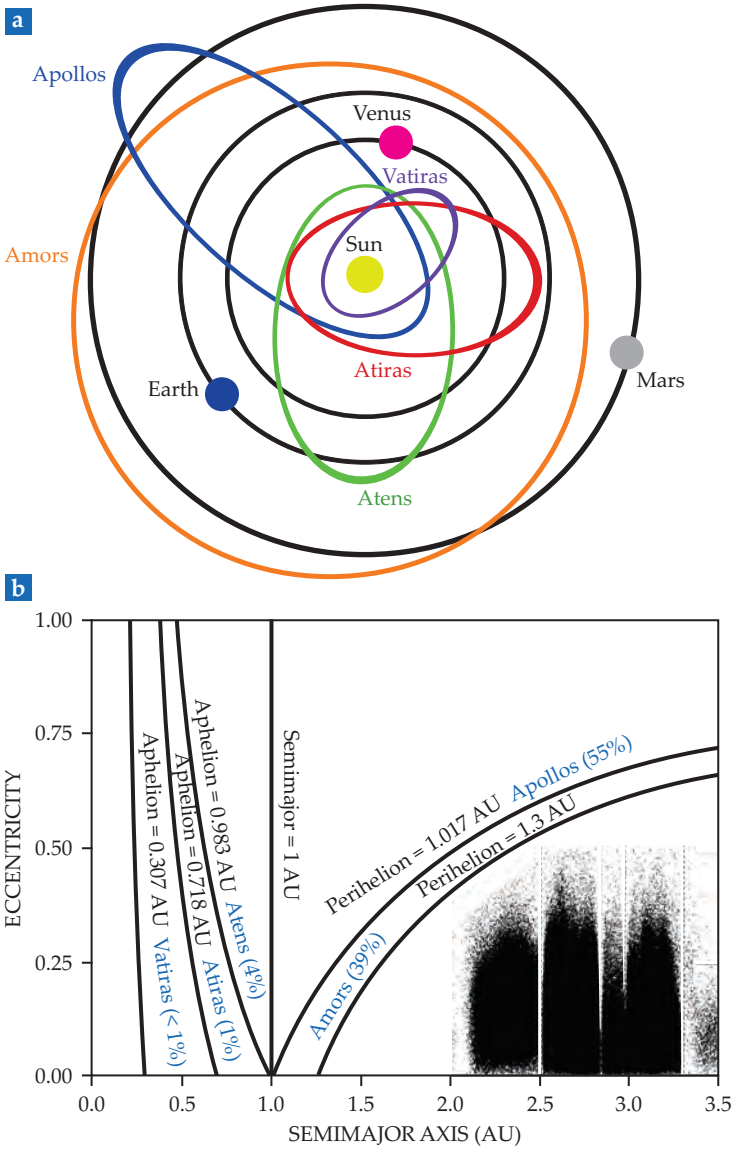

FIGURE 2. SCHEMATIC ORBITS of near-Earth-asteroid classes. **(a)** Those of Apollos and Atens cross Earth's orbit. Amors orbit the Sun entirely outside Earth's orbit, and Atiras orbit the Sun completely inside Earth's orbit. Vatiras are on orbits entirely inside Venus's orbit. **(b)** This projection shows the inner solar system in a plot of near-Earth asteroid eccentricities versus their semimajor axes. At the lower right are the known main-belt asteroids. The vast majority (Apollos and Amors) in the inner solar system reside outside Earth's semimajor axis (1 AU). The fraction of near-Earth asteroids in each subpopulation and the limits on their aphelia or perihelia are shown by their names. (Image by Sarah Greenstreet.)

Their orbital parameters make Apollos and Atens Earth-crossing. Atiras must have aphelia that are smaller than Earth's perihelion to stay closer to the Sun than Earth's orbit is at all times. Lastly, Vatiras have aphelia that are inside Venus's perihelion (0.718 AU) and outside Mercury's perihelion (0.307 AU). Any asteroids with aphelia inside Mercury's perihelion would remain closer to the Sun than Mercury's orbit is. Another reason Amors and Apollos are the most numerous NEAs is because they overlap the resonances where asteroids enter the NEA population. That overlap greatly enhances their number over the Atens, Atiras, and Vatiras, which lie much closer to the Sun than those resonances.

Generally, asteroids can reach the Aten, Atira, and Vatira subpopulations only through a series of planetary close encounters that cause their semimajor axes to jump to increasingly smaller values. The close encounters are more frequent in the inner solar system because of higher orbital speeds. But for the encounters to push asteroids into the three innermost NEA populations, they must occur in such a way that they cumulatively decrease, not increase, an asteroid's semimajor axis. As you can imagine, that process becomes increasingly difficult as asteroids reach smaller orbits and encounter fewer planets. Thus a large drop-off in asteroid population occurs between the Apollos and the Atens.

Likewise, it becomes more difficult to gravitationally scatter asteroids onto orbits decoupled from the planets—that is, orbits that are no longer planet-crossing—at the increasingly smaller orbits entirely interior to the orbits of Earth and Venus. For those reasons, Atiras are rare and Vatiras even rarer among the NEAs. And although it is theoretically possible, asteroids almost never reach orbits completely interior to Mercury's orbit.

Dynamical behavior

Despite the rarity of Atiras and Vatiras, they provide a unique glimpse into the dynamic environment of the innermost regions of our solar system. Any given asteroid that becomes a Vatira will have passed through the Amor, Apollo, Aten, and Atira populations to reach its eventual small orbit. Each Atira and Vatira will have taken a unique path from the main belt, often over tens of millions of years, and will have spent varying amounts of time in each population along the way.

Asteroids do not remain in the Atira and Vatira populations for long. Detailed dynamical simulations of Atira asteroids performed by Anderson Ribeiro of the Geraldo Di Biase University Center in Brazil and his colleagues indicate that the very planetary close encounters required to enter those hard-to-reach orbits are responsible for continually scattering the asteroids into and out of the Vatira and Atira populations many times during their lifetimes.[5] Those events keep the asteroids from lingering in either of the planet-decoupled populations.

As Gladman, Ngo, and I discovered in our simulations,[3] the asteroids typically spend only a couple million years—integrated over their lifetimes—as Atiras and a few hundred thousand years as Vatiras. It is possible for asteroids to enter the Vatira region and to remain there for more than a million years before leaving. However, such long-lived Vatiras are extremely rare. If most of those asteroids don't remain in the Atira and Vatira populations, where do they go? The frequent planetary close encounters generally push the asteroids outward, over tens of millions of years, back onto Venus- and Earth-crossing orbits. (The asteroids become Atens and Apollos.) Because the vast majority of Atiras and Vatiras do not remain

FIGURE 3. THE ZWICKY TRANSIENT FACILITY is located at the Palomar Observatory's 48-inch Samuel Oschin Telescope. The facility's twilight observing program is responsible for finding the three near-Earth asteroids with the shortest orbital periods known to date. (Image courtesy of Palomar/Caltech.)

decoupled from Earth and Venus, most eventually collide with one of those planets or with Mercury. Any that remain are frequently pushed onto Sun-grazing orbits, and some are even scattered back out to Mars-crossing orbits and potentially beyond the asteroid belt.

Dynamical simulations reveal the orbits in which Atiras and Vatiras spend most of their time and thus where it is best to look in the night sky to find them. Their rarity has made them of particular interest to telescopic surveys focused on asteroid discovery. Many of those surveys have dedicated time to searching for asteroids near the Sun, and some telescopes, such as the space-based *Near-Earth Object Surveillance Satellite* (*NEOSSat*),[6] were specifically designed to discover new Atens, Atiras, and Vatiras.

Not only are Atiras and Vatiras a rare part of the NEA population because of their difficulty in gravitationally scattering to small, planet-decoupled orbits, they are also challenging objects to observe in the night sky because of their close proximity to the Sun. The asteroids are never farther from the Sun than is Earth, so ground-based telescopes—which make most asteroid discoveries—must aim near the horizon during a brief period of time shortly after sunset and shortly before dawn to have any hope of capturing one in an image. Considering that observational limit, when new discoveries of such asteroids are made, it is quite exciting.

Atira discoveries

To date, 23 known asteroids orbit the Sun in the Atira population. They range in size from 50 m to 5 km. Both the Granvik and Greenstreet models estimate the existence of 10 Atiras[3,4] with diameters larger than a kilometer. Beyond the six known Atiras in that size range, few large ones are likely left to be discovered. The number of Atiras with increasingly smaller diameters is much greater, so many more remain to be found.

The first confirmed Atira asteroid was discovered in 2003 by the Lincoln Near-Earth Asteroid Research program at the MIT Lincoln Laboratory near Socorro, New Mexico. Called 163693 Atira, it was named after the Pawnee goddess of Earth. The asteroid follows a highly inclined orbit with an aphelion just inside Earth's perihelion—the cutoff for orbits interior to Earth's. Because the asteroid's aphelion is so close to Earth's perihelion, it is possible for the Atira to have close encounters with Earth. In January 2017 one such encounter occurred when the asteroid passed close enough for the Arecibo Observatory to capture it in a series of radar images.

Radar astronomy uses reflected microwaves from nearby solid targets to constrain the shape, size, and spin state of an asteroid. As reported by Edgard Rivera-Valentín and colleagues, all at Arecibo Observatory at the time, the radar measurements revealed an unexpected finding—that 163693 Atira is a binary system.[7] It consists of two objects, a primary and a smaller secondary, that orbit each other. The diameter of the primary was measured at 4.8 ± 0.5 km with an elongated and very angular shape; the diameter of the secondary was 1.0 ± 0.3 km. The semimajor axis of the binary was fit at near 6 km with an orbital period of roughly 16 hours.

Astronomers are not lucky enough to get radar measurements of many asteroids, but telescopic observations reveal many of their features. The asteroids' brightness, distance, and reflectivity reveal their size. The periodicity at which that brightness changes reveals their rotation periods. And spectral analysis reveals their surface composition. Using dynamical simulations of an observed orbit, astronomers can learn where an asteroid likely came from, how long it is likely to stay on its current orbit, and what its most likely future trajectory will be. Using our dynamical model of the NEA orbital distribution,[3] we can say that 163693 Atira probably entered the NEA population through the inner portion of the main asteroid belt and likely took tens of millions of years to scatter down to its current region. It will probably scatter into and out of the Atira population several times with an integrated lifetime in the Atira region of a couple million years before most likely colliding with a terrestrial planet.

Over time, more Atira-class asteroids have been discovered that have increasingly smaller orbits. In 2019 astronomers found two Atiras that have the smallest semimajor axes known and aphelia that put them near the Atira–Vatira boundary (Venus's perihelion). The first, 2019 AQ3, was discovered on 4 January by the twilight observing program at the Zwicky Transient Facility[8] at Palomar Observatory, shown in figure 3. The second, 2019 LF6, was discovered five months later, on 10 June.

The first Vatira

Within a year of the discoveries of 2019 AQ3 and 2019 LF6, the first Vatira-class asteroid was spotted by the same program at the Zwicky Transient Facility that had discovered the two Atiras. Figure 4 shows the asteroid appearing as a tiny dot in the night sky four days after its discovery. Designated 2020 AV2, the asteroid has an aphelion well inside the Venus perihelion cut-off, which makes its orbit entirely inside Venus's orbit. As estimated by Marcel Popescu of the Astronomical Institute of the Romanian Academy and colleagues, 2020 AV2 is roughly 1.5 km in diameter.[9] And to judge by the Greenstreet and Granvik dynamical models,[3,4] it is likely one of two Vatiras of that size currently in existence.

Popescu and colleagues classified the composition of 2020 AV2 as one that dominates the inner main belt.[9] The composition is consistent with our model prediction that the asteroid most likely originated at the inner edge of the main belt before making the long journey to the Vatira population.[3,10] It will likely remain a Vatira for a few hundred thousand years before scattering back out through a Venus-crossing Atira orbit to the Earth-crossing region, where it will most likely collide with Venus or Earth several million years from now.[10] The current orbit of 2020 AV2 puts it very close to the 3:2 resonance with Venus.[10,11] Unlike the resonances located in the main-belt Kirkwood gaps, that resonance with Venus is relatively stable, given the scarcity of resonances in the innermost portion of the solar system. Vatiras can remain in the resonance for millions of years, making the Venus resonance a likely place where other Vatiras are lurking and thus a good hunting ground for discovering more asteroids in that class.

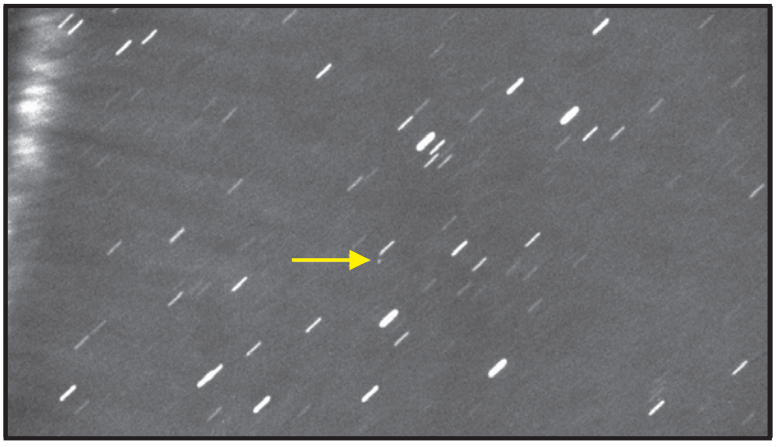

FIGURE 4. A VATIRA ON FILM. The Virtual Telescope Project took this image on 8 January 2020. It shows the average of 14 60-second exposures. They were combined to track the motion of 2020 AV2—the white dot, marked by an arrow—across the sky to reveal the asteroid as a point source, against which the stars streak. (Image courtesy of Gianluca Masi, Virtual Telescope Project.)

Asteroid surveys, such as the twilight observing program at the Zwicky Transient Facility and the space-based *NEOSSat*, are ongoing. In addition, two large observing programs—the Vera C. Rubin Observatory's Legacy Survey of Space and Time and NASA's Near-Earth Object Surveillance Mission—are upcoming. Those new programs are likely to vastly increase the number of known NEAs, particularly given the new software being developed to prepare for the deluge of data from the new surveys. For example, using a program[12] built by the University of Washington's Dirac Institute, the cloud-based Asteroid Decision Analysis and Mapping platform will allow the B612 Asteroid Institute to extract even the trickiest-to-find asteroids among the data.

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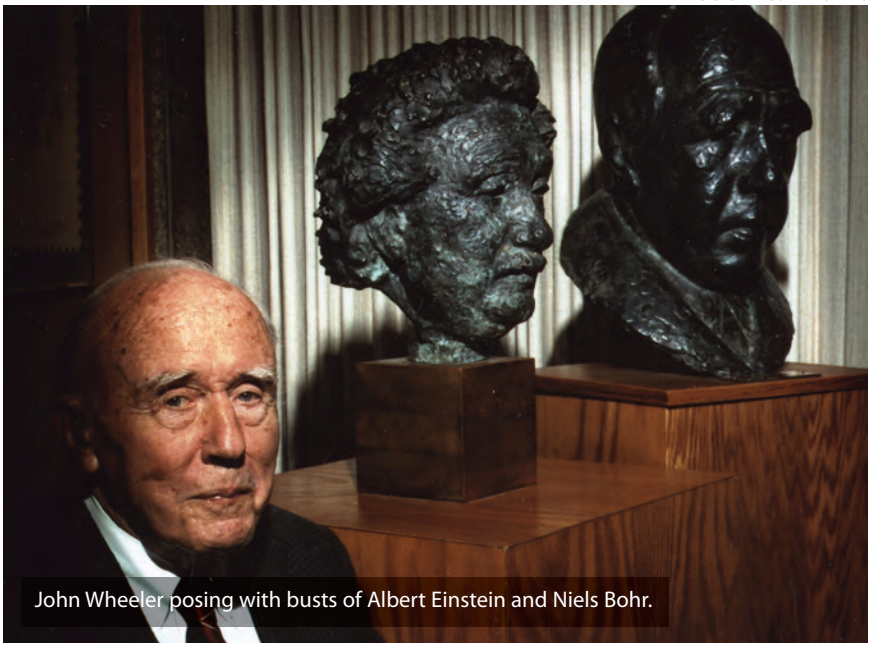
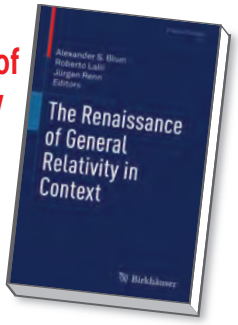


John Wheeler posing with busts of Albert Einstein and Niels Bohr.

Einsteinian ebbs and flows



The Renaissance of General Relativity in Context
Alexander S. Blum, Roberto Lalli, and Jürgen Renn, eds.
Birkhäuser, 2020.
$119.99

One might wonder what it means for a theory to have a "renaissance." After all, we tend to think of them as binary—proven or not. Once we know that one is right, it goes into the textbooks and becomes part of the body of accepted knowledge. *The Renaissance of General Relativity in Context*, though, contends that theories' fortunes can change long after they are verified. Consider, for example, general relativity. The theory was accepted following the 1919 eclipse expeditions that measured the gravitational deflection of starlight by the Sun. Didn't that establish its status as a pillar of modern physics?

The real story is more complicated. Historians of science have noticed that Albert Einstein's theory had an unusual trajectory after its verification: decades of stagnancy and disinterest—the "low-water-mark" period—followed by a resurgence of interest and activity, the "renaissance" of the book's title. The present volume is the result of several years of examination of that renaissance by researchers connected to the Max Planck Institute for the History of Science. Authored by some of the world's leading experts on general relativity, the essays are deeply researched and tightly argued pieces of scholarship that combine approaches from history, sociology, physics, and big data.

The group's first task was to establish whether general relativity had such a renaissance and, if so, what exactly it entailed. That is where big data and similar innovative tools helped create a new kind of history. They allowed the authors to discern connections between scientists working in particular areas that would otherwise be difficult to notice. For instance, the vague sense that general relativity was not in vogue between 1920 and 1950 can now be replaced with a precise statement: Plenty of people were working on the theory, but they were generally working independently. Moreover, their efforts were tangential to the core of contemporary physics.

The Renaissance of General Relativity in Context shows, in beautiful graphs, how the theory went from idiosyncratic to the cutting edge of research. It even exposes novel kinds of networks—not just social networks of coauthors, but semiotic networks of scientific representations and semantic networks of research agendas and conceptual interpretations.

Once uncovered, those networks can point to fascinating developments. For example, most of the physicists working on relativity before World War II were pursuing alternatives to Einstein's theory, whereas research in the 1950s and 1960s marked a return to the "original" version—and a renewed sense that its physical consequences were worth looking for. Particularly interesting is the role of humble postdocs in connecting disparate researchers in the networks that were the essence of the renaissance. In addition to those network studies, the book includes focused explorations of many of the major figures, concepts, and projects involved in the renaissance, such as Vladimir Fock, Leopold Infeld, Peter Bergmann, gravitons, the cosmological constant, dark matter, and the Virgo interferometer.

Appropriately, John Wheeler gets particular attention. His conversion in the 1950s from nuclear physics to general relativity is a microcosm of the field's resurgence. The success of quantum electrodynamics drove him to look for new approaches that might be equally successful. He took advantage of his position at Princeton University—namely, being near Einstein and his friends at the Institute for Advanced Study—and developed both a research program and one of the first courses in general relativity. He trained new students in the fundamentals of the theory and illustrated the benefits it might bring to physics. New textbooks, publications, and conferences followed, and they provided the infrastructure necessary for the theory to thrive.

Wheeler's story is also helpful in answering one of the great questions about the renaissance: Why did it happen when and where it did? Was it because of Wheeler's connections to the resources of the military-academic-industrial complex, what the volume calls the "sugar daddy" scenario, or was it due to his aesthetic embrace of a beautiful, rediscovered theory, the "sleeping beauty" scenario? Both possibilities are explored in

some detail, along with other important factors, such as private patronage from wealthy figures who were unhealthily obsessed with the hypothetical phenomenon of antigravity.

The renaissance of general relativity provides a rich case study for thinking about fundamental problems of scientific change. How are theories used and not used? What is the difference between healthy and withering research programs? Can the resurgence of a theory be explained by new observational discoveries? Technological advances? Individual personalities? Social and political developments? The book is a great cross section of those different approaches, which will make it valuable to scholars in history and sociology of physics—although it might set a fairly high methodological barrier to entry for nonspecialist readers. Nevertheless, *The Renaissance of General Relativity in Context* will quickly become a classic in the history of the field, and it will perhaps spur new research programs of its own.

Matthew Stanley
New York University
New York City

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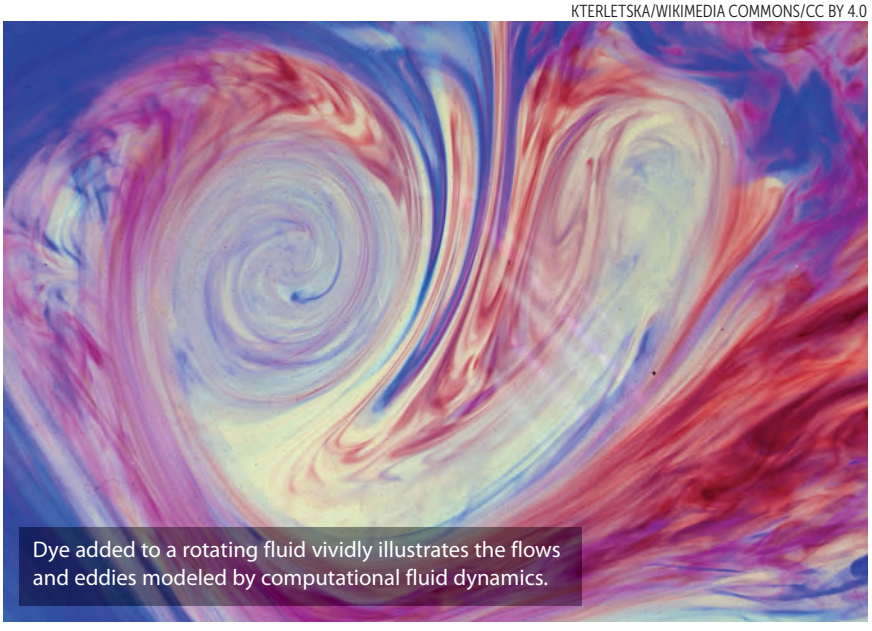
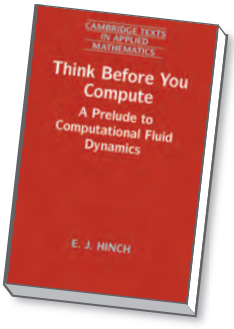


Dye added to a rotating fluid vividly illustrates the flows and eddies modeled by computational fluid dynamics.

Numerical methods: A user's guide

Think Before You Compute
A Prelude to Computational Fluid Dynamics

E. J. Hinch
Cambridge U. Press, 2020. $79.99



The equations governing the flows of fluids are inherently nonlinear, so exact solutions are rare and gemlike. Approximate solutions of the equations are thus critical to understanding most of the interesting behaviors seen in fluids. Although analytic approximations have been used to glean insight into fluid phenomena since the field's beginning in the 19th century, numerical approximations provide a complementary way to learn about the behaviors of the solutions. In his new book, *Think Before You Compute: A Prelude to Computational Fluid Dynamics*, renowned fluid dynamicist Edward John Hinch provides an introduction to those techniques.

The titular exhortation outlines the book's objective: To help readers develop intuition about the physics and the mathematics necessary to formulate a problem, learn the techniques and algorithms used to solve the equations approximately, and understand the meaning of the results. The product of decades spent teaching the subject, *Think Before You Compute* is a superb introduction to the basic methods underlying the theory and practice of computational fluid dynamics (CFD).

The book is split into three parts. The first part starts with an invitation to jump directly into the deep end of the pool and solve the two-dimensional Navier–Stokes equations for flow in a cavity with a driven lid, which is a classic problem that encompasses and highlights all the major issues of CFD. The section discusses different formulations of the problem; issues associated with the pressure singularity at the corners; questions of stability, consistency, and accuracy in the finite difference discretization; and various iterative and projection-based methods. Helpful ready-to-run MATLAB codes are available on the author's website. (A better solution might be to host the code on GitHub and permanently link to the repository from the publisher's site.)

Hinch makes the case for part 1 to be covered in about three lectures and a few exercises. I tried that recently, and it works. The approach of using a single example to illustrate the main difficulties of the field is a refreshing change from other books in the genre that often take too long to spin up.

Part 2 presents a broad but succinct introduction to different CFD approaches, including methods based on compact finite differencing, finite elements, spectral techniques, and the many ways of time stepping. It concludes with a chapter on numerical linear algebra that starts with a very apt caution to readers: "HEALTH WARNING. Do not do it." Each topic is presented concisely, and the exposition is uniformly lucid.

The final third of the book is a discursive amble through such topics as hyperbolic problems and shock capturing, boundary integral methods, interface tracking, lattice- and particle-based methods, numerical continuation, and wavelets. Throughout, Hinch shows readers how to think via examples embedded in the text. Those include the use of scaling estimates for real and spurious instabilities and singular behaviors, how to separate the behavior of the algorithm from that of the continuum equations, and a discussion of convergence and speed of computation. Part 3, however, is probably too brief to be useful for a beginner except as an appetizer.

Overall, the relatively short book strikes a good balance by being neither too technical nor too recipe driven, and it imparts key concepts and practical details without a fuss. Adding an online supplement with examples of when the maxim in the title was not followed would illuminate the teachable moments at the origin of the amusing and occasionally inscrutable pronouncements sprinkled throughout the book.

In our digital age, the firepower afforded by cheap and fast computing is immense, and it is easy to generate Colored Fanciful Displays; this minimalist book has none and is none the worse for it. CFD has succeeded—and will continue to do so—because it augments physical experimentation and analytic approximation. Hinch's direct and informal writing style and his emphasis on understanding fluid dynamics via a recursive loop—think, compute, and think again—make *Think Before You Compute* an attractive textbook for a standalone course on CFD or an excellent supplement for a graduate course that includes conceptual, analytic, and numerical approaches.

L. Mahadevan
Harvard University
Cambridge, Massachusetts

NEW BOOKS & MEDIA

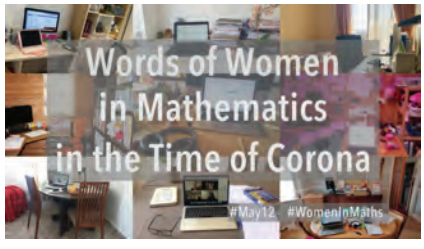
Voyagers

Neil Burger
AGC Studios/Fibonacci Films/Ingenious Media/Thunder Road Films, 2021

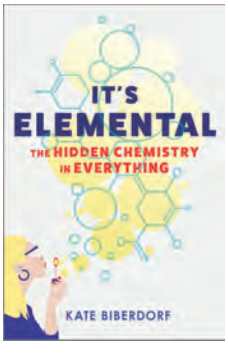
How do you train a crew to travel to another solar system if most of them won't be alive at the end of the 86-year-long trip? In *Voyagers*, the solution is to keep them isolated from Earth, so they never know any environment other than their spacecraft. And to keep them incurious, the fix is to ban art, theater, and music that portray humanity's quest to understand the deep questions of existence. But the spacefarers are a bunch of highly intelligent young people. They soon realize that their emotions are being managed and attempt to break their conditioning. As some of the systems fail on the spacecraft, the crew's reaction to the changing environment brings the mission to the brink of failure and radically changes their societal dynamics. Colin Farrell, Tye Sheridan, and Lily-Rose Depp do an excellent job capturing the awareness of what it means to be human in this unusual take on an interstellar journey. —PKG

Words of Women in Mathematics in the Time of Corona

Irina Linke
Vimeo, 2021



The pandemic has been an opportunity to learn new technologies. It's a time to rethink priorities. It makes concentration difficult. It's isolating. Remote interactions broaden communication. Forming new collaborations is nearly impossible. It's a time of anxiety and uncertainty. Those are among the sentiments conveyed in *Words of Women in Mathematics in the Time of Corona* by German documentary filmmaker Irina Linke. The film, available on Vimeo, features 86 women from 37 countries who speak 25 languages (most of which are accompanied by English subtitles). In vignettes that range from a few seconds to about a minute long, the women describe how the pandemic has affected them professionally and personally. The montage of comments, faces, and surroundings paints a moving and memorable picture. The film was released on 12 May, the birthday of mathematician Maryam Mirzakhani, who died in 2017 at age 40. —TF



It's Elemental

The Hidden Chemistry in Everything

Kate Biberdorf
Park Row Books, 2021. $27.99

From brewing our morning coffee to working out at the gym and cooking dinner, chemistry is everywhere in our daily lives. Yet the atomic and molecular processes and phenomena underlying those and other activities remain a mystery to many people. Chemistry professor Kate Biberdorf of the University of Texas at Austin seeks to rectify that with her latest book. Part primer, part personal narrative, *It's Elemental* takes the reader through some of the typical activities most humans engage in and explains in detail diverse concepts, such as how pain medicines work inside our bodies and how shampoos clean our hair. Her nontechnical text and everyday analogies make the material easily accessible to a general audience, and she provides some useful tips along the way, including why you shouldn't mix household cleaning products. —CC

Black Holes

The Edge of All We Know

Peter Galison
Collapsar/Sandbox Films, 2020

This documentary from Harvard University's Peter Galison—a physicist, historian of science, and filmmaker—takes viewers inside the quest to understand black holes. The film crosscuts between two scientific collaborations: a massive international effort, the Event Horizon Telescope, which involves more than 300 scientists and in 2019 produced the first-ever image of a black hole; and a smaller partnership between theorists Stephen Hawking, Malcolm Perry, Andrew Strominger, and Sasha Haco, who published a paper, Hawking's last, on the black hole information paradox. By focusing on the extensive efforts of the two groups, the film impressively documents the complications of such undertakings. The Event Horizon Telescope collaboration stitched together observations of the supermassive black hole Messier 87, which were taken simultaneously by eight telescopes across the globe. Similarly, the four theorists initially anticipated that they would quickly resolve their problem, but it took more than a year of work to tackle it. The film is available to stream on Netflix. —RD

Reimagining Time

A Light-Speed Tour of Einstein's Theory of Relativity

Tanya Bub and Jeffrey Bub
Yale U. Press, 2021. $24.00

This enjoyable exploration of the strange consequences of Albert Einstein's theory of relativity is coauthored by artist Tanya Bub and her father, theoretical physicist Jeffrey Bub. The book was inspired by Tanya's reading of Einstein's famous 1905 paper on special relativity, "On the electrodynamics of moving bodies," which prompted her to envision two trains moving in opposite directions. Without including equations, the authors use the two-train metaphor to explore enduring paradoxes of the famous theory, including time dilation, length contraction, and mass–energy equivalence. Creative illustrations bring the various scenarios to life. For those interested in digging deeper into the physics, a section at the end cheekily titled "Geek Notes for the Skeptical Relativist" contains the relevant calculations. —RD

The Curie Society

Heather Einhorn, Adam Staffaroni, Janet Harvey, and Sonia Liao
MIT Press, 2021.
$18.95 (paper)

In this graphic novel, three first-year university students are drafted into a secret science society for women that was founded by Marie Curie. Roommates Maya, Simone, and Taj couldn't be more different from one another, yet each has a unique ability in science, math, or technology. When cutting-edge de-extinction research is stolen from the society's remote science lab by an industrial-espionage ring, the three overcome their differences and pool their STEM abilities to take on the thieves at a national symposium. With its predominantly female cast, colorful graphics, and action-packed narrative, *The Curie Society* seeks to inspire young readers and bring some much-needed diversity to the spy thriller genre. —CC PT

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NEW PRODUCTS

Focus on lasers, imaging, microscopy, and nanoscience

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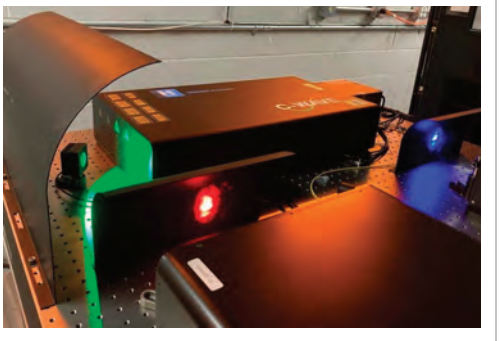
Andreas Mandelis

Tunable laser for holography



Hübner Photonics and Metamaterial Inc (META) have announced the installation at META (Halifax, Canada) of Hübner's C-Wave GTR/NIR (green-to-red/near-IR) tunable laser. The new system—the first of its kind in the world, the companies say—features a broad color palette from three tunable Hübner sources. Crucially, it covers a significant gap in the green region that is costly and complex to address with alternative narrow-bandwidth lasers. With the C-Wave GTR/NIR, META will be able to record holograms at any desired wavelength across the entire visible spectrum and, therefore, potentially accelerate holographic product development. The new full-spectrum capability will allow the company to craft full-color red, green, and blue holograms at any combination of wavelengths users may require for optical combiners in augmented reality and head-up display applications. ***Hübner Photonics Inc****, 2635 N 1st St, Ste 202, San Jose, CA 95134, https://hubner-photonics.com*

Superresolution microscope for life sciences

Bruker's Vutara VXL superresolution fluorescence microscope for nanoscale biological imaging incorporates the company's single-molecule localization technology in a streamlined, cost-effective system. Designed to serve as a biological microscopy workstation for research on DNA, RNA, and proteins, the Vutara VXL also supports advanced biological and biomedical research imaging. When combined with Bruker's microscope fluidics unit, it enables multiplexed imaging for targeted proteomics research. It can also perform optical nanoscopy. The Vutara VXL offers a large field of view, high-throughput data acquisition, and multimodal capabilities. Users can obtain intrinsic 3D superresolution data and achieve 20 nm localization precision in the *xy*-direction, 50 nm in the *z*-direction for organic dyes, and even finer with DNA PAINT probes. A proprietary emission path allows the system to achieve low background fluorescence, even in thick samples. ***Bruker Nano Surfaces****, 3400 E Britannia Dr, Ste 150, Tucson, AZ 85706, www.bruker.com*

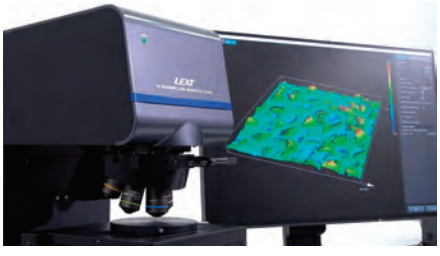
Dilution refrigerator for quantum computing

The ProteoxLX is the latest innovation in cryogen-free dilution refrigerator technology for quantum computing scale-up from Oxford Instruments NanoScience. The LX system can maximize qubit counts with its large sample space and ample coaxial wiring capacity, low-vibration features for reduced noise and support of long qubit coherence times, and full integration of signal conditioning components. Its flexible modular format makes it adaptable to various application requirements. Two fully customizable secondary inserts let users optimize the layout of cold electronics and high-capacity input and output lines. They allow full experimental setups to be installed and exchanged. The ProteoxLX delivers greater than 25 μW cooling power available at 20 mK and a low base temperature at less than 7 mK. Twin pulse tubes provide several watts of cooling capacity at 4 K. ***Oxford Instruments plc****, Tubney Woods, Abingdon OX13 5QX, UK, https://nanoscience.oxinst.com*

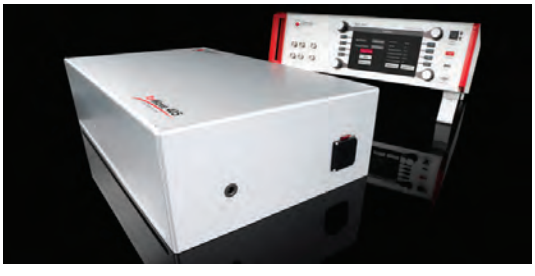
Crystallographic microcomputed tomography system

The Xradia CrystalCT microcomputed tomography system from Zeiss Research Microscopy Solutions enables 3D crystallographic imaging of polycrystalline materials for metal and alloy, additive manufacturing, ceramic, and pharmaceutical samples. In what the company claims is the world's first commercial implementation, the Xradia CrystalCT delivers diffraction contrast tomography on a traditional computed tomography system, which allows researchers to complement absorption contrast tomography data with crystallographic information in 3D. Seamless large-volume grain mapping increases data volume capacity compared with destructive 3D crystallographic methods. It is facilitated by advanced acquisition modes that provide stitch-free scanning for fast, accurate 3D grain data. Advanced scanning modes further remove size and acquisition-speed limitations for a wide range of common samples. ***Zeiss Research Microscopy Solutions***, *Carl-Zeiss-Promenade 10, 07745 Jena, Germany, www.zeiss.com*

Highly precise and accurate laser microscope



According to Olympus, its LEXT OLS5100 laser microscope delivers the high levels of accuracy and precision required for submicron 3D observation and surface roughness measurement, and its smart features accelerate and optimize experiment workflows for materials science applications. In three simple steps, the Smart Lens Advisor assists in the selection of the correct objective lens to measure surface roughness. The Smart Experiment Manager helps users handle the planning, acquisition, and analysis phases of their experiments. The microscope scans samples according to a software-generated customized experiment plan, which helps prevent users from missing data or having to redo work. Once users place a sample on the stage and press the start button, the microscope makes all necessary setting adjustments and acquires the data. During analysis, the software's trend visualization tools help users spot problems. ***Olympus Corporation of the Americas***, *3500 Corporate Pkwy, Center Valley, PA 18034-0610, https://olympusamerica.com*



Gas laser alternative

With its new TopWave 405 model, Toptica presents a cost-efficient alternative for the bulky, power-hungry krypton-ion-gas lasers commonly used in lithographic and holographic applications. The TopWave 405 provides 1 W output power at 405 nm and excellent beam quality. Beam diameter and M^2, which is typically 1.15, are designed to match the established gas laser parameters, which allows for easy integration without significant changes to the optical system. The higher coherence length—greater than 100 m—is well-suited for stable pattern generation in interference lithography or holography. The all-semiconductor TopWave 405 draws less than 100 W and does not require water cooling, which reduces the cost of ownership. Fully automated, push-button optimization of the optomechanics and of the output power stabilization allows for easy, hands-off, remote operation via the included graphical user interface or via users' control software. ***Toptica Photonics Inc***, *5847 County Rd 41, Farmington, NY 14425, www.toptica.com*

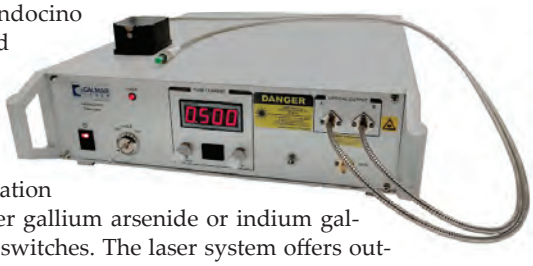
Interband cascade lasers

Boston Electronics now offers broad-gain interband cascade laser (ICL) chips from Alpes Lasers (St-Blaise, Switzerland). Developed for use in external cavity systems, the ICLs allow emission at shorter wavelengths than do traditional quantum cascade lasers, which is particularly relevant to hydrocarbon detection. The chip initially offered by the company covers the 3.2–3.6 μm (2820–3070 cm^{-1}) range, which contains absorption lines mainly for formaldehyde, as well as for methane, ethane, and hydrogen chloride. The ICLs deliver optical power up to 10 mW. ***Boston Electronics Corporation***, *91 Boylston St, Brookline, MA 02445, www.boselec.com*

Scientific SWIR camera

With a 640 pixel × 512 pixel sensor and 15 μm × 15 μm pixel size, the Ninox 640 SU from Raptor Photonics offers very high spatial resolution. According to the company, the indium gallium arsenide camera offers an ultralow dark current reading of less than 300 e/p/s at −80 °C and read noise of less than 56 e^- in high gain, which makes it one of the most sensitive scientific shortwave IR (SWIR) cameras currently available and appropriate for imaging weak signals using longer exposure times. It is vacuum cooled to −80 °C for ultralong exposures of up to 5 min. To enable simultaneous capture of bright and dark portions of a scene, the camera also offers a wide intrascene dynamic range of 56 dB in high gain. The Ninox 640 SU is suitable for staring applications in SWIR wavelengths (900–1700 nm), including near-IR II *in vivo* imaging, fluorescence imaging, and astronomy. ***Raptor Photonics Ltd**, Willowbank Business Park, Larne, Co Antrim BT40 2SF, Northern Ireland, UK, www.raptorphotonics.com*

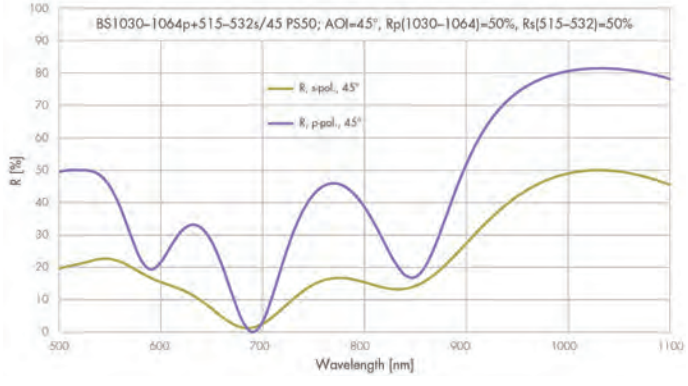
Laser for terahertz-radiation generation



Calmar has expanded its Mendocino benchtop family of femtosecond fiber lasers by adding a dual-wavelength 780/1550 nm system designed for researchers in the terahertz-radiation field. It is a suitable source for the generation of terahertz radiation with either gallium arsenide or indium gallium arsenide photoconductive switches. The laser system offers output power levels up to 200 mW. It features convenient armored-fiber-cable beam delivery, a simple optical switch to select the required wavelength, and user-friendly front-panel controls. With Calmar's proprietary saturable absorber technology, the system delivers reproducible mode-locking with high stability and reliability soon after the laser is turned on. ***Calmar Laser**, 951 Commercial St, Palo Alto, CA 94303, http://calmarlaser.com*

Ultracompact UV nanosecond lasers

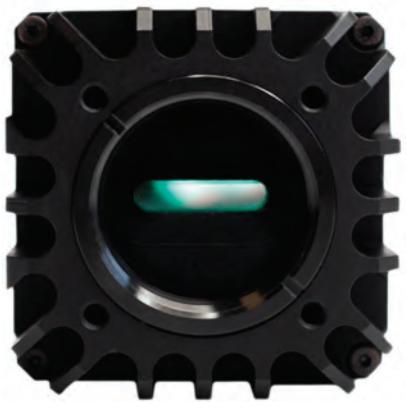
The latest entry in the Spectra-Physics Explorer One HP line of ultracompact actively Q-switched lasers from MKS Instruments delivers 3.5 times as much pulse energy as existing models. The Explorer One HP HE 355-200 UV laser offers pulse energies of greater than 200 μJ, pulse widths of less than 15 ns, and average power of greater than 4 W. User-adjustable repetition rates range from single shot to 200 kHz. For optimal process control, the E-Track active pulse-energy control features a closed-loop algorithm that enables dynamic pulse-energy adjustment with various gating operations. A single lightweight package houses the electronics and laser cavity, which facilitates fast, straightforward integration into compact tools and desktop instruments. The high-energy laser is suitable for precision industrial-manufacturing applications such as structuring and ablating thin films in displays and photovoltaics and trimming of microresistors and capacitors. ***MKS Instruments Inc**, 2 Tech Dr, Ste 201, Andover, MA 01810, www.mksinst.com*



Two-wavelength and polarization beam splitter

Laser Components has developed a beam splitter in which the combined beam of a frequency-doubled laser is divided such that 50% of each of the two wavelengths is split off, even if the beams have different polarizations. The polarization remains the same for both beams. Previously, a beam splitter and a retardation plate were required for that process. The company has been able to combine both functions into one optic, which significantly accelerates setup and maintenance. The original design is for 1030 nm and 515 nm incident beams. However, wavelengths, polarization, and the reflection/transmission ratio can be individually adapted depending on the application. ***Laser Components USA Inc**, 116 S River Rd, Bldg C, Bedford, NH 03110, www.lasercomponents.com*

Compact SWIR camera for quality control



New Imaging Technologies has launched a line of shortwave IR (SWIR) indium gallium arsenide cameras. The LiSaSWIR is optimized for applications that require short exposure times and high-accuracy line rates. According to the company, the line-scan array camera delivers high SWIR image quality while maintaining cost and integration advantages in quality-control systems. The SWIR spectrum simplifies obtaining more invisible data during real-time monitoring. The first version available is the light, compact LiSaSWIR 2048M-STE with 2048 pixels × 1 pixel at a 7.5 μm pitch, a speed of 60 kHz at full line, and a readout noise of 250 e^- in high gain. It features bad pixels replacement, embedded nonuniformity correction, and CameraLink interface. Applications include the inspection of semiconductor, wafer, and solar cell panels. ***New Imaging Technologies***, *1 Impasse de la Noisette, 91370 Verrières-Le-Buisson, France, https://new-imaging-technologies.com*

Wavelength-tunable picosecond laser

EKSPLA's PT403 series tunable picosecond laser, which integrates a diode-pumped solid-state laser and an optical parametric oscillator into a single housing, provides 210–2300 nm output from one box. Compared with two-box systems, the PT403 has a footprint almost half the size, a shorter installation time, better stability, and other benefits. The optical design is optimized to produce low-divergence beams with moderate linewidth—typically less than 8 cm^{-1}—at approximately 15–20 ps of pulse duration. Featuring a 1 kHz repetition rate, the PT403 tunable laser is a versatile, cost-effective tool for scientists in such disciplines as time-resolved fluorescence, pump–probe spectroscopy, laser-induced fluorescence, and IR spectroscopy. ***EKSPLA***, *Savanoriu Ave 237, LT-02300 Vilnius, Lithuania, https://ekspla.com* PT

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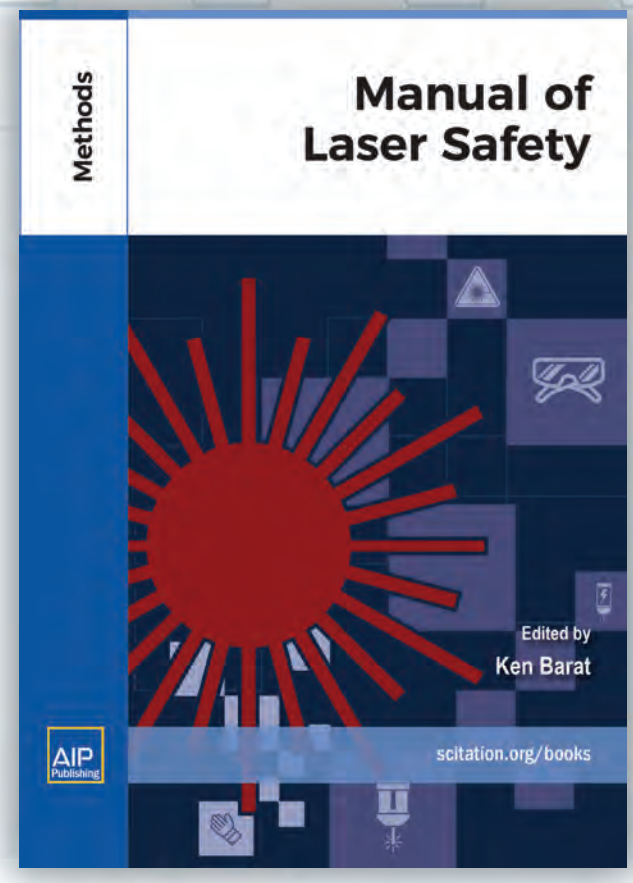
Recently published

A concise guide for anyone using lasers in R&D labs, academia, or industry



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Neil William Ashcroft

Neil William Ashcroft was born in London on 27 November 1938. He had childhood memories of blackouts and bombings during World War II. Two years after the war, his family settled in New Zealand, where he received BSc and MSc degrees in mathematics and physics from what is now the Victoria University of Wellington. He did his 1964 PhD at Cambridge University with John Ziman and Volker Heine. His thesis contained one of the earliest calculations of the Fermi surface of aluminium. In the US he enjoyed explaining that aluminium was a "transatlantic isotope" of aluminum.

In 1965 Neil went to Cornell University as a postdoc. He joined the faculty in 1966, and he remained a member of the physics department for the rest of his life. After a long, debilitating illness, he died of pneumonia in Ithaca, New York, on 15 March 2021.

Neil's wide-ranging research included density functional theory, matter under extreme pressures, high-temperature superconductivity, metallic hydrogen and its alloys, and metal–insulator transitions. After his retirement in 2006, he joined the Cornell research group of Roald Hoffmann and collaborated on almost 50 joint papers. Roald said that "Neil was wise and perceptive, fascinated by the border between chemistry and physics. We valued his physical insight and remember his gentle wit."

In 1968 Neil proposed that hydrogen would become metallic, and a high-temperature superconductor, at ultrahigh pressures. Three decades later experimentalists showed that hydrogen molecules did indeed metallize. When Neil's research group predicted in the 1990s that highly compressed lithium would change from a highly symmetric, close-packed structure to a less symmetrical form with more conduction electrons per atom, that surprising transition was quickly confirmed. Two decades ago he predicted that hydrogen-enriched metallic elements would become ultrahigh-temperature superconductors under extreme pressures. In the past six years, that, too, has been confirmed: Several research groups achieved record high temperatures—room temperature and above—with superconducting LaH_{10} and SH_3.

Neil was a talented administrator. He was director of Cornell's Laboratory of Atomic and Solid State Physics in 1979–84 and of the Cornell Center for Materials Research in 1997–2000. He played a vital role in launching the Cornell High Energy Synchrotron Source and served as its coprincipal investigator and associate director in 1978–89 and its deputy director in 1990–97.

We became close friends soon after Neil arrived at Cornell. The happiest years of my professional life were 1968–76 when we wrote and saw into print our book, *Solid State Physics*. Neil was fascinated with materials: Each was like a personal friend. I had little interest in or knowledge of particular materials, but I was fascinated by the conceptual structure that encompassed them all.

So Neil wrote almost all the first drafts. I would rarely understand what general issue he was trying to get at and would revise it into something that made sense to me. Neil would then correct all the mistakes I had introduced. Back and forth we went, slowly converging on something that looked good to us both. That was before the age of personal computers. I typed every page on a state-of-the-art IBM bouncing-ball typewriter, making revisions with a white "erasing ribbon" and redoing entire pages when revisions were major.

Neil had a wonderful sense of humor. He was a fine mimic and did a superb Hans Bethe. We had great fun dealing with each other's idiosyncrasies throughout the process, and our fun permeates the book. That might explain why it's still thriving, still in its original edition, 45 years after it came out. In 1990 I remarked to Hans that Ashcroft and Mermin, as the book became known, was still in its first edition. He said it showed "the stability of the subject." True enough, but I believe it's also because unlike almost all technical books, ours *entertains* the reader just as Neil and I entertained each other during our six years of writing.

Neil William Ashcroft

LINDSAY FRANCE/CORNELL UNIVERSITY

We even had fun reading page proofs and making our enormous index. Every entry was written by hand on "3-by-5 cards." If we stacked them, the pile would have been a couple of meters high. Neil's favorite index entry is "Cart, before horse, 92," followed nine pages later by "Horse, after cart, 92." My favorite, on page 808, is "Exclamation marks, 61, 185, 219, 224 (twice!), 291, 305, 403, 808." You see here the difference in our styles. The book itself has a uniform tone that is neither of ours, because we negotiated almost every word.

My only other collaboration with Neil was a short memorial article in 2006, "Hans Bethe's contributions to solid-state physics." Our revisions, re-revisions, and re-re-revisions were unbelievably easier in the modern era, but just as extensive. We realized that we no longer had the energy to write a second edition of our book, even had we thought one was needed.

PHYSICS TODAY does not list professional honors in its obituaries, but the distinction of Neil that I really envy is "Foreign Member of the Russian Academy of Sciences." (Russia, are you listening?)

He would have enjoyed this joke. I miss Neil enormously.

N. David Mermin
Cornell University
Ithaca, New York

Masatoshi Koshiba

Nobel laureate Masatoshi Koshiba, professor emeritus at the University of Tokyo, died on 12 November 2020 in Tokyo.

Koshiba was born in Toyohashi City in central Japan on 19 September 1926. Two years after getting his BS in physics from the University of Tokyo in 1951, Koshiba enrolled in the graduate program at the University of Rochester. He received his PhD in 1955 under the supervision of Morton Kaplon, with a thesis entitled "High energy electron–proton cascade in cosmic radiation."

For the next three years, Koshiba worked as a research associate at the University of Chicago. After returning to Japan and spending a year as an associate professor at the University of Tokyo's Institute for Nuclear Study, he went back to Chicago, where he was the principal investigator of a balloon-borne cosmic-ray experiment using emulsions. In 1962 Koshiba again returned to the University of Tokyo as an associate professor of physics. After retiring in 1987, he taught at Tokai University for 10 years.

Koshiba recognized the potential of conducting experiments with high-energy electron–positron colliders. In the early 1970s, his collaboration with Gersh Budker, a particle-accelerator pioneer in the Soviet Union, was cut short, so Koshiba looked to Europe to find new partners. He connected with Erich Lohrmann, a good friend from Chicago who was director of research at the German Electron Synchrotron (DESY). Koshiba and his University of Tokyo group worked on the DORIS e^+e^- storage ring at DESY as part of the DASP experiment.

In 1974 in the US, researchers at Brookhaven National Laboratory and at SLAC independently discovered the J/ψ resonance. That detection led DESY scientists to build PETRA, a higher-energy e^+e^- collider. Koshiba joined with others from Japan, Germany, and the UK to form the JADE collaboration. In 1979 JADE and other experiments at PETRA discovered the gluon.

Koshiba founded the Laboratory for International Collaboration on Elementary Particle Physics (now the International Center for Elementary Particle Physics) at the University of Tokyo in 1977. In the 1980s Koshiba and his team worked on the OPAL collaboration at CERN's Large Electron–Positron Collider. Additionally, he dedicated his time to promoting the construction of the International Linear Collider.

In 1978 Koshiba got a phone call from theoretical physicist Hirotaka Sugawara, who asked him to devise a proton-decay experiment and present it at a KEK workshop. Koshiba immediately recalled an idea he had during his time in the US and designed an experiment with a large amount of water and photomultiplier tubes (PMTs). Soon after, Koshiba heard that a similar but potentially larger experiment, later known as IMB (Irvine-Michigan-Brookhaven), was being planned in the US. He revisited his original design and came up with the idea to develop PMTs with a 50 cm diameter. He thought that even if the IMB experiment discovered proton decays, his experiment could study the branching ratio of the proton decays that result from high photon-detection efficiency. In the end, his experiment, eventually named Kamiokande, brought many important results.

The Kamiokande experiment was constructed 1000 m underground at the Mozumi mine in Kamioka. It started in July 1983, but no convincing proton decay signal was observed. Koshiba noted, however, that the 50 cm PMTs performed superbly. In the fall of 1983, Koshiba proposed improving the Kamiokande detector so it could observe solar neutrinos. At that time, the Homestake experiment in South Dakota was the only one to have successfully detected solar neutrinos, but the observed number of events was only about 30% of the expectation.

After undergoing several years of improvements, the Kamiokande experiment restarted at the beginning of 1987 with a lower energy threshold to observe solar neutrinos. Then, on 23 February 1987, a supernova explosion was detected in the Large Magellanic Cloud. Kamiokande recorded a neutrino burst that beautifully confirmed the basic mechanism of the supernova explosion. In addition, Kamiokande detected solar neutrinos and confirmed the solar neutrino deficit in 1989. Koshiba was a corecipient of the 2002 Nobel Prize in Physics "for pioneering contributions to astrophysics, in particular for the detection of cosmic neutrinos."

In 1983 Koshiba came up with the Super-Kamiokande experiment. When he originally proposed that Kamiokande should observe solar neutrinos, he realized that the event rate would be low because of the detector's limited mass. He thought that a much larger and higher-sensitivity detector was necessary to advance "neutrino astronomy." The 50-kiloton Super-Kamiokande has also been successful in obtaining many important neutrino-physics and astrophysics results, including the discovery of neutrino oscillations.

Masatoshi Koshiba

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Koshiba was a great physicist who was able to feel the direction of physics. He told his younger colleagues that they should always have several "eggs" of research ideas because some of them could hatch in the future.

Takaaki Kajita
University of Tokyo
Kashiwa, Japan
Sachio Komamiya
Waseda University
Tokyo, Japan PT

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PHYSICS TODAY | JOBS

Tomoyuki Endo is at the National Institutes for Quantum and Radiological Science and Technology in Kyoto, Japan. **Chen Qu** is at the University of Maryland, College Park. **Heide Ibrahim** is at INRS in Varennes, Quebec, Canada.



A molecular road movie

Tomoyuki Endo, Chen Qu, and Heide Ibrahim

As a photoexcited molecule breaks apart, we can see not just where the fragments are but also whether they are departing from the beaten path.

The development of instantaneous photography in the 19th century brought new understanding of human and animal movements that were too rapid to observe with the naked eye. Suddenly, it was possible to see with certainty that all four hooves of a galloping horse left the ground at once. Similarly, a central theme of modern physical chemistry is the observation of chemical reactions at the molecular level and in real time. So-called molecular movies allow researchers to view the intermediate steps of a reaction, not just its results (see PHYSICS TODAY, August 2003, page 19, and April 2011, page 13).

In the conventional view of chemical reactions, atoms follow straight, predictable paths, and one knows exactly where to find them. In a photodissociation reaction, in which a molecule breaks apart upon excitation with light, that simple picture gives rise to two basic types of reaction pathway: Either a single bond stretches until its breaks, or the atoms efficiently rearrange to form a new chemical bond while breaking two others. For the dissociation of formaldehyde (H_2CO), those pathways are represented by the green and blue arrows, respectively, in figure 1. They're easily distinguished because they lead to different sets of products: H and HCO in the first case, H_2 and CO in the second.

Sometimes, however, atoms slip loose and wander off into the wild. Their destinations are unknown, and their trajectories can be all over the map. Tracking their unpredictable paths is not easy, even when using the best time-resolved spectroscopic methods. We need to turn to powerful techniques sensitive to single molecules.

Roaming atoms

The elusive phenomenon now termed "roaming" surprised researchers when they discovered it in the dissociation of H_2CO in 2004. It is illustrated in figure 1 by two example trajectories

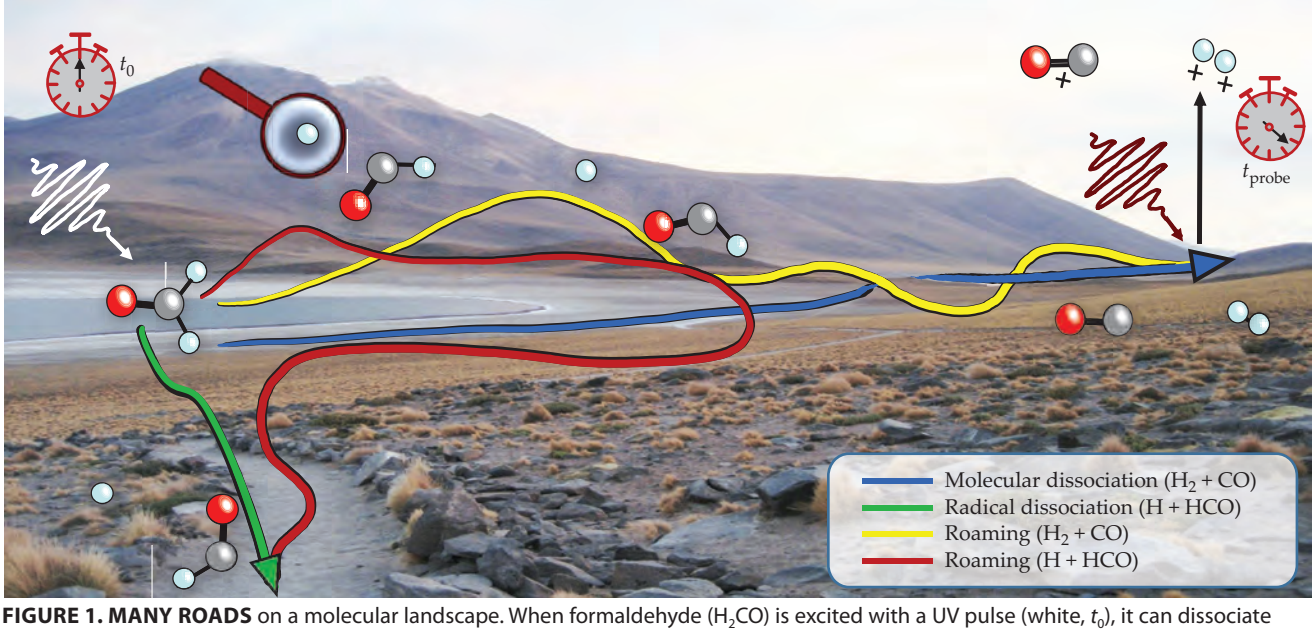

FIGURE 1. MANY ROADS on a molecular landscape. When formaldehyde (H_2CO) is excited with a UV pulse (white, t_0), it can dissociate into either H + HCO or H_2 + CO. Conventionally, those reactions were thought to follow straight paths, as represented by the green and blue arrows, but it's now known that they can follow more tortuous roaming trajectories. To catch the roamers on the road, we ionize the dissociating molecules with a probe pulse (brown, t_{probe}) and reconstruct their geometry from the ensuing Coulomb explosion. We found that roaming trajectories can lead not only to molecular products (yellow line) but also to radical products (red line). (Image by Heide Ibrahim, adapted from *A molecular road movie*, https://youtu.be/CQ3Cril0YSA.)

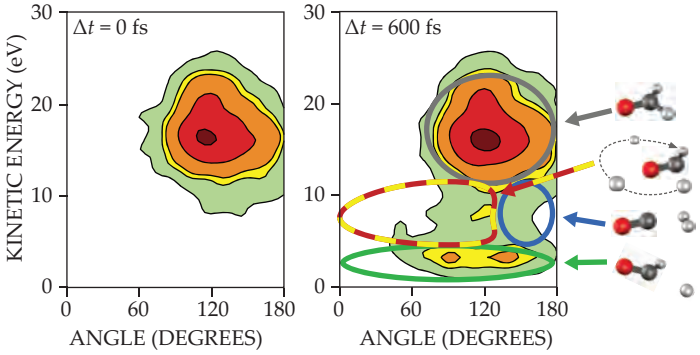

FIGURE 2. SNAPSHOTS of dissociating D_2CO molecules, with the total kinetic energy released in the Coulomb explosion plotted against the angle between the two deuteron momentum vectors. Geometries that correspond to different molecular roads are marked by the colored curves: gray, equilibrium; red–yellow dash, roaming; blue, molecular dissociation; green, radical dissociation. (Figure by Tomoyuki Endo and Heide Ibrahim.)

shown in yellow and red. In each case, the molecule undergoes a hindered dissociation that strays from the conventional paths. Molecular fragments orbit each other at large interatomic distances for hundreds of femtoseconds before finally going their separate ways. Along the roaming path, one H atom might detach from the molecule, roam around the remaining HCO fragment, and then abstract the other H atom to yield H_2 and CO—but via a different path than the conventional one. (See the article by Joel Bowman and Arthur Suits, PHYSICS TODAY, November 2011, page 33.)

Roaming is now known to occur in many molecular systems. It's generally observed indirectly, through the spectroscopic imprint it leaves on the reaction products. When H_2CO dissociates into H_2 and CO, roaming reveals itself through the distributions of H_2 vibrational states and CO rotational states. However, such indirect detection provides little information about the exact molecular pathway and the dynamics of the moving fragments. Even time-resolved experiments have, until now, been limited to the indirect observation of the outcome of processes that involve roaming. To observe roaming in real time, we must expand the concept of the molecular movie into a molecular-road movie: to identify not just the individual moving fragments but also the different roads they travel.

Directly observing roaming in dissociating H_2CO is challenging because of the unpredictability of the process. Each roaming fragment follows its own path, no two of which are alike. Furthermore, although the roaming process itself lasts just a picosecond or less, it could take up to tens of nanoseconds to get started, so at any given instant, only a tiny fraction of molecules might be caught in the act of roaming. Finally, many of the molecules still follow the conventional, direct dissociation pathways, which cross the roaming pathways and can therefore be difficult to distinguish. We needed a way to extract the roaming dynamics hidden behind the overwhelming statistical background.

Explosive imaging

We chose Coulomb-explosion imaging, an established technique in which a short, intense laser pulse ejects several of a molecule's electrons at the same time. The ionic fragments repel one another and fly apart, and from their trajectories toward a detector, we can reconstruct the molecular geometry at the time of ionization. Not only is the technique sensitive to single molecules, but we can also isolate specific channels from the background by using ion correlations and thus select statistical events. At the Advanced Laser Light Source, headed by François Légaré, we have filmed the roaming dynamics of deuterated formaldehyde (D_2CO), which we chose over H_2CO for experimental reasons.

We can capture a snapshot of an ensemble of dissociating molecules at any desired moment with femtosecond precision by adjusting the time delay between the photoexcitation pulse and the ionization pulse and then correlating the signals from the D^+, D^+, and CO^+ ion fragments. Supported by the theory groups of Michael Schuurman, Paul Houston, and Joel Bowman, we distinguished the possible pathways by plotting the kinetic energy released in the Coulomb explosion against the angle between the two deuterons' momentum vectors as they fly apart. We cannot sharply separate all the regions, because deuterons undergoing conventional dissociation must pass through the same configurations as roaming ones. But for the most part, we can classify the pathways according to the outlines in figure 2, whose colors correspond to the trajectories in figure 1.

The gray circle marks the region of undissociated D_2CO molecules. Before ionization, their atoms are bound together, so in the Coulomb explosion, the charged fragments strongly repel one another for a large kinetic energy release.

The blue circle indicates molecules following the conventional dissociation pathway to D_2 + CO: The two deuterons are near one another but far from the CO fragment, so they fly apart in nearly opposite directions. The green ellipse represents the conventional pathway to D + DCO: The departing D atom is already almost gone, so its repulsion in the Coulomb explosion is small, and its momentum direction is almost uncorrelated with the other D atom's.

The red and yellow dashed curve shows molecules in the act of roaming, with one deuteron roaming around the remaining DCO fragment. That configuration leads to a larger kinetic-energy release than the conventional D + DCO pathway but a smaller D–D angle than the D_2 + CO pathway.

With this work, we generalized the definition of roaming to include processes recognized by their transient features, not just their outcomes. Because we catch the roamers on the road, we can detect them whether they complete the roaming path or end up in a conventional dissociation channel. Previous measurements of roaming in H_2CO relied on the quantum states of CO and H_2, so they were sensitive only to roaming pathways that yield those products, like the yellow trajectory in figure 1. But by tracking roaming populations over time, we found that some roamers, in fact, dissociate into D + DCO. Their trajectories, exemplified by the red path, have been invisible until now. The results introduce a new paradigm for detecting roaming dynamics and, more broadly, for detecting weak statistical dynamics hidden under a large stochastic background.

Additional Resources

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- A. G. Suits, *Annu. Rev. Phys. Chem.* **71**, 77 (2020).
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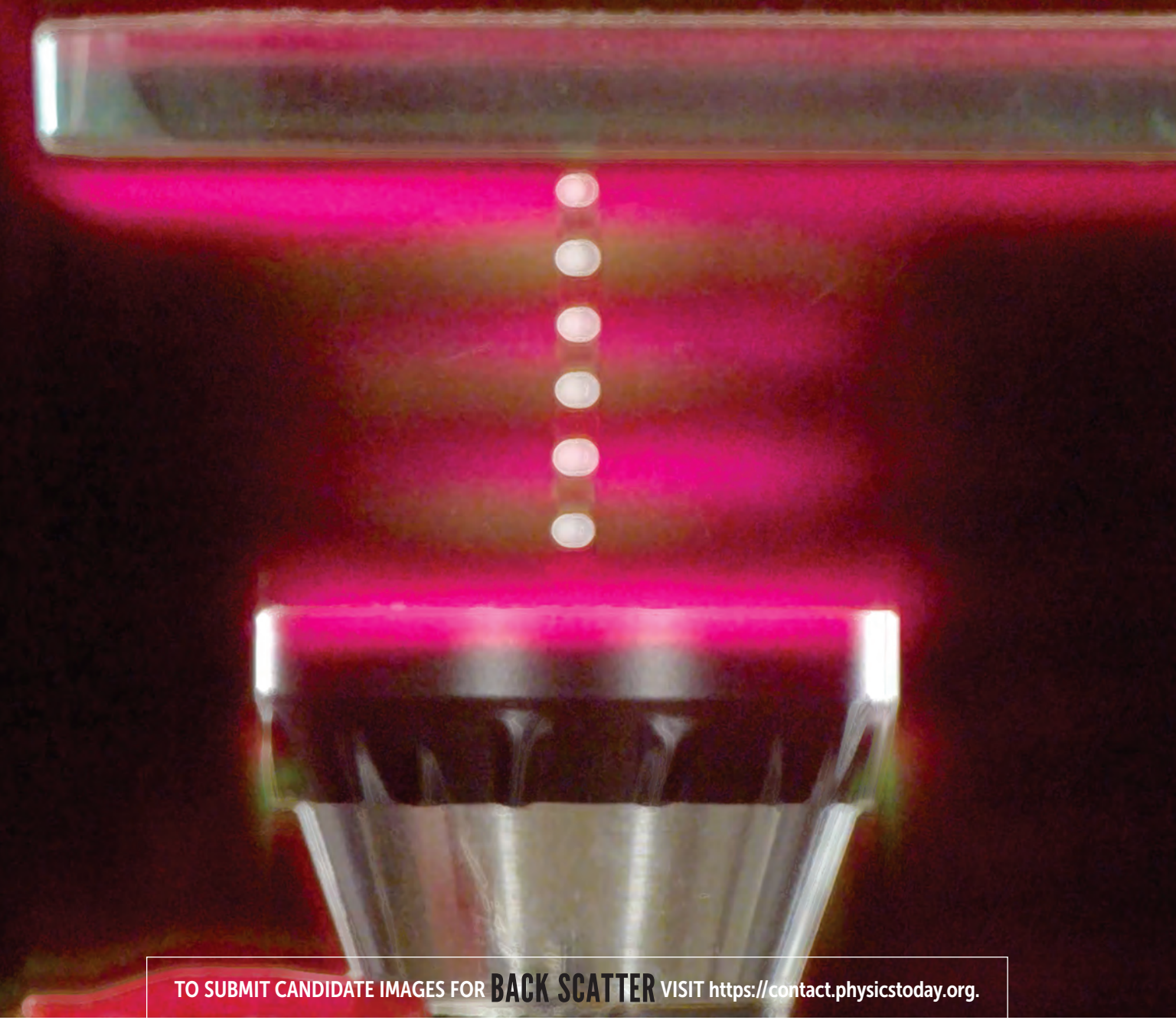
PT

Visualizing acoustic levitation

The six polystyrene foam balls in the middle of the photo are levitated in air by an acoustic standing wave, formed between an ultrasonic transducer below and a glass plate above. David Jackson of Dickinson College in Carlisle, Pennsylvania, and Ming-Hua Chang (now at the Pennsylvania State University) made the wave visible at a specific phase of its cycle by strobing a light source at the same frequency as the acoustic wave. The air's density gradients cause the light to refract and pass through colored filters on either side of a light block. The pink areas designate nodes where pressure is increasing with height, and the green areas indicate nodes of decreasing pressure.

A simple analysis of the linearized fluid equations predicts that an acoustic ponderomotive force would push levitating objects into pressure antinodes. But the observations—including the image here—show levitating balls in both colored bands, which correspond to pressure nodes. Jackson and Chang's experimental results are consistent with a more complex nonlinear effect called the acoustic radiation force. Much stronger than the ponderomotive force, it traps particles at the nodes of the standing pressure wave. (D. P. Jackson, M.-H. Chang, *Am. J. Phys.* **89**, 383, 2021; image courtesy of David Jackson.) —AL



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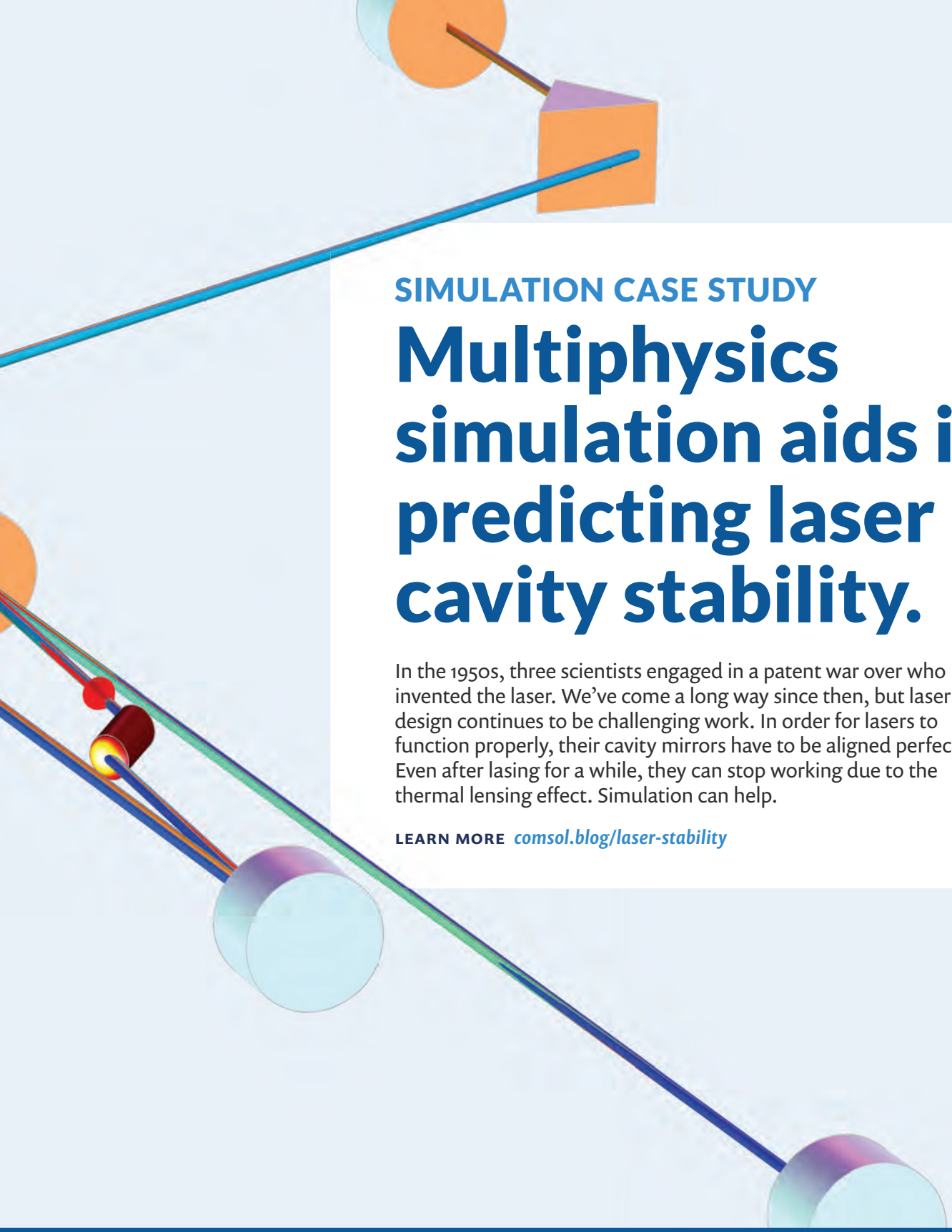

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