PHYSICS TODAY

February 2018 • volume 71, number 2

A publication of the American Institute of Physics

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Cell membrane thermodynamics

Modeling social behavior

Quantum interference in chemical reactions

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FEATURES

ON THE COVER: Gorgeous symmetric snowflakes form when water vapor condenses in a cloud. The details of their shapes reflect not only the changing environment the ice crystals experience as they travel through the cloud but also the molecular structure of the crystal surface. Nonequilibrium effects are important, too, and for that reason, snowflakes formed in clouds and single-crystal ice condensed from liquid water grow differently. To learn more, turn to the article by Mary Jane Shultz on **page 34**. (Photo courtesy of Kenneth Libbrecht.)

Recently on PHYSICS TODAY ONLINE

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▶ Nemtsov, physicist

Before Boris Nemtsov became the political adversary of Russian president Vladimir Putin, he was an ambitious physicist who developed a concept for an acoustic laser. Richard Blaustein profiles Nemtsov the physicist nearly three years after his assassination in Moscow.

physicstoday.org/Feb2018a

ROBERT LANG

▶ Origami master

In 2001 Robert Lang switched careers from laser physicist to origami entrepreneur. It was a wise decision. In a PHYSICS TODAY Q&A, Lang describes his folding work for such clients as NASA and national labs and his origami-inspired advances in computational geometry.

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NAT'L PORTRAIT GALLERY, LONDON

▶ Lonsdale, FRS

From its founding in 1660 until 1945, the Royal Society of London did not admit a single woman fellow. Books editor Melinda Baldwin profiles one of the first women—and the first woman physicist—elected: Kathleen Lonsdale, the Irish crystallographer who confirmed the structure of benzene.

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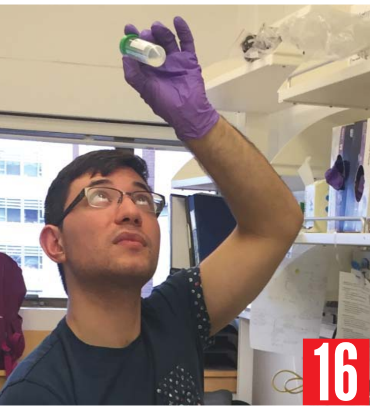

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FROM THE EDITOR

In praise of preprints

Charles Day

When it's my turn to write for the magazine's Physics Update department, I visit the arXiv.org preprint server. There, I browse the latest papers in the astrophysics of galaxies, medical physics, and fluid dynamics—to name just three of arXiv's categories. My goal: To find an interesting paper that can be adequately summarized in 250–400 words.

Of course, arXiv does more than provide source material for science writers. Since its inception in August 1991, arXiv has served as a public library for papers before their peer review and publication. In the early years, astrophysics, condensed-matter physics, and high-energy physics predominated. In 2017, mathematics (25.6% of all papers) and computer science (21.9%) held the top two spots. High-energy physics (7.8%) slipped to fifth place behind condensed matter (11.7%) and astrophysics (10.7%).[1]

I'm not surprised that mathematicians have embraced arXiv. Referees check every equation. Papers can take years to be published. For example, the most cited paper of 2017 in *Journal of the American Mathematical Society*, "Canonical bases for cluster algebras,"[2] was received by the journal in November 2014 and published in November 2017.

Even in fields with speedier publication, the prompt posting that arXiv affords is an attractive advantage, especially when a topic is hot. In February 2008, Hideo Hosono published his discovery of a new family of iron-based superconductors in the *Journal of the American Chemical Society*. In a news story about it, I wrote: "Within weeks, physicists who'd read the *JACS* paper or who'd heard about it from chemists had started making samples, measuring properties, and posting papers on arXiv. The first band-structure calculations showed that the superconducting phase is two-dimensional, as in the cuprates, and occupies the FeAs planes." (See PHYSICS TODAY, May 2008, page 11.)

The quest to find new members of the superconducting family, to reach higher critical temperatures, and to understand the superconductivity was intense. In posting to arXiv, competitive condensed-matter physicists aimed to establish the priority of their results.

Another motivation to post on arXiv is to share ideas with a wide audience. In 1997 Alexei Kitaev posted his 13 000-word treatise "Fault-tolerant quantum computation by anyons." The paper helped to launch the new field of topological quantum computing. Kitaev didn't submit it to a journal, *Annals of Physics*, until 2002.

ArXiv has been an integral part of the physics landscape for so long that it's worth taking a look back at what the preprint scene was like before it came along. When I was an astronomy grad student in the 1980s, preprints were paper copies bound between card stock and distributed by mail. Some institutions even had branded covers. Given that some of us print out electronic preprints, having them preprinted might seem an advantage, provided only one person at a time wanted to read them.

But the paper preprint system had a serious shortcoming. If your institution wasn't on other institutions' mailing lists, you wouldn't see the preprint. With its free online distribution, arXiv is fairer and more democratic. Anyone with an internet connection can download and upload the latest research.

Preprints continue to evolve. Crossref, the nonprofit that facilitates the interlinking of scholarly research online, has developed a way to assign digital object identifiers, or DOIs, to preprints in such a way that preprints are as fully citable as the final, published versions of record. Last year the National Institutes of Health, the Wellcome Trust, and other big biomedical funders announced they would allow grant applicants to cite preprints. Also last year the American Chemical Society launched its own preprint server, ChemRxiv.

I learned of those and other developments from a blog post on the Scholarly Kitchen by Judy Luther.[3] One of her crossheads neatly captures why preprints benefit science and scientists: "Preprint servers put authors in control of when their research is released."

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1. These and other statistics can be found at https://arxiv.org/help/stats.
2. M. Gross, P. Hacking, S. Keel, M. Kontsevich, *J. Am. Math. Soc.* (2017), doi:10.1090/jams/890.
3. J. Luther, "The stars are aligning for preprints," Scholarly Kitchen (18 April 2017).

PT

READERS' FORUM

Commentary

Thinking differently about science and religion

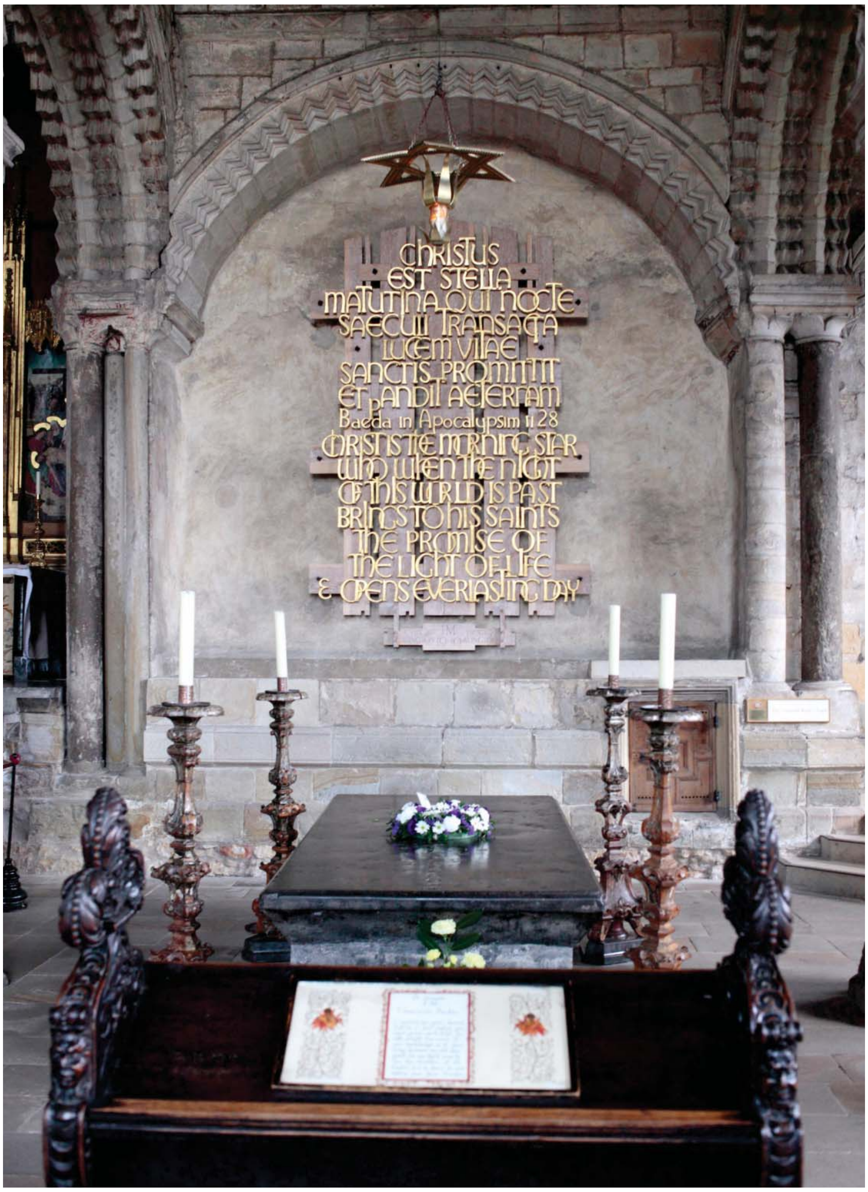
Maintaining the "alternative fact" that science and religion, and in particular Christianity, are in conflict is hurting science. Over the past year, three occasions have left me with strong visual memories and deep impressions that point towards a better approach.

The first, held at St John's College of Durham University in the UK, was a debate on the sensitive topic of fracking—shale-oil recovery by hydraulic fracturing. I have witnessed several such discussions, both live and broadcast, and they rarely succeed in anything except escalating entrenched positions and increasing misinformation and fear; few participants bother to treat the science with respect.

This gathering was different. Strongly opposing views were expressed, but their proponents listened to each other. Everyone was keen to grasp both the knowns and the uncertainties of the geological science and technology. Social science and geophysics both drew sustained civil dialog. The notion of different priorities was understood—and some people actually *changed* their views.

The second occasion was some reading I have been doing for a book on the role of creativity and imagination in science. Research for one chapter had led me to connections between the explosion of new science in the 17th century and ideas from the same period expressed in literature, art, and theology. Those ideas included a discussion of the nature of God to a depth unseen since the fourth-century ecumenical councils. One treatise impressed me hugely with its author's detailed knowledge of textual analysis, variants in New Testament manuscripts, and nuances of Greek; it would rival any current scholarship. Furthermore, it evidenced a scientific logic and a perception of the revolutions in natural philosophy that is very rare in theological writing today.

A one-act play I attended in my hometown of York in the UK supplied the third occasion. I'd heard that a respected national theater company had long wanted to create a work based on the ancient book of Job. I admit to a personal love for that ancient poem. No one really knows where it came from, but for my money it contains the most sublime articulation of the innate curiosity into nature that still drives science today but that has clearly deep human roots. Its



IVAN VDOVIN/ALAMY STOCK PHOTO

TOMB OF THE VENERABLE BEDE, Durham Cathedral, UK. Bede (AD 673–735) was an English monk and author of *De Natura Rerum* (*On the Nature of Things*), a book motivated by its author's conviction that it is important for the church to teach the workings of nature, so that people are less frightened by them.

probing questions seek answers to where hail, lightning, and clouds come from; why stars can be clustered together; how birds navigate huge distances; how the laws of the heavens can be applied to Earth; and so on.

Common across the three occasions is the theme of surprisingly deep and constructive mutual engagement of science and religious belief. The conference on shale-gas recovery was between academic Earth scientists and a few dozen senior church leaders, including bishops of the Church of England. The author of the impressive New Testament scholarship was Isaac Newton. And the play that so impressed me, staged by the Riding Lights Theatre Company in the elegant renaissance church of St Michael le Belfrey in York, featured a 20th-century Job as a research physicist. After the performance a panel of scientists discussed how their faith supports their scientific research. Anyone who has not read beyond the superficial yet ubiquitous stories of conflict between science and religion that receive so much airtime today would be surprised to see such deep entanglements of scientific and religious thinking, from the ancient past of the book of Job to current scientifically informed political decision making.

Between the ancient and the contemporary lies the history of early modern science. There, too, the public sphere today seems dominated by a determined program of misinformation. Newton himself is testimony to the deep formative role of Christian theology in the rise of experimental and mathematical sciences. Far from being a sort of secular triumph over centuries of dogmatic obscurantism, the writings of early modern scientists such as Newton and Robert Boyle make it clear that they were motivated by the theological philosophy of Francis Bacon.

For Bacon, science became the gift by which humankind restores an original knowledge of nature, lost as a consequence of rejection of God. The truth that faith conveyed direct motivation and influence for many great scientists can be uncomfortable. Historian of science and biographer Geoffrey Cantor, author of *Michael Faraday: Sandemanian and Scientist—a Study of Science and Religion in the Nineteenth Century* (1991), still receives "hate mail" from readers incensed at the suggestion that such a scientific mind

READERS' FORUM

might also have been a Christian one.

We are even learning to readjust our schoolbook picture of the Middle Ages as a period of intellectual stagnation, generally repressive of science. History is far more interesting. The scientific enlightenment that gave birth to the Copernican Revolution, the Royal Society of London, the universal theory of gravitation, and the telescope and microscope did not, of course, arise from nowhere. The long fuse for that intellectual fireworks display was lit in 12th-century Europe through the movement to translate Aristotle's scientific texts. They were mostly lost to the West since late antiquity but were preserved and developed by brilliant Islamic scholars in Baghdad, the Levant, and Spain.

Arab natural philosophers Al-Kindi, Averroës, Alhazen, and Avicenna ought to be far better known as beacons in the long history of science; they, too, saw their task of comprehending the cosmos as God-given. The consequent scientific awakening in the West saw the new learning about the cosmos not as conflictual with the Bible but as a "second book" to be read alongside it.

The scholars' work allowed 13th-century English thinkers Robert Grosseteste, Roger Bacon, and others to develop theories of light, color, and motion. Their work led, for example, to the first complete theory of the rainbow at the level of geometric optics, from the laboratory of Theodoric of Freiberg around 1310, and to the first mathematical articulation of accelerated motion by Nicole Oresme of Paris in mid-century. Small wonder that Nicolaus Copernicus saw his astronomical work as a form of worship and that Galileo Galilei viewed his as reading God's second book.

Maintaining the view that science and religion are in conflict does no one any favors and is hurting science. The damage comes not only through a warped transmission of history but also because it suggests to religious communities that science is a threat to them rather than an enterprise they can celebrate and support. The bishops' fracking conference is just one example of how the quality of social support of and discussion around science can be raised once churches get involved. After all, a community with a commitment to core values of truth and a banishment of fear might well offer the clarity and calm needed in a public debate currently marked by far too much falsehood and fear.

Equally tragic is that in families with a faith tradition, even very young children may receive the idea that science is not for them or that it somehow threatens their community. The truth is that throughout most of history, scientific investigation has gone hand in hand with a commitment to theism, at least in the three Abrahamic faiths. It is, sadly, possible to invent conflict where none needs to be.

The "literal" reading of texts such as Genesis—as if they were scientific documents rather than part of a story in which we inquire about the universe—is a 20th-century aberration away from orthodox Christianity. Conversely, misrepresenting faith as mindless adherence to beliefs in the face of evidence to the contrary needs to give way to a more thoughtful understanding. The term can describe painstaking engagement with the world through the true stories we are part of. Reflecting the vital presence of what we might call "reasoned hope," faith is not so very far from descriptions of the experience of doing science.

Driving an unhistorical and unrealistic wedge between science and religion has got to stop. It leads, in part, to the optionalism that we see in some public and political attitudes toward science, from climate change to vaccination. It damages the educational experience of our children, and it impoverishes our understanding of our own science's historical context. Human beings live not only in a physical world but within historical narratives that give us values, purpose, and identity. Science sits on the branches and draws from the sap of many of those stories whose roots are anchored in the great themes of creation, redemption, and renewal that course through our religious traditions and endow us with humanity. We are still looking for answers to some of the questions God asks of the luckless Job:

Have you comprehended the vast
expanses of the Earth? . . .
What is the way to the place where
lightning is dispersed . . . ?
Can you bind the beautiful
Pleiades?

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LETTERS

Physics education reform in lab and classroom

As a retired college physics teacher, I found the article "The past and future of physics education reform" by Valerie Otero and David Meltzer (PHYSICS TODAY, May 2017, page 50) well written and important. As a longtime member of the American Association of Physics Teachers, I have had many discussions with high school physics teachers, and I often found that their concerns are similar to those of instructors of introductory college physics.

I agree that students can learn from discoveries made in physics laboratories. However, because only a limited amount of time, often only about two hours per week, is allotted for a physics lab, we must be realistic about our goals. It is also important to remember that students have access to so much information on the internet that they can learn about an experiment and its results well before they enter the lab. And when courses have multiple sections, students can learn from those who took the lab on a previous day, which ruins the experience of discovery.

To properly revise physics courses, schools must consider more flexible scheduling instead of brief, specific blocks of time. A longer laboratory session would probably give students a more meaningful experience.

I have one further comment: Aspects of the scientific method should not be restricted to science courses. The process of theorizing and logically following implications of theories can be applied to

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history, political science, sociology, and other subjects. For example, instead of just teaching about the history of World War II and asking students to repeat information on tests or in term papers, we could ask them what might have happened if the US had entered the war at a different point in time or not at all and then have them consider the logical consequences of each possibility. Getting students to hypothesize and follow a logical sequence should begin well before they study physics or any other science.

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Magnetic monopoles and a cheap detector

The letters from Ken Frankel and Christopher Harrison (PHYSICS TODAY, June 2017, page 13) in response to Arttu Rajantie's article on the history of searches for magnetic monopoles (PHYSICS TODAY, October 2016, page 40) brought back a memory. After Blas Cabrera's 1982 publication of a candidate monopole event detected with a superconducting loop,[1] three groups[2]—a University of Chicago, Fermilab, and University of Michigan collaboration; IBM; and Imperial College London—built Faraday induction detectors with larger areas. Using a coincidence technique of two gradiometer detectors in a nonzero but pinned magnetic field, Joe Incandela and coworkers showed that a likely explanation of the candidate event was a flux jump rather than the transit of a monopole.[3] I was invited by the organizers of the First Aspen Winter Conference to give a review talk of the hot though cryogenic topic.[4]

I had been a graduate student at the University of California, Berkeley, and had great admiration for Luis Alvarez, so I sent him a draft asking for comments. I had leaned over backwards to give him credit for inventing the Faraday induction technique, as my looking in depth at monopole detection by ionization brought home that there was no way to calibrate the ionization detector, and hence a nondetection could never be definitive. Faraday detection, however, can be calibrated with a "pseudopole," a very long but small-diameter, tightly wound, magnetic solenoid much akin to a Dirac string.

I was working at my desk when my phone rang, with a furious Luis on the other end. Without any introduction, he barked, "Henry, this was my idea, and I should be the first reference." I was stunned, as I thought I had done him proud, but I managed to say, "Luis, the guys ahead of you are not to be sneezed at—Faraday, Maxwell, Dirac. . . ." Still angry, he said, "Yes, but who are these other guys?" Luis later sent a nice note praising the review, and all was well.

A brief addendum: Sunil Somalwar's PhD thesis followed up on Incandela's superconducting gradiometers by showing that using just copper wire and a field-effect transistor operating at liquid nitrogen temperature, one could build an inexpensive detector, capable of covering large areas and sensitive to a single Dirac charge.[5]

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The problem of the electron's mass

As I read "An electron–proton collider could bridge the gap between the LHC and its successor" (PHYSICS TODAY, May 2017, page 29) and how it would serve in high-precision studies of Higgs decays as a portal to new physics, I was disappointed. I saw no mention of a long-standing problem in connection with the electron: What fraction of the electron's mass is due to its interaction with the quantized electromagnetic field? Despite its enormous success in quantum electrodynamics, renormalization does not solve the problem, nor does it even tell us how to tackle it. Furthermore, the Higgs contribution to the electron's mass is unknown. We also don't know how to measure those respective contributions. Perhaps in thinking about the electron–proton collider, one should be thinking about opening portals to these long-neglected areas as well.

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Energy efficiency in motion and thought

Simon Sponberg's article (PHYSICS TODAY, September 2017, page 34) addresses important topics in the physics of insect locomotion in terms of muscle motion, sensing, and information processing. However, one especially important and astonishing aspect of physics, common to living objects and unattainable by manmade machines, is the energy efficiency in both muscle motion and information processing. One impressive example is the energy consumed by the human brain in playing Go or chess with a supercomputer. Although humans now lose both games, the energy consumed by the human brain while playing is five to six orders of magnitude less than that of the supercomputer.[1]

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1. See, for example, Y. Yanagida, Y. Ishii, *Proc. Japan Acad. B* **93**, 51 (2017).

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SEARCH & DISCOVERY

East Antarctica's past foreshadows an uncertain future

Although it's now relatively stable, the immense ice sheet was sensitive to climate fluctuations millions of years ago.

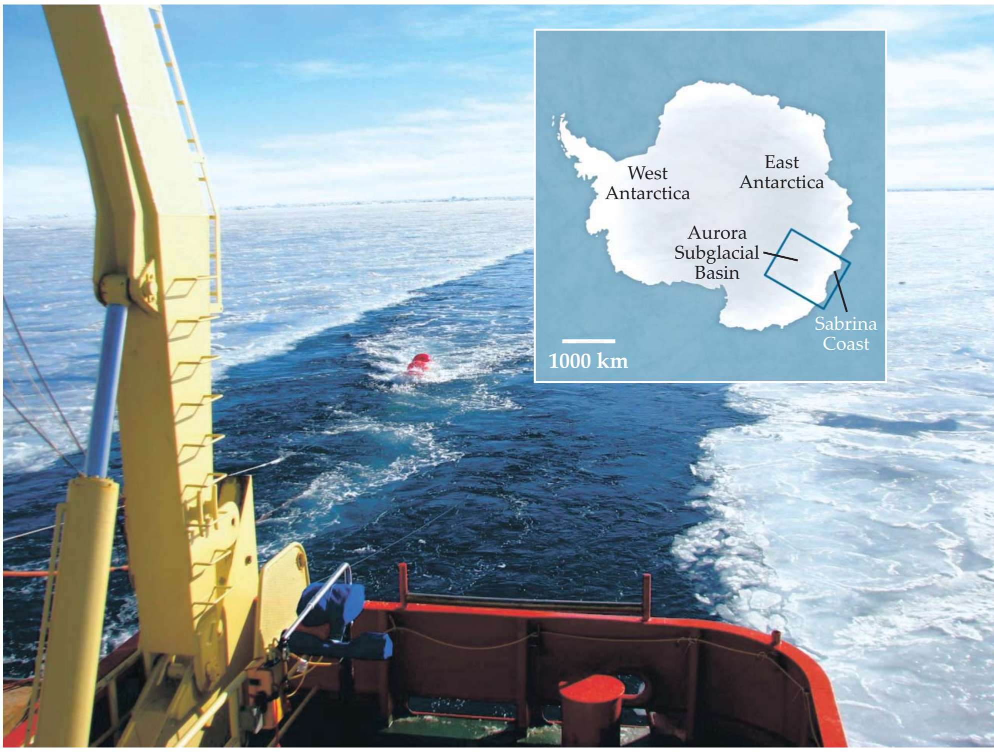

FIGURE 1. OFF THE COAST OF THE AURORA SUBGLACIAL BASIN in East Antarctica, researchers used seismic instruments deployed from the back of this icebreaker to acoustically probe the seafloor and the rock below it. (Photo by Sean Gulick; map courtesy of the University of Texas at Austin, Jackson School of Geosciences.)

The glaciers of Greenland and Antarctica together contain enough water to raise global sea levels by more than 60 meters. With so much human infrastructure having been planned around current sea levels, if all the polar ice were to melt, the effect on human society would be devastating.

But Earth has seen warm climates and high seas before. During the Mesozoic era—the time of the dinosaurs, which ended 66 million years ago—the planet was far hotter than it is today. The polar regions were ice free.

Since then, temperatures and sea levels have generally been on the decline, and polar ice caps have grown to cover the Antarctic continent and Greenland. That overall trend was punctuated by dramatic bouts of warming and cooling, with glacial periods coming and going. More than a century of Antarctic exploration, on land and by sea, has built up a body of knowledge of how the ice sheet formed and how it has behaved. Geological records of past periods of ice instability during warm times are especially important for estimating the future consequences of anthropogenic climate change.

But there is still a lot more to discover. Global temperature and polar ice coverage aren't related by a simple one-to-one correspondence. Air and ocean temperatures don't always move in tandem, and a glacier can respond to changes in either or both. The collapse of a glacier is a mechanical process that, once initiated, takes time to play out. Glaciers don't all necessarily behave the same way, even in the same part of the world. The local details are important—and in a continent as vast as Antarctica, knowledge of them is incomplete. Much of the Antarctic coast has never been visited by a research vessel.

Four years ago Sean Gulick (University of Texas at Austin), Amelia Shevenell (University of South Florida), and their colleagues undertook the first foray into one of those previously unexplored areas: the Sabrina Coast continental shelf off the shore of the Aurora Subglacial Basin (ASB) in East Antarctica, as shown in the map in figure 1. They've now analyzed the data they collected.[1]

From a combination of seismic measurements and sediment samples retrieved from the seafloor, the researchers found that the ASB glaciers had a dynamic past, advancing and retreating at least 11 times over a period of 30 million years. During much of that time, the atmospheric carbon dioxide concentration was close to what it is today, and the average global temperature was at a level it may reach again by the end of this century. And the ASB and other East Antarctic regions seem to have responded differently to past climate fluctuations.

Uncharted waters

Most attention to the future of Antarctic glaciers has focused on the precarious situation of West Antarctica. Because of the topography of the underlying rock, much of the West Antarctic ice is dangerously unstable, and some glaciers may have already entered a state of irreversible decline (see PHYSICS TODAY, July 2014, page 10).

The larger, thicker East Antarctic ice sheet rests on firmer foundations, but it's not immune to changes in climate. Evidence has been accumulating that parts of East Antarctica have been responsive to climate in the geological past, including under conditions not too far from what's expected in the coming decades.[2] But the studies are still few and scattered.

When they set out to add another data point to the map, in the austral summer of 2014, Gulick, Shevenell, and colleagues

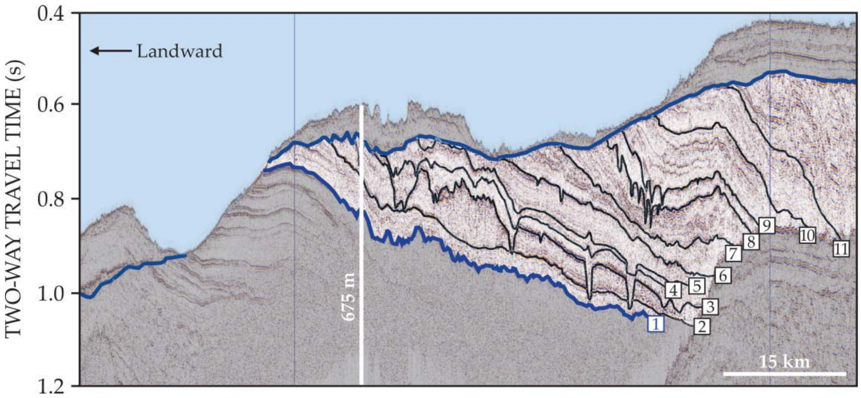

FIGURE 2. A SEISMIC PROFILE tells the history of glacial ice on the Sabrina Coast continental shelf, now underwater. The region between the two blue lines represents a period when the ice was responding dynamically to fluctuations in climate; each of the bold lines marked 1–11 is an erosion surface created by glacial advance and retreat. (Adapted from ref. 1.)

had their sights on Totten Glacier, on the western edge of the ASB. Aerial measurements had shown that Totten Glacier was losing mass faster than anywhere else in East Antarctica, and they wanted to know why. But polar field research doesn't always go according to plan. Sea ice and icebergs dictated where they could go and what they could do—sometimes on an hourly basis. Although conditions precluded reaching Totten Glacier, the researchers found a gap in the heaviest ice on the eastern portion of the Sabrina Coast. For four weeks they zigzagged over the continental shelf, gathering data and sediment samples.

A complicated past

As ice, meltwater, ocean currents, and accumulating debris shaped the continental shelf over tens of millions of years, they created layers of material with different acoustic properties. Seismic profiling—projecting sound waves toward the seafloor and recording their reflections—can uncover that structure, as shown by the profile in figure 2. The highlighted region corresponds to the period of glacial dynamicism: The layers below it formed before the arrival of ice to the continent, and the layers above formed after the East Antarctic ice sheet stabilized as a polar ice cap. The rough surfaces marked 1 through 11 were created by glacial erosion and correspond to periods of glacial advance and retreat. The layers between them are unusually thick. That means that when the glacier retreated, it must have pulled back far enough—hundreds of kilometers—to leave behind an open marine environment unsheltered by an overhanging ice shelf.

Some of the erosion surfaces are marked by narrow V-shaped gouges. Those so-called tunnel valleys are a common feature associated with glaciers in the Northern Hemisphere. But they're unusual for Antarctica, with only one known location in West Antarctica and no others in East Antarctica. They're attributed to surface meltwater that seeps through the porous glacial ice and gushes out the bottom. The formation of such deep tunnel valleys means that the ASB was exposed to warm air—as opposed to warm ocean water—for prolonged periods. Surface melting is thought to have little effect on Antarctic glaciers' behavior today. But it must have been a significant driver of glacial dynamics in the past—at least in the ASB.

Converting the seismic profile to a chronology is more complicated than counting layers like tree rings. Erosion surfaces form at irregular intervals, and there's no obvious connection between the features in the profile and events elsewhere on Earth. To pin down the timeline, the researchers collected sediment cores.

Because the ship wasn't equipped with a drill, the samples were collected with a piston corer, a long, heavy tube that plunges into the seafloor sediment like a straw into a milkshake. The cores, therefore, extended just a meter or two beneath the seafloor, so they had to be taken from just the right places where the strata of interest were naturally exposed. And the researchers had to choose those locations on the fly, without the benefit of a full analysis of their data. In fact, they didn't even get access to their sediments until almost six months later, back in their home labs.

Happily, the researchers succeeded in obtaining sediment cores from key moments in the history of the Sabrina Coast, including one core that recorded the transition from the dynamic period to the polar ice-sheet regime. That crucial core was rich in the fossils of ancient silica-shelled diatoms, such as the ones in figure 3. Many of the microfossils were broken or degraded, but some were sufficiently intact to be identified by species. The diatoms in figure 3 are of different species, but they both roamed the seas at about the same time: between 8.6 million and 4.8 million years ago. Once the researchers had taken into account the species they didn't find in the core, the researchers concluded that the ASB glaciers probably settled down sometime between 6.9 million and 5.6 million years ago.

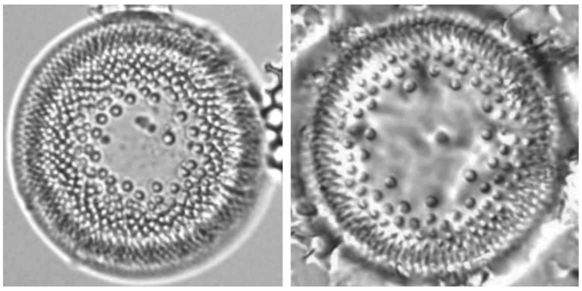

FIGURE 3. THESE FOSSIL DIATOMS, each 30 µm in diameter, were recovered from the sediments of the Sabrina Coast continental shelf. Their species—*Thalassiosira oliverana* (left) and *Actinocyclus ingens* (right)—flourished more than 4.8 million years ago. (Adapted from ref. 1.)

The result puts the ASB in an interesting contrast to other parts of East Antarctica. The nearby Wilkes Subglacial Basin, for example, seems to have still been advancing and retreating in response to climate fluctuations as late as 3.3 million years ago.[3] Still, it's hardly surprising that different parts of the East Antarctic ice sheet—a complex continent-scale system—don't all move in concert.

Estimates of atmospheric CO_2 levels from millions of years ago are subject to large uncertainties, but the past 25 million years have almost certainly included periods when the concentration exceeded the 400 ppm seen today. The global average temperature at the end of the ASB's dynamic period was likely 4 °C warmer than today, well within the span of projections for the year 2100 if drastic action is not taken to limit greenhouse emissions.

The broad similarities between past and future conditions are not predictive, but they are suggestive. Even the possibility of East Antarctic destabilization highlights the need for more data to better understand the ice sheet's vulnerability. Indeed, several more interdisciplinary expeditions will be visiting East Antarctica in the next few years, and Gulick, Shevenell, and colleagues have a pending proposal with the International Ocean Discovery Program to return to the Sabrina Coast with a scientific drilling rig. The longer cores that they can obtain with a drill could fill in the timeline and help the researchers understand exactly when and how the ice advanced and retreated in the past.

Johanna Miller

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Laser cooling delivers a Bose–Einstein condensate

The new, faster path to condensation could vastly speed up some quantum experiments.

It's been more than two decades since Carl Wieman, Eric Cornell, and their coworkers created the first Bose–Einstein condensate (BEC), confirming that a macroscopic population of integer-spin particles will pile into a single quantum ground state if cooled below some critical temperature. (See PHYSICS TODAY, August 1995, page 17.) After all those years, the recipe for creating the condensates remains virtually unchanged: Laser cooling chills the cloud of atoms as close to the critical temperature as it can, and when that technique can go no further, evaporative cooling does the rest.

Experimenters have long sought to bypass the evaporative cooling step, a slow process that jettisons most of a cloud's atoms in order to cool the remaining few. The process can take seconds, sometimes more than a minute, to unfold. Afterward, typically less than 1% of the original atoms remain.

Now MIT researchers led by Vladan Vuletić have used a laser technique known as Raman sideband cooling to take a cloud of rubidium atoms all the way to the condensation threshold—no evaporation needed.[1] From an initial gas of 2000 atoms, they can generate a BEC of more than 500 in just 300 ms—about the time it takes to blink an eye.

The Doppler limit

The threshold for Bose–Einstein condensation is often expressed in terms of a critical temperature. But a more fundamental quantity is the dimensionless phase-space density, the peak occupation per quantum state. Roughly speaking, that quantity describes the extent to which atoms' wavefunctions overlap. It grows as a cloud of atoms becomes colder and denser. As it surpasses a value of one, a BEC forms.

At the outset of their experiment, the MIT researchers' vapor of rubidium atoms has a phase-space density near 10^{-20}. To boost that value, the team captures the atoms in a magneto-optical trap and applies a standard laser cooling technique: Doppler cooling.

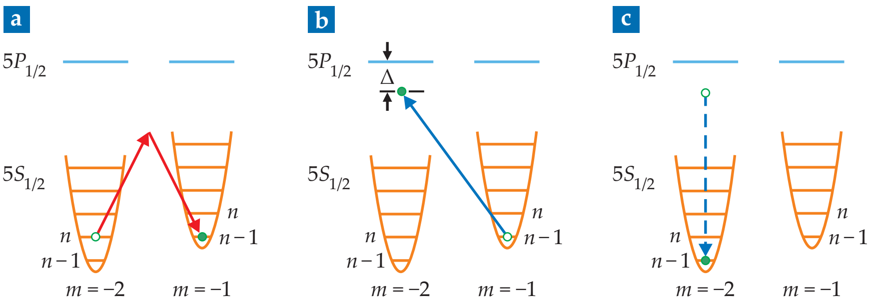

FIGURE 1. RAMAN SIDEBAND COOLING. When its magnetic hyperfine sublevels *m* are appropriately split by an applied magnetic field, a rubidium atom can be cooled via an optical cycle that toggles the atom between those sublevels. **(a)** A two-photon Raman transition induced by IR trapping beams transfers an atom having *n* vibrational quanta in the $m = -2$ sublevel to a degenerate $m = -1$ state having $n - 1$ vibrational quanta. **(b)** A pump beam, red-detuned by an amount Δ from the 5*S*–5*P* electronic transition, transfers the atom to an excited $m = -2$ state. **(c)** The atom decays back to the $m = -2$ ground state, arriving with one less vibrational quantum than it started with. (Adapted from ref. 1.)

First demonstrated in the 1970s, Doppler cooling exploits the frequency shifts that an atom sees as it moves toward or away from a light source. When two counterpropagating lasers are tuned just below an electron resonance, the atom will preferentially absorb light—and momentum—from the laser it's traveling toward, since that light is slightly blueshifted to higher energy. The net effect, regardless of which source the atom moves toward, is to slow the atom's momentum. If three such sets of counterpropagating beams are arranged orthogonal to one another, they brake the atom's motion in every direction.

But there's a catch. As absorbed photons are reemitted, the atoms suffer random recoils. Below a certain temperature, typically a few hundred microkelvin, those recoils are large enough to offset the cooling effect of the lasers, and Doppler cooling is rendered ineffective. After just a millisecond or so of cooling, Vuletić and his colleagues reach that Doppler limit, with their cloud's phase-space density still seven or eight orders of magnitude below the condensation threshold.

That's when conventional experiments would switch to evaporative cooling. Instead, Vuletić and his colleagues turn off the Doppler cooling beams, release their atoms from the magneto-optical trap, and recapture them in a two-dimensional optical lattice—a square array of potential wells formed by the interference of two orthogonal retroreflected IR beams. Now, instead of sharing one large trap, the team's atom cloud is dispersed among hundreds of tiny traps. The tight spatial confinement creates large spacings between the atoms' vibrational energy levels. And that sets the stage for Raman sideband cooling.

Cool, compress, repeat

Developed in the 1990s by Stanford University's Steven Chu and Mark Kasevich, Raman cooling siphons away a trapped atom's vibrational energy by converting it to magnetic energy and then to light.[2] Figure 1 illustrates the basic scheme. An applied magnetic field is tuned to split the energies of two of the atom's magnetic hyperfine sublevels *m* by an amount precisely equal to a vibrational quantum. In this case the energy of the $m = -1$ sublevel is raised above that of the $m = -2$ sublevel.

Then, when an atom with *n* vibrational quanta in the $m = -2$ state is transferred to the degenerate $m = -1$ state, it arrives with $n - 1$ vibrational quanta; that step, driven by a two-photon interaction with the trapping light, is known as a Raman transition. A shorter-wavelength pump beam then transfers the atom to an excited state with $m = -2$. When the atom decays to the electronic ground state, it does so with $n - 1$ vibrational quanta.

Raman sideband cooling can easily chill an isolated atom to the ground state. But two issues that arise in dense gases of atoms have foiled previous attempts to use the technique to create BECs. First, in atomic clouds, photons emitted by one atom can scatter off neighboring atoms and generate heat-inducing recoils. Second, pairs of nearby atoms can be excited to repulsive molecular states that, upon decaying, give each atom a jolt of kinetic energy. Both effects produce unwanted heat that can make the ground state inaccessible.

In 2000 a group at the University of California, Berkeley, led by David Weiss showed that by detuning the pump beam from the atomic transition, one can suppress scattering and all but eliminate recoil heating.[3] But it wasn't obvious how to solve the molecular-excitation problem. Near the atomic resonance frequency, the molecular-excitation rate scales identically to the rate of the atomic excitation used in the cooling cycle. Although detuning could in theory reduce the rate of heat-generating molecular excitations, it would slow the cooling rate by just as much. Vuletić eventually realized that if he red-detuned the pump beam far from the atomic resonance, he could find gaps in the molecular spectrum—special detunings where atomic excitations win out over molecular ones.

In their experiment, the MIT researchers set the pump beam to one of those special detunings. After just 100 ms of sideband cooling, the temperature of the rubidium cloud falls to 10 μK—cold enough that nearly all 2000 atoms are in their vibrational ground states. Even still, the phase-space density only reaches 0.02. To create a BEC, the researchers must compress the cloud.

To do so, they borrow a trick developed by Weiss:[4] They turn off one of the trapping beams, transforming the square array of 2D potential wells to a row of 1D wells, as illustrated in figure 2. Because the light that forms those wells is more intense near the beam axis, the wells slope downward toward the axis. As a result, atoms that had been trapped in the outer wells of the 2D trap fall inward in the newly 1D trap. If the 2D lattice is restored at just the right moment, those atoms can be recaptured in the low-lying potential wells near the lattice's center.

Unfortunately, that "release-and-retrap" trick doesn't increase phase-space density; the compression-induced warming negates the rise in spatial density. So after each compression, Vuletić and his coworkers must sideband cool the atoms anew.

With two rounds of compression—one in each trap direction—the MIT researchers boost the cloud's density nearly 50-fold. And near the end of the third 100 ms round of cooling, the phase-space density nudges past one. Barely 300 ms after the start of their experiment, Vuletić and his colleagues have their BEC.

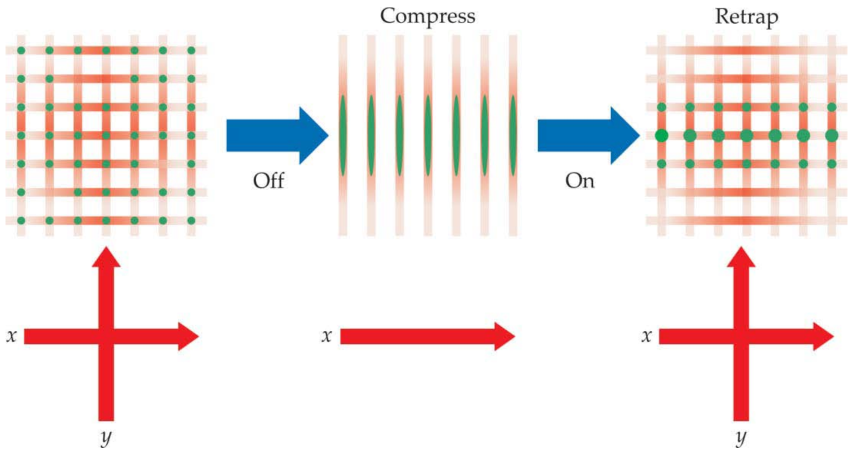

FIGURE 2. RELEASE AND RETRAP. A gas of atoms (green) trapped in a two-dimensional optical lattice (red) can be compressed by briefly turning off one of the trapping beams. Here, when the *y* beam is turned off, atoms are driven by intensity gradients toward the axis of the *x* beam. If the *y* beam is restored at just the right moment, the gas of atoms is retrapped in a smaller region of the optical lattice. The process can then be repeated with the *x* beam. (Adapted from ref. 1.)

A matter of time

The MIT team isn't the first to laser-cool atoms to the condensation threshold. Five years ago an Austrian team led by Florian Schreck created a BEC of strontium atoms in just 100 ms using only Doppler cooling.[5] But their approach relied on an extraordinarily narrow-linewidth transition that gives strontium an unusually low Doppler limit; it can't be translated to most atoms of interest in quantum experiments.

The MIT group's method, by contrast, doesn't use anything special about the rubidium atom. For JILA's Jun Ye, who has helped pioneer the development of optical-lattice atomic clocks, that's welcome news.

Atomic clocks keep time by syncing an oscillator with the frequency of some reference atomic transition. To maximize precision, one wants to measure that transition in large atomic ensembles and to repeat the measurement as many times as possible. Last October, Ye's group reported that they could keep time to a record precision of better than one part in 10^{18} by measuring transitions of a quantum degenerate gas loaded in an optical lattice.[6] But because the researchers used evaporative cooling to generate their quantum gases—and because the protocol calls for creating a new gas for each measurement—they could make just a few measurements per minute. Says Ye of Vuletić's sideband-cooling approach, "We could benefit from the much shorter preparation time."

Vuletić thinks the shorter preparation times will also benefit quantum-gas microscopy, where high-resolution optics are used to image tunneling and other phenomena in lattice-confined gases designed to mimic strongly correlated condensed matter. (See PHYSICS TODAY, October 2010, page 18, and August 2017, page 17.) But his ultimate dream is to send the technique into orbit, where BECs have been proposed for use in space-based gravitational-wave detectors, among other applications. There, the method's chief virtue would be its economy. One wouldn't need the powerful magnetic coils used for evaporative cooling, Vuletić explains: "You could use modest magnets and standard laser beams."

Ashley G. Smart

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Membrane phase demixing seen in living cells

A simple physical phenomenon underlies the complex organization of some biological systems.

GLENNIS RAYERMANN

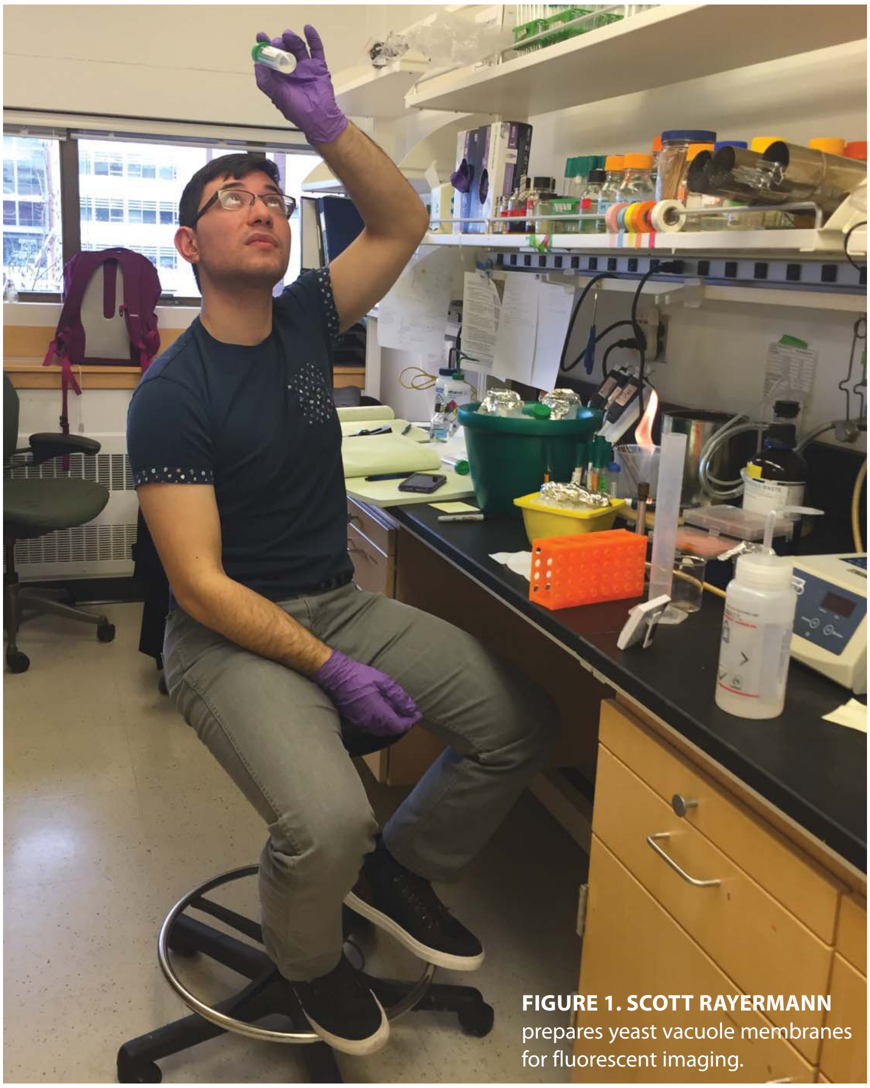

FIGURE 1. SCOTT RAYERMANN prepares yeast vacuole membranes for fluorescent imaging.

To keep their insides in and their outsides out, cells and their substructures are enveloped by lipid bilayer membranes. The membranes have the consistency not of rubbery balloons but of thin liquid films: Proteins and other molecules embedded in the membranes can diffuse from place to place. But despite that diffusion, the membranes are compositionally heterogeneous, not uniformly mixed, and they sometimes appear to host discrete domains enriched in particular molecules.

Biologists and biophysicists have long debated the mechanism of membrane organization—and, in particular, whether it has anything to do with thermodynamic phase separation, the same physics that drives the demixing of a shaken bottle of vinegar and oil. Now Sarah Keller, Alexey Merz, and their colleagues at the University of Washington in Seattle have shown that membrane domains do indeed form through phase separation, at least in some living cells.[1]

Keller's interest in the problem was

from a physics point of view: How can cell membrane organization be understood in terms of what's known about phase separation in other liquids? Merz came to the topic from a cell biology perspective: How might membrane structure relate to the formation and function of cells and organelles? Together, they co-mentored the brother–sister team of graduate students Scott Rayermann (pictured in figure 1) and Glennis Rayermann, the joint lead authors on the new paper.

The Seattle researchers looked at the membranes that enclose vacuoles—a type of organelle—in single-celled budding yeast. They sought and found two telltale hallmarks of phase-separation dynamics. First, when two domains with the same composition coalesced, the surrounding domain boundaries quickly rearranged to minimize the overall energy due to line tension. Second, when the yeast cells were heated and cooled, the domains disappeared and re-formed—and the transition consistently happened at a single characteristic mixing temperature.

Vesicle models

One reason membrane organization has been so difficult to study is that the putative domains are so small. Experiments to date on the membranes that surround whole cells tend to rule out domains larger than tens of nanometers. That's too small to see with conventional optical microscopy. Superresolution techniques can help to bring tinier structures into view, but the gain in resolution is accompanied by a loss of speed, so crucial information about dynamics is lost.

Cell membranes, however, are not free-standing bubbles. They are anchored to the cytoskeleton inside, and the anchoring points may be preventing domains from growing any larger than the distance between attachments.

For a simpler system, researchers have turned to synthetic membranes. Under some conditions, lipids in water spontaneously assemble into bubble-like membranes called vesicles. And with some coaxing, vesicles can be grown to sizes of 100 µm or more, so they and their correspondingly larger domains can be optically imaged with ease. It's been observed since the early 2000s that vesicles made from a combination of lipids—one of the simplest formulations is two lipids with

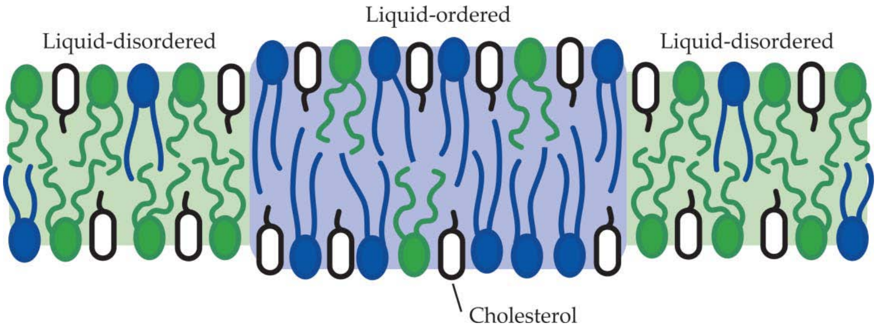

FIGURE 2. IN A MODEL SYNTHETIC MEMBRANE made of two types of lipid (green and blue) and cholesterol (white), the components separate into immiscible liquid-ordered and liquid-disordered phases below a characteristic mixing temperature. In biological membranes, which contain proteins embedded in the lipid layers, those molecules may be preferentially partitioned into one phase or the other. (Courtesy of Sarah Keller.)

different melting points plus cholesterol—exhibit complex phase behavior, with the components mixing at high temperatures and segregating into immiscible domains when cooled.[2] Those compositionally distinct ordered and disordered phases, shown schematically in figure 2, are both two-dimensional fluids.

The synthetic vesicles were an interesting model system that yielded new physics discoveries.[3] But the question remained of their relevance to biology. Living cell membranes contain not just lipids and sterols but a multitude of embedded proteins. Certain biological membranes showed phase-demixing behavior similar to that seen in vesicles, but only when they'd been removed from their cellular environment or otherwise perturbed from their physiological state. And they had some curious properties: Membranes taken from a culture of zebrafish cells, for example, consistently underwent phase demixing at temperatures 17 °C below the cell-growth temperature—even when the cell-growth temperature was changed.[4] But observing a demixing transition *in vivo*, or even under physiological conditions, remained frustratingly elusive.

A turning point came in 2013. Alexandre Toulmay and William Prinz, of the National Institutes of Health in Bethesda, Maryland, noticed that when yeast cells entered the stationary growth phase—when a dearth of nutrients prompted the cells to temporarily give up on trying to reproduce—their vacuole membranes formed micron-sized domains strikingly similar to the liquid-ordered and liquid-disordered phases in synthetic vesicles.[5] Moreover, when the researchers fluorescently labeled 14 different membrane proteins, they found that each one was enriched in one of the two membrane regions and depleted in the other.

Vacuole phases

Just because the vacuole domains looked like liquid-ordered and liquid-disordered phases, however, doesn't necessarily mean that they were. Although Toulmay and Prinz tried heating and cooling the cells, they saw no signs of a mixing transition.

The Seattle researchers were inspired to pick up where the NIH team left off: If a phase-separation mechanism was responsible for the vacuole domains, they were determined to see dynamic proof of it. "Two of our assets are stubbornness and optimism," says Keller. "According to Toulmay and Prinz's paper, our experiments should not have worked. We did them anyway."

The biggest challenge was in imaging the tiny structures. The vacuole domains were bigger than the diffraction limit of conventional microscopy, but seeing them clearly still required sophisticated optical tricks.

Vacuoles are spherical and transparent. Typically, a reconstructed projection of a 3D object would comprise superimposed images of the front and back hemispheres, which could have obscured important features. So the researchers used deconvolution microscopy to obtain stacks of 2D slices, from which they painstakingly reconstructed images of just one hemisphere.

Figure 3, obtained in such a way, shows what happens when a boundary

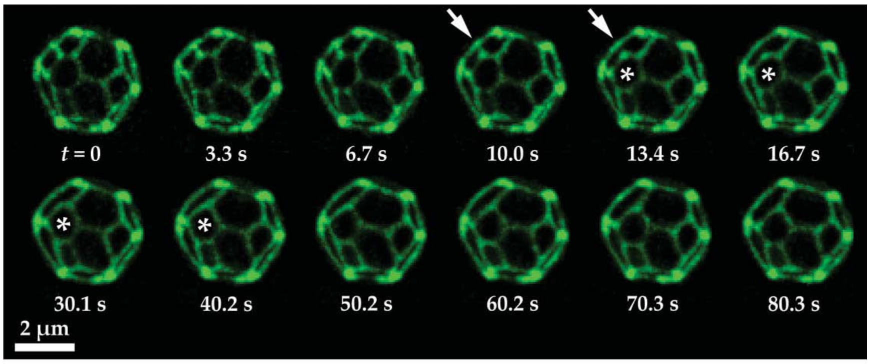

FIGURE 3. DOMAIN COALESCENCE on short time scales in this series of optical micrographs demonstrates that the domains are liquid. The green lines mark the distribution of a fluorescently labelled protein that's partitioned into one of the two membrane phases; the green phase forms thin boundaries between domains of the other phase. When the boundary indicated by the arrows breaks, the surrounding domains quickly rearrange. In particular, the domain marked by the star changes from hexagonal to pentagonal. (Adapted from ref. 1.)

breaks between two domains of the same phase and the domains merge. Domain coalescence isn't a common spontaneous occurrence *in vivo*, but the researchers found that they could provoke it by flowing water over the cells to increase the vacuoles' volume by osmosis. In the seconds after the domains coalesce, as marked by the arrow, the surrounding boundaries rearrange—in particular, the starred domain transforms from a hexagon to a pentagon, which lowers the interface energy.

To observe the other manifestation of liquid phase separation—the mixing and demixing of domains—the researchers turned to a version of light-sheet microscopy[6] that conferred the necessary combination of low noise and high imaging speed. Above the transition temperature of about 38 °C, the domains mixed and the vacuoles fluoresced a uniform pale green. Below the transition temperature, dark domains on a green background reemerged.

Useful transitions

The results confirm that vesicle models are indeed relevant to at least some biological systems, but it remains to be seen whether membrane domains in other organelles and species form by the same mechanism. "Our work implies that all biological membranes have the opportunity to employ miscibility phase transitions," says Keller. "However, there's no obligation for them to do so."

What does it mean for a cell to employ a phase transition? If each membrane protein is confined to either the liquid-ordered or the liquid-disordered domains, domain formation brings some proteins closer together and keeps others farther apart. If a cellular process is helped or hindered by contacts between particular membrane proteins, then the demixing transition could serve as a way to switch the process on or off in response to changes in temperature. In fact, recent work by Jodi Nunnari and collaborators suggests that a critical cell-growth pathway in budding yeast may be regulated in just that way.[7]

In nature, yeast cells encounter a wide variety of environmental conditions, and they may sometimes benefit from switching at temperatures other than 35–40 °C. Keller, Merz, and colleagues are planning to investigate whether and how the transition changes in different yeast strains to help them adapt to different environments.

Johanna Miller

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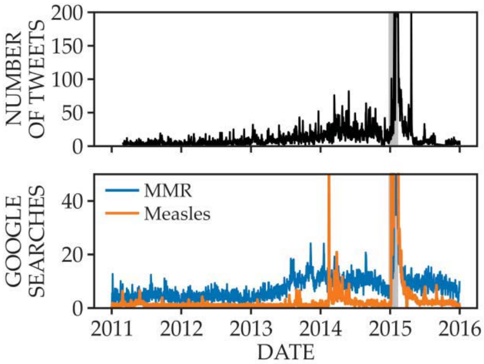
PHYSICS UPDATE

These items, with supplementary material, first appeared at www.physicstoday.org.

VACCINATION BEHAVIOR AS A CRITICAL PHENOMENON

The 2014–15 measles outbreak at Disneyland in California brought heightened attention to the decision by some people to refuse vaccination for themselves and their children. Such personal decisions play into the complex relationship between vaccination behavior and disease dynamics, which influence each other in a nonlinear feedback loop that also incorporates societal norms and perceived risks. Chris Bauch and his colleagues at the University of Waterloo, Dartmouth College, and École Polytechnique Fédérale de Lausanne have now analyzed Twitter and Google search data related to measles and the measles-mumps-rubella (MMR) vaccine before and after the outbreak. Treating trends in the social-media data as a proxy for trends in the evolution of people's attitudes toward vaccination, they find signs that the coupled vaccination–disease system was approaching a critical transition, a tipping point leading to a new dynamical regime—in this case an epidemic. The numbers of tweets and Google searches containing measles-related terms peaked sharply in early 2015, just after the outbreak began. For several years leading up to the outbreak, a period in which the vaccination rate was decreasing, the variations in the data from both platforms revealed so-called critical slowing down—a declining rate of recovery from small perturbations that is a signature of critical phenomena. In the wake of the outbreak, the vaccination rate increased and the system moved away from the tipping point, even before new requirements went into effect in California. The team's mathematical model qualitatively reproduces both trends. Since statistical indications of an approaching tipping point appeared well before it was evident in the raw time series, the researchers suggest that online social data can provide early warning signals of approaching outbreaks in vaccination and disease dynamics. (A. D. Pananos et al., *Proc. Natl. Acad. Sci. USA* **114**, 13762, 2017.) —RJF



GRAVITY HERALDED THE MIGHT OF THE 2011 JAPAN EARTHQUAKE

US AIR FORCE/TECH. SGT. DENORIS A. MICKLE

Ruptures in Earth's crust—earthquakes—generate elastic waves that travel through the crust and upper mantle at speeds of several kilometers per second. When observed at seismic stations, those waves provide information about the interior structure of the planet and the magnitude of the quake that generated them.

The earthquake's initial rupture and subsequent seismic waves redistribute mass and thus alter Earth's gravitational acceleration, or field. The change in the field, like an electromagnetic disturbance, propagates at the speed of light, and a seismometer feels it almost immediately. The perturbed gravitational field also induces small mass redistributions, which generate their own mini seismic waves that jiggle the ground at seismic stations before the arrival of the main elastic waves. The two tiny effects combine to give a seismometer reading of something like 1 nm/s^2 for the largest of earthquakes. If only its magnitude mattered, such a small gravitational effect would be swamped by the elastic waves generated at the epicenter, which show up as ground displacements five orders of magnitude greater. But thanks to their earlier arrival, the gravitational perturbations can, in principle, be registered by seismometers.

Now Martin Vallée (Institut de Physique du Globe de Paris) and his team have revisited the data taken by 11 seismic stations located 427–3044 km from the site of the 2011 Tohoku earthquake in Japan and have teased out the combined gravitational signal. Given that the quake had a magnitude of 9.1, the researchers' numerical modeling matched the observed data well. The researchers hope that, in the future, information carried by the gravitational signal can be inverted to give a prompt estimate of a large earthquake's magnitude. (M. Vallée et al., *Science* **358**, 1164, 2017.) —SKB

WHAT CAUSES MEGADROUGHTS?

The severe and prolonged drought that beset North America in the 12th century likely caused the collapse of the Ancestral Puebloan and some other civilizations on the continent. Given that no megadroughts of comparable magnitude have yet recurred, evaluating their likelihood is challenging as well as prudent. Rare events can arise either from purely statistical fluctuations or as the result of rare exogenous events, such as a prolonged yet transient uptick in solar activity. Toby Ault of Cornell University and his collaborators set out to determine the causes of megadroughts using a so-called linear inversion model (LIM), which presumes that a system's dynamics consist of a linear deterministic component and a nonlinear component of random fluctuations. Feeding the LIM with data yields the two components. Recent, well-sampled measurements of Earth's sea-surface temperatures and other climate variables can be used to investigate past climates—provided the underlying dynamics have remained the same. Indeed, Ault and his collaborators explicitly assumed that was the case. They found that their LIM could reproduce the 12th-century megadrought, but not the four other megadroughts that clustered in the preceding five centuries during the Medieval Climate Anomaly. The researchers conclude that the megadroughts were caused by external forcing or by a type of internal climate behavior that was quiescent in the recent past and therefore not manifested in the data fed to the LIM. (T. Ault et al., *J. Climate* **31**, 3, 2018.) —CD PT

ISSUES & EVENTS

Trump shows his apathy for science

Climate skepticism, budget cuts, and regulatory rollbacks dominated the federal scientific landscape during the first year of his administration.

PRESIDENT TRUMP receives a NASA flight jacket after signing the NASA Transition Authorization Act this past April.

Whatever one's political views, few would argue that President Trump hasn't left a lasting mark on science, technology, and environmental policies one year into his presidency. From his neglect in appointing a science adviser and other key subcabinet-level officials with science and technology (S&T) responsibilities, to his rejection of the scientific consensus on climate change and his attempts to reverse carbon emissions limits imposed by Barack Obama, Trump's actions have diminished the importance of science in the federal government.

Trump's fiscal year 2018 budget plan, which hewed closely to a blueprint advanced by the conservative Heritage Foundation, proposed big reductions to all nondefense agencies having an S&T mission, save for NASA. (See PHYSICS TODAY, July 2017, page 34.) It included a $5.6 billion, 17% cut to the National Institutes of Health and a $1.4 billion, 70% rollback to the Department of Energy's energy efficiency and renewable energy programs. For NSF, he proposed an 11% cut, and DOE's Office of Science, which provides most of the funding for basic research in the physical sciences, faced a 16% cut.

John Holdren, Obama's science adviser, noted that absent a capable scientist in the White House, the president might not see the relevance of S&T to the choices before him. He might not know when he needs to ask a question of a science-related agency or what question to ask. Holdren added that it's helpful for the president to have a trusted source of S&T information independent of the agendas of the particular agencies.

The White House science adviser, who also serves as director of the Office of Science and Technology Policy (OSTP), is one of a few dozen presidentially appointed S&T positions that have yet to be filled. Others include the four associate directors at OSTP, the director of the Department of Energy's Office of Science, the director of the US Geological Survey, the administrator and chief scientist at NOAA, the undersecretary of defense for research and engineering, and the deputy director of NSF. (A more precise listing of vacancies would depend on how broadly or narrowly those responsibilities are defined.) Trump has yet to assemble a presidential council of S&T advisers or to convene the National Science and Technology Council, the cabinet-level entity that coordinates federal S&T policy.

Many of the administration's appointments have been controversial. "The list of conflicted or unqualified appointees is extremely long, when they bother to fill the positions at all," says Michael Halpern of the Union of Concerned Scientists. He points to the naming of Albert Kelly, a disgraced Oklahoma banking executive with no environmental background, to head the Superfund program at the Environmental Protection Agency, and William Wehrum, who was confirmed in November as EPA assistant administrator of air and radiation. Wehrum, a lawyer who represented the oil and gas, chemical, and manufacturing industries in contesting EPA actions, had been forced to withdraw his nomination to that same post by President George W. Bush due to Senate opposition.

The Interior Department ordered the National Academies of Sciences, Engineering, and Medicine in August to end a study already under way on the health risks of surface mining on communities in Appalachia and in December to end another study on Interior's safety inspections of offshore oil and gas operations. Later in December the National Academies issued a statement urging resumption of the surface-mining study and added that some private donors have indicated interest in funding its completion.

Halpern notes that implicit or explicit hiring freezes at the EPA and other

PAUL WILLIAMS, WHITE HOUSE PHOTO

regulatory agencies have left them with diminished scientific and analytic capacities needed to develop and enforce environmental laws.

Climate change and the EPA

Nowhere has the contrast between the Obama and Trump administrations been starker than on climate change and other environmental policies. Trump reconfirmed his personal denial of climate change as recently as 28 December. Commenting on a cold snap gripping the eastern half of the US, he posted to Twitter, "Perhaps we could use a little bit of that good old Global Warming that our Country, but not other countries, was going to pay TRILLIONS OF DOLLARS to protect against. Bundle up!"

On 18 December Trump issued a statement that removed climate change as a national security threat, undoing the Obama-era designation. Yet a week earlier, he signed into law the voluminous FY 2018 National Defense Authorization Act, which included a provision declaring climate change a "direct threat to the national security of the United States." The legislation requires the Pentagon to prepare a report on how military installations and overseas staff may be vulnerable to climate change over the next 20 years. It's not unusual for a president to assent to must-pass bills containing provisions he objects to. But significantly, 46 House Republicans voted against a GOP-sponsored attempt to remove the climate change measure from the final bill.

Trump has named climate change skeptics to prominent positions in his administration; most notable was his appointment of former Oklahoma attorney general Scott Pruitt as Environmental Protection Agency administrator. Others include Interior secretary Ryan Zinke, Energy secretary Rick Perry, and Office of Management and Budget (OMB) director Mick Mulvaney. His nominee for NASA administrator, Representative Jim Bridenstine (R-OK), and his choice for chair of the White House Council on Environmental Quality, Kathleen Hartnett White, a former chair of the Texas Commission on Environmental Quality, also are acknowledged climate change skeptics.

An exception is Barry Myers, Trump's nominee for NOAA administrator. Myers, the founder of the private weather service AccuWeather, told lawmakers during his nomination hearing that he accepts the peer-reviewed literature showing the scientific consensus that human activity is mainly responsible for climate change.

In June Trump announced that the US will withdraw from the 2015 Paris climate change accord that Obama had helped to secure. That move leaves the US as the only nation not to have backed the pact. Soon thereafter Trump ordered the rescinding of the Clean Power Plan (CPP), which would have imposed limits on greenhouse gas emissions from existing fossil-fuel power plants (see PHYSICS TODAY, December 2016, page 26). Pruitt told the House Energy and Commerce Committee on 7 December that his opposition to the CPP was grounded in his conviction that the EPA had overstepped its constitutional authorities in regulating states. "Rule of law will again take center as we make decisions around the responsibilities that I have as administrator," he told lawmakers.

In April the EPA took down the climate change page of its website to update the language "to reflect the approach of new leadership." The page has yet to be

SCOTT PRUITT, Environmental Protection Agency administrator

MITCHELL RESNICK, WHITE HOUSE PHOTO

restored, though some climate change information remains accessible through a subject index on the EPA site.

The Environmental Data and Governance Initiative, an organization of academics and employees of nonprofits, documented the removal of climate change pages from the Interior Department's websites. Information about international obligations regarding climate change has been excised from the EPA, DOE, and State Department websites, and online descriptions of agencies' priorities have shifted to emphasize job creation and downplay renewable fuels, the group said in a report released last month. On DOE's website, mentions of "clean energy" were removed, as were explanations of the harmful effects of fossil fuels.

Pruitt made a name for himself in Oklahoma by suing the EPA more than a dozen times in attempts to halt implementation of several air and water regulations, notably the CPP. Pruitt has proposed conducting a "red team–blue team" debate-like exercise often used by the military; in a process open to the public, it would pit a team of climate change science skeptics against a team that holds the consensus view. Floated last year by physicist and former undersecretary of energy Steven Koonin, the idea is to identify weaknesses in the scientific consensus where additional research may be desirable before implementing policies that could have negative economic or environmental repercussions.

The administration's undoing of Obama-era climate change efforts isn't limited to the EPA. For example, in December the American Geophysical Union magazine *Eos* reported that DOE will shut down this year what was to be a $100 million, 10-year effort to improve the accuracy of modeling how tropical forests will respond to climate change, after just three years.

Pruitt further shook up critics by declaring that scientists who are receiving EPA grants cannot serve on any of the agency's 22 scientific advisory committees. In announcing that decision in October, Pruitt estimated that 20 grantees who sat on three committees had collectively received $77 million in agency awards while serving on those panels. "That causes a perception or an appearance of a lack of independence," he told the December House hearing; he said that the affected scientists could continue to serve if they terminated their grants.

On 21 December three former EPA advisory committee members joined a lawsuit brought by Physicians for Social Responsibility, the National Hispanic Medical Association, and the International Society for Children's Health and the Environment. The suit challenges the new policy, calling it an "illegal attempt to override federal ethics rules." Charging that the exclusion of grantees "is arbitrarily biased in favor of polluting industries," the plaintiffs warned the policy "will undermine the integrity of EPA science and introduce pro-polluter bias into agency decisions and programs."

Former EPA administrator Gina McCarthy says that to avoid conflicts of interest, the Obama administration followed detailed procedures when identifying scientists to serve on advisory panels. "No scientist who gets funding for their project is able to advise the agency on anything related to that particular work," she says. Industry lobbyists and state officials who serve on the commit-

KEN SHIPP, DOE

RICK PERRY, secretary of energy

tees under Pruitt undergo no similar review for vested interests they might have, she and others note.

McCarthy says the Trump administration will find it difficult to roll back some Obama-era regulations, such as the 2015 Waters of the United States rule that Trump ordered to be revisited shortly after taking office. Altering environmental rules requires identifying a flaw in either the underlying science or the law or finding that the administrative procedures weren't followed during the rulemaking process. McCarthy says she can't predict whether courts will accept Pruitt's federal overreach argument on the CPP but adds that the trend to cleaner energy sources is irreversible with or without the plan. Harvard Law School, Columbia Law School, and other groups are tracking the Trump administration's rollback of environmental regulations. A *New York Times* analysis from December reports 29 overturned rules, 24 rollbacks in progress, and 7 rollbacks in limbo.

The *Times* and *ProPublica*, citing information obtained under the Freedom of Information Act, reported in December that more than 700 EPA staff, including more than 200 of its 1600 scientists, had quit, retired, or taken a buyout since the onset of the Trump administration.

McCarthy says the cutbacks in staff and resources to the EPA's S&T programs are what concern her the most. "One thing we all know for sure is that the role of the federal government in terms of science and technology cannot be duplicated at the state level. You need a strong science component and capability at the federal level, and you need good labs and technical folks who can work through crises, like the Flint water problem."

Department of Energy

Trump's appointment of former Texas governor Perry as secretary of energy was in the mold of his naming Pruitt: Perry had famously pledged during his short-lived 2012 presidential campaign to abolish DOE—but then couldn't remember the agency's name. Perry reassured senators at his confirmation hearing that he had changed that view and that he would do what he could to mitigate Trump's proposed budget cuts.

Aiming to help prop up the ailing coal and nuclear power generation industries, Perry proposed a rule to the Federal Energy Regulatory Commission (FERC) to help them compete in the bulk electricity markets, primarily with low-cost natural gas. The controversial proposal, which FERC commissioners unanimously denied last month, would have provided a subsidy to nuclear and coal generation plants for storing a 90-day supply of fuel onsite. That would supposedly provide resilience to the grid in the event of a crisis, Perry had argued.

Trump proposed eliminating the Advanced Research Projects Agency–Energy, a small DOE office that supports development of innovative, high-risk, high-payoff, clean-energy technologies. Trump did propose maintaining US participation in ITER, the seven-party international effort to construct an experimental fusion reactor in southern France, albeit at a lower level than last year.

NASA

Trump spared NASA from the budget cuts he put forward for other science agencies. He reinstated the Moon as the next destination for human exploration beyond low-Earth orbit and thereby rejected the Obama administration's plan to forgo the Moon in favor of sending astronauts to an asteroid that would be brought closer to Earth by a robotic mission. Trump, however, didn't set a timetable or specify the level of funding to be devoted to the Moon mission.

Consistent with his climate change views, Trump proposed cutting NASA's Earth science program by 9% and canceling multiple Earth-observing missions.

Trump's choice of Bridenstine for NASA administrator appeared in jeopardy at press time. At least one GOP senator, Marco Rubio of Florida, has indicated he may not vote to confirm Bridenstine, who has no science or engineering background. With Republicans now holding a slim one-vote margin in the Senate, another GOP defection would deny Bridenstine the job—a tie would presumably be broken by Vice President Pence.

Scientists push back

Trump's policies have engendered a new activism among scientists, a community traditionally averse to political participation. "There's a thirst for engagement that I haven't seen in 15 years . . . , and a lot of scientific societies are stepping up to the plate," says Halpern. "Ensuring the federal scientific enterprise continues to thrive has become a big priority of many scientists across the country." Most visibly, hundreds of thousands of scientists and their advocates rallied in April in Washington, DC, and at dozens of other March for Science events held around the world (see physicstoday.org/MarchForScience).

Reacting to Pruitt's ban on grantee participation on EPA science advisory committees, the Association of Environmental Engineering and Science Professors in November announced that it would create a shadow environmental committee to review the work of EPA advisory panels.

In December, 42 scientific societies and universities wrote to OMB director Mulvaney objecting to news reports that the Centers for Disease Control and Prevention had banned the use of certain terms, including "science-based" and "evidence-based" in budget documents. While noting the CDC director's denial that there had actually been a ban, the signatories added, "Our community remains concerned and requests you encourage the heads of all federal agencies to support the use of science in decision making."

The Data Refuge project was organized by librarians, archivists, and scientists to archive terabytes of climate data threatened for removal from the websites of NOAA, the EPA, and other agencies (see PHYSICS TODAY, March 2017, page 31).

Through it all, scientists have continued doing science. "In many ways this has been a good year for science. There has been great research with important results," says Rush Holt, CEO of the American Association for the Advancement of Science. That includes yet more evidence that climate change is occurring and, he adds, that "its effects will be on the greater, not lesser, side of the range of expectations."

David Kramer

Google Lunar X Prize hopefuls struggle to lift off

The finalists face long odds to land a rover on the Moon in time to claim the $20 million grand prize.

It's been more than 10 years since Google and the X Prize Foundation (now XPrize) announced the Lunar X Prize, which offered $20 million to the first privately funded team to land a spacecraft on the Moon, navigate 500 m across the lunar surface, and beam high-definition images back to Earth. Of the competition's initial field of 29 teams, 5 confirmed their launch plans in time to make the cut as finalists: teams from India, Israel, Japan, and the US, and an international team that boasts members from six continents. To have a chance of claiming the grand prize, one of them will have to get its spacecraft off the ground before 31 March.

Lunar X Prize or no, the teams are determined to reach the Moon. As they hustle to complete preflight testing, raise last-minute funds, and prepare for launch, some are already setting their sights on a more distant and potentially more lucrative prize: a foothold in the burgeoning commercial space industry.

EDITORS' NOTE: *As this issue went to press, XPrize announced that none of the remaining teams would launch their spacecraft by the contest deadline. The $20 million grand prize will therefore go unclaimed. Read more at* ***www.physicstoday.org.***

The new space race

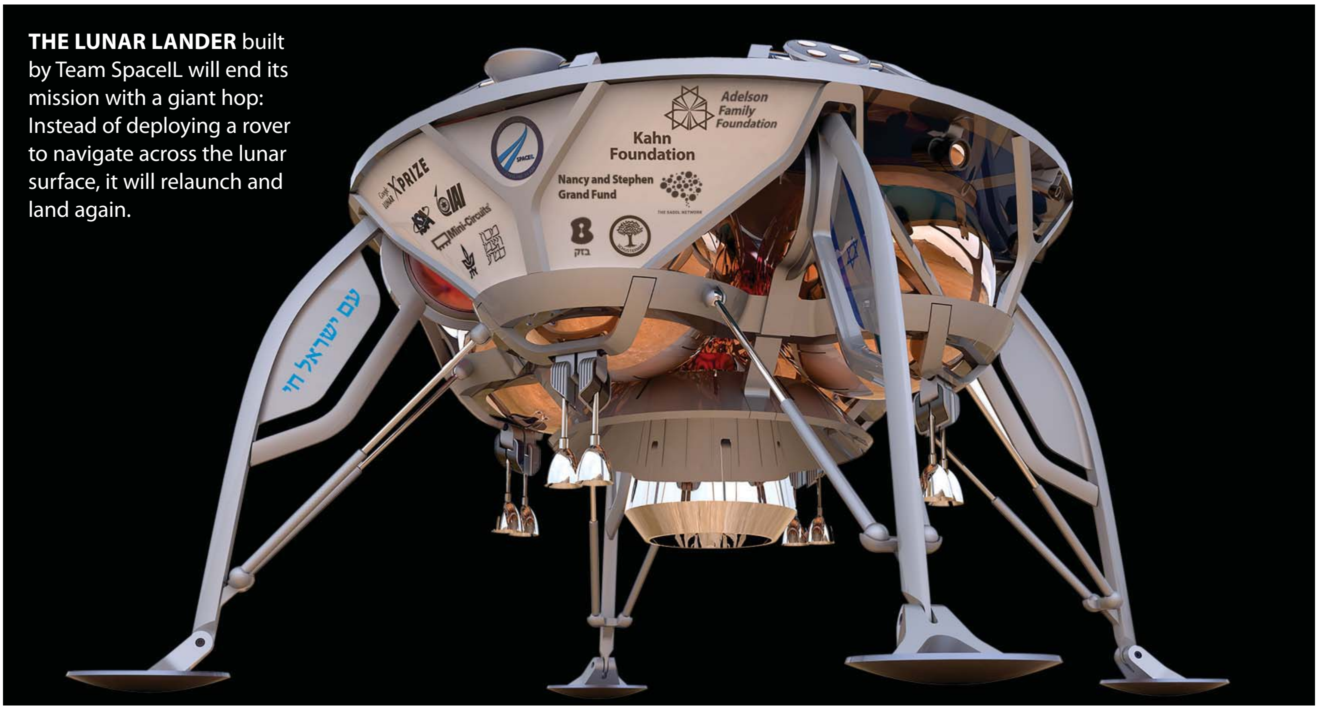
The task the contestants face is immense. Since the culmination of the Cold War–era space race, nearly 50 years ago, only China has soft-landed a spacecraft on the Moon. And its *Yutu* rover, after touching down in late 2013, wheeled less than 120 m across the rugged lunar surface before malfunctioning and losing mobility.

Although China hasn't disclosed the cost of the mission that carried *Yutu* to the Moon, the US Apollo program and its Soviet counterpart, Luna, each cost billions of dollars. In essence, the X Prize is challenging teams composed largely of academics, space entrepreneurs, and neophyte rocket scientists to reach the Moon at a minute fraction of that cost.

To keep their budgets lean, all but one of the finalists have opted to hitchhike their way to space: Instead of flying on a dedicated rocket, their lunar landers and rovers will nestle inside commercial

© HAKUTO

TEAM HAKUTO, one of five teams still vying for the Lunar X Prize, tests its *Sorato* rover on a simulated moonscape.



SPACEIL

THE LUNAR LANDER built by Team SpaceIL will end its mission with a giant hop: Instead of deploying a rover to navigate across the lunar surface, it will relaunch and land again.

rockets alongside communications satellites, CubeSats, and other payloads. The rockets will deposit the spacecraft in Earth orbit. The teams will have to complete the rest of the 380 000 km journey to the Moon on their own.

"With one stage of spacecraft, we need to get from Earth orbit to a lunar orbit, do the energy-intensive lunar-capture maneuver, and then land—which itself requires lots of energy," says Eran Privman, CEO of the Israel-based finalist SpaceIL. "That mission has never been done."

SpaceIL has contracted to launch its lunar lander to geostationary orbit on a SpaceX Falcon 9 rocket. Once the lander touches down on lunar soil, it will use an unorthodox approach to complete the final 500 m leg of the Moon race: Instead of deploying a rover, it will relaunch and touch down again at a distant site.

"The team joined the competition on the last day of registration, without any knowledge of space rovers or Moon rovers," Privman explains. By skipping the development of the rover, he says, they were able to make up for lost time and inexperience.

The US-based finalist, Moon Express, founded by space entrepreneur Bob Richards, will also forgo a rover in favor of a "hop" strategy. But the team's launch provider, RocketLab, will deposit the lander not in a 35 000-km-altitude geostationary orbit but in low-Earth orbit, some 33 000 km below, where it will still need to expend considerable energy to escape Earth's gravity well.

The Indian and Japanese finalists, Teams Indus and Hakuto, won't have that problem. Both teams contracted to launch their spacecraft to geostationary orbit on one of the Indian government's Polar Satellite Launch Vehicles. And the teams will share more than just a rocket: The Indian contestants will allow Hakuto's rover to ride all the way to the lunar surface on their lander, in return for an undisclosed transport fee.

"That's allowed us to focus on miniaturizing our rover," says Takeshi Hakamada, team leader of Hakuto. The final version, *Sorato* ("space rabbit") weighs just 4 kg and is about the size of a microwave oven.

If *Sorato*'s wheels ever do kick up lunar dust, the vehicle will find itself in a 500 m dash against Team Indus's *ECA*, short for Ek Choti si Asha ("a small hope"). The two rovers will squeeze into Team Indus's 2-m-tall lunar lander along with a soda-can-sized biology experiment that was designed by high school students as part of the team's Lab2Moon contest.

Only Synergy Moon, the international finalist, has dared to build its own rocket. The brainchild of adventurer and documentary filmmaker Nebojša Stanojević, the team formed when Stanojević's Human Synergy Project merged with US team Interplanetary Ventures in the early days of the contest. Since then, the collaboration has incorporated a dozen teams and companies representing 15 countries.

One of those companies, the US aerospace manufacturing firm Interorbital Systems, has been working for years to develop a series of inexpensive, modular rockets. Synergy Moon is counting on one of those rockets to fly its three-wheeled rover to the Moon.

Flight delays

When the Lunar X Prize was announced in 2007, contestants had only until the end of 2012 to claim the $20 million grand prize. After that, the reward would drop to $15 million, and if no team reached the Moon by the end of 2014, the competition would end altogether.

When it became clear, however, that none of the entrants could meet the ambitious deadlines, contest organizers kept the prize at $20 million and granted a string of extensions. They eventually gave teams until 2017 to complete the mission, provided they had secured launch contracts by the end of 2016. Last August, when the five remaining teams still weren't ready to hurl their crafts into space, XPrize granted one last reprieve, to 31 March 2018.

If the deadline slips again, the competition risks losing some of its thunder;

the Indian government is planning to send its own rover to the Moon in early 2018 as part of its Chandrayaan-2 mission. Why is it taking so much longer than expected for X Prize contestants to get to the Moon?

"Missions are planned by optimists but executed by pessimists," says Scott Hubbard, Stanford University adjunct professor and former director of NASA's Ames Research Center. As teams come to realize that a single misstep can scuttle an entire mission, he explains, corner-cutting measures that initially seemed prudent are often deemed too risky. Not only does that send teams back to the drawing board, Hubbard adds, "it leads to cost growth."

Indeed, most of the finalists have seen their budgets swell to more than double the $20 million payout. And those unexpected costs present their own challenges. "The difficulty is not in the technology," explains Team Hakuto's Hakamada. "It is in the fundraising."

Hakamada recalls that several teams struggled to raise money during the early days of the competition. But he and his colleagues largely avoided that fate by limiting their scope to rover design. As the Moon race enters the homestretch, Hakuto finds itself in the enviable position of being ahead of schedule and in the black: The team has raised the roughly $10 million it needs to cover costs, completed testing of its rover, and shipped it to the planned launch site in Bangalore, India. All that remains is to blast the diminutive robot into space.

There's just one big problem: Its ride, Team Indus, is reportedly still scrambling to raise the $70 million it needs to complete its own rover and lander. As PHYSICS TODAY went to press, an Indian news publication reported that India's space agency had canceled Team Indus's launch contract due to missed payments.

The other finalists also face potentially show-stopping delays. As this year began, SpaceIL was still assembling its lander, which would then need months of preflight testing; Moon Express's launch provider, RocketLab, had yet to demonstrate that it could deliver a payload into orbit; and Synergy Moon had yet to demonstrate that it could even get its rocket off the ground.

Moon or bust

If the Lunar X Prize is canceled after March, it wouldn't be the first time XPrize called off one of its global challenges: In 2013 the foundation abandoned a $10 million competition to spur rapid human-genome sequencing, citing that technological innovations in the field had rendered the contest unnecessary.

Still, the Lunar X Prize hopefuls say they would rather miss the March deadline—and launch later—than rush an unproven craft into space. In fact, some teams have already shifted their sights to a more distant reward: a stake in the emerging lunar exploration industry.

According to the nonprofit Space Foundation, space has become a $300 billion economy, driven mostly by commercial activities at geostationary altitudes and below. With the commercialization of the Moon, that market could grow substantially.

Space entrepreneurs have floated proposals to mine the Moon for water that could one day support lunar colonies, harvest helium-3 for use on Earth, and establish the Moon as a waystation for missions to Mars and other deep-space realms. Hakuto is eyeing the Moon for many of the same reasons. Its parent company, the Japanese startup Ispace, recently raised $90 million to develop a lunar lander for two return trips to the Moon by 2020.

Meanwhile, Moon Express has already lined up paying clients for its maiden lunar voyage: It will deliver a telescope for the nonprofit International Lunar Observatory Association; a laser array for scientists from the University of Maryland and Italy's National Laboratory of Frascati; and cremated remains for Celestis, a Texas-based company that offers memorial spaceflights and space burials. Only after the team's spacecraft completes those deliveries will it attempt the 500 m scamper to win the Lunar X Prize.

Even SpaceIL, the lone nonprofit among the finalists, would be undeterred by the prize's cancellation. Funded largely by Israeli philanthropist Morris Kahn and the Adelson Family Foundation, the team hopes it can create an "Apollo moment" that will inspire young Israelis to pursue careers in science.

"Because of that, we are going even if we launch after the end of the competition," says the team's CEO Privman. "And it will be very worth it."

Ashley G. Smart PT

CRYSTAL GROWTH IN ICE AND SNOW

Mary Jane Shultz

Surface molecular structure is the arbiter in the contest between energy and entropy that largely determines how ice and snow crystals develop.

ICE AND SNOW in Eyjafjallajökull, Iceland. Photo by Andreas Tille.

Mary Jane Shultz is a professor of chemistry at Tufts University in Medford, Massachusetts.

Ice shapes our world. The water-to-ice phase transition tempers the climate, fractures rock, and squeezes material caught in interstitial ice grain boundaries. The vapor-to-ice transition produces symmetric snowflakes that are both beautiful and fascinating. These phenomena and more have their roots in the building blocks—made from water molecules—that compose ice and snow.

More than 400 years ago, well before scientists knew about molecules, Johannes Kepler pondered the relationship between building-block packing and the hexagonal shape of snowflakes.[1] We now know that the core of a snowflake consists of a single crystal of so-called hexagonal ice, I_h, the first elaborated of 17 known phases of ice. The lacy structure of snowflakes builds on that single-crystal core as additional vapor molecules condense on the surface. The growth of single-crystal ice from liquid water also proceeds from sequential condensation events, but in ways significantly different from snowflake growth.

The internal structure of ice has been known since the advent of x rays. But the surface binding that grows ice and snowflakes is different from binding in the bulk. In due course, I'll present a molecular-level model that elucidates the surface growth process. The laboratory environment in which researchers grow single-crystal ice is quite different from the clouds in which vapor condenses into snowflakes, and I'll also discuss how the different environments affect the growth process. But first, I invite you to join me on a visual tour of snowflake structure at multiple scales—from the macroscopic hexagonal prism that is the core of all the observed shapes, to the microscopic surface structures revealed by etching single crystals, to the molecular-level surface configuration detected by atomic scattering.

Symmetry within chaos

Snowflake growth starts with a surface on which water vapor can condense. In the environment, seeds are provided by many kinds of particulate matter, including pollen, mineral dust, and salts created when ammonia neutralizes acidic gases in the atmosphere. Exactly how the nascent snowflake forms on the solid seed remains uncertain, as demonstrated by the still not quite successful efforts to seed clouds.[2] Nonetheless, if conditions are right, a perfect hexagonal ice crystal nucleates on the seed and the nascent flake grows.[3] Usually the mature flake has six elaborate and nearly identical sides, but as figure 1 shows, nature can display other forms.

The symmetry and variety of snowflakes have fascinated scientists and nonscientists alike. How can molecular forces that act on the subnanometer-to-nanometer scale operate so that parts of the crystal literally billions of molecules away assemble in the same way, yet any two snowflakes are highly unlikely to be identical? The first steps toward answering the question came in the 1930s, when Ukichiro Nakaya diagrammatically cataloged the importance of temperature and relative humidity on crystal morphology.[4] In brief, he found that thin plates form at −2 °C, long needles at −5 °C, thin plates again at −15 °C, and thick plates and columns at −25 °C. He also observed that at low relative humidity, the crystals grow slowly and develop few branches. Conversely, high relative humidity supports more rapid growth and more abundant branches.

Although the relative humidity and temperature vary from location to location in a cloud, on the tiny scale of a snowflake they are constant. As a result, snowflake growth is essentially perfectly symmetric. On the other hand, as tiny snowflakes blow around in the chaos of the cloud, buffeted by the wind and perhaps warmed by the Sun, individual flakes are highly unlikely to experience exactly the same set of varying conditions. As a result, pretty much every snowflake is unique.

Nakaya's morphology diagram is observational. It does not explain why the structure changes with temperature from plates to needles to columns or why high relative humidity supports dendritic growth. Ultimately, the answers lie in energy and kinetics considerations at the nanoscale. Before arriving at the nanoscale, however, we will take a detour to the microscopic level to see the context in which the nanoscale physics operates.

Etch pits

The heart of every snowflake is a single, hexagonal prism ice crystal. Figure 2a shows the geometry and identifies three distinct types of crystal face: the hexagonal basal faces that cap the prism, the rectangular primary faces on the sides, and the secondary faces formed by cleaving along the line connecting alternate hexagon points. Snowflake cores are micron sized, delicate, and ephemeral, but to get at their microscopic structure, it is not necessary to deal with such fragile systems. Instead, one can explore etch pits created by the sublimation of material from the surface of a larger, single crystal.

First, cleave a flat surface on the crystal and coat it with a thin polymer film that naturally forms with minute pinholes. Water molecules sublimate through the pinholes. Etching is thus the reverse of the process by which snowflake cores develop by condensing vapor-phase water molecules onto the growing surface. Suppose, for example, that the crystal is cleaved along a basal face. Then the etch pits will be tiny hexagons, just

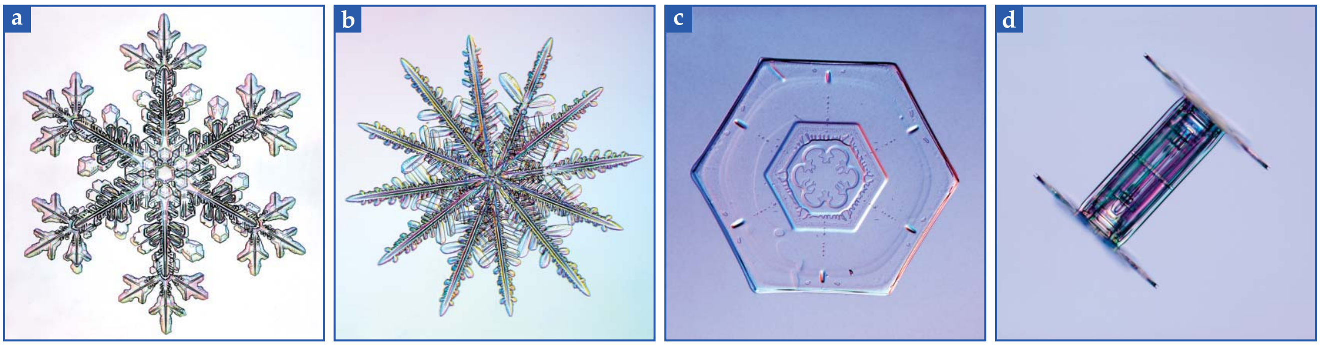


FIGURE 1. SNOWFLAKES FORM A RICH VARIETY OF STRUCTURES. (a) Elaborate dendrites sprout from the hexagonal points of the snowflake core. **(b)** In a 12-sided flake, growth originates from the hexagonal points and from the hexagonal sides. **(c)** A plate-form snowflake has defects where crystal domains meet. **(d)** A hexagonal column snowflake is capped with larger hexagonal ends. (All photos courtesy of Kenneth Libbrecht.)

like the cores of snowflakes. The etch pits that arise if the crystal is cleaved along a primary or secondary face are perhaps harder to visualize, but they are shown in figure 2b, along with the basal hexagons. For me, the etch pits illustrate one of the satisfying aspects of ice research: the visual connection between macroscopic and microscopic structure.

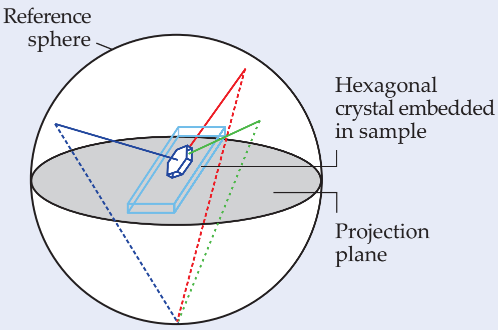
The basal, primary, and secondary faces are the major characters in the story of growing ice. Usually, lacy snowflake structures originate at the hexagonal prism points. Thus the advancing ends are secondary prism faces. When single-crystal ice is produced in the lab, the secondary prism face is again most likely to propagate. To understand why requires an exploration of ice at the molecular scale, the next step in our tour.

A hidden hexagon

Consideration of the molecular-level ice structure raises a question, only recently answered, that is directly relevant to face stability and growth out of the hexagonal corners.[5,6] The question may be stated with the help of figure 3a, which shows two distinct hexagonal structures in the ice basal face. The first hexagon structure (red and white in the figure) is familiar to students of chemistry and molecular physics. The second (blue) is larger, is rotated by 30° with respect to the other hexagons, and consists of six water molecules surrounding a central water molecule. Which hexagon structure coincides with the snowflake core?

Last year my colleagues and I reported an answer to the question.[6] Part of the reason it took so long is that substrate preparation is difficult. Crystal impurities and stresses found in the environmental ice used in previous work muddied the data interpretation, but the advent of laboratory methods for growing large, optically perfect single crystals[7] enabled us to clear away the mud. Our approach was to carefully ensure the same sample orientation for etching and for probing with electron backscatter diffraction and then to correlate the resulting etch pits and orientation density functions (see the box). By doing so, we could establish that the hexagonal prism at the core of a snowflake corresponded to the larger of the micro-

THE ORIENTATION DENSITY FUNCTION



Quantum mechanics teaches us that electrons are waves, so electrons scattering from crystal planes produce constructive and destructive interference if the electron wavelength is comparable to the crystal lattice spacing. The scattering pattern can be interpreted to find the normals to the scattering planes. Three normals are relevant; they are called *a* (red), *b* (green), and *c* (blue) crystallographic axes. The *c*-axis is perpendicular to the basal plane of a snow crystal. Crystallographic *a*- and *b*-axes are defined in figure 3a; *a priori* one doesn't know which of those two axes is directed toward the hexagonal points of an actual snow-crystal core. But—spoiler alert—the illustration shows the proper correspondence.

In our work, we present the scattering information as a two-dimensional figure called an orientation density function (ODF). Imagine that the sample is enclosed in a sphere. At least some of the outward-directed normals intersect the northern hemisphere; the figure shows one example for each crystallographic axis. Connect the intersection points to the south pole and mark where the connecting line crosses the equatorial plane. Repeat the procedure over hundreds of scattering events, express the likelihood that a given equatorial point is crossed, and you've got an ODF.

A tight clustering of equatorial crossings indicates a single crystal, and the specific crossing spots indicate how the crystal is oriented. For example, if the basal plane is parallel to the projection plane, the ODF associated with the *a*-axes would display six equatorial crossings that correspond to the directions of the six vertices of the blue hexagon shown in figure 3a. (In this idealized special case, the northern hemisphere intersections would correspond to the equatorial crossings.) Indeed, figure 3b shows an ODF for a crystal with almost that perfectly basal orientation.

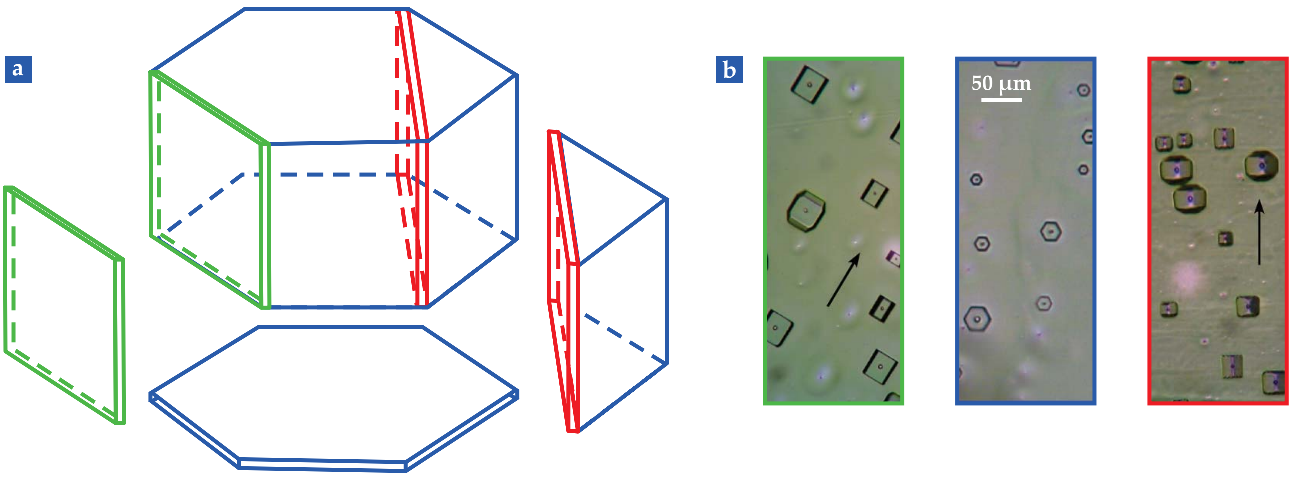


FIGURE 2. SINGLE-CRYSTAL ICE ETCH PITS reflect the geometry of the hexagonal prism lattice. **(a)** Surfaces parallel to the rectangular prism sides are primary prism faces (green), those parallel to the top and bottom caps of the hexagonal prism are called basal faces (blue), and those cut perpendicular to the line joining opposite hexagon points are secondary prism faces (red). **(b)** Etch pits such as shown here form when a crystal is cleaved and small bits of the surface sublimate away. The color-coded photos show the etch pits that result from cleaving along a primary, a basal, and a secondary surface. They look, respectively, like flat-bottom boats, hexagons, and V-bottom boats; the features visible in the pits lie below the plane of the page. Black arrows indicate the prism axis. Because the sample is a single crystal, the etches that occur in different places all have a similar shape and are aligned in the same way.

scopic hexagons in figure 3a. Figures 3b and 3c show some of our results.

A more detailed look at snowflakes at the molecular level illuminates why dendrites typically grow out of the hexagonal points. Specifically, I will examine the molecular structure of the primary and secondary prism faces. A primary face, we now know, corresponds to a flat side of the blue dashed hexagon in figure 3a. As figure 4 shows, the face's top layer consists of pairs of water molecules in a row structure. A secondary prism face corresponds to a flat side of the red-and-white hexagon in figure 3a. Its top layer has chains of water molecules. To successfully dock onto the growing surface, the incoming water molecule must orient to complement the existing surface. That is, a covalently bonded hydrogen atom of the incoming molecule must link with an open valence (unshared electron pair) of a surface oxygen atom. Conversely, an open valence on the incoming molecule must link with an O–H group dangling from the surface.

The pair configuration of the primary face affords greater flexibility in forming a successful dock than does the chain configuration of the secondary face. More precisely, the surface entropy is greater for the primary face. But entropy is just one component of a surface's free energy. The other is enthalpy—the heat of fusion released when vapor condenses to grow the snowflake. Enthalpy favors docking at the secondary prism face, which has a greater valence density. Most of the time, snowflakes grow by advancing the secondary prism face.

However, the free energies of the three major prism faces are nearly the same, and small temperature and humidity variations in a cloud encourage different kinds of growth. Each snowflake experiences a unique history, and thus each snowflake is unique.

Having completed our multiscale tour and looked at some of the thermodynamics of ice, let us review some of the varied snowflake forms shown in figure 1. In the humid conditions that favor highly branched structures, the secondary prism face gathers water molecules rapidly and grows branches. Released heat of fusion maintains the high humidity in a positive feedback loop. The growth is actually so rapid that the branches develop imperfections that send them in a new direction oriented 60° away, in accord with the ice crystal's hexagonal symmetry. The result is beautiful dendrites, as depicted in figure 1a.

The existence of 12-sided snowflakes, as in figure 1b, indicates that if the temperature and humidity are right, the primary prism face can ably compete with the secondary face to grow dendrites. Again, a positive feedback loop maintains growth.

Ridged snowflakes, as in figure 1c, form in calm conditions with constant temperature and relatively low humidity. In such an environment, domains sprouting from adjacent hexagonal points grow large enough to fill in the space between them. Crystal imperfections resist the smooth joining of adjacent domains. Water molecules bridge the domains, but stress from the bridging creates ridges at the domain junctions.

Columnar snowflake crystals, as in figure 1d, start life in a cold, low-humidity environment that favors growth of the primary prism face. As the snow crystal grows, it is blown to a region of the cloud with more typical conditions, and there it becomes capped with a large basal face. Nakaya's morphology diagram shows that the temperature variation between growing a long ice crystal and capping the ends with plates can be as little as 3 °C. Those little barbell-shaped snowflakes are excellent thermometers.

Laboratory-grown ice

Our experiments to answer the hexagon riddle of ice structure were possible only because we could grow single-crystal ice in the laboratory. Fabricating such a crystal might seem to be a trivial task; just put some water in the freezer. Alas, water contains dissolved gases, which is why ice cubes typically have bubbles in them. Furthermore, ice cubes consist of thousands of small crystallites. Another approach is needed to grow a single crystal.

At the macroscopic stop of the multiscale tour, I noted that

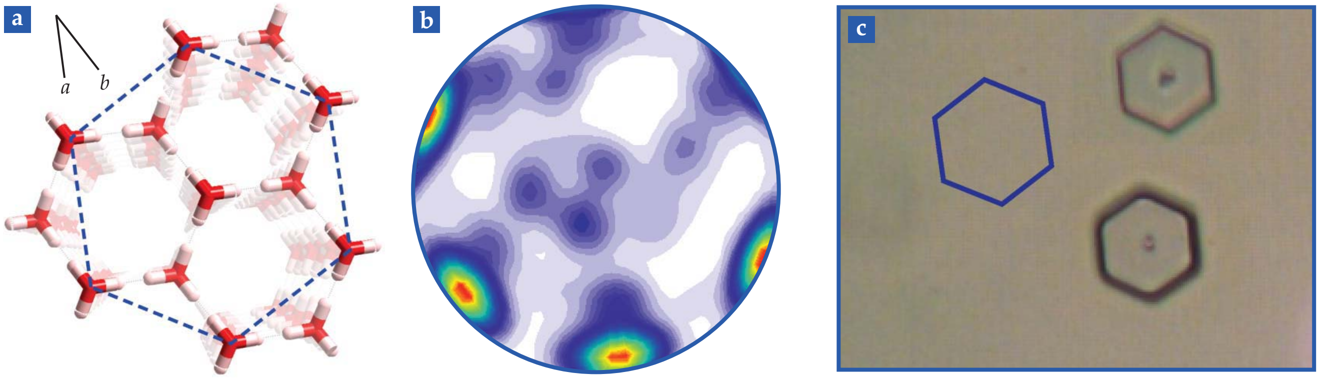


FIGURE 3. A TOP VIEW OF THE ICE BASAL FACE reveals two hexagonal structures. **(a)** One type of hexagon is illustrated with a red-and-white molecular model, in which the red junctions are oxygen atoms and the white capsule-shaped regions indicate possible locations of hydrogen atoms; an O atom is always bound to two H atoms and only one H atom lies between any pair of O atoms. The blue dotted shape indicates a second structure, a crystallographic hexagon consisting of six water molecules surrounding a central water molecule. Black lines show the crystallographic *a*- and *b*-axes. Which hexagon corresponds to the core of a macroscopic snowflake? To answer the question, we compare **(b)** an orientation density function (ODF; see the box) that reveals the directions of the *a*-axes with **(c)** etch pits of the basal face of an ice crystal. Since the *a*-axes point to the vertices of the crystallographic hexagon in panel a, the match between the hot spots in the ODF and the vertices of the etch pit demonstrates that the basal face corresponds to the crystallographic hexagon. Note that some of the hexagonal points in panel b are hidden because the sample is slightly tilted; it is raised a little at the seven o'clock location and depressed a little at one o'clock. For the same reason, the two center spots in panel c—the lowest points in the hexagonal pits—are slightly off center.

snowflakes require a seed to initiate growth. That is because clean water supercools—remains liquid—to temperatures as low as −46 °C. So, like snowflakes, laboratory-grown ice requires a seed. Once nucleated, water and other supercooled materials solidify rapidly and generate many crystal domains.

To make single-crystal ice, we started with a polycrystalline seed, grew at 0 °C, and took advantage of competitive growth to winnow down to just one domain. Winnowing begins with a short capillary that connects the seed bulb to a growth tube. As the frozen front advances through the capillary toward the growth tube, the lowest-free-energy, most stable face occupies a larger and larger fraction of the liquid–solid interface. A length of 5 millimeters accommodates a million layers—a million generations—which is ample opportunity for survival of the stablest. Then a flared-out crucible region of the growth tube magnifies the one to five domains that typically survive the capillary stage. Final selection occurs as the crucible constricts to a narrow neck and spatially filters out one domain that seeds the main body. Voilà, a single crystal.

Because the ice sample takes on the shape of its container, it does not reveal the orientation of the ice lattice; etch pits do. If the surface of the single-crystal happened to be precisely aligned along a basal, primary, or secondary face, the etch pit would look like one of the examples in figure 2. In general, such a fortuitous orientation is not the case, and determining the actual orientation is an exercise in three-dimensional geometry.

Imagine a virtual hexagonal prism partially embedded in the surface, as shown in figure 5. Removing the prism leaves a pit whose profile reveals the orientation of the original prism. To specify the orientation, first consider the so-called tilt angle θ between the axis of the growth tube, or boule, and the axis of the hexagonal prism. In the figure, the tilt angle is about 80°, which is a typical result. Indeed, the most likely tilt angles are in the range of 70°–90°, and tilt angles less than 45° are never observed. The boule cross section is a frozen record of the growth front. Given that the tilt angle is not zero, the basal face is not that front. It is, in fact, the least stable of the three major ice faces. If snow ice grew from the liquid rather than from the vapor, snowflakes would all be columnar.

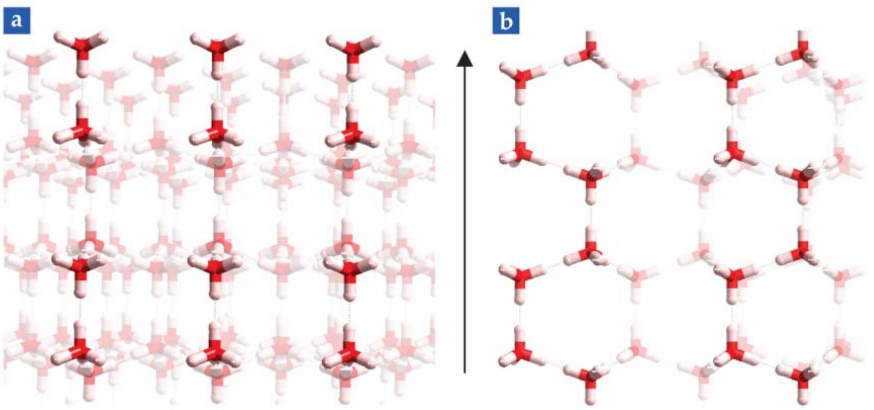


FIGURE 4. THE MOLECULAR STRUCTURES of ice's primary and secondary faces govern the faces' thermodynamic properties. These views from above show the locations of oxygen (red) and hydrogen (white) atoms in the surface layer of water molecules, as described in figure 3a. Atoms in deeper layers are faded out so that the top layer is more clearly visible. **(a)** The top layer of the primary prism face features pairs of water molecules. Shown here are two rows each with three oxygen pairs. The primary face's pair configuration contrasts with **(b)** the secondary face's chain structure. Those different molecular arrangements result in different entropy and enthalpy for the two faces. The black arrow indicates the crystal prism axis.

Rotation about the prism axis is called the roll angle α. It is measured from a hexagonal point to the surface-normal plane, which is determined by the boule and prism axes. For example, if the point faces directly into the boule, the roll angle is 0° and the growth front is a secondary prism face. A roll angle of ±30° indicates that the primary prism face is the growth interface. In observations of growth in hundreds of boules, about 60% of the growth fronts have roll angles near 0°, 30% have angles near ±30°, and 10% are between those extremes.

The near-equilibrium growth of single-crystal ice in boules favors the secondary prism face, though the primary face offers reasonable competition. The secondary prism face is thus the most stable face for the liquid–solid interface. The results are not surprising in light of the entropy and enthalpy of the faces' molecular structures. Entropy favors the primary face over the secondary one, and both of those are favored over the basal face. The secondary prism face has a slight enthalpy edge over the primary prism face, and both have an advantage over the basal face. At the 0 °C temperature of the growth front, enthalpy slightly edges out entropy.

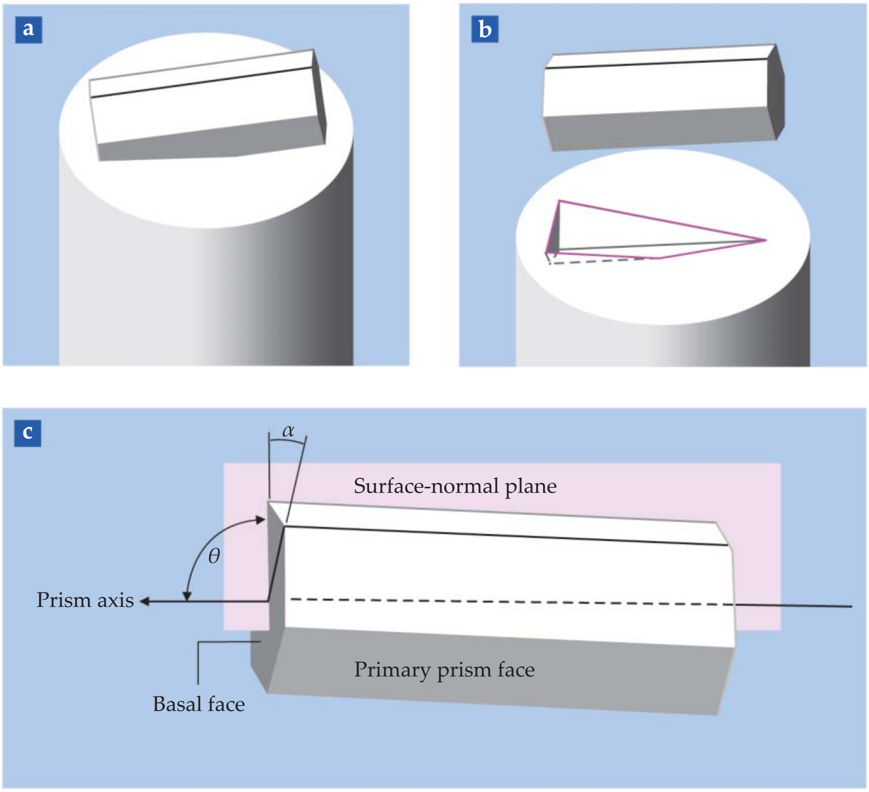


FIGURE 5. THE ORIENTATION of ice grown in the lab can be determined from etch pits. The ice takes on the shape of the container it is grown in, here a cylinder, but the ice crystal itself is a hexagonal prism. **(a)** The orientation of the prism with respect to the container surface can be arbitrary. **(b)** The etch pit formed by the lab-grown ice corresponds to the submerged part of the prism shown in panel a. **(c)** The orientation revealed by the etch pit can be specified by the tilt angle θ and the roll angle α illustrated here and defined in the text. The surface-normal plane is the plane that includes the container cylinder axis and the crystal prism axis.

In retrospect, the development of the snowflake seems odd. If the secondary prism face has the lowest free energy and indeed is often the advancing front, why is the area of a snowflake dominated by the basal face, with the secondary face occupying only a small fraction of the area? One key is heat conduction. For ice grown in liquid, the growth front has good thermal contact with the ice and water baths on either side of it. The baths easily conduct away heat of fusion provided the growth is slow enough. In snow clouds, one side of the growth front is vapor, a poor heat conductor, and the other is a thin dendrite, which is hardly a heat sink. As a result of inefficient heat conduction and high heats of fusion, the primary and secondary fronts vaporize and the basal face of the snowflake has a relatively large area. Topology may also be important. The surface of a snowflake is a closed 2D area in 3D space. In contrast, the liquid–ice system is enclosed in a boule; the growth face is planar. I also note that the theoretical modeling of ice and water is quite challenging, in part because of the quantum nature of the proton.

Tools of the trade

Particularly in the atmosphere, ice likely shapes the world in ways that are not yet appreciated but that are amenable to explorations with the tools now available to researchers. Single-crystal ice samples can be grown in the laboratory in a reasonable time. Etching serves to determine crystal lattice orientation, and by cutting the sample appropriately, investigators can generate whatever faces they want to look at.

Nearly any molecular-level question of interest is still open. Secondary prism face chains have been detected spectroscopically,[8] but the primary face pairs have not been probed. Chemistry on either of the two faces is yet to be explored. Dangling valences on the ideal prism faces seem to be oriented in a manner nearly perfect for small-molecule docking, a phenomenon that could have a profound effect on the environment. The future looks bright for ice researchers, who can look forward to learning much more about one of our most common and fascinating materials.

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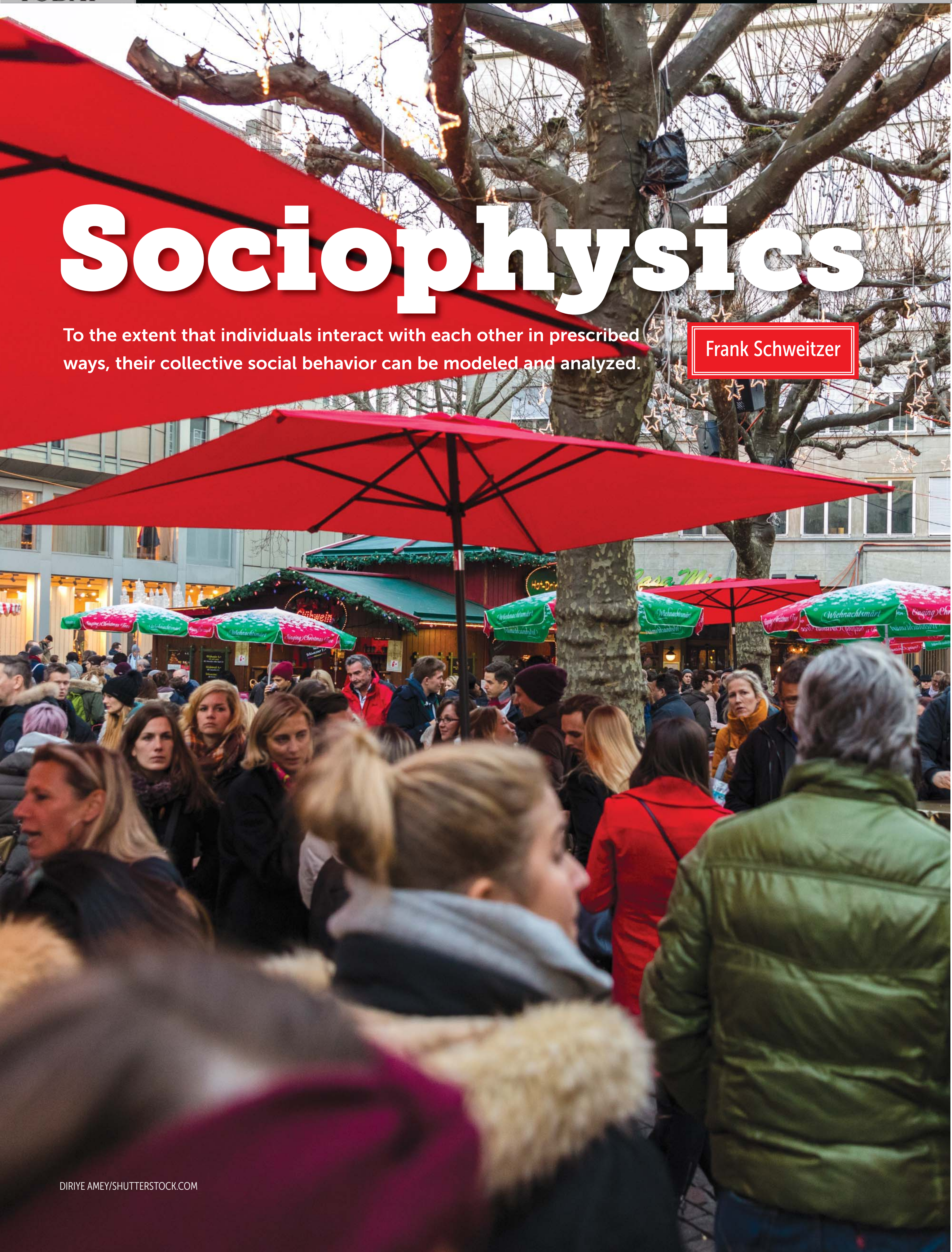
Sociophysics

To the extent that individuals interact with each other in prescribed ways, their collective social behavior can be modeled and analyzed.

Frank Schweitzer



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Twenty-four years ago Paul Krugman, who went on to receive the 2008 Nobel Prize in Economic Sciences, wrote, "Economics is harder than physics; luckily it is not quite as hard as sociology."[1] Thirteen years ago Doyne Farmer, Martin Shubik, and Eric Smith posed the question, Is economics the next physical science? (see PHYSICS TODAY, September 2005, page 37). If you were skeptical then about sociology as the next physical science, you may be even more skeptical now.

A healthy skepticism regarding those two fields may indeed be better than the unhealthy optimism found in some of today's physics publications. But between physics and the social sciences there are signs of fruitful encounters, most of which are related to the emerging field of computational social science. The trend is driven by new social data provided by engineers, who build the sensors that increasingly log our everyday lives, and by computer scientists, who build the software that harvests the data. To elucidate those developing relations, it is helpful to start with a historical perspective.

In *A Treatise of Human Nature*, Scottish philosopher David Hume (1711–76) proposed establishing a new science of man in the spirit of mathematics and physics. During the 19th century, new physical theories emerged. Electromagnetism showed that two seemingly different phenomena could be understood from a general perspective. Thermodynamics introduced a new and rather abstract concept of "systems." French philosopher Auguste Comte (1798–1857) proposed that society follows general laws much as the physical world does. To determine the laws' empirical basis, Belgian statistician Adolphe Quetelet (1796–1874) applied probability theory to data about humans. In his *Essays on Social Physics* (1835), he derived statistical laws for the average human based on the normal distribution. For example, he defined the body-mass index to quantify obesity. He also analyzed crime and public health. After discovering that Quetelet had appropriated the term "social physics" for his statistical approach, Comte decided to coin, for his new science of man and society, the term "sociology."

Physics served again as a role model in the 20th century when new fundamental theories were devised. Relativity, with its revision of the concepts of space and time, and quantum mechanics, with its introduction of the uncertainty principle, both shed new light on the role of the observer and the process of observation. Modern physics had a broad impact on philosophy and the social sciences to a degree that can seem surprising nowadays. By the second half of the 20th century, the impact was no longer through general theories but through generic and abstract modeling approaches. Already during the 1940s, lattice models, later generalized as cellular automata (CA), were being used to study social segregation. The models had tunable parameters, such as migration distance and the ratio of tolerated and untolerated inhabitants in a person's neighborhood.

The value of CA was readily apparent in its ability to simulate and visualize social dynamics. However, some CA also made it possible to conduct formal analysis. The Ising model, put forward in 1924 by Ernst Ising, was developed as an abstract spin system to explain ferromagnetism. Spins with a value of either +1 or −1 are positioned on a one- or two-dimensional lattice. Depending on the strength of the pairwise coupling constant between neighboring spins, Ising's solution yielded ferromagnetic phases, in which spins are aligned in the same direction, or antiferromagnetic phases, in which neighboring spins are antiparallel. The generic model later became the paragon for opinion dynamics, with the positive and negative spins representing opinions. But the insights gained with respect to social phenomena were rather limited. In opinion dynamics, one tends to be interested in the conditions under which consensus is obtained (the ferromagnetic phase) or in how a stable coexistence of opinions is reached.[2] The voter model and other simplified models formalized that type of analysis and extended it to various topologies, including networks. But voters do not vote in those models. Rather, they copy the "opinion" of a randomly chosen spin.

Such models gratified the sociophysicist, but they did not impress the sociologist. Generic modeling approaches that replicate physics insights, such as phase transitions and scaling laws, may reveal a lot about statistical physics but little about social dynamics. Merely using physical metaphors and analogies does not make physics applicable. Noticeable exceptions were obtained only in rare cases in which physicists paid attention to existing social theories. One such example was social impact theory, which was developed by social psychologists in the 1980s to describe how individuals act as sources and targets of social influence. Underlying the theory is the concept of a social force that acts very much like a physical force. Individuals are able to persuade others with opposite opinions and support those with the same opinion, but their influence scales with social distance. When such interactions are simulated, one

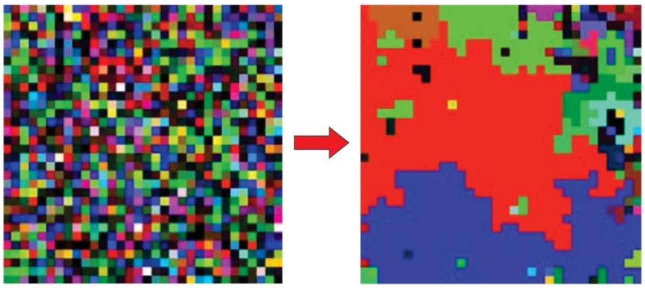


FIGURE 1. CULTURE DYNAMICS. Each agent on a two-dimensional regular lattice is characterized by a vector of features that represents its culture. Features could be cuisine or religion, whose different possibilities—Cantonese, say, or Buddhism—are termed traits. Different cultures are denoted here by different colors. The probability of an agent's interaction with its neighbors increases with the overlap of traits. Agents are therefore more likely to interact if they already share many traits, and this interaction leads agents to become even more similar. Assigning random traits to agents at the start of a simulation (left) leads in most cases to coexisting domains of agents that share the same culture (right). Other simulations lead to monocultures. (See ref. 4.)

still observes the formation of domains with like-minded individuals, but the phenomena are much richer than in Ising-like models.[3]

Another example of the fruitful adoption of a social theory in sociophysics is the model of cultural dissemination, which was originally proposed in 1997 by political scientist Robert Axelrod (see figure 1). Its sociophysics version[4] can be seen as a generalization of opinion dynamics in a Potts model, whose spins can have more than two values. The cultural dissemination model aims to incorporate social mechanisms, such as assimilation (individuals become more similar when they interact) and homophily (individuals interact more often if they are similar).

A different class of sociophysics models came into full swing during the 1970s when concepts of self-organization, the forerunners of today's theories of complex systems, were formalized. Self-organization was seen as a universal concept: What matters for system dynamics is not the system's elements but their dynamic interactions. Consequently, insights into the principles of structure formation in, say, the Belousov–Zhabotinsky reaction and other physicochemical systems can be generalized and extended to biological or social systems. Self-organization theory indeed found applications in sociophysics, mostly as a formal approach to social dynamics.[5] Its applications included migration and opinion dynamics. But, as was typical of its time, it lacked a link to social data.

In the decade 1995–2005, as cheap computing power became available for modest simulations, sociophysics topics burgeoned in the physics community. Then, almost everything was modeled and simulated. Opinion dynamics, marital infidelity, sexual reproduction, the evolution of languages, the emergence of hierarchies—all those phenomena and more received sociophysicists' attention (see references 6 and 7 for overviews). The advantage and disadvantage of those models was their simplicity. For example, in modeling how children acquire language, generative mechanisms—that is, the processes that cause the effect—were assumed rather than justified. The mechanisms' influence and the role of certain feedback processes for the system's dynamics could then be studied without the need to incorporate all details of the problem at hand.

Computational social science

The more recent interest of physicists in socioeconomic problems is driven in part by the availability of so-called Big Data. In the mid 1990s, physicists started to analyze Big Data from financial markets with the same enthusiasm they had in the mid 1980s for Big Data from experiments in high-energy physics. The development of econophysics was the result. In the mid 2000s, physicists became interested in the Big Data available through the internet in general and through online social networks in particular. Much as was the case in econophysics, the early forays were preoccupied by searches for characteristic patterns in the data and universal statistical laws.

That quest in econophysics nicely echoed Quetelet's early attempts to identify statistical laws, and it led to several interesting findings. For example, one aspect of human communication, the time interval between two consecutive messages, turns out to be described by a power-law distribution (see figure 2). The exponent seems to be universal across different communication media. Other examples of universal distributions that were uncovered include votes in elections that use proportional representation and citations of scientific publications.[7]

The findings illustrate what British economist Nicholas Kaldor (1908–86) called "stylized facts"—regularities in the social world that are robust across different observations. Physicists identified dynamic mechanisms that could conceivably reproduce such regularities but did not claim that the mechanisms capture the gist of social interactions. Still, the universality emphasized by physicists provoked economists and sociologists and raised questions about its importance and origin. What does it mean to be human if social phenomena fall into physical universality classes? And what does it mean when they don't?

The current trends in sociophysics are closely related to what is now called computational social science, which denotes a data-driven approach to social phenomena. The data in question manifest what humans do electronically as they use mobile phones, online social networks, search engines, online banking, and so on. Sociology did not ask for that trove of data, which extends the reach of previous empirical analyses by orders of magnitude, nor was it prepared. This generated a void that is now filled by engineers who build and install more sensors and by computer scientists who gather and process ever more massive amounts of data.

Alex Pentland's book *Social Physics*[8] and other recent publications about the topic have little to do with physics and more to do with the analysis of Big Data. In that respect, they share the original intention of Comte's philosophy—to build knowledge on observation and experiment. But instead of understanding the generative mechanisms underlying a phenomenon, the focus of Big Data analysts is on regulating processes such as traffic flow, on developing apps such as Uber that make use of Big Data, and on solving problems such as predicting what customers will order online.

Despite the lack of emphasis on understanding phenomena, recent trends in Big Data have raised hopes for a new kind of social science based entirely on data processing. In 2008 the former physicist and editor-in-chief of *Wired* magazine, Chris Anderson, wrote that "faced with massive data, this approach to science—hypothesize, model, test—is becoming obsolete." What his magazine projected instead was a petabyte age: "Sensors everywhere. Infinite storage. Clouds of processors. Our ability to capture, warehouse, and understand massive amounts of data is changing science. . . . As our collection of facts and figures grows, so will the opportunity to find answers to fundamental questions. Because in the era of Big Data, more isn't just more. More is different."[9]

There's nothing wrong with Anderson's claim that the new science is driven by data and by technology. But the most important ingredients of science are, and always have been, the research questions. Data science may help to answer some fundamental research questions, but it cannot develop such questions by itself. The practice of first collecting data and then seeing what patterns can be extracted will identify new—and mostly spurious—correlations. But it will not lead us to an understanding of causal relationships. In sociology, questions are not just about the how, but also about the why. Thus we need new types of models that embody the "reasoning" that underlies the dynamics of social systems.

Data-driven modeling

Developing such models is not just a technical challenge but also a conceptual one that physics can meet. We physicists can build on the generic understanding of complex systems that we developed in collaboration with researchers in other disciplines. Complex systems consist of a large number of strongly interacting elements, generally denoted as agents. In the tradition of statistical physics, approaches in complex systems aim to predict the collective effects that arise from the agents' interactions. Physicists have contributed both formal methods—for example, stochastic equations to derive a system's macroscopic dynamics—and computational approaches to model such systems. In fact, particle-based simulation methods used in computational physics have much in common with agent-based models developed not only in sociology and economics but also in computer science.

As mentioned above, most sociophysics models of the past aimed at revealing generic insights. The limited complexity of the models did not reflect the complexity of any particular social system. For that reason, they could not be calibrated and validated against real data. Big Data cannot cure the validation problem. We need models that are expressly developed with their calibration and validation against real data in mind.

Another problem, also mostly ignored in previous sociophysics models, pertains to the complexity of the agents themselves. Agents that purport to represent humans can barely be captured by up and down spins. Human decisions reflect personal preferences, social norms, and the influence of others. Accommodating those factors is not just a matter of adding degrees of freedom. Agents in socioeconomic systems are also

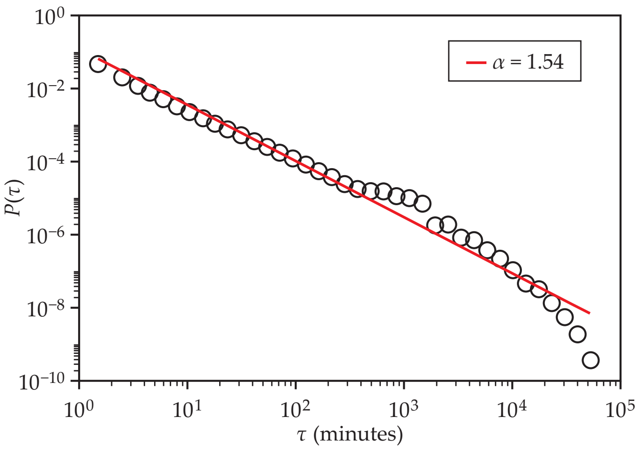


FIGURE 2. HUMAN COMMUNICATION seems to be a scale-free phenomenon. The time lapse between two consecutive messages sent by the same person, also known as the inter-activity time interval, τ, follows a power-law distribution, $P(\tau) \propto \tau^{-\alpha}$ with $\alpha \approx 3/2$.[13] The finding is quite robust no matter what medium analyzed, whether letters, emails, or online chats (shown in the figure). The slight bulge at 10^3 minutes indicates a daily rhythm. (Adapted from A. Garas et al., *Sci. Rep.* **2**, 402, 2012.)

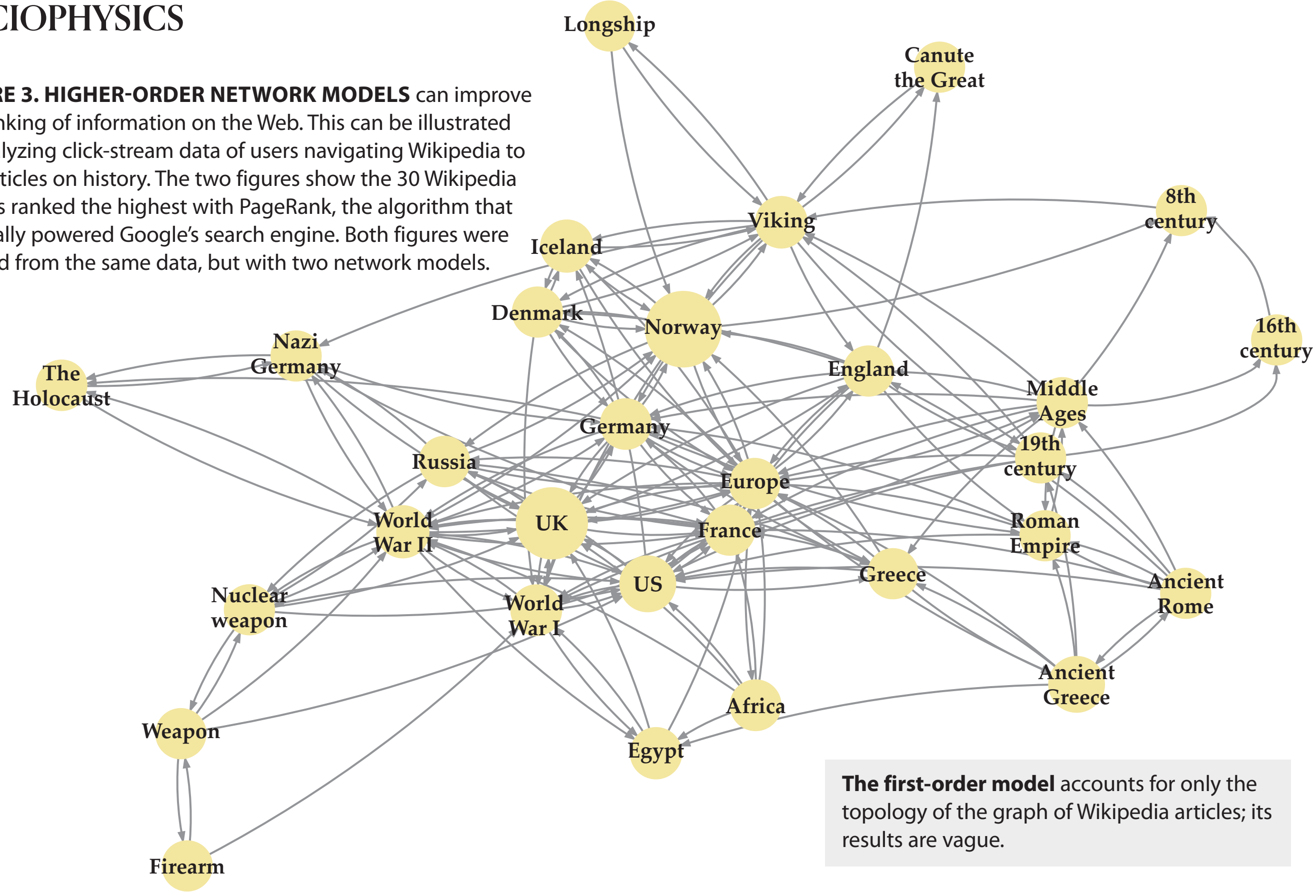
heterogeneous—they vary widely in how they interact under similar situations. They are also adaptive. They respond to incentives and to changes in the system by learning from their experiences. At the same time, they also change the system—for example, by consuming resources or by making innovations. Heterogeneity and adaptivity make the prediction of socioeconomic systems difficult.

Successful sociophysics models tend to have interfaces with both empirical data and social theories. Without the second interface, one may still find interesting phenomena and new results. But how they relate to existing disciplinary knowledge will not be clear, and the findings' impact may be low. The first interface helps to define the problems that the models are designed to solve, most often in terms of new data that need to be explained or even created. Although machine learning approaches can, by themselves, classify the same data and make predictions, they lack the ability to model the underlying generative mechanisms.

Successful sociophysics models also bridge the micro and the macro. That is, they link interacting agents on small, local scales to dynamics on large, system-wide scales—and they do so in a concrete and testable manner. Ideally, such sociophysics models follow principles of data-driven modeling: Agents are modeled according to the standards in the relevant discipline, such as linguistics or anthropology, and the agent-based model admits the calibration of the interaction mechanisms against empirical data. The model is then validated by a quantitative comparison of the simulated system dynamics with observations.

One application of that approach is to pedestrian dynamics.[10] Models of agents take into account social forces between pedestrians, preferred moving directions, and obstacles. The result is a realistic simulation of pedestrians' collective dynamics, which can then be used to simulate escape dynamics in case of a terrorist attack or other panic, or to optimize the design of buildings and streets. Similar models describe biological

FIGURE 3. HIGHER-ORDER NETWORK MODELS can improve the ranking of information on the Web. This can be illustrated by analyzing click-stream data of users navigating Wikipedia to find articles on history. The two figures show the 30 Wikipedia articles ranked the highest with PageRank, the algorithm that originally powered Google's search engine. Both figures were derived from the same data, but with two network models.



The first-order model accounts for only the topology of the graph of Wikipedia articles; its results are vague.

swarming phenomena across different branches of the animal kingdom.

Another example of successful data-driven modeling is forecasting the spread of an epidemic through, say, global aviation traffic.[11] Based on the calibrated model, control strategies for epidemics have been proposed. A third example is the modeling of collective emotional dynamics (see box), for which hypotheses about the emotional interactions of agents have been tested against data. The calibrated model correctly reproduces large-scale emotional influence in various online platforms.

Complex networks

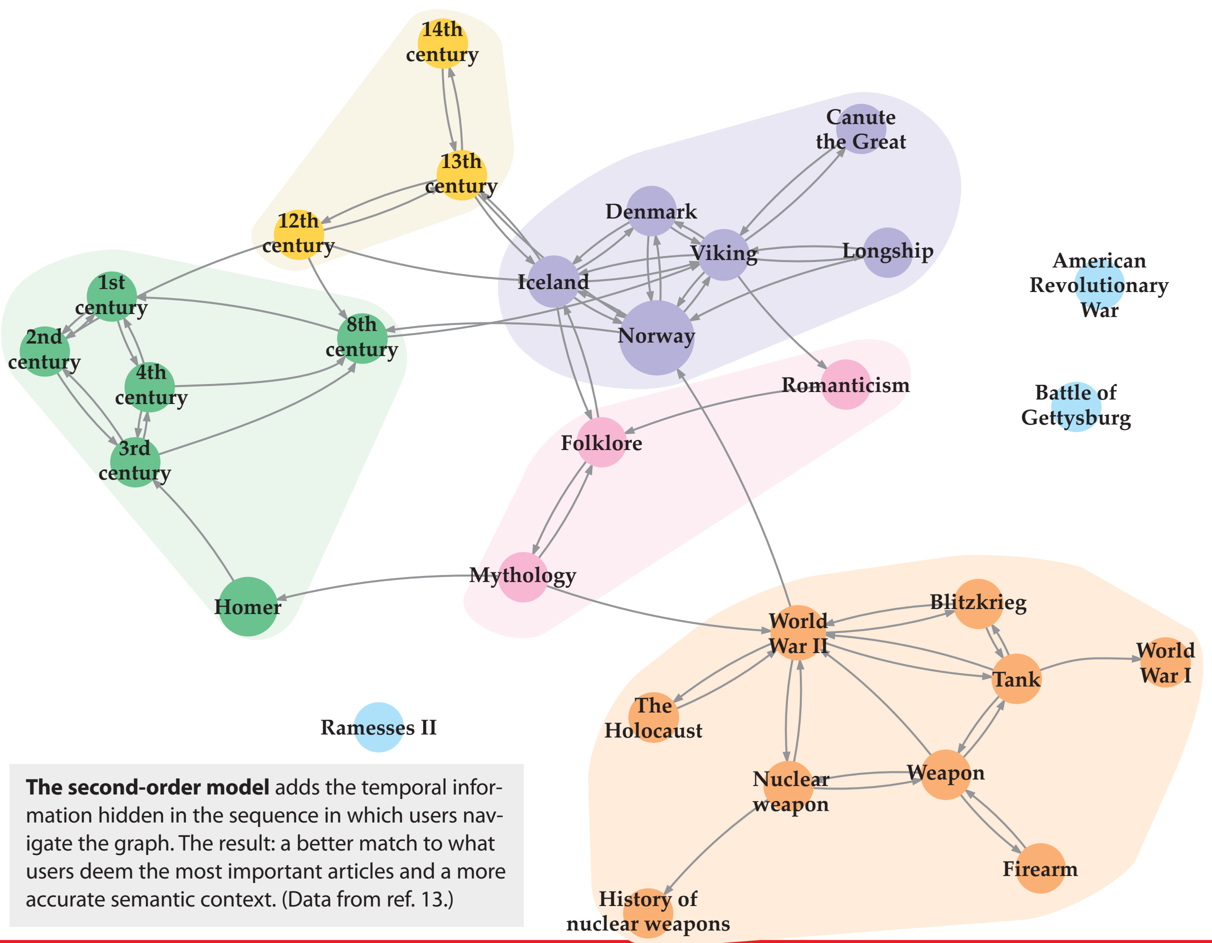
Models of pedestrians, epidemics, and emotional dynamics might seem distant from electromagnetism, thermodynamics, and other branches of physics. Nevertheless, those models, like traditional physics, lead us closer to understanding real-world phenomena—in our case, social phenomena. Although physics concepts may not be generalizable to other disciplines, physics methods can contribute, in a general manner and with great benefit, to system modeling in the social sciences. The methodological contributions are not restricted to interactive systems, of which agent-based models are prominent examples. Rather, they also extend to so-called statistical models that test assumptions about data-generating processes.

Such models belong in the field of machine learning, which became even more important as massive amounts of data became available. Although handling terabytes of data efficiently is a technical challenge, an additional, scientific challenge arises from handling modestly sized but structurally complex data sets because of the relational information they contain. Examples include online social networks of friends and family members, citation networks among scientific papers, and navigation patterns through a patent database and other knowledge repositories. Physicists contribute information-extraction methods that go beyond those provided in computer science or the social sciences. The methods belong to another domain of sociophysics, complex networks, which are now discussed in more detail.

Complex networks are one way to represent complex systems. Agents are represented by nodes, and their interactions by links in the network. Systemic properties are then accounted for by the interaction structure—that is, by the network's topology. Compared with agent-based models, network models have different strengths and weaknesses. The internal dynamics of the network's nodes, the agents, are not explicitly modeled. What's more, all types of interaction are decomposed into binary interactions between two agents. If agents act in groups larger than pairs, the applicability of the approach is limited.

On the other hand, using topology to model complex systems has led to applicable, impactful insights in the social sciences. One example is the small world network,[12] which emerges on a regular lattice topology when some links between a node and its local neighbors are reconnected to distant nodes. The rewiring creates short path lengths (connections between any two nodes) and high clustering coefficients (the links between three neighboring nodes form triangles). Because social scientists had independently discussed similar properties, they could relate their theoretical foundations to an explicit generative mechanism, the rewiring.

Another topological example is Google's PageRank. The algorithm quantifies the importance of a given webpage based on the number and importance of other webpages that link to



The second-order model adds the temporal information hidden in the sequence in which users navigate the graph. The result: a better match to what users deem the most important articles and a more accurate semantic context. (Data from ref. 13.)

it. Formally speaking, the algorithm embodies the solution to an eigenvalue problem, well known in physics, and the importance metric relates to eigenvector centrality. Because of the general nature of the eigenvalue problem, PageRank evaluates websites' relevance based on their interconnections and not on their content.

Such topological analyses require knowledge of the network, which has to be reconstructed from data. By default, the networks are time aggregated. They do not take into account, say, the sequences of other webpages that users visit before they arrive at a given webpage. However, if such temporal correlations are included, the importance ranking changes drastically and context-dependent behavior can be captured (see figure 3). Formally, the temporal conditions are calculated using higher-order Markov models, in which the order represents the persistence of memory in navigation paths. From the Markov models, we can also determine under what conditions temporal correlations can be safely neglected in reconstructing networks. Recent findings in temporal networks have considerably enhanced existing methods to characterize how people navigate Wikipedia and other social-knowledge spaces.

Sociologists have long used social network analysis to characterize the topological position of nodes in static networks. The physics contribution mainly comes with the ensemble approach. As in statistical thermodynamics, such ensembles define what topological configurations are compatible with specific constraints, the likelihood of their occurrence, and expected properties of networks. Using such methods, we can, for instance, identify which node characteristics, such as gender, common friends, and hobbies, influence the formation of links. Such results can be used to form hypotheses about causal mechanisms that social scientists can test in the field.

Beyond disciplinary borders

What are the challenges and barriers to further advance research in sociophysics and computational social science such that all disciplines involved—physics, the social sciences, computer science, and engineering—can benefit?

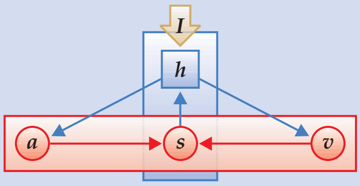
Certainly, there are institutional imperatives. University education has to be developed such that curricula and academic degrees reflect the specialized knowledge needed in sociophysics. Existing curricula in the areas of network science and complex systems can serve as starting points. But sociophysics also needs high-quality journals centered around topics and problems rather than methods and disciplines. Such journals would serve as homes for scientific results that would otherwise fall between disciplinary cracks and fail to gain wide recognition. Hiring and tenure committees should also recognize the value of the extra miles that scientists with a multidisciplinary profile have traveled.

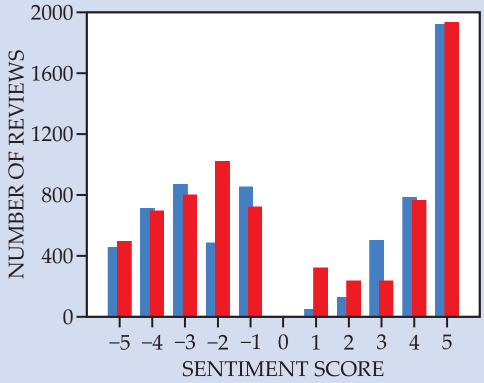
Mutual respect for the different scientific contributions each discipline provides has to be encouraged and developed. A starting point could be the admission that at this time no single discipline has all the tools, methods, theories, and knowledge needed to really understand a realm as complex as human society. Data mining, natural language processing, machine learning, and other applications of artificial intelligence are not currently among the core methods of physics. But they should be welcomed, as they give physicists access to data and to analytics that they would not ordinarily have.

Physicists with a real interest in social phenomena should also acquire a deeper knowledge of the tremendous body of

EMOTIONAL INFLUENCE

When people read reviews of books and other products on Amazon, they can choose to rate the review as helpful or unhelpful. They might also be inspired to write and submit their own review, which, in addition to carrying a rating of 0 to 5 stars, may range in sentiment from damningly negative to gushingly positive. To what extent do Amazon customers influence each other emotionally?





To address that question, my colleague David Garcia and I analyzed 1.8 million anonymized Amazon reviews of 16 670 products.[14] We used a sentiment detector to automatically rate the reviews on a 10-point scale from −5 (highly negative) to +5 (highly positive). Zero was omitted. Then we set ourselves the challenge of reproducing the collective sentiment distributions with a Brownian agent framework.

The framework, depicted schematically on the left, incorporated a well-established psychological model of emotional influence, the circumplex model. The emotional state of an agent is quantified by valence (*v*), which represents the pleasure associated with an emotion and ranges from −5 (highly negative) to +5 (highly positive). Arousal (*a*) represents the activity induced by the emotion, such as purchase or rating a review. When *a* exceeds a threshold, the agents express themselves with a level of sentiment (*s*). Agents transmit and receive emotional information (*h*) through social media and other means, and they are subject to external emotional influences (*I*) such as coverage of products in mainstream media.

The graph on the right shows the result of running the model on one product, the book *Harry Potter and the Deathly Hallows* (2007). The blue bars are the real sentiment values for the reviews. The red values are the agent-based simulation. Our study reveals, among other things, that individual reviewers are indeed influenced by other people.

work that the social sciences have accumulated. Indeed, the lack of awareness and of understanding of their work is one of the major criticisms raised by social scientists when confronted with the papers of sociophysicists. For their part, sociologists should recognize, much more than they have in the past, their need to collaborate with researchers in other disciplines, in order to make computational science a social one. Their aversion to stylized facts and universal distributions could be overcome by formal models, jointly developed, that explain such findings based on disciplinary theories.

And realistic expectations about multidisciplinary collaboration should be established before a collaboration gets under way. It's naïve to assume that scientists from different disciplines simply fill each others' knowledge gaps to then jointly create results that define the state of the art in their area of collaboration. Success is never guaranteed, and many collaborations ultimately fail because of barriers between their scientific languages, differences in their scientific cultures, and disagreements about where to publish and publicize results. Fostering multidisciplinary collaborations should involve raising awareness of the inevitable hurdles.

Individual scientists should also be realistic in their expectations. Confronted with the challenge of turning from a method-driven to a problem-driven perspective, many sociophysicists eventually find out that their true motivation lies in physics-based methods rather than in social phenomena or data processing. As a result, the potential sociophysicist might withdraw from making the upfront investment to gather the requisite knowledge from social science and computer science. That effort comes with considerable risk of not being rewarded by social scientists, physicists, or institutions. An informed decision is paramount.

Those willing to make the effort, however, can be motivated and guided by the increasing number of successful applications in sociophysics. They can draw inspiration from fascinating findings, sophisticated methods, and real-world problems. And they can contribute to the foundations of computational social science, which are still being laid.

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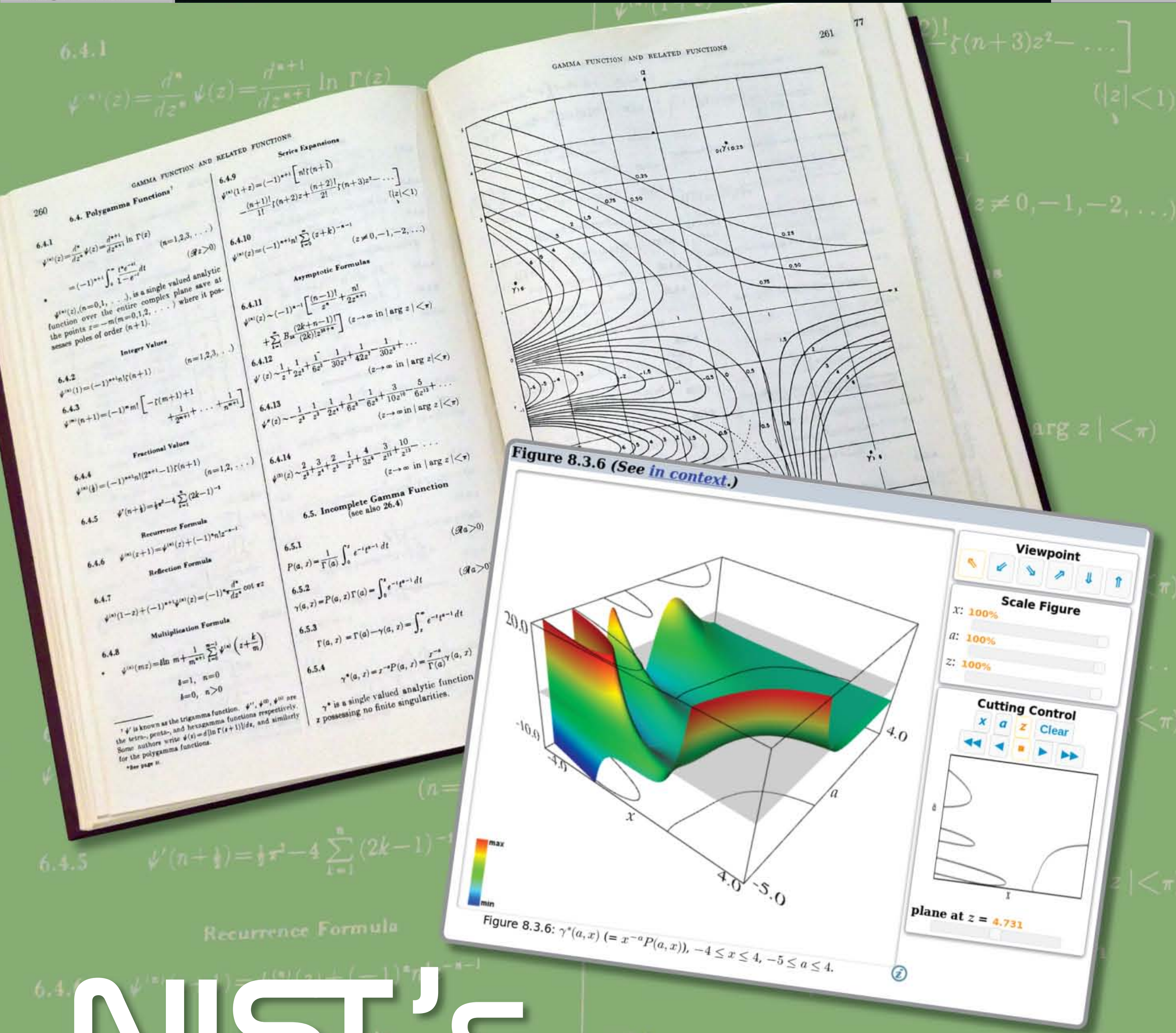
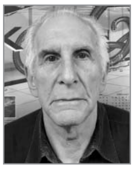


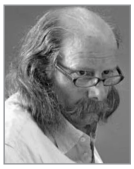
NIST's Digital Library of Mathematical Functions

Barry I. Schneider, Bruce R. Miller, and Bonita V. Saunders

The half-century-old handbook commonly known as *Abramowitz and Stegun* enters the 21st century.

Barry Schneider, **Bruce Miller**, and **Bonita Saunders** are scientists in the applied and computational mathematics division at the National Institute of Standards and Technology in Gaithersburg, Maryland. They are part of a team responsible for the design, expansion, and maintenance of NIST's *Digital Library of Mathematical Functions*. They welcome any comments or corrections to the *DLMF* at dlmf-feedback@nist.gov.





Several years ago, I was invited to contemplate being marooned on the proverbial desert island. What book would I most wish to have there, in addition to the Bible and the complete works of Shakespeare? My immediate answer was: A&S [Abramowitz and Stegun].

—Michael Berry, "Why are special functions special?" PHYSICS TODAY, April 2001, page 11

The information technology revolution is creeping into all aspects of our lives. Today more of us rely on digital information for personal and professional purposes than ever before. It is so much easier to search the Web to locate that information or to purchase the widget of one's desire than to go to a library or a retail store. And for scientists, journal articles and books are far easier to access online than anywhere else. Although there are many examples of online scientific material that go beyond their print equivalents—for instance, specialty dictionaries, encyclopedias, and millions of journal articles—the power of the Web to transcend the printed page is still in its infancy.

One classic scientific reference that the revolution has radically affected is the *Handbook of Mathematical Functions*, familiarly known as *A&S*, edited by Milton Abramowitz and Irene Stegun.[1] In this article we discuss how *A&S* was transformed into an online 21st-century resource known as the *Digital Library of Mathematical Functions*, or *DLMF*, and how that new, modern resource makes far more information available to users in ways that are quite different from the past. The *DLMF* also contains far more material—in many cases updated—than does *A&S*. (For a brief history of the evolution of *A&S* to the *DLMF*, see box 1.)

To set the stage for what follows—and to provide practical context for appreciating the utility of the *DLMF* for research and education—consider this hypothetical situation. Many years ago a researcher—let's call him Bill—was working on finding solutions to the radial Schrödinger equation for the attractive and repulsive Coulomb potential in terms of a set of square-integrable orthogonal functions. He had previously shown that it was indeed possible to expand the solutions in some complete, discrete set of functions and to relate the expansion coefficients to some set of orthogonal polynomials. For the Coulomb potential, the expansion coefficients satisfy a three-term recursion relationship described by so-called Pollaczek polynomials. When *A&S* was written, little was known about those polynomials, and Bill had to work out their properties largely on his own or with colleagues.

When Bill recently decided to generalize his older results to physical parameters not part of the original work, he found, much to his surprise and delight, that the *DLMF* has a much more extensive and up-to-date treatment of many special functions, orthogonal polynomials included, and treats the Pollaczek polynomials in some detail. Had that information been accessible when Bill first began the project, his work would have been significantly easier. Bill also found many useful references and notes in the metadata that are listed in the *DLMF*'s "info boxes." He is now actively extending the earlier research to the physically important ranges of the nuclear charge and energies for the attractive Coulomb potential.

Not your thesis adviser's handbook

Once you broaden your perspective of "a book on the Web" to include potentially much more than the adaptation of a traditionally printed book for a computer screen and embrace it as a full-fledged electronic resource on the internet, the power of hypertext and the vast computational capabilities of the Web open a rich tableau of possibilities for enhancing the book's content, utility, and ease of use. For the developer, that abundance can be frustrating, as there are so many choices and possibilities to explore; moreover, the Web's evolution takes place in fits and starts, with promising technologies sometimes stalling and at other times becoming suddenly essential.

Yet the traditional handbook has virtues, such as conciseness, stability, and permanence, that are worth preserving in a Web-based resource. By adopting an enriched authoring markup language for the source documents and by leveraging hypertext links, we and other *DLMF* developers have been able

BOX 1. ABRAMOWITZ AND STEGUN AND THE *DLMF* PROJECT

In 1964 the National Bureau of Standards (NBS) published the *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables,*[1] edited by Milton Abramowitz and Irene Stegun, as volume 55 of its *Applied Mathematics Series*. Originally intended as a compendium of numerical tables for evaluating the special functions—including gamma, Legendre, Jacobian, Bessel, and more than a hundred other functions commonly used in applied mathematics—it was augmented with selected properties and identities to make the tables easier to use. Ironically, that additional material was what led to the handbook's long-term popularity. Fondly referred to as *Abramowitz and Stegun*, and even simply *A&S*, it became the most widely distributed and cited NBS publication in the first 100 years of the institution's existence.

At a hefty 1046 pages, the handbook did more than concisely provide critically useful mathematical data. It served to standardize definitions and notations for special functions. Both services were at the heart of NBS's mission. And yet by the late 1990s, *A&S* was showing its age and was due for more than a simple update with errata. Important advances in the special functions had taken place: More properties of many functions had been discovered, and advances in applied mathematics had considerably enlarged the field to include many new and useful functions.

The advent of the Web had also opened unique opportunities for publishing. In 1998 NIST (the name NBS had adopted a decade earlier) initiated an effort to assemble the available information on the current state of the special functions into a freely accessible online resource that would take advantage of the then relatively new potential of the Web. Over the ensuing decade, with the generous sponsorship of NSF's Knowledge and Distributed Intelligence Initiative and with continuing internal support from NIST, 29 experts in the various special functions were contracted to write material for the new handbook.

Whereas roughly half of *A&S* had consisted of numerical tables, the revision would have none. Instead, the amount of mathematical content doubled. New chapters on Lamé, Heun, and Painlevé functions were included; so were integrals with coalescing saddles. The result was 36 chapters long (compared with 29 in *A&S*) and boasted a more extensive bibliography. Since it was a handbook, mathematical proofs were not included, but great care was taken to clarify any constraints on the validity of all formulas and to reference their original sources. Significantly more graphs and visualizations were also included. In 2010, after 11 years of dedicated effort, the enhanced online resource was released as the *Digital Library of Mathematical Functions* at https://dlmf.nist.gov. The printed companion handbook was published as the *NIST Handbook of Mathematical Functions*.[7]

to layer the presentation of information. For users interested in browsing, we strove to preserve the book's concise, telegraphic style, which emphasizes the essential, selected properties of the functions. Most users will find the information they need simply by scanning the relevant sections. When that is insufficient, they can turn to our search engine.

Once our friend Bill realized that Pollaczek polynomials were relevant to his problem, for instance, he searched for "pollaczek recurrence" to locate the specific relation he needed. That's fine as far as it goes, but in a context so full of mathematical formulas and bereft of text, the usual text search is insufficient; the search cries out for a math-aware search engine. Our search tool[2] recognizes not only mathematical notations but also the semantics of the symbols as well. Thus, as exemplified in box 2, the proper and common names of functions or their classifications can be used as search terms.

For researchers interested in digging a bit deeper, an additional layer of information reveals the symbols used, the sources of the material, cross-references, and so forth. The mathematical symbols themselves are linked to their definitions to reduce ambiguities of notation. The selective nature of a handbook virtually guarantees that not every useful relation will be presented. But by providing the specific source of each equation, the methods by which it can be derived, and other relevant expository annotations, the *DLMF* offers a researcher alternative sources of information or guidance on how to derive what she needs for her application.

What kind of enriched markup can enable those features? Most mathematicians prefer to write using LaTeX, a powerful, expressive markup system that provides high-quality typesetting, particularly for mathematics. That the system is extensible—armed with tools developers can use to define new descriptive terms and shorthands as needed—makes it notoriously difficult to convert to HTML for the Web. And yet that is exactly its strength for the *DLMF*. A system of semantic macros for many mathematical functions and concepts ensures that the functions and concepts retain their underlying meaning.

Converting that enriched LaTeX markup into an intermediate XML representation allows for the layering of information to capture a surface presentation of the functions for users and yet still provide them with access to a database that can be mined for additional details about the functions and their connections to other, related mathematics. Those extra details, or metadata, are what we use to link symbols to their definitions and to populate indices, notation lists, and info boxes. Because the tools needed for that job are not available off the shelf, we created a system called LaTeXML (see http://dlmf.nist.gov/LaTeXML), which converts the author's LaTeX into XML and thence into HTML and the mathematical markup language MathML. Box 2 illustrates the benefits of that approach.

The stability of a traditional handbook is maintained by securing, across updates and even new editions of the *DLMF*, the connection between equations, their reference numbers (such as equation 14.3.6 in box 2), and permanent URLs (so-called permalinks, such as http://dlmf.nist.gov/14.3.E6 in box 2), so that the *DLMF* can be used as a resource for decades to come. The permalinks, moreover, provide a convenient way for researchers to exchange information from the *DLMF*.

Behind the plots

The graphs and visualizations in the *DLMF* are hidden gems, often overlooked as researchers peruse the website. A re-

BOX 2. A MATH-AWARE SEARCH ENGINE AND LAYERED INFORMATION

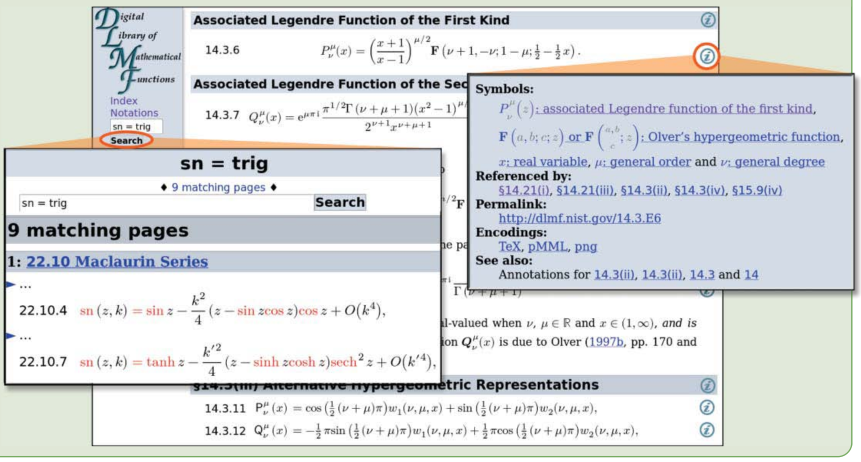
NIST's *Digital Library of Mathematical Functions* (*DLMF*) has a sophisticated search engine. Like other search engines, it can retrieve information using textual terms, but it also recognizes queries phrased as math operators, symbols, or conventional LaTeX commands. The latter are then matched against mathematical expressions in the *DLMF*.

Moreover, the search engine recognizes the meaning of the symbols. For example, both "*J*" and "Bessel" match the Bessel function J_ν. The figure's left inset shows the result of searching for the Jacobian elliptic function sn(z, k) in terms of trigonometric functions. While the "sn" matches the appropriate elliptic function, the term "trig" or "trigonometric" matches any trigonometric function, such as sine, cosine, or hyperbolic tangent. One benefit of such technologies as the mathematical markup language MathML is that the search engine can highlight the portions of formulas that match the query terms and provide some reassuring feedback to users.

On any given webpage of the *DLMF*, there's more than meets the eye. Hovering over or clicking on the information icon ⓘ next to a formula reveals a variety of metadata (right inset)—data about the data—associated with the formula. In this case, the metadata include listings of defined symbols, links to original sources, cross-references, and alternative formats, such as TeX code, MathML, and images.

The permalink gives the permanent URL for the formula; here it indicates that 14.3.E6 will always refer to this formula, independent of errata, updates, or future editions of the *DLMF*. Other metadata include any relevant keywords, links to *A&S*, notes on the formula's derivation, and any other annotations, classifications, or errata.

In addition to the list of symbols shown in the info boxes, individual symbols in the formula hyperlink to their definitions in the *DLMF*—another benefit of MathML. Clicking on a symbol will clarify and disambiguate it from similar-appearing notations. One must, as the saying goes, know one's *P*s and *Q*s, as there are several distinct functions denoted by each.



searcher can use many strategies to gain insight into a function that describes physical phenomena. She might study its differential equation, compute its zeros using Newton-type methods or asymptotic expansions, or use some other numerical and analytical technique to examine the function. However, an accurate graphical representation can provide that aha moment or quickly send her back for more analysis or computation when the plot differs from what is expected. Indeed, our own plots of the complex zeros of Bessel functions of positive integer order alerted us to inaccuracies in diagrams published in Frank Olver's 1954 asymptotic expansion paper[3] and repeated in *A&S*. The new plots showed that the arrangement of zeros needed to be moved to the opposite side of their asymptotes (see http://dlmf.nist.gov/10.21.ix).

As technology has evolved for viewing graphics on the Web, so has our development of graphics for the *DLMF*. That evolution made it possible to replace the static graphs in the original handbook with close to 600 2D and 3D figures, including 200 that can be interactively rendered by users as 3D visualizations. The clarity and responsiveness of the visualizations are a product of so-called WebGL-based technology[4] and our own careful attention to plot and data accuracy. The JavaScript-enabled WebGL application programming interface (API) provides portability and allows users to view the visualizations in major Web browsers without downloading a 3D graphics plug-in.

We achieved plot accuracy—that is, accurate graphical representation of function features—by designing computational grids, or meshes, that effectively capture key function attributes, such as zeros, poles, and branch cuts.[5] To tackle the issue of data accuracy, we computed function values using at least two different methods, with codes from reliable repositories, from standard computer algebra packages, or even from *DLMF* chapter authors. We resolved any discrepancies through discussions with the chapter author and a close examination of function definitions and properties.

Although illustrative diagrams and graphs appear throughout the *DLMF*, most figures that represent function curves or surfaces can be specifically found in the graphics sections of each chapter. Clicking on a static 3D image opens a page with an array of interactive options that allow users to rotate, scale, zoom, or otherwise manipulate the graphs. Figures 1, 2, and 3 exemplify some of the capabilities.

The future of the *DLMF*

NIST is committed to the *DLMF*'s long-term maintenance and further development, both in the evolution of its mathematical content and in its presentation on the Web. We issue quarterly updates, including errata, corrections, and clarifications. As we track the evolving Web technologies—for example, HTML5, MathML, and WebGL—and different usage patterns, we add new features and capabilities. Over time, we plan to make the site increasingly accessible and to add support for mobile devices.

Occasionally, new material becomes relevant to applications and is added to the website. A revision of the chapters on orthogonal polynomials and Painlevé transcendents is under way, and a completely new chapter on orthogonal polynomials of several variables is in progress. We also continue to improve the metadata associated with functions. The metadata are now presented in human-readable form, but we are exploring ontologies to recast the data in machine-readable forms, an advance that will strengthen and extend our search engine's

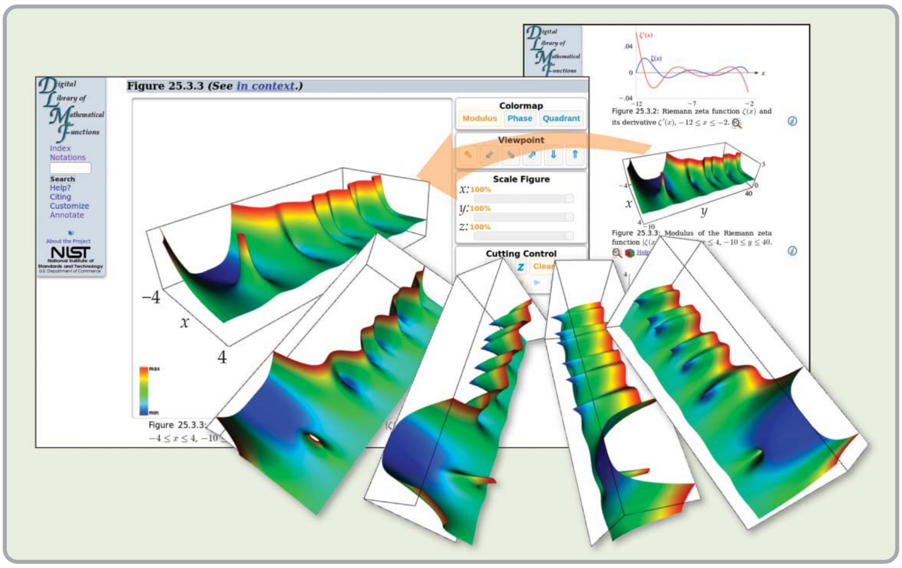


FIGURE 1. INTERACTIVE VISUALIZATIONS in the *Digital Library of Mathematical Functions* (*DLMF*). The complex shape of the modulus of the Riemann zeta function $|\zeta(x + iy)|$, an important function in number theory, quantum field theory, and other areas of mathematics and physics, illustrates the difficulty in displaying key features of a function surface with a single static image. The *DLMF* allows users to rotate a function surface in any direction and manipulate it with other tools to explore it. Clicking on the static image of the Riemann zeta function in one webpage (top right) opens a new page (top left) containing an embedded figure with control side panels. The original static image shows the simple pole at $x = 1$, $y = 0$, but obscures the nontrivial zeros on the critical line at $x = 0.5$, where the Riemann hypothesis asserts they lie. Such visualizations were designed using WebGL-based technology, which lets one view the graphics on different platforms without downloading a special browser plug-in.[4] (Adapted from *DLMF* screenshots. See chapter 25, "Zeta and Related Functions," for more information.)

capabilities and improve the ability of other, external search engines to mine features and data in the *DLMF*. In our first efforts we used MathML technology (more specifically, Presentation MathML) to represent the mathematical formulas for display in browsers. But our longer-term goal is to use Content MathML to encode representations that could be exported to applications for direct use in computations and that could further improve accessibility.

Several spin-off projects have also begun. The motivation for one—the *DLMF* Standard Reference Tables on Demand Project—is described succinctly by the feedback we received from a user in September 2016:

> It is no longer useful to include large tables of function values for the purpose of interpolation. But a set of test values for each function with various decimal precisions would be useful for developers as they try to test implementations of special functions. This could be the beginning of a benchmark for numeric software. —E. Smith-Rowland

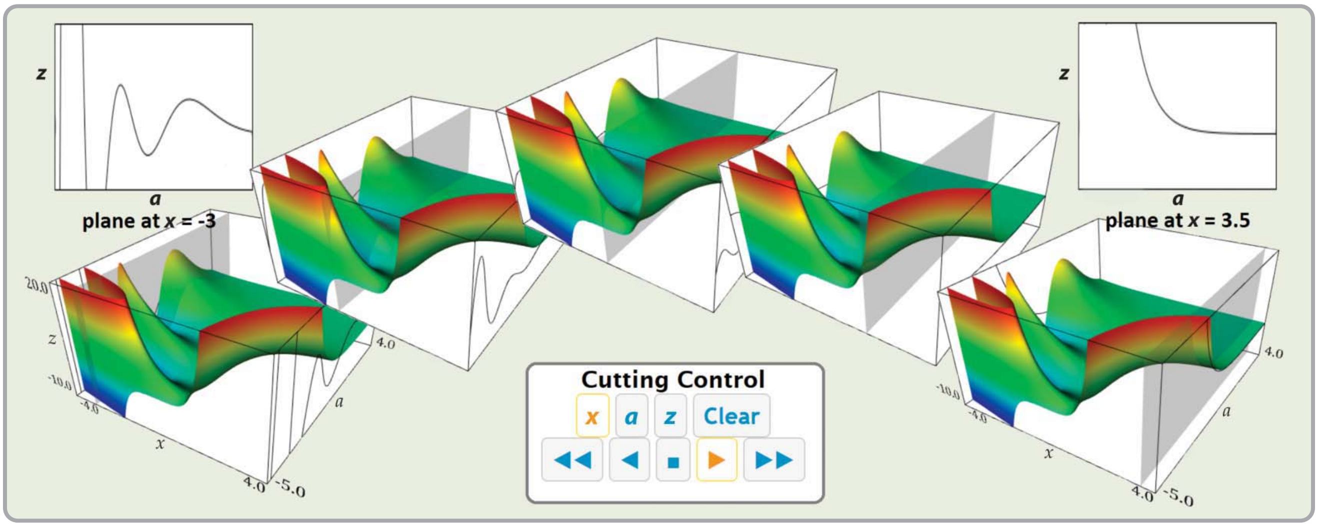


FIGURE 2. CUTTING THROUGH A SURFACE. One of the visualization options offered in the *Digital Library of Mathematical Functions* (*DLMF*) is cutting-plane control. Observing how a plane intersects a function surface can provide users with a unique perspective. These images show a cutting plane moving in the *x*-direction through a surface that represents the incomplete gamma function $\gamma^*(a, x)$. The two-dimensional curves that mark the intersection of the plane with the surface are projected onto opposite ends of each bounding box and displayed in a pop-up window. Users can manipulate standard media controls to create an animation or manually move the plane using a slider bar. In the case of figure 1's Riemann zeta function surface, a view of nontrivial zeros is revealed by cutting the surface with a plane at $x = 0.5$. (Adapted from *DLMF* screenshots. See chapter 8, "The Incomplete Gamma and Related Functions," for more information.)

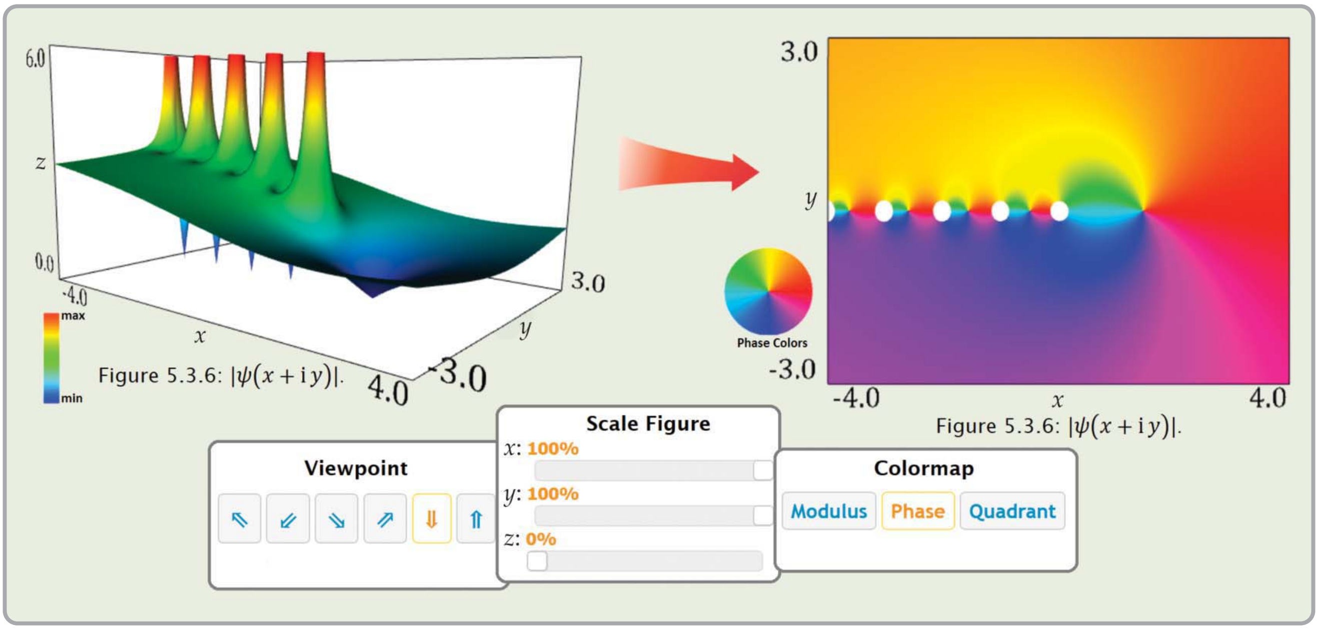


FIGURE 3. CREATING A PHASE DENSITY PLOT. One may use interactive control options to produce graphical displays that reveal significant features of a function. One display (left) represents the modulus of the complex digamma function $\psi(x + iy) = \Gamma'(x + iy)/\Gamma(x + iy)$, where Γ denotes the complex gamma function. Users can construct a phase density plot (right) of ψ by setting the controls as shown: phase colormap, top view, z scaled to zero. Like the gamma function, the ψ function has simple poles (seen as circular holes) at the nonpositive integers along $y = 0$. The phase changes by 2π radians as one completely circles any of those poles. Circling the zeros between those poles in the opposite direction yields the same 2π phase change. The phase-reversal pattern between successive poles and zeros is analogous to that of a fluid flow produced by a semi-infinite line of vortices with alternating directions of flow. (Adapted from screenshots of the *Digital Library of Mathematical Functions*.)

Our eventual goal is an online testing service, by which users can generate high-precision tables of special-function values with certified error bounds that can be compared with their own uploaded function data. A collaborative effort between the NIST applied and computational mathematics division and the University of Antwerp computational mathematics research group has already produced a fully operational beta version of the site. It's publicly available at http://dlmftables.uantwerpen.be.

Yet another project is the Digital Repository of Mathematical Formulae (DRMF), a wiki-based compendium of formulas for orthogonal polynomials and special functions to promote interaction in the OPSF community. The *DRMF* will be expandable but moderated, so that new formulas from the literature can be added to it after they have been reviewed. To create a solid foundation, the wiki is being seeded with formula data from the library and other sources, which require the extension and development of various format-conversion processors.[6]

Come explore!

With the *Digital Library of Mathematical Functions*, NIST has attempted to preserve the best attributes of *A&S*, while adapting them to the tools and technologies of the Web. It is a vibrant and evolving product that draws on new knowledge of special functions discovered since 1964 and corrects and expands the older material in the handbook. A group of associate editors who are experts in various special functions provide continuing advice on individual chapters, and a group of senior associate editors provide overall advice to the project.

We invite readers to explore the library: Hover the mouse over intriguing objects, symbols, and graphics to see behind the scenes. Open the info boxes to see what other possibly useful data may be available. We believe that the library will prove as useful to scientists and engineers of today and tomorrow as *A&S* has been since 1964.

We appreciate the helpful comments and suggestions of Eric Shirley (NIST) and William Reinhardt (University of Washington). We also acknowledge the efforts of the more than 50 authors, validators, editors, and developers of the DLMF. *A complete list of them is at http://dlmf.nist.gov/about/staff.*

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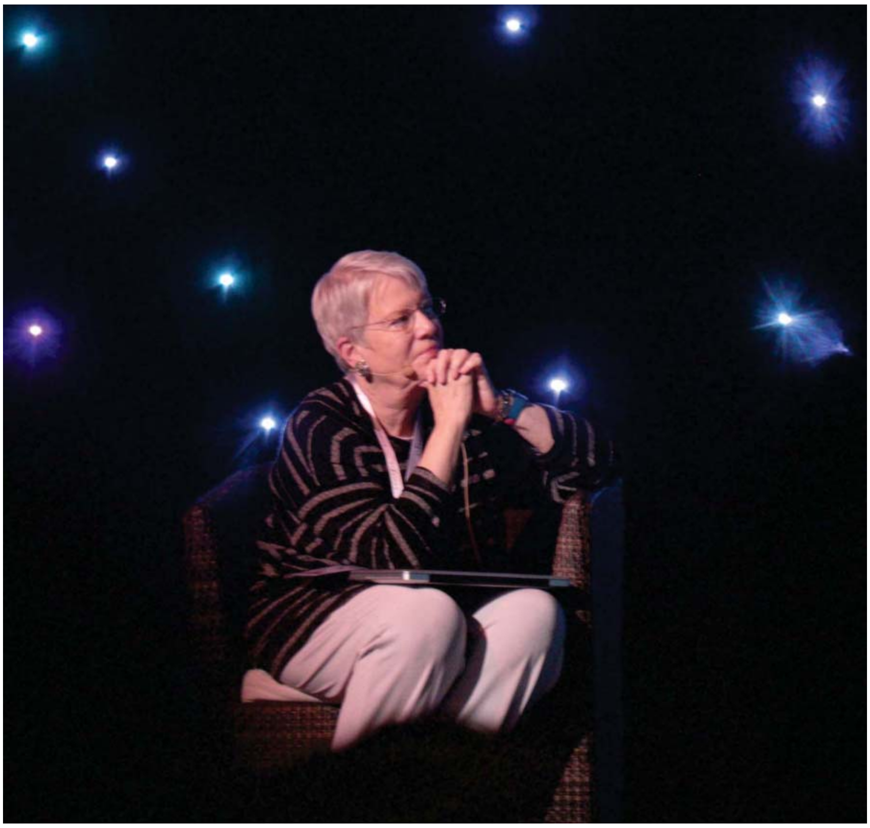
BOOKS



WIKIMEDIA COMMONS VICTOR R. RUIZ

Jill Tarter, role model and SETI pioneer

Capturing science as a human endeavor is at the core of *Making Contact: Jill Tarter and the Search for Extraterrestrial Intelligence*. Sarah Scoles's biography deftly and entertainingly tells the story of groundbreaking scientist Jill Tarter, whose work has been pivotal to SETI.

Tarter is no stranger to battles. She was the first woman to receive a degree in engineering from Cornell University, where she completed her bachelor's in 1965. *Making Contact* astutely highlights the nuances and challenges of being a female scientist at that time, a heroic achievement in itself. Tarter's role in inspiring new generations of women to join the ranks of scientists, engineers, and mathematicians is significant. Scoles, an accomplished science writer, acknowledges that Tarter is a personal hero who inspired her own career in science, and countless other women have pointed to Tarter as a role model.

Making Contact
Jill Tarter and the Search for Extraterrestrial Intelligence
Sarah Scoles
Pegasus Books, 2017. $27.95

But Tarter's significance is not just about her success as a woman in science. Occasionally a remarkable scientific mind demonstrates insight beyond that of the collective consciousness and is able to push both scientists and the public in new directions. In my view, Tarter is such a person. Despite widespread public skepticism about the project, SETI is important for humankind. As Scoles puts it, "SETI holds up a mirror, showing us how we look from a cosmic perspective." Tarter has made it her life's pursuit to prepare us—not just scientifically but emotionally—for the answer to whether we are alone.

Making Contact tells the story of Tarter's ambition and interminable curiosity and of her fortuitous stumble into the new field of SETI in 1969 during her second year of graduate school at the University of California, Berkeley. A trained engineer and radio astronomer, Tarter found she was not fulfilled by traditional research. She was, however, hooked when she learned of the work of early SETI scientists, and she became determined to pursue a scientifically rigorous investigation into the possibility of alien life.

Scoles skillfully weaves explanations of the science behind SETI into the story of Tarter's life. Her witty style leavens the potentially dry engineering and astrophysics discussions to create a text that will engage both amateur science enthusiasts and the most seasoned physicists. Readers learn about the fundamental principles to consider when looking for life in the universe and how scientists might communicate over vast interstellar distances with today's technology. They also hear about Tarter's first pivotal meetings with Carl Sagan, foreshadowing her role as the inspiration for the protagonist in Sagan's beloved novel *Contact* (1985). The book, and the 1997 film adaptation starring Jodie Foster, made Tarter a scientific star across the globe.

On more than one occasion, Tarter found herself at the center of congressional ideological and budget crosshairs. Readers learn of SETI researchers' head-on collision with the political establishment and follow their fight to save the federal funding line for SETI investigations. After Congress cut off SETI funding in the 1990s, Tarter and her colleagues navigated the waters of private philanthropic financing, a voyage that ultimately led to the launch of the SETI Institute. That tale will seem all too familiar to researchers facing battles over funding today, and such stories are important to document because they show how budget debates can fundamentally alter our collective scientific pursuit.

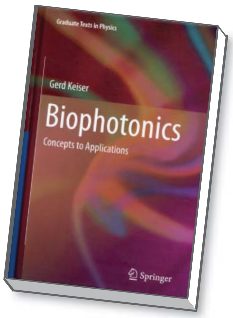
Although Scoles does not provide a historical account of SETI's origins or future direction, she does present important episodes in SETI's history through the lens of Tarter's experience. Those include the launch of second-generation SETI searches with Project Phoenix, in which the Parkes Observatory telescope in Australia and the Robert C. Byrd Green Bank Telescope in West Virginia were used to search millions of frequencies for advanced extraterrestrial signatures. Scoles also discusses Tarter's grandest SETI ambition: the Allen Telescope Array. She doesn't shy away from describing the intricate details of the project and the tumultuous financial and experimental road that finally led to commissioning tests and initial observations in 2007.

Scoles also highlights connections between SETI's fascinating research and the broader interdisciplinary science of astrobiology. She stresses that we now know that the universe is teeming with potentially life-supporting planets. That truth, she continues, only bolsters Tarter's determination to find other civilizations in the universe.

Jill Tarter's life is now woven into the arc of SETI history and will be reflected on for years to come. Her story reminds us to keep pursuing answers to pivotal scientific questions, regardless of the ideological barriers. Tarter's life's work has made us better prepared to continue the search for extraterrestrial life and better prepared for actual cosmic contact.

Shelley Wright
University of California, San Diego

Biophysical optics in a single voice



Biophotonics
Concepts to Applications
Gerd Keiser
Springer, 2016.
$99.99

Biophotonics, or biomedical optics, is a rapidly growing interdisciplinary field. Its research encompasses optical imaging, spectroscopy, and therapeutics of biological materials ranging in size from subcellular scales to organ systems. Its applications include cancer detection and diagnosis, noninvasive tissue biopsy, functional brain monitoring, image-guided surgery, light-based therapeutics, and microscopies of many types targeting biomarkers in cells and tissues. *Biophotonics: Concepts to Applications*, a new volume by Gerd Keiser, aims to serve as a course textbook for advanced undergraduate and graduate students and to be a working reference for biomedical and biophysical researchers.

Presently, most books covering biomedical optics are edited volumes with chapters on different topics written by different authors. Comparatively few textbooks have been written in a single voice about the whole field. In my view, we need more single-author books, and I enjoyed working through Keiser's text.

The 11 chapters of *Biophotonics* systematically take the reader from underlying concepts about light, including the basic optical techniques needed for most biomedical measurements, to a discussion of light–tissue interactions that carefully builds from basic physics to therapeutics. The early sections set up a series of chapters about increasingly modern advances, including fluorescence techniques, photon correlation spectroscopy, optical coherence tomography and microscopy, linear and nonlinear spectroscopy, interferometry, and optical trapping. In total, the material is covered in less than 350 pages.

Some of the book's sections are more successful than others, which is not surprising given its ambitious scope. I found the three chapters on optical fibers, light sources, and optical detectors to be a strength. These tools are important to the field, and the author guides the reader step-by-step through a

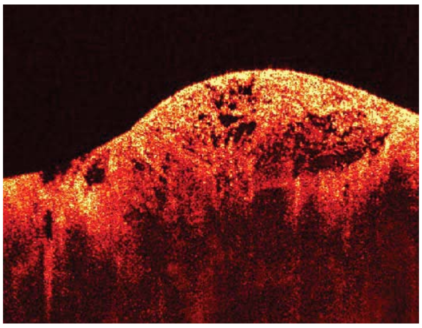


IMAGE OF A SARCOMA, or muscle tumor, obtained using optical coherence tomography. (Wikimedia Commons, courtesy of Dr Stephen Boppart, Biophotonics Imaging Laboratory, UIUC.)

plethora of devices of increasing complexity. Light collection and detection methods and signal-to-noise in the detection process are well explained, and the systematic description of light sources (with extensive and useful references) and their characteristic features is excellent.

Throughout, Keiser introduces and explains useful formulas and then cements the discussion by working out sample problems. I found the worked examples to be very helpful. The chapter on light–tissue interactions provides essential results compactly and has an interesting subsection on interaction mechanisms. The remaining chapters teach new material and provide the interested reader with valuable references for further exploration. However, in my view those chapters would have benefited from more extensive discussions of diffuse optical spectroscopy and tomography and of functional near-IR spectroscopy, which are especially important for probing deep tissues such as brain, breast, and muscle.

Biophotonics is a good textbook and will undoubtedly be a valuable lecture supplement in an advanced undergraduate or graduate-level course. However, because the text covers so much in so few pages, it sometimes lacks the rigor I prefer. Courses in biomedical optics are challenging to teach because the students typically come from multiple fields and have different scientific and mathematical backgrounds. Therefore, I tend to rely on texts with comprehensive discussions of fewer topics. For example, I have found the recent textbook *Quantitative Biomedical Optics: Theory, Methods, and Applications* by Irving Bigio and Sergio Fantini (2016) particularly well-suited for such courses; another older but still excellent text is *Biomedical Optics: Principles and Imaging* by Lihong Wang and Hsin-i Wu (2007).

On the other hand, scientists, engineers, technicians, and clinicians working in the biomedical optics community will find that *Biophotonics* offers quick, quantitative insight into many important topics, especially in connection with light sources, light detection, light guiding, and light–tissue interactions. In all the book's chapters, the material is pertinent and is presented clearly enough to provide a springboard for further study. Researchers will appreciate its reasonably complete and up-to-date accounting of state-of-the-art biomedical optics techniques and applications.

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University of Pennsylvania
Philadelphia

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Field theory with French flair

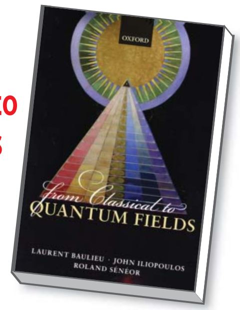
Since Denis Diderot's 1772 *Encyclopédie*, French textbooks have often been characterized by a wealth of topics. Examples that many physics students have encountered include classics such as Albert Messiah's *Quantum Mechanics* (1961) and the two-volume *Quantum Mechanics* (1977) by Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloë. Now a new French book stands out with its wide range: *From Classical to Quantum Fields* by Laurent Baulieu, John Iliopoulos, and the late Roland Sénéor.

This 992-page book takes the reader on a theorist-guided journey into the standard model of particle physics. The trip begins with a lengthy review of concepts in classical physics. From there, the authors proceed to the main attraction and explore our current understanding of fundamental interactions; they then lead the reader all the way to the uncertain terrain of physics beyond the standard model. *From Classical to Quantum Fields* has a distinctly French feeling, as it pays particular attention to the mathematical aspects of its topics. The authors successfully present the mathematical structures underlying quantum field theory without sacrificing the clarity and fluidity of the exposition. On the other hand, extensive physical applications are sparse.

From Classical to Quantum Fields

Laurent Baulieu, John Iliopoulos, and Roland Sénéor

Oxford U. Press, 2017. $120.00



The encyclopedic aspirations of the book are evident early: The first chapters include the electromagnetic and the gravitational classical fields along with a review of spacetime symmetries that allows the authors to offer a first look at the relativistic field equations and introduce spinors and the notion of physical state. The book's early chapters were originally designed as a master's-level course, in which students with a background in physics and those trained in mathematics would find a common language to proceed further into modern topics in theoretical physics.

The presentation of the concepts is clear and never redundant. The authors aim to provide a compact path through basic topics rather than offer a complete course on them. Each chapter ends with a few problems suitable for a reader with some previous background on the subjects. The book is enriched with historical notes that provide pleasant interludes.

The highlights of the book come when the authors address more specialized topics, including ones to which they themselves made essential contributions. Those subjects are presented in greater detail than is found in most textbooks. The clear discussion of the path integral, for example, includes fermionic variables. The Euclidean path integral, instead of being relegated to an appendix, rightly finds a dedicated chapter. Also excellent are the explanations of the quantization of gauge theories, symmetry breaking, and Becchi-Rouet-Stora-Tyutin symmetry, in which the authors pay tribute to their friend and mentor Raymond Stora.

Even better is the material on renormalization, the authors' field of expertise. The chapters on the renormalization group and IR divergences are truly outstanding and original. *From Classical to Quantum Fields* also includes a useful presentation of Bargmann coherent states, which unfortunately is missing in many other texts.

At the end of the tour, have the authors passed over any points of interest? One topic that deserves more than a brief mention is extended field configurations such as instantons, monopoles, and skyrmions. What else? The authors say in the prologue that they "decided to leave out subjects, such as the attempts to obtain a quantum theory of gravity based on string theories, because, although they involve very beautiful modern mathematics, they have not yet been directly connected to concrete experimental results." Although sensible, that decision is not consistent with the inclusion of a chapter on supersymmetry, which also lacks concrete experimental results.

That kind of blind spot is one of the drawbacks of the book's theoretical-particle-physicist viewpoint. The limited perspective also undermines the material on gravity. The chapter on general relativity is quite dry and feels disconnected from the rest of the book. Al-

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though *From Classical to Quantum Fields* presents many useful observations about the difficulties of achieving general covariance in a quantum field theory, it does not deal with the problem of quantizing gravity.

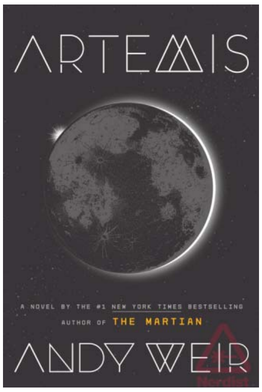
Unfortunately the authors also share two misconceptions common among particle physicists. The first concerns the phenomenological accessibility of quantum gravitational effects. The authors discuss how far particle accelerators are from reaching the energy scale of quantum gravity, but forget that we have already obtained important results from other kinds of experiments. We have more than just accelerators! For example, astrophysical and cosmological observations place strong constraints on violations of Lorentz invariance.

The second misconception in the book is that string theory is the only theory addressing the problem of quantum gravity. It is certainly not the only one, and today perhaps not even the most promising.

Despite a few flaws, *From Classical to Quantum Fields* makes for a fine companion for students and an excellent general reference for researchers in theoretical physics.

Francesca Vidotto
University of the Basque Country
Vizcaya, Spain

NEW BOOKS & MEDIA



Artemis

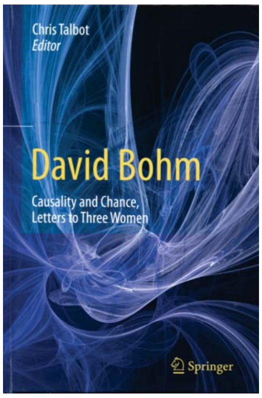
Andy Weir
Penguin Random House, 2017. $27.00

In 2014, first-time novelist Andy Weir had an unexpected smash hit with *The Martian*, a sci-fi adventure about a stranded astronaut who uses his wits and engineering skills to survive on the harsh surface of Mars. *Artemis*, Weir's sophomore novel, moves us from Mars to the Moon. Weir's worldbuilding is top-notch; he's thought through both the technical and economic challenges of life in the lunar city of Artemis, and the result is a rich and fascinating setting. The characters don't quite live up to the same standard, unfortunately, and protagonist Jazz Bashara is particularly underdeveloped. Fans of *The Martian*'s scientific detail, however, will still find much to like here. For a full review and interview with Andy Weir by National Air and Space Museum curator Matthew Shindell, visit http://physicstoday.scitation.org/do/10.1063/PT.6.3.20171215a/full/. —MB

David Bohm

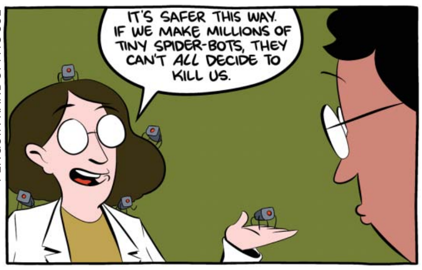
Causality and Chance, Letters to Three Women

Chris Talbot, ed.
Springer, 2017. $199.00



The life and career of US theoretical physicist David Bohm spanned some of the most politically fraught periods in the country's history. Fired from his position at Princeton University after a federal investigation into his Communist ties, Bohm relocated to Brazil, where he became known for advocating an unusual causal interpretation of quantum mechanics. Editor Chris Talbot, a retired physicist, argues that understanding Bohm's Marxism is essential to fully appreciating his physics, and offers selections from Bohm's correspondence to support his thesis. Talbot features three Bohm correspondents in particular: Hanna Loewy, a former girlfriend; fellow physicist Melba Phillips, also a former student of Robert Oppenheimer; and mathematician Miriam Yevick. The fascinating letters deserve publication, but historians will be left wondering if these letters are representative or unusual for Bohm. —MB

BOOKS



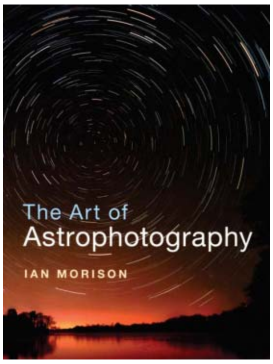
PENGUIN RANDOM HOUSE

Soonish

Ten Emerging Technologies That'll Improve and/or Ruin Everything

Kelly Weinersmith and Zach Weinersmith
Penguin Random House, 2017. $30.00

Ecologist Kelly Weinersmith and cartoonist Zach Weinersmith (best known for his web comic *Saturday Morning Breakfast Cereal*) have joined forces to create this entertaining and highly readable take on cutting-edge scientific innovation. Focusing on 10 emerging fields—including asteroid mining, fusion power, augmented reality, and synthetic biology—the authors discuss the science behind some of the latest technologies, the state of their development, and the possible ramifications should they come to fruition. Aimed at a general audience, the text uses Zach Weinersmith's whimsical cartoon drawings (left) to illustrate key points. —CC



The Art of Astrophotography

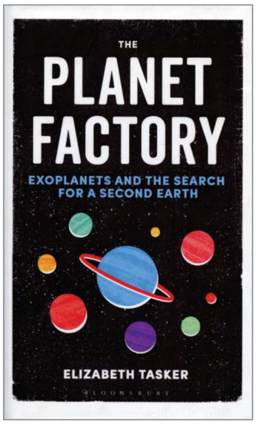
Ian Morison
Cambridge U. Press, 2017. $44.99 (paper)

Written for photography enthusiasts who want to capture images of the night sky, *The Art of Astrophotography* walks the reader through the equipment and techniques required to photograph astronomical phenomena. Author Ian Morison, an emeritus professor of astronomy at the University of Manchester, also provides step-by-step instructions for post-processing the raw photographic data. The book progresses from simple equipment to more elaborate hardware and software. Photographs and images of the equipment illustrate each chapter. —CC

The Planet Factory

Exoplanets and the Search for a Second Earth

Elizabeth Tasker
Bloomsbury Sigma, 2017. $27.00



In 1992, astronomers made the first confirmed detection of a planet orbiting a star outside our solar system. Twenty-five years later, exoplanets have captured the imaginations of scientists and nonscientists alike. In *The Planet Factory*, astrophysicist Elizabeth Tasker discusses the different ways exoplanets are formed and the techniques used to detect them. She then explores what conditions are required to make a planet Earth-like and why we are so eager to find more. Aimed at a general audience, the book provides an introduction to one of the fastest growing fields in astronomy. —CC PT

NEW PRODUCTS

Focus on analytical equipment, sensors, and instrumentation

The descriptions of the new products listed in this section are based on information supplied to us by the manufacturers. PHYSICS TODAY can assume no responsibility for their accuracy. For more information about a particular product, visit the website at the end of the product description. For all new products submissions, please send to ptpub@aip.org.

Andreas Mandelis

Software for layer analysis

Bruker's XMethod software can be used to analyze the composition and thickness of single and multiple layers. Analyses are based on data obtained by sample excitation with the company's XTrace microfocus x-ray source for scanning electron microscopes. The software enables the characterization of thin films and multilayer structures with thicknesses ranging from a few nanometers to 40 μm. There is no need to cross-section the sample. Bruker claims that x-ray excitation yields improved limits of detection over those achieved by sample excitation that uses high-energy electrons. It lets users obtain information on material several tens of microns beneath the surface. Applications include the analysis of coatings on solar cells and of connector pins and solder bumps on printed circuit boards, lead frames, and chip carriers. ***Bruker Nano GmbH**, Am Studio 2D, 12489 Berlin, Germany, www.bruker.com*

Flow cell for electrochemistry

By agreement with Lawrence Berkeley National Laboratory and the University of California, Berkeley, Hiden Analytical is commercializing a novel differential electrochemical mass spectrometry (DEMS) cell for use with its HPR-40 DSA membrane inlet mass spectrometer. The DEMS technique characterizes electrocatalytic performance, which has special relevance to fuel-cell chemistry. It allows for fast, *in situ* identification of gaseous and volatile products and intermediates generated during the electrochemical faradaic reactions taking place directly at the electrode–electrolyte interface. The benchtop system provides real-time multispecies analysis, high sensitivity, and detailed characterization as it monitors evolved and adsorbed species across the atomic mass range from 1 amu to 300 amu. ***Hiden Analytical Inc**, 37699 Schoolcraft Rd, Livonia, MI 48150, http://hideninc.com*

Dual-wavelength x-ray diffractometer

Rigaku Oxford Diffraction has introduced a compact, high-flux single-crystal diffractometer for 3D chemical structure analysis. The XtaLAB Synergy-DW features a hybrid photon counting detector and is configured with a fast, efficient, four-circle kappa goniometer compatible with a wide range of detectors. The versatile diffractometer combines the increased flux of a rotating anode source—Rigaku's MicroMax-007 HF-based microfocus rotating anode x-ray generator—with the flexibility of two wavelengths. The target is constructed with copper and molybdenum source materials and is coupled with an auto-switching dual wavelength optic. According to Rigaku, the system offers up to 12× higher flux compared with standard sealed tube sources, but maintenance requirements are reduced because only a single generator is used. ***Rigaku Americas Corporation**, 9009 New Trails Dr, The Woodlands, TX 77381-5209, www.rigaku.com*

Magnetron and power supply packages

The Kurt J. Lesker Company (KJLC) has released its Research Advantage magnetron and power supply packages, or RAPs. They include all the cables and connectors necessary to integrate the RAP into an existing sputtering system and enable users to create a complete magnetron and power supply system. RAPs offer a choice of a 2-, 3-, or 4-inch Torus Mag Keeper sputtering source; each features KJLC's latest design technology, which has quick target capability and UHV-compatible operation. The magnetrons come with a flexible assembly and standard magnets, and the Mag Keeper source can be packaged with a DC or RF power supply. Users who choose a DC supply have the option of adding one of KJLC's Impulse high-power magnetron sputtering power supplies. ***Kurt J. Lesker Company**, 1925 Rte 51, Jefferson Hills, PA 15025, www.lesker.com* PT

PHYSICS TODAY PRODUCT PICKS

Gas Analyzer – PrismaPro®

The Pfeiffer Vacuum PrismaPro quadrupole mass spectrometer is designed for both qualitative and quantitative gas analysis as well as leak detection. The PrismaPro is built rugged and features a distinctive combination of high sensitivity with a detection limit of <3E-15 mbar, maximum stability, and intelligent operation. It's based on Pfeiffer Vacuum's over 50 years of proven success in the field of mass spectrometry.

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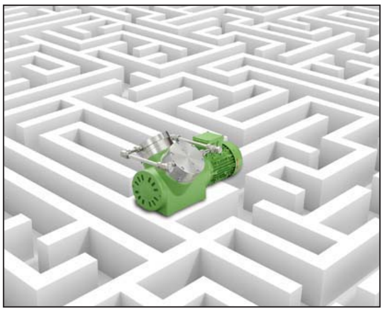

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OBITUARIES

To notify the community about a colleague's death, send us a note at http://contact.physicstoday.org. Recently posted notices will be listed here, in print. Select online obituaries will later appear in print.

Nicolaas Bloembergen

Nicolaas Bloembergen, a Dutch-born US physicist and Nobel laureate, died from cardiorespiratory failure on 5 September 2017 in Tucson, Arizona. Generally regarded as the father of nonlinear optics, Nico will be remembered not only for his groundbreaking scientific achievements but for his great perseverance and genuine concern for others.

Born in Dordrecht, the Netherlands, on 11 March 1920, Nico grew up in Bilthoven, a residential suburb of Utrecht. His innate curiosity about the correspondence between mathematics and physical facts led him to study physics at the University of Utrecht. He received his bachelor's degree in 1941 and completed the equivalent of a master's degree in science in 1943; he passed his doctoral qualifying exam just three months before the university was closed later that year by German forces occupying the country. For the remaining two years of World War II, everyday liberties were greatly restricted, forcing Nico to hide indoors most days. During the winter of 1944–45, known as the Dutch Hunger Winter, Nico's family ate tulip bulbs to survive, and at night, using a storm lamp, Nico read Hendrik Kramers's book on the basics of quantum theory.

Nico always thought he would start work on his PhD thesis outside the Netherlands. Because of Europe's devastation, in 1945 the US seemed to be the most promising place to conduct research. At the suggestion of his older brother, Nico applied to the University of Chicago, which never replied; to the University of California, Berkeley, which wrote that it was not admitting foreign students at the time; and to Harvard University, which accepted him after receiving additional recommendations.

Luckily for Nico, he arrived at Harvard six weeks after Edward Purcell, Robert Pound, and Henry Torrey had detected an NMR signal in condensed matter. He was hired as a graduate assistant to develop the early NMR device. "The hitherto unexplored field of nuclear magnetic resonance in solids, liquids and gases yielded a rich harvest," Nico wrote in his biographical Nobel sketch. That research resulted in his 1948 *Physical Review* paper with Purcell and Pound, now commonly referred to as BPP, which became one of the most-referenced physics papers ever.


Nicolaas Bloembergen

Nico returned to the Netherlands in 1947 to submit his PhD thesis, "Nuclear magnetic relaxation," at the University of Leiden. After receiving his degree in 1948, Nico worked as a postdoc for Cornelius Gorter at the Kamerlingh Onnes Laboratory for a year, and then he returned to Harvard to join the Society of Fellows. Although Nico also studied nuclear physics and microwave spectroscopy at the Harvard cyclotron, he ultimately chose to work on smaller-scale spectroscopy experiments.

In 1956 Nico created the crystal maser, which grew out of his work in microwave spectroscopy. In the early 1960s, soon after Theodore Maiman unveiled the laser, Nico extended his spectroscopy work into tunable lasers and developed a high-precision technique to observe atomic structure. His work on laser spectroscopy in turn led to his conception of nonlinear optics, in which he created a new theoretical way to analyze how electromagnetic radiation interacts with matter. "In fact, what we did was quite simple," Nico told the Dutch newspaper *de Volkskrant* in 1990. "We took a standard textbook on optics and for each section we asked ourselves what would happen if the intensity was to become very high. We were almost certain that we were bound to encounter an entirely new type of physics within that domain."

Nico became an intellectual force at Harvard and rose quickly through the academic ranks. He became an associate professor in 1951 and received named professorships in 1957, 1974, and 1980. Nico retired from Harvard in 1990 as Gerhard Gade University Professor Emeritus.

Among the many honors Nico received for his work were the American Physical Society's 1958 Oliver E. Buckley Prize for Solid State Physics and the 1974 National Medal of Science. In 1981 the Nobel Prize in Physics was awarded to Nico and Arthur Schawlow for developing laser spectroscopy and to Kai Siegbahn for developing high-resolution electron spectroscopy.

Despite receiving such impressive honors, Nico continued to dedicate himself to teaching and mentoring. Throughout his life, he retained an attitude of sincere modesty. Harvard professor Eric Mazur, a postdoc of Nico's, recently said of his mentor, "Even though he received the Nobel Prize . . . he always remained one of the humblest people I have ever known. . . . He considered the success of the people around him his biggest accomplishment."

John Armstrong, a retired IBM vice president of science and technology, also worked in Nico's lab. He recalled the profound influence Nico had on his career: "It was the formative experience in my life as a scientist to have worked with him in [nonlinear optics] as a postdoc. He provided crucial support at an early stage in my career, and I believe this was true for many of his former students and postdocs."

Nico remained active at Harvard until he and his wife moved to Tucson in 2001. He was appointed as a professor of optical sciences at the University of Arizona. Refusing a salary, Nico was given an office, a computer, and a parking spot next to the optical sciences building. As only an academic could appreciate, the nearness of the parking space was the most important part of the arrangement.

For his entire scientific career, Nico kept his high level of productivity and enthusiasm for science. Until his health started to decline during the last year of his life, he went to his office several days a week. He welcomed any opportunity to meet with visitors, students, and faculty. His standing in the optics community and the respect he inspired were evident at his 90th birthday party in 2010. In addition to the many former PhD students and postdocs who came to celebrate their mentor, Nobel laureates Roy Glauber, John Hall, and Charles Townes attended. Loved by many for his generosity, playfulness, and kindness, Nico will be greatly missed.

James C. Wyant
Tammy Orr
University of Arizona
Tucson

Cécile DeWitt-Morette

Cécile DeWitt-Morette passed away on 8 May 2017 in Austin, Texas. She is perhaps best known for establishing the Les Houches School of Physics, located in the French Alps, and for having thus contributed greatly to the development of physics during the second half of the 20th century. Over the years the school attracted prominent teachers, and many students later became prominent scientists in their own right. Recent Nobel laureate Kip Thorne attended Les Houches first as a student and then as a lecturer; he is one of 50 participants who have earned a Nobel Prize or Fields Medal.

Cécile DeWitt-Morette

AIP EMILIO SEGRÈ VISUAL ARCHIVES

Born in Paris on 21 December 1922, Cécile grew up in Caen, and she obtained her bachelor's degree in science from the university there. On 6 June 1944, the day of the Normandy landing, while Cécile was taking her master's exam at the University of Paris, bombs destroyed her home in Caen and killed most of her family.

Soon after, Cécile was hired by Frédéric Joliot-Curie to assist with tasks requiring theoretical knowledge. However, France lagged significantly in theoretical physics: No structured course on quantum mechanics had yet been offered. A conversation she had with Paul Dirac while visiting the UK led Cécile to realize her ignorance. Like other graduate students, she was expected to be trained abroad, and thus she prepared her doctoral thesis in Dublin under the direction of Walter Heitler. After she defended her thesis on the production of mesons, she left Paris for Copenhagen; in 1948 she went to the Institute for Advanced Study in Princeton, New Jersey. There she met a young physicist, Bryce DeWitt, who was as tall as she was short.

In the spring of 1951, Cécile married Bryce, which meant she would live outside of France, and she imposed on herself a condition to contribute to the redevelopment of physics in her motherland. Having experienced firsthand the deficiency of modern-physics instruction in France, she set out to remedy that. Through her energy, courage, and vision, she invented the concept of an autonomous international summer school with specific features: gathering a small group of carefully selected, promising students and eminent professors engaged in cutting-edge research; letting them work, live, and eat together for two-month sessions in a secluded and beautiful location; delivering extensive courses that progress from basic physics to recent advances; and publishing the lecture notes.

By the summer of 1951, Cécile was already able to launch the first session. Using her unique power of persuasion—Pierre-Gilles de Gennes said that no one could resist her "blue-eyed stare"—she garnered support for the project from influential physicists such as Louis Néel and Yves Rocard, obtained funds from the French government, found assistants, recruited outstanding lecturers, and advertised the school. Through a Girl Guide friend whose father had bought them in the 1920s, she borrowed several ancient alpine chalets overlooking the village of Les Houches and facing the Mont Blanc chain. She installed rudimentary housing and a classroom in a hayloft.

For two summer months that year, about 30 students—half French, half foreign—who paid only for their meals, were introduced to modern physics by an impressive list of teachers, including Léon van Hove, Walter Kohn, Wolfgang Pauli, Emilio Segrè, and Victor Weisskopf (shown in the photo with Cécile at Les Houches). Some students slept on straw, but the lack of comfort and the intensive work were balanced by a congenial atmosphere and mountain hiking or climbing during free time. Lasting relationships were created.

From 1951 to 1972, Cécile directed and developed her school with tireless energy; she spent every summer at Les Houches with her four daughters and often with Bryce. She transformed the school into an official institution, installed a scientific and administrative board, and obtained funding from various sources, including the NATO Science Committee after 1958. Over time, she organized the purchase of the school property, the remodel of old farms, and the construction of modern chalets for housing and a building with a classroom, a library, and working spaces.

As graduate-level instruction in Europe improved, the yearly sessions increasingly focused on specific themes and were organized by a scientific director, but Cécile resisted overspecialization. In 1958 she entrusted Philippe Nozières with an eight-week session on the many-body problem, at which I had the marvelous experience of discovering living physics. Other institutes created throughout the world since 1953 have used Les Houches as a model.

In parallel with the development of the Les Houches School, Cécile pursued her physics career in the US and eventually became the Jane and Roland Blumberg Centennial Professor at the University of Texas at Austin. She produced foundational work on path integrals, their classical limit, and their interplay with topology. She published articles on wave propagation and on general relativity, measured the deviation of the light of stars by the Sun during the 1972 eclipse, and directed the work of many students. She edited numerous volumes of the Les Houches proceedings, and with Yvonne Choquet-Bruhat she wrote an excellent two-volume book, *Analysis, Manifolds and Physics*.

Cécile offered me the great honor and pleasure of succeeding her in 1973 as director of the Les Houches School, which she had always regarded as her "child." After retiring, she remained an active member of its board. Her successors, while following the advances of science, have preserved the spirit she instilled. Her school will remain her living legacy.

Roger Balian
Academy of Sciences
Paris
Institute of Theoretical Physics
Saclay, France

Jerry Earl Nelson

UNIVERSITY OF CALIFORNIA, SANTA CRUZ

Jerry Earl Nelson

Jerry Earl Nelson, the father of the segmented-mirror telescope and a towering figure in the history of telescope building, passed away on 10 June 2017 at his home in Santa Cruz, California.

Jerry was born on 15 January 1944 in northern Los Angeles County to a father who was a machinist and a mother who ran a children's center. He was introduced to astronomical research as a high school student in 1960 at the renowned Summer Science Program in Ojai (then in its second year) and to telescope building as an undergraduate physics major at Caltech when he assisted Gerry Neugebauer with the construction of a 1.5-meter IR telescope. Jerry so impressed his Caltech lab instructor and future colleague Eric Becklin with his experimental skill and thoroughness of approach that Becklin was still marveling about it 50 years later.

After graduating from Caltech in 1965, Jerry went on to graduate school at the University of California, Berkeley, where he shifted his interest to experimental particle physics. He received his PhD in 1972 under the direction of Burton Moyer. Staying on as a postdoctoral fellow at Lawrence Berkeley National Laboratory, Jerry returned to astrophysics. In particular, he applied his expertise in particle-physics electronics to a series of ingenious timing experiments at Lick Observatory that involved the Crab and other optical pulsars.

In 1977, University of California astronomers formed a committee to investigate what telescope to build as a successor to the Lick 3-meter. Jerry, who had caught the attention of some committee members with his optical pulsar work, was appointed to provide an outsider's perspective. Astronomy would never be the same.

Jerry had an abiding love of first principles and a remarkable ability to see both their furthest reaching implications and a path to getting there; his mantra was, "It's just freshman physics!" Preventing a mirror from distorting under gravity requires that its thickness increase as the square of the diameter, a fact that led Jerry directly to the concept of segmented mirrors. However, the idea of building a 10-meter-diameter mirror out of 36 segments raised some formidable problems.

Working with Terry Mast, who would be his close collaborator for 40-plus years, Jerry proceeded to solve those problems. In particular, his development, with Jacob Lubliner, of stressed mirror polishing solved the problem of how to fabricate large nonaxisymmetric optical segments, and his and Mast's development of active electromechanical control systems allowed large numbers of such segments to remain locked together and function as a single, continuous optical surface. The first Keck telescope was such a success when it went into scientific operation in 1993 that by 1996 there was a second, virtually identical Keck. Within a few more years, Jerry was at work, again with Mast, on designing what is now the Thirty Meter Telescope (TMT), which is scheduled to begin construction later this year.

Jerry recognized that the enormous collecting area of the Keck telescopes made each photon more precious, not less. He worked tirelessly to help design and develop state-of-the-art instruments and to improve the telescopes' performance. Every morning he reviewed the Keck night logs. He was a fixture as an outspoken member of the Keck Science Steering Committee.

Not only a truly great physicist, Jerry was a remarkable electrical engineer and a world-class mechanical engineer as well. He received both the 2010 Kavli Prize in Astrophysics and the 2012 Benjamin Franklin Medal for electrical engineering. His personality was as impressive as his professional accomplishments. The courage he manifested in the face of criticism and personal adversity was remarkable and inspiring. Although he had a physically debilitating stroke in late 2011, Jerry still went to work every day, including holidays, and was making essential contributions to both Keck and the TMT up until his final days. His optimism was relentless—he was undeterred by people constantly telling him he was trying to do the impossible—and his intellectual curiosity was legendary. He was a mentor of uncommon patience and generosity, and it is doubtful whether anyone, with the possible exception of his colleague Mast, got more joy out of his work.

Jerry's vision, expertise, technical knowledge, and leadership made the twin Keck telescopes the first of the 8- to 10-meter telescopes to go into operation. The two Kecks, together with Jerry's efforts as the founding director of the Center for Adaptive Optics at Santa Cruz, helped to usher in an unprecedented era of astronomical discovery that covered such diverse phenomena as exoplanets, the formation and evolution of galaxies, the acceleration of the expansion of the universe, and the black hole at the galactic center. Jerry had a profound influence on the careers of a hundred astronomers and telescope engineers. His continuing influence can be seen in the segmented-mirror design of ongoing telescope megaprojects, including the *James Webb Space Telescope*, the European Southern Observatory's Extremely Large Telescope, and the TMT.

Gary Chanan
University of California, Irvine

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academic positions

Positions at Shanghai Center for Complex Physics (SCCP), School of Physics and Astronomy, Shanghai Jiao Tong University (SJTU), Shanghai, China

SCCP at SJTU (**http://sccp.physics.sjtu.edu.cn**) with **Prof. Tony Leggett** of University of Illinois, a part-time faculty member of SJTU, as its director, announces 2 faculty (tenured or tenure-track) and 4 postdoctoral openings in theoretical and experimental condensed matter physics. Salary, start-up funds, housing allowance, and other provided benefits, are competitive with those offered by other leading universities in mainland China. The working language of the Center is English. Interested candidates of all nationalities are encouraged to initiate the application process by sending a CV (including a full list of publications) to **sccp@sjtu.edu.cn** before **April 15, 2018**.

Ruhr Explores Solvation (RESOLV), a joint scientific research project comprising 50 research groups from the Ruhr area, is funded by the German Excellence Initiative. The mission of RESOLV is to understand the impact of solvation on reactions, the function of biomolecules, and processes at liquid/solid interfaces in the field of Solvation Science. RESOLV aims to create a multidisciplinary framework for understanding solvent processes that is universal and adds predictive capabilities. To achieve the goals of RESOLV, the current faculty will be reinforced by the following vacancy in the **Department of Physics** at the **University of Duisburg-Essen**:

University Professor (W3 level) in "Interface-Sensitive Probing of Surface/Liquid Interfaces"

Close collaboration with the RESOLV Cluster of Excellence (**www.solvation.de**) expected. Applicants are expected to have an excellent, internationally recognized academic standing and an outstanding publication record. The successful candidate will be appointed to a tenured position, supported by scientific and technical staff at the Duisburg campus, provided with funding for dedicated instrumentation, and will strongly benefit from state-of-the-art equipment at ZEMOS, a research facility at the Ruhr University of Bochum (www.rub.de/zemos).

Further requirements:
- The candidate's ability and the willingness to collaborate with existing groups in the RESOLV Cluster of Excellence.
- Participation in interdisciplinary academic work.
- Substantial commitment to teaching and graduate education.
- Research and instruction in physics

Publications in international peer-reviewed journals and experience with the acquisition and management of third-party projects, ideally in the field of publicly funded research projects, are expected. The University Duisburg-Essen places great emphasis on the quality of teaching. Candidates must present didactical concepts for teaching - with consideration of the profile of the University Duisburg-Essen and the Faculty of Physics. The hiring requirements comply with § 36 of the University Directive North-Rhine Westphalia.
The University Duisburg-Essen pursues the objective of promoting the diversity of its members (see **http://unidue.de/diversity**). The university strives for an increase of the share of women among the academic staff and therefore emphatically invites qualified women to apply. Natalie Velibeyoglu, the faculty's equal opportunities representative, is available as contact person and can be reached by e-mail at **gleichstellungsbeauftragte.physik@uni-due.de**. In case of identical qualifications, female candidates will be considered with preference as per the measure of the Equal Opportunities Act. Applications from qualified severely disabled persons and equivalents as per § 2 Sect. 3 SGB IX are welcome.
Applications with the usual supporting documents should be sent within one month of the publication of this advertisement to the **Dean of the Faculty of Physics of the University of Duisburg-Essen, Prof. Dr. Michael Schreckenberg, Forsthausweg 2, 47057 Duisburg, Germany.** The supporting documents should include: a detailed resume, a list of publications highlighting the five most important ones, documentation describing scientific and professional development, details of externally funded projects and information on past academic duties and activities, teaching concepts and previous teaching experience, and a two-page research plan for the next five years at the Physics Department of the University of Duisburg-Essen and in Solvation Science. Further information on the position is available at **www.uni-due.de/physik/dekanat/stellen.php**. Please direct any questions about this position to **Prof. Dr. Uwe Bovensiepen** (**uwe.bovensiepen@uni-due.de**).
Further information about
- RESOLV is available at **https://www.solvation.de/**
- Universitätsallianz Ruhr (UA RUHR) is available at **http://www.uamr.de/en/**

Scientific/Computational Science/Postdoctoral Positions
US - NY - Long Island
Brookhaven National Laboratory

Comscope, the BNL Computational Material Science Center aims to develop and disseminate methodologies (theory, algorithms, and codes) to accurately describe the physical properties of complex strongly correlated materials. This includes in particular developing for public dissemination a number of first principle and DMFT based codes. To support this effort it has opened a number of positions including post-docs in electronic structure, quantum many-body theory, and multi-scale modeling, a code base developer position, and two staff positions involving electronic structure and software engineering. For further information see positions 779, 1117, 1143, 1164, 1165, and 1166 at **https://jobs.bnl.gov**. For queries please contact **rmk@bnl.gov** or **kotliar@physics.rutgers.edu**. These positions are based at BNL but will involve close interactions with other scientists in the center. Applications consisting of a cover letter, curriculum vitae with publication list, a brief (1-2 page) description of research interests and accomplishments, and three letters of recommendation should be submitted to through the BNL website. Please indicate in your cover letter when you would be available to begin employment. Review of applications will commence immediately and continue until the position is filled. Members of underrepresented groups are particularly encouraged to apply. Applicants are encouraged to contact **Dr. Robert Konik** (**rmk@bnl.gov**) or **Prof. Gabriel Kotliar** (**kotliar@physics.rutgers.edu**) for further information. At Brookhaven National Laboratory we believe that a comprehensive employee benefits program is an important and meaningful part of the compensation employees receive. Our benefits program includes but is not limited to: •Medical Plans •Vacation •Holidays •Dental Plans •Life Insurance •401(k) Plan •Retirement Plan •Swimming Pool, Weight room Tennis Courts, and many other employee perks and benefits. To be considered for the above positions, please apply online at BNL Careers and enter the job title into the Keyword Search (or follow the links provided). *Brookhaven National Laboratory (BNL) is an equal opportunity employer committed to ensuring that all qualified applicants receive consideration for employment and will not be discriminated against on the basis of race, color, religion, sex, sexual orientation, national origin, age, disability, or protected veteran status. BNL takes affirmative action in support of its policy and to advance in employment individuals who are minorities, women, protected veterans, and individuals with disabilities.*

Lecturer Position in Physics
College of Sciences and Mathematics
Auburn University

The Physics Department at Auburn University is seeking a highly qualified individual for a Lecturer position. This is a nine-month, non-tenure track position, renewable on a yearly basis. The expected salary range is between $46,000 and $50,000 for the nine month appointment. The successful candidate will be expected to: (1) teach introductory and upper-level undergraduate courses in physics and astronomy, (2) interact with other faculty and staff to contribute to current and future innovative pedagogical efforts in undergraduate teaching, and (3) supervise graduate teaching assistants. Experience in physics education research (PER), lecture demonstration activities, and teaching large lecture classes is desirable. Applicants must possess a Ph.D. or equivalent degree in Physics or a related field. Applicants to the position in the Department of Physics must apply online at: **http://aufacultypositions.peopleadmin.com/postings/2624**. Candidates need to include in their application a cover letter, curriculum vitae, statement of teaching philosophy, and the names and contact information for three professional references. More information on these positions can be found at: **http://www.physics.auburn.edu**. Review of applications will begin **15 February 2018** and will continue until the position is filled. The desired starting date is 16 August 2018. The candidate selected for this position must be able to meet eligibility requirements to work in the United States at the time the appointment is scheduled to begin and continue working legally for the proposed term of employment. Excellent written and interpersonal communication skills are required. *Auburn University is an EEO/Vet/Disability Employer.*

Faculty Position
Izmir Institute of Technology

Department of Physics is seeking an experimental physicist with proven expertise in using Molecular Beam Epitaxy (MBE) growth techniques to fabricate compound semiconductor-based epitaxial thin films (Group II-VI or III-V), and using them in optoelectronic device applications. The faculty position is available in all ranks; however, applications at the Assistant Professor level will be given priority. Applicants should send their documents, including curriculum vitae, a publication list, and a statement of teaching and research interests to **apply-physics@iyte.edu.tr**. For further details please visit: **http://physics.iyte.edu.tr/facultypositionmbe**. *Turkish citizens will be given priority.*

Max-Planck-Institut für Dynamik und Selbstorganisation

Max Planck Institute for Dynamics and Self-Organization

The Max Planck Institute for Dynamics and Self-Organization (MPI-DS) at Göttingen, Germany, is an international, inter-disciplinary and collaborative environment offering an exceptional research setting. It hosts a range of experimental and theoretical fundamental scientific research, and it currently employs a diverse group of researchers of about 280 people. The MPI-DS has recently appointed Oxford University theoretical physicist Prof. Ramin Golestanian as a new Director, and he is currently in the process of establishing the Department of Living Matter Physics. The new department will engage in a wide range of theoretical research aimed at a multi-scale under-standing of the dynamics of living systems from a physical perspective. In connection with the launch of this major re-search initiative at MPI-DS, we expect to have several open positions at a variety of levels.

Group Leader positions (m/f)
Reference no. MPIDS-W005

We are looking for excellent and highly motivated researchers with some postdoctoral research experience in the gen-eral area of Nonequilibrium Statistical Physics of Biological Systems and Soft Matter to join our department. Our aim is to understand the complex dy-namics of living matter well enough to be able to make it from the bottom-up; i.e. from molecules to systems. This theo-retical and conceptual challenge will require the use of the full spectrum of analytical and computational techniques. We aim to build the necessary all-encompassing technical expertise in the department, and invite applicants with the relevant experience in any part of the spectrum to apply. The Group Leaders are expected to help set up and maintain the tech-nical expertise, pursue research at the highest standards in their own respective areas, and contribute actively to collab-orative and complementary research across the department.

The Group Leader positions are limited to five years with some flexibility and their holders are expected to be able to use the well-supported positions to develop their careers to the level that will make them qualify for competitive international academic or senior research positions elsewhere. The candidate should hold a PhD/DPhil degree with a background in theoretical physics, applied mathematics, or a related field, have prior experience with nonequilibrium statistical physics of biological systems and soft matter, and be fluent in English language. Salary is in accordance with the German state public service salary scale (E14 TVöD-Bund) and the corresponding social benefits, and is commensurate with experi-ence. The earliest starting date is **1st March, 2018**.

Our offer
The Max-Planck Society is committed to increasing the number of individuals with disabilities in its workforce and there-fore encourages applications from such qualified individuals. Furthermore, the Max Planck Society seeks to increase the number of women in those areas where they are underrepresented and therefore explicitly encourages women to apply.

Your application: To apply please follow the link below. Applications in writing will not be sent back.
Group Leader positions (m/f):https://s-lotus.gwdg.de/mpg/mpsf/perso/mpids_w005.nsf/application

Please send your CV, publication list, a statement of research interest and at least two letters of reference. Your state-ment of research interest should be commensurate with the position you are applying to. In addition to the description of your proposed research if relevant (depending on the position you are applying to), it should also briefly describe your past and current research interests and why you are interested in joining our department. The positions are open until they are filled. Once a position is filled, all applicants will be informed about the final decisions.

Please contact **Prof. Ramin Golestanian** (ramin.golestanian@ds.mpg.de) if you should have further questions.
MPI for Dynamics and Self-Organization, Prof. Dr. Ramin Golestanian, Am Faßberg 17, 37077 Göttingen, Germany, ramin.golestanian@ds.mpg.de

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Max-Planck-Institut
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Gauss Fellows (m/f)
Reference no. MPIDS-W006

The department will have up to two research positions entitled Gauss Fellows. These prestigious positions are aimed at postdoctoral researchers who have shown exceptional promise in their doctoral or early postdoctoral work, which needs to be in a relevant field. Gauss Fellows are expected to perform research of the highest standards in physics of living matter, and will have the freedom to join any active research area in the department. Our aim is to understand the complex dynamics of living matter well enough to be able to make it from the bottom-up; i.e. from molecules to systems.

The candidate should hold a PhD/DPhil degree with a background in theoretical physics, applied mathematics, or a re-lated field, have prior experience with nonequilibrium statistical physics of biological systems and soft matter, and be fluent in English language. The Gauss fellowship is limited to two years with the possibility of extension. Salary is in accordance with the German state public service salary scale (E13 TVöD-Bund) and the corresponding social benefits. The earliest starting date is **1st March, 2018**

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Please send your CV, publication list, a statement of research interest and at least two letters of reference. Your state-ment of research interest should be commensurate with the position you are applying to. In addition to the description of your proposed research if relevant (depending on the position you are applying to), it should also briefly describe your past and current research interests and why you are interested in joining our department. The positions are open until they are filled. Once a position is filled, all applicants will be informed about the final decisions.

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MPI for Dynamics and Self-Organization
Prof. Dr. Ramin Golestanian
Am Faßberg 17, 37077 Göttingen, Germany
ramin.golestanian@ds.mpg.de

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Postdoctoral Researcher positions (m/f)
Reference no. MPIDS-W007

The department will have a number of open postdoctoral researcher positions. These positions are aimed at excellent and highly motivated researchers with relevant background, who will join the wide spectrum of research in the depart-ment aimed at understanding the physics of living matter. Our aim is to understand the complex dynamics of living matter well enough to be able to make it from the bottom-up; i.e. from molecules to systems.
The ideal candidate should hold a PhD/DPhil degree with a background in theoretical physics, applied mathematics, or a related field, have prior experience with nonequilibrium statistical physics of biological systems and soft matter, and be fluent in English language. The postdoctoral position is limited to two years with the possibility of extension. Salary is in accordance with the German state public service salary scale (E13 TVöD-Bund) and the corresponding social benefits. The earliest starting date is **1st March, 2018**.

Our offer
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Your application
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Postdoctoral Researcher positions (m/f):
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MPI for Dynamics and Self-Organization
Prof. Dr. Ramin Golestanian
Am Faßberg 17, 37077 Göttingen, Germany
ramin.golestanian@ds.mpg.de

Assistant Professor
California State University, LA

Ad: Assistant Professor in Experimental Physics The Department of Physics and Astronomy seeks an Assistant Professor in Experimental Physics. Cal State LA is located 5 miles east of downtown Los Angeles, and is a recognized leader in achieving upward mobility for its diverse and multicultural student body. Position duties include teaching and research. The Department seeks a candidate who will develop innovative instructional labs for introductory physics and include students in his/her research. Full text of job ad appears at http://www.calstatela.edu/2018/college-natural-social-sciences/nss-phys-ttf. Review of applications begins **February 20, 2018**, and continues until position is filled. For information contact **Dr. Konrad Aniol, Search Committee Chair,** kaniol@calstatela.edu.

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QUICK STUDY

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Quantum interference in chemical reactions

F. Javier Aoiz and Richard N. Zare

Interference much like that observed in two-slit experiments can be seen in the outcomes of chemical processes in which multiple reaction mechanisms lead to the same final state.

Thomas Young conducted his celebrated double-slit experiment in 1801. Nowadays, quantum physicists pass not only light through screens with slits cut out but also electrons, neutrons, and even molecules as big as the soccer-ball-like fullerene C_{60}. In all cases we see the same kind of interference. Moreover, the interference is observed even if the particles are shot one at a time. However, if the apparatus is modified to register which slit each particle passes through, the interference is destroyed, as shown in figure 1a.

The double-slit experiment, as Richard Feynman observed in his famous *Feynman Lectures*, "has in it the heart of quantum mechanics. In reality, it contains the *only* mystery, . . . the basic peculiarities of all quantum mechanics." The question we and our colleagues have addressed is whether chemical reactions, studied one collision at a time, display a behavior analogous to that of the particles impinging on a pair of slits. The answer is a resounding yes. When more than one reaction trajectory leads to the same final outcome, interference appears as an oscillatory pattern in the angular distribution of the collision products.

Pass the deuterium

The specific process we considered is an exchange reaction in which a hydrogen atom impinges on a diatomic deuterium molecule and plucks off one of the deuteriums: $H + D_2(v = 0, j = 0 \text{ or } 1) \rightarrow HD(v', j') + D$. The symbols v and j denote vibrational and rotational quantum numbers, respectively, of the reagents; v' and j' refer to the products. We produced the H atoms by photolyzing hydrogen bromide molecules. By choosing specific laser wavelengths, we could control the velocity of the emitted H atom and hence the collision energy in the exchange reaction. The laser light needed to ionize the molecule determines the vibrational–rotational state of the HD product; the technique is called REMPI (resonance-enhanced multiphoton ionization). A position-sensitive detector records the HD angular distribution.

Figure 1b presents the $HD(v' = 1, j' = 1)$ angular distribution from an experiment with a collision energy of 1.97 eV. We have obtained similar results for different energies, for different vibrational–rotational states, and in reactions involving heavier atoms. The distribution is compared with the predictions of a full quantum calculation (black) and with those from a quasi-classical trajectory (QCT) calculation (red), a procedure that runs classical trajectories on an accurate potential energy surface and bins the results into different vibrational–rotational quantum states of the HD product. The experimental data and quantum calculation agree fairly well, but the QCT calculation does

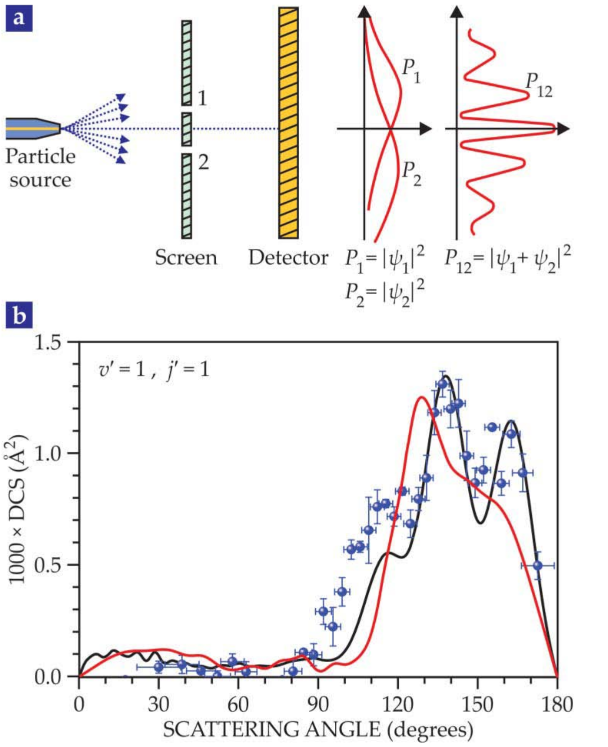

FIGURE 1. INTERFERENCE. When a quantum particle is shot through a single slit, **(a)** the probability that it is detected at a specified location is the absolute square of the quantum amplitude ψ. The probability distributions P_1 and P_2 show the results when, respectively, slit 1 or slit 2 is open. When both slits are open, the amplitudes are added first and then squared to give the probability P_{12}. (Adapted from *The Feynman Lectures on Physics*.) **(b)** Shown here is the angular distribution of hydrogen deuteride formed when H collides with D_2. Blue points are data, the black curve is a quantum mechanical simulation, and the red curve is a classical simulation. In all cases the HD produced had a specific, well-measured rotational–vibrational state. The oscillatory structure of the experimental results and quantum calculation is in stark contrast with the classical prediction. The differential cross section (DCS) is the particle physicists' measure of the probability distribution of the scattering angle.

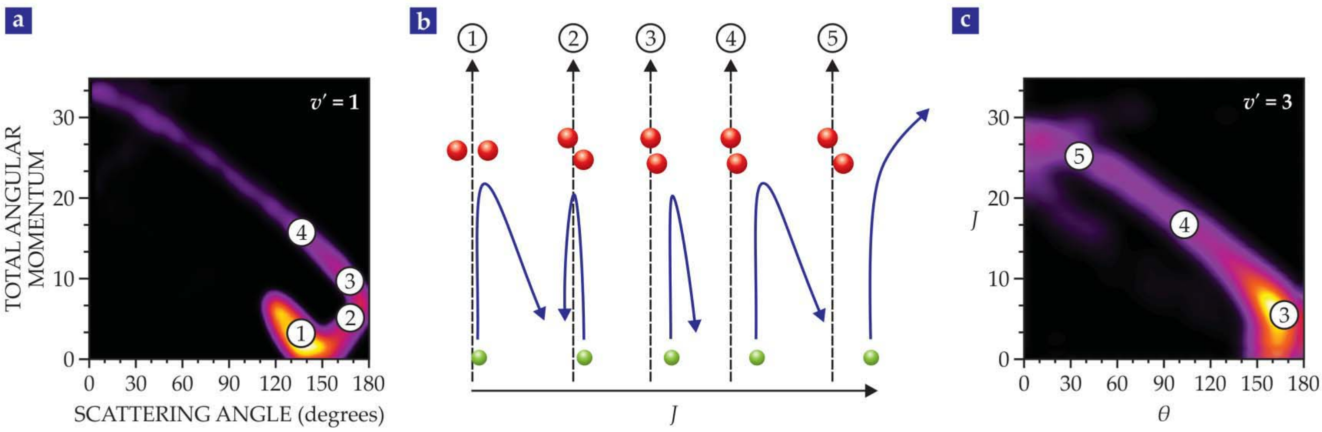

FIGURE 2. THE DEFLECTION FUNCTION. The joint distribution for scattering angle θ and total angular momentum J is expressed by the deflection function. **(a)** Shown here is the deflection function for the exchange reaction $H + D_2 \rightarrow HD + D$. The HD vibrational state is $v' = 1$, as in figure 1b. Probability increases as color changes from black-purple to yellow-white. **(b)** The numbered regions in panel a correspond to the same-numbered reaction pathways shown here. **(c)** Shown here is the deflection function when the HD vibrational state is $v' = 3$; again, numbers indicate reaction pathways shown in panel b.

a disappointing job and fails to capture the fingerlike pattern in the angular distribution. What is the origin of those oscillations? It certainly lies outside classical mechanics. Nonetheless, to understand the origin of the quantum phenomenon, we will turn to the classical world.

Different impact, same scattering

The crucial mathematical quantity we turn to is the classical deflection function, which maps the dependence of the scattering angle θ on the total angular momentum J. For many reactions, including the ones we studied, θ and J are strongly correlated. In joint distributions, such as those presented in figure 2, the correlations appear, roughly speaking, as a band that moves from low J (small impact parameters) and backward scattering angles close to 180° to high J and scattering angles in the forward region.

Close examination of the deflection function gives valuable information not only about the possible concurrent dynamical mechanisms that govern the reaction but also about the relative importance of those mechanisms. Figure 2a shows the function for the exchange reaction in which $D_2(v = 0,\ j = 0)$ goes to $HD(v' = 1,\ j' = 1)$. The several dynamical paths encoded in the deflection function are depicted in panel b. Panel c refers to $HD(v' = 3,\ j' = 1)$. In that case, high values of J are associated with forward scattering, and as J decreases, scattering tends toward increasingly backward angles, as described above. For the $v' = 1$ state of figure 2a, however, several mechanisms associated with different sets of J contribute to backward scattering, and sometimes different mechanisms lead to the *same* backward scattering. When that happens, the two reactions lead to interference in the real, quantum world.

For example, mechanism 1 of figure 2b, which makes the greatest contribution to the scattering intensity, leads to θ near 130° and occurs when the H collides almost side-on with the D_2. But mechanism 4, with its larger impact parameter and near head-on collision, also leads to θ near 130°. Scattering at 130° could be caused by reactions with $J \approx 3$ or $J \approx 15$ to 18. Similarly, reaction paths 2 and 3 lead to the same scattering angles. In a classical world, we could say from which J the scattering occurred, but as in the case of the double slit, the quantum world denies us that knowledge. For the $v' = 3$ case, mechanisms do not superpose; hence no interference is observed in the differential cross section (DCS).

Small mixing, big effect

Because quantum mechanics adds amplitudes first and then squares to get probabilities, a small amount of one mechanism mixed with a large amount of another leads to appreciable interference. For example, suppose mechanism 1 of figure 2b has 10 times the amplitude of mechanism 4 and that mechanism 1 alone leads to a DCS of 100 units. If the probabilities of the two processes add incoherently, then the DCS varies from $10^2 + 1$ to $10^2 - 1$; that is, the DCS varies from 101 to 99, which is a ±1% effect. However, if the two processes are coherent, the probability varies from $(10 + 1)^2$ to $(10 - 1)^2$—that is, from 121 to 81, which is a ±20% effect.

In a sense, the potential energy surface that is the basis for any dynamical calculation acts as an interferometer. The reaction paths on the surface are analogous to particle trajectories passing through slits cut into a screen. Interference is observed whenever two distinct reaction mechanisms lead to products scattered into the same angle at the same total energy and with the same internal states. The result is general: Oscillatory behavior in the DCS caused by interference is not limited to collisions between hydrogen atoms and hydrogen molecules, but it should occur in any scattering system in which the initial collision partners have a well-defined energy and the final scattering partners are observed in a state-selective manner, whether the collisions are reactive or inelastic. Classical scattering pictures are appealing and intuitive tools for describing chemical reactions, but there is no escaping that we live in a quantum world.

We thank Pablo Jambrina and Mahima Sneha for their inestimable contributions to the work described in this Quick Study.

Additional resources

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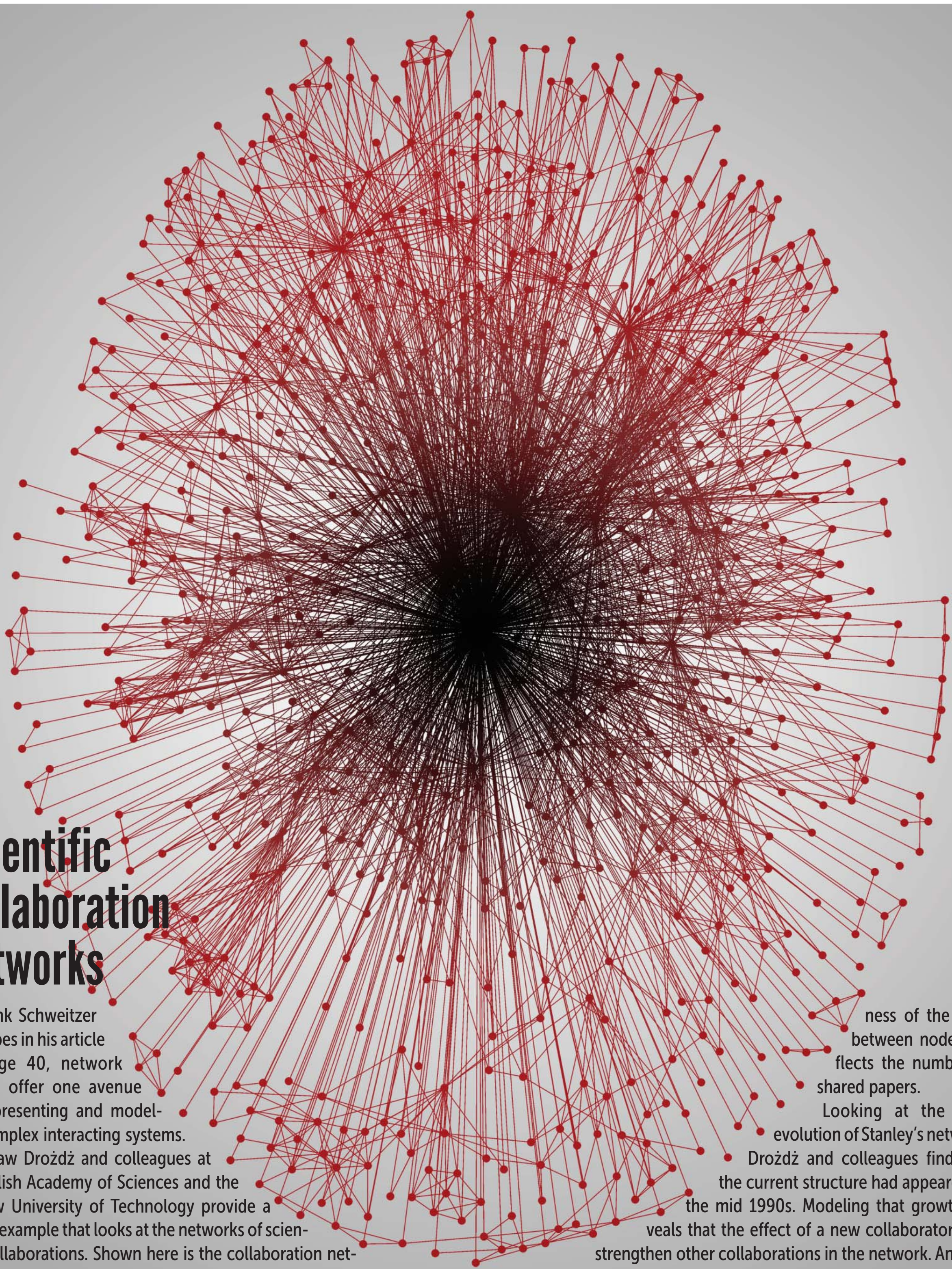

Scientific collaboration networks

As Frank Schweitzer describes in his article on page 40, network graphs offer one avenue for representing and modeling complex interacting systems. Stanisław Drożdż and colleagues at the Polish Academy of Sciences and the Cracow University of Technology provide a recent example that looks at the networks of scientific collaborations. Shown here is the collaboration network of H. Eugene Stanley of Boston University, who is represented by the node in the center. The other nodes are the 738 scientists who had coauthored at least one paper with him through March 2016. The thickness of the links between nodes reflects the number of shared papers.

Looking at the time evolution of Stanley's network, Drożdż and colleagues find that the current structure had appeared by the mid 1990s. Modeling that growth reveals that the effect of a new collaborator is to strengthen other collaborations in the network. And the eigenvectors that emerged from the team's spectral analysis of Stanley's network revealed collaborative subnetworks and relations among them. (S. Drożdż et al., *J. Informetrics* **11**, 1114, 2017.)

—RJF

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