made repeated measurements to monitor the characteristic time over which the spin-state oscillations decayed. That work now sets the stage for statistical studies that explore the link between an NV center's decoherence and local magnetic fluctuations in processes such as the charge transport through ion

channels in a cell membrane. Last year Hollenberg and colleagues calculated that ion-channel dynamics could, in principle, be detected with millisecond resolution by monitoring the probe's decoherence.⁴ The issue is not just academic; ion channels are important drug targets.

Mark Wilson

References

- 1. J. R. Maze et al., Nature 455, 644 (2008).
- 2. G. Balasubramanian et al., *Nature* **455**, 648 (2008).
- 3. L. P. McGuinness et al., *Nat. Nanotechnol.* **6**, 358 (2011).
- L. T. Hall et al., Proc. Natl. Acad. Sci. USA 107, 18777 (2010).

Kinetic experiments shed light on protein-folding thermodynamics

Perturbing biomolecules and then watching them relax may be the kind and gentle way to determine their free-energy landscapes.

In its native state, the treasure trove of nutrients and biochemical machinery known as egg white is a slimy, translucent soup of proteins. Heat it atop a stove, however, and the proteins unfold, coagulate, and collectively morph into an opaque white solid. The unraveled proteins are said to have denatured. The enzymes among them, although well-suited for a cheese omelet, are in no shape to usher along biochemical reactions.

The proteins would have suffered a similar fate had the egg white been whipped into a foamy meringue or soaked in lime juice. Indeed, the precise biological work of folding a protein can be undone by any number of environmental stresses, including heat, acidity, and mechanical strain. Proteins, like all molecules, tend to adopt the shape that minimizes their free energy. In some circumstances, a compactly folded state makes thermo-

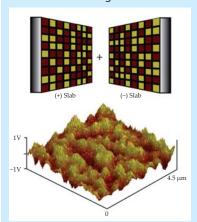
dynamic sense; in others, it doesn't.

To characterize the influence of environment on a protein's shape, biologists construct a free-energy landscape. They typically do so by performing titrations, experiments not all that dissimilar to frying an egg: A protein solution is subjected to a gradual ramp in some input variable—perhaps temperature, perhaps some other quantity—and monitored for physical changes indicative of folding or unfolding.



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

A nanoscale mosaic model of static electricity. Rub a balloon against your hair or rub any two nonconducting materials together, and as any high school physics student knows, the surfaces develop opposing static charges. Theoretical models of that process, known formally as contact electrification, have long assumed that the material properties of each surface are spatially homogeneous and that the post-contact charge distributions are uniform. If those assumptions were correct, then identical materials rubbed together should not transfer any charge. But



they do, as was demonstrated by Northwestern University researcher Bartosz Grzybowski and colleagues roughly two years ago with identical polymer slabs. They predicted then that charge is transferred through a random mosaic of oppositely charged submicron-scale domains, shown in the schematic, generated by inhomogeneities in the materials' surface properties.

Now, Grzybowski and other Northwestern researchers have experimentally verified the mosaic model by imaging contact-electrified polymer slabs with an atomic force microscope; the AFM-generated surface potential map shown here revealed multiple positively and negatively charged nanometer-sized domains. Probing further, the researchers found possible evi-

dence of surface inhomogeneities: Raman spectra indicated that some bonds were cleaved or oxidized, and x-ray photoelectron spectra of dissimilar polymer slabs that had been in contact revealed nonnative elemental peaks, which suggests material transfer. Their next goal is to probe other local surface properties to find out how bond breaking and material transfer influence domain size and overall charge. (H. T. Baytekin et al., Science, in press, doi:10.1126/science.1201512.)

Tantalizing and rare neutrino oscillation. The first appearance of electron neutrinos amidst an underground beam of muon neutrinos has been reported by Japan's T2K collaboration. The three "flavors" of neutrinos—electron, muon, and tau—can quantum mechanically swap identities in transit as long as all three neutrino masses are different. To date, those so-called flavor oscillations have been detected mainly by observing the disappearance, rather than the appearance, of neutrinos of a given flavor; the assumption is that some of the missing neutrinos changed identity en route from their source. Originating at the Japan Proton Accelerator Research Complex (J-PARC), the T2K muonneutrino beam traveled 295 km to Japan's Super-Kamiokande detector, where 88 neutrino-interaction events were detected. Of those 88 events, 6 appear to come from electron-type neutrinos. Only 1.5 such events would be expected if the elusive flavormixing parameter θ_{13} were zero. The θ_{13} result, based on only 2% of the data originally expected from the experiment, is considered preliminary. But it is being published because J-PARC was damaged by eastern Japan's massive earthquake and tsunami on 11 March 2011 and will remain offline for many more months. If confirmed, the result will have profound implications: A nonzero θ_{13} makes possible *CP* violation with leptons, which might then explain the cosmic matter-antimatter imbalance. (K. Abe et al.: T2K collaboration, http://arxiv.org/abs/1106.2822.)

Houston's structures thwart cleansing breezes. On 30 August 2000, as the Sun beat down on Texas's largest city, ozone

But as Martin Gruebele of the University of Illinois at Urbana-Champaign can attest, the titration approach has its limitations. Gruebele is one of a growing number of biophysicists who are interested in understanding how proteins fold inside living cells and organisms. He and his coworkers have learned firsthand that many cells, including the cancer cell shown in figure 1, can't survive the considerable knob-turning required to complete a titration.

Now a team led by Gruebele and Yann Chemla (also at the University of Illinois) has arrived at a potentially less destructive way to generate folding free-energy landscapes.¹ The researchers' theory, simulations, and experiments endorse a counterintuitive strategy: To get the clearest picture of a protein's folding equilibria, force it out of equilibrium.

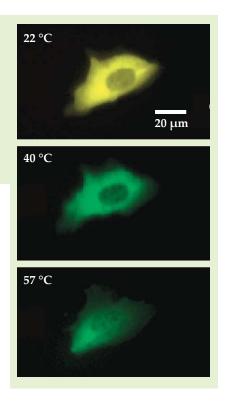
The baseline problem

The dramatic change in texture and appearance that befalls a frying egg is only a crude and indirect indicator of protein denaturation. To precisely characterize

Figure 1. The structure of the fluorescent-tagged phosphoglycerate kinase enzymes in this bone-cancer cell can be inferred from their emission spectrum. The cell's yellow appearance at 22 °C indicates the enzymes are in their native, folded state. The green emission at 40 °C signals that several of the enzymes have unfolded. But at 57 °C, a measurement point needed to round out the titration data, the cell has already died. (Images courtesy of Martin Gruebele.)

folding transitions, biologists look for more subtle clues, such as a shift of a peak in the protein's vibrational spectrum or a change in the emission of a fluorescent probe.

Ideally, the observed property would produce an output signal *B* that changes only when a protein folds or unfolds. Plotted as a function of the input variable, *B* would describe a sigmoid curve. The two horizontal tails would correspond to folded and unfolded states. The transition point, at which half the proteins are folded and



concentrations soared to unhealthy levels. Usually in summer, as the city heats up, sea breezes blowing in from nearby Galveston Bay and the Gulf of Mexico refresh the air. But the prevailing winds over Houston, although mild, tend to counteract the sea breeze. Thus, if the breeze collides with the prevailing winds, stagnation sets in over the city and pollutants can build up. Now a numerical study led by Fei Chen of the National Center for Atmospheric Research suggests that the materials of the urban environment are partly to blame for ozone pollution. Chen and colleagues validated their computer model by com-



paring their simulation of the August 2000 pollution event against extensive data collected in the Texas Air Quality Study 2000. Then, to understand how various environmental features affect the development of the sea breeze, they simulated conditions that were wetter or dryer than normal, and in one simulation they replaced

the urban landscape with cropland. The substitution of crops for concrete had the greatest impact on boosting the sea breeze and reducing periods of stagnation. (It also increased the efficacy of the nighttime land breeze that blows pollutants out to sea.) Compared with green space, the researchers found, the urban environment is hotter. That effect actually tends to enhance the sea breeze, but the enhancement is more than offset by the frictional damping from Houston's buildings. (F. Chen et al., *J. Geophys. Res. [Atmospheres]*, in press, doi:10.1029/2010JD015533.)

Stirring superfluids. If you chill fermions enough, they can pair up to form bosons and settle into a single collective ground

state, a Bose–Einstein condensate. In the case of helium-3 atoms, the resulting BEC is a superfluid that flows without dissipation—provided the flow is not so energetic that it breaks the pairs apart or destroys the ground state's coherence. Until now, theorists could characterize placid flows in fermionic superfluids, but not the vigorous turbulence that results from shaking or stirring. Aurel Bulgac of the University of Washington in Seattle and his colleagues have adapted density functional theory—a computational approach originally devised to calculate molecular energy levels—and applied its time-dependent extension to model turbulent fermionic superfluids. Although the underlying quantum mechanical equations are straightforward, solving them required the use of one of the world's most powerful supercomputers, Jaguar at Oak Ridge National Laboratory in







Tennessee. In their simulations, Bulgac and his colleagues agitated a fermionic superfluid by shooting spherical projectiles through it or by stirring it with a laser beam. Turbulent superfluids are known to harbor tubes of quantized vorticity. As the figure shows, the simulation could track how two vortex tubes (marked a and b) joined to form a ring, which then opens in a manner reminiscent of the unzipping of a DNA molecule during transcription. Bulgac's model could help astronomers understand another agitated superfluid: the interior of a rapidly spinning neutron star. For more on quantum turbulence, see PHYSICS TODAY, April 2007, page 43. (A. Bulgac et al., *Science* 332, 1288, 2011.)

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