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Stirring superfluids

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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 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

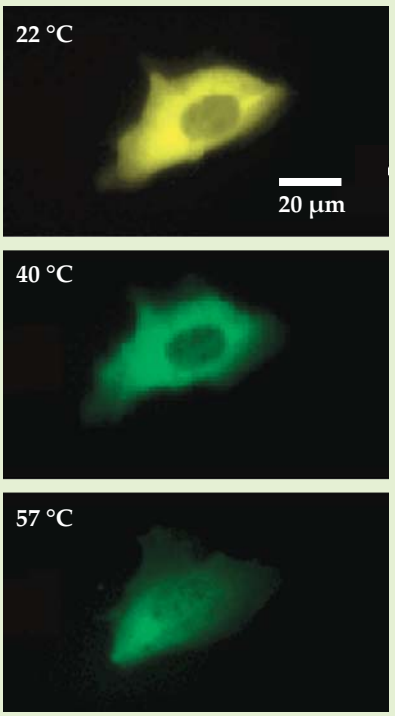

Figure 1. The structure of the fluorescent-tagged phosphoglycerate kinase enzymes in this bone-cancer cell can be inferred from their emission spectrum. The cell's yellow appearance at 22 °C indicates the enzymes are in their native, folded state. The green emission at 40 °C signals that several of the 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.)

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 comparing 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.) —SKB

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.) —CD