FLIES, WEEDS AND STATISTICAL MECHANICS

The flies are two species of fruit flies of the genus Drosophila; the weeds are two species of mustards of the genus *Arabidopsis*; the statistical-mechanical techniques are applied by a six-person Harvard-Cornell-Washington University-North Carolina State team (Bustamante, Nielsen, Sawyer, Olsen, Purugganan, Hartl) and the results are reported in the April 4 2002 *Nature.* The goal is to tease out the pressure of natural selection on individual genes; they use a sophisticated "analytical method that borrows information from all the genes to make inferences about the magnitude of selection for any individual gene." The method, a "hierarchical bayesian analysis", leads to analytically intractable calculations. The authors handle them with Monte Carlo Markov Chain computation scheme borrowed from thermodynamics. The title of the work is "The cost of inbreeding in Arabidopsis".

The Erdös Prizes

In the April 5 2002 Science Charles Seife has a News Focus piece entitled "Erdös's Hard-to-win Prizes Still Draw Bounty Hunters." Paul Erdös died in 1996, but his personal, quirky influence lives on through the prizes he offered for solutions to problems he found intriguing. The prize would be proportional to the difficulty of the problem. There are \$10 problems, \$25 problems, and a couple worth over \$1000. Since his death the prizes have been administered by his long-time friend and associate Ronald Graham (U. C. San Diego), who will send a winner an Erdös-signed check ("suitable for framing") and another of his own, suitable for cashing. Graham "estimates that the outstanding bounties on unsolved problems total about \$25,000 " but does not seem to be worried about a run on the bank. A special case of a \$1000 problem was worth a Fields Medal for Klaus Roth (University College, London) in 1958.

DNA Computer solves a hard problem

Here's the problem: assign values 0 (False) or 1 (True) to the 20 variables A, B, C, D, E, F, G, H, I, J, K, L, M, N, O, P, Q, R, S, T so that the following 24-fold product gives the value 1:

 $\begin{array}{l} (c+p+R)(E+L+i)(m+b+T)(L+h+e)(S+d+F)(I+L+e)(a+D+k)(M+b+s)(E+Q+I)(O+I+q)(e+i+l)(F+K+D)(o+q+G)(f+S+M)(l+i+E)(L+A+N)(T+C+B)(J+g+h)(e+I+l)(R+t+C)(j+r+p)(A+k+n)(H+g+o)(H+P+j) = 1, \end{array}$

where a = 1 - A, b = 1 - B etc., and + stands for the logical "or".

The (unique) solution (A = 0, B = 1, C = 0, D = 0,E = 0, F = 0, G = 1, H = 1, I = 0, J = 1, K = 1,L = 1, M = 0, N = 0, O = 1, P = 1, Q = 1,R = 0, S = 0, T = 0) was found by a DNA computer in Pasadena, programmed by a Cal Tech - USC team (R. S. Braich, N. Chelyapov, C. Johnson, P. W. K. Rothemund, L. Adelman). "The DNA computation ... exhaustively searched all 2^{20} (1,048,576) possible truth assignments in the process of finding the unique satisfying assignment." The work, described in a Research Article in the April 19 2002 Science, was picked up in the March 19 2002 New York Times, in a piece by George Johnson: "In Classic Math Riddle, DNA Gives a Satisfying Answer" available online. After joking about Mick Jagger and "Can't get no satisfaction," Johnson gives an apt real-world interpretation, corresponding to (a+C+b)(c+E+F)(e+a+B)...:

"Suppose Alice will attend a party only if Caroline does and Bobby doesn't, while Caroline insists that Eric and Francesca be there. Eric, though, refuses to be in the same room with Alice unless Bobby is there to distract her attention. Try to accommodate 20 such prima donnas and there are more than a million (2 to the 20th power) possible combinations to consider."

He notes that "The computation, which took four days of lab work to carry out, would have gone much faster with a regular old computer." In fact the team's report ends by saying "Despite our successes, and those of others, in the absence of technical breakthroughs, optimism regarding the creation of a molecular computer capable of competing with electronic computers on classical computational problems is not warranted." The team goes on to suggest specialized contexts in which molecular computation, as we know it today, might nevertheless be valuable. Johnson's take on the experiment: "What was remarkable was that a swarm of DNA molecules could be coaxed into solving a problem that would flummox an unaided human brain." POINCARÉ CONJECTURE ON NPR, AND IN THE TIMES

On Tuesday morning April 16 2002, listeners to National Public Radio's Morning Edition would have heard Bob Edwards say: "A British mathematician says he's found a way to solve a 100-year-old math mystery. Martin Dunwoody at Southampton University has been working on something called 'the Poincaré conjecture;' it suggests a kind of universal quality of multidimensional space. For example, mathematicians inspired by the conjecture already have proven that in two dimensions the surface of objects like a sphere and a tabletop are similar, but no one has proved the conjecture true in 3-dimensional space. If Dunwoody has solved it, he'll win a million dollars, but not until people such as Arthur Jaffe say it's correct. Jaffe is Professor of Math at Harvard and President of the Clay Mathematics Institute. The Institute will award the million-dollar prize for solving of one of seven math mysteries." Their minds befogged with images of tabletops and spheres, they would have heard Arthur Jaffe explain that the Poincaré conjecture "is regarded as one of the major outstanding problems of the field." Edwards questions him on the status of Dunwoody's claim. Jaffe: "There's a little skepticism." Edwards asks about the other six mysteries, and then "Shouldn't these great minds be working on cancer, or something?" Jaffe answers: "We feel that mathematics is really at the basis of all of science. Cancer of course is important. But these fundamental questions in mathematics have a way of coming up in every field of life." And he ends with: "We think it's very important that the brightest young people in the country, some of them, think about these questions which don't get quite as much publicity as cancer or other medical research at the moment."

Cellular automata at the seashore

A "letter to *Nature*," appearing in the October 25 2001 issue (and picked up in the March 29 2002 email journal Science Week) explains how "an empirically derived cellular automaton model of a rocky intertidal mussel bed based on local interactions correctly predicts large-scale spatial patterns observed in nature." The thick-andthin pattern of mussel colonisation on a typical mussel bed has a fractal-like aspect. J. Timothy Wooton (Chicago) analysed the factors affecting the spread of a mussel colony, including competition from other organisms, the impact of waves, and the tendency of mussels to attach themselves to other mussels. He gathered data for six years at 1400 reference points in a mussel bed on Tatoosh Island, Washington, used the data to specify transition probabilities for a cellular automaton model of the bed, and ran the model for 500 (simulated) years. At the end, the patterns exhibited by the model were THE DIFFERENTIAL EQUATIONS OF PATHOGEN VIR-

quote from *ScienceWeek*).

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found to be in excellent agreement with those occurring in on the site, showing that in this case "processes such as species interactions that occur at a local scale

can generate large-scale patterns seen in nature" (the

An imperfect vaccine can lead to increased virulence in a pathogen to the point where "overall mortality rates are unaffected, or even increase, with the level of vaccination coverage." This in a letter to Nature (Imperfect vaccines and the evolution of pathogen virulence, December 13 2001) from an Edinburgh team led by Sylvain Gandon and Margaret Mackinnon. Gandon, Mackinnon and their collaborators drew their conclusions from the long-term behavior of a system of differential equations, which were set up to analyze the long-term effect of vaccines designed to reduce pathogen growth rate and/or toxicity (as opposed to "infection-blocking" vaccines). The equations are nonlinear but simple in form. The population has two classes of hosts: those that are fully susceptible to the pathogen (density of uninfected x and infected y) and those that are partially immune (density of uninfected x' and infected y'). The system is a set of four differential equations in these unknowns.

Dynamic Catastrophe Theory

The September 14 2001 *Science* has an article by David J. Wales (Universal Chemical Laboratories, Cambridge UK) on a new application of catastrophe theory to the study of the kind of potential energy "landscapes" that occur in complicated energy-minimization problems like protein folding. His principal result in this context is "a quantitative connection between the potential energy barrier, the path length, and the lowest vibrational frequencies for a steepest-descent path linking a minimum and a transition state. This result may appear counterintuitive, for one might suppose that these quantities are independent." In a commentary piece ("Flirting with Catastrophe") in the same issue of Science, Robert Leary (San Diego Supercomputing Center) explains Wales' result in these terms: "He shows that neighboring stable states and the reaction paths that connect them can often be described by universal functional forms dictated by catastrophe theory." He mentions that "The results are validated with large databases of paths for various potentials, with excellent agreement where the minimum lies in close vicinity of the transition point" and concludes "Wales' application of catastrophe theory, an analytical tool not widely familiar to the scientific community, to energy landscapes is an exciting new development."

TINY COMPUTER FACTORS 15

The December 20/27 2001 Nature ran a "letter to Nature" from an IBM Almaden/Stanford University team describing their implementation of Peter Shor's quantum factoring algorithm using a molecule as quantum computer. (Ancillary details appear in an IBM Research News item: IBM's Test-tube Quantum Computer Makes History.) It takes 7 "qubits" to factor 15; Isaac Chuang and his team-mates custom synthesized a special molecule to accomodate and process them. In this molecule, a perfluorobutadienvl iron complex, the computing is done by the five Fluorine atoms and the two Carbon-13 atoms in the center. Those seven nuclear spins carry the qubits of a quantum computation. They can be programmed by radio pulses, they can interact, and they can be read out by nuclear magnetic resonance instruments.

The experiment depends crucially on properties of this special molecule, e.g.: "All seven spins in this molecule

are remarkably well separated in frequency." But "the demands of Shor's algorithm clearly push the limits of the current molecule, despite its exceptional properties." And in fact the IBM News release concedes that "... it will be very difficult to develop and synthesize molecules with many more than seven qubits." This is still significant as the first physical realization of Shor's algorithm. The answer, 3 times 5, was obtained in about 720ms.

WAVES OF MEASLES

An article in the December 13, 2001 Nature applies wavelets to the study of measles epidemics. In "Travelling waves and spatial hierarchies in measles epidemics," Bryan Grenfell (Cambridge), Ottar Bjornstad (Cambridge, Penn State) and Jens Kappey (Penn State) "use wavelet phase analysis" to "demonstrate recurrent epidemic travelling waves in an exhaustive spatio-temporal data set for England and Wales." One of their observations is that the increase in the vaccinated population from 1968 to the late 1980s generates a progressive increase in the period of this wave phenomenon.

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