Satisfied with Physics

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S tatistical physics is one of the pillars of modern physics, explaining the macroscopic world on the basis of the dynamics of its microscopic components. But methods from statistical physics can also foster a deeper understanding of computational phenomena. On page 812 of this issue, Mézard et al. (1) use this approach to characterize the properties of random instances of the satisfiability problem in unprecedented detail. They also introduce a novel strategy for finding solutions to this problem.

Satisfiability (SAT) is a logical reasoning problem defined in terms of Boolean variables \(a, b, c,\) and so forth) and logical constraints describing the relation between these variables. Each variable can be either “True” or “False.” An example of a constraint is

\[
a \text{ OR } (\text{NOT } b)
\]

A SAT problem is solved by assigning truth values to the variables such that all constraints are satisfied simultaneously. For example, the constraint in Eq. 1 is satisfied if \(a\) is “True” or \(b\) is “False.”

The SAT problem plays a central role in the quest for more efficient ways of solving large-scale computational problems, such as planning and scheduling, finding the folded state of a protein, and determining whether a computer chip design meets its specification. These problems are called “NP-complete.” Thousands of NP-complete problems are known; all can be encoded as SAT problems (see the second figure).

It is widely believed that there does not exist an efficient algorithm for solving NP-complete problems. Formally proving that no such algorithm exists is one of the main open problems in modern computer science (2). NP-completeness is, however, a worst-case notion, capturing the computational cost of the very hardest possible instances of the problem. In practical applications, one may not encounter instances that are quite that hard. What, then, is the computational cost of “typical” instances? One can obtain important insights into typical case complexity by considering randomly generated SAT problems.

Mézard et al. (1) consider random instances of a particular case of SAT, the K-satisfiability problem (K-SAT), in which each constraint contains exactly \(k\) variables. Such randomly generated instances exhibit a “phase transition” as a function of the ratio \(\alpha\) of constraints to variables (3). K-SAT problems with a small \(\alpha\) value almost all have one or more satisfying assignments, whereas problems with a large \(\alpha\) value have too many constraints and become unsatisfiable (that is, no setting of the variables simultaneously satisfies all constraints). As the number of variables grows, the transition from almost always satisfiable to almost always unsatisfiable becomes very sudden (see the first figure). For 3-SAT (that is, \(k = 3\)), the transition occurs at \(\alpha = 4.25\). The exact location of the phase transition threshold has not yet been derived rigorously (4–8).

Many of the computationally hardest problem instances appear to lie in this phase transition area. Hence, a better understanding of the phase change in the K-SAT problem may also provide new insights into its computational properties and strategies for solving it.

References and Notes
11. M. Mande, personal communication.
14. We thank J. Picaut for discussions about ENSO and PDO.
An approach that is often effective for solving the K-SAT problem is called local search. The search starts from a randomly generated truth assignment. One then changes or “flips” the truth value of one of the variables to try to satisfy more of the constraints. Such flips are repeated until a satisfying assignment is found. However, the set of possible truth assignments is exponentially large—$2^N$ truth assignments for $N$ variables. A large number of flips may be required, depending on the structure of the search space (9).

Mézard et al. (1) provide a remarkably detailed picture of the search space of a random K-SAT problem and introduce a new algorithm for finding a satisfying assignment. The algorithm is based on the cavity method from statistical physics. In this approach, the concept of a cavity field is used to measure the tendency of a variable to be “True” when one of the clauses containing the variable is removed from the SAT problem. In effect, the method exploits the topology of the search space to navigate efficiently through the exponentially large set of assignments.

The authors show how the search space for $k \geq 3$ changes dramatically when one approaches the phase transition region. For $k = 3$ and $\alpha < 3.92$, the search space is globally smooth, with the solutions grouped together. A basic local search method can find a satisfying assignment relatively quickly. However, for larger values of $\alpha$, the space breaks up into a number of metastable states, signaling the onset of search complexity. A basic local search method will get “stuck” at assignments with a nonzero number of unsatisfied clauses. In such cases, Mézard et al.’s method still has a high probability of finding a satisfying assignment.

Mézard et al.’s technique is general and holds promise for a wide range of hard computational problems. However, because SAT problems in real-world applications are not random, the approach may have to be adapted for SAT problems that are more structured (10–13). The work illustrates the power of bringing together ideas and techniques from statistical physicists interested in disordered systems, mathematicians studying combinatorial structures, and computer scientists studying computational complexity.

References and Notes
2. See www.claymath.org/prizeproblems/pvsnp.html.
11. See also www.cs.cornell.edu/gomes/demos.
13. See also www.satlive.org.

PERSPECTIVES: SILICON CHEMISTRY

R₃Si⁺—Free at Last

Peter P. Gaspar

Cations containing a tri-coordinate silicon atom, R₃Si⁺, well separated from counterions and solvent molecules have been avidly sought for decades (1). On page 825 of this issue, Kim et al. (2) bring this search to a successful conclusion by presenting the crystal structure of the salt of such a cation.

Silicon is in the same group as carbon and shares some of its chemical characteristics. But silicon chemistry often follows pathways different from those of carbon. To understand reaction mechanisms for silicon compounds, one must synthesize and study silicon analogs of the reactive intermediates of organic chemistry.

The trivalent silyl cation R₃Si⁺ has been particularly challenging. To solve this problem, chemists have had to view the covalent bond in shades of gray rather than black and white—as a continuum of electronic interactions of varying strength, rather than as a link between atoms that is either present or absent. New quantitative probes for the extent of bonding of ions with surrounding species had to be developed, and a seeming paradox had to be resolved: Why are R₃Si⁺ cations difficult to detect in solution, yet comparatively easy to make in the gas phase (3)?

In normal organosilicon compounds, R₃Si-Z, silicon is attached to four groups.

How can an Si-Z bond be broken in such a manner that a trivalent silicon cation is created? Researchers have looked to analogous carbon compounds, RₓCₓ–, for answers. But most Z groups that easily ionize from RₓCₓ–Z to form RₓC⁺ do not readily depart from the silicon compound because the Si-Z bonds are stronger than the equivalent C-Z bonds.

Hydrogen is unusual in that C-H bonds are stronger than Si-H bonds. Hence transfer of a hydride ion, H⁻, from RₓSiH to a carbon cation could lead to the formation of a silyl cation. But when the salt of a carbon cation was used as a hydride acceptor (4), the products proved to be silyl esters (5). If a silyl cation formed at all, it was immediately consumed by the counterion.

Why can a carbon cation, Ph₃C⁺, persist in the presence of ClO₣⁻, but a silyl cation, R₃Si⁺, is immediately captured by this anion? Silicon forms a much stronger bond with oxygen than does carbon, and silicon cations are stabilized to a lesser ex-