

dominantly X-H... σ hydrogen bonds at all. Could it be that they are really N-H...M hydrogen bonds where the true acceptor function is a nonbonding pair of electrons on the metal itself and the short H...H distance is merely a consequence of the short H...M distance?

Moving to B-H bonds as acceptor entirely removes this ambiguity because boron has no nonbonding electrons but only has the σ -bonding electrons of the B-H bond, so an N-H... σ bond is the only type of interaction that can be considered. Borane-ammonia, H_3BNH_3 , attracted our attention because, although it is isoelectronic with a gas, ethane (H_3CCH_3 , melting point 183°C), it is a solid with a melting point of $+109^\circ\text{C}$. Just as the classical H bonding in water is thought to be responsible for elevating its melting point by nearly 100° from what it would be in the absence of H bonding, the melting point elevation in H_3BNH_3 seemed abnormally high unless dihydrogen bonding were important. Although the reported x-ray structures of H_3BNH_3 indeed indicated close H...H distances, the conformation of the

N-H...H-B unit was the exact reverse (namely, structure **6**, with $Y = \text{N}$ and $X = \text{B}$) of the expected conformation, (structure **6**, with $Y = \text{B}$ and $X = \text{N}$). The expected conformation (**6**, with $Y = \text{B}$ and $X = \text{N}$) was indeed found in a Cambridge Crystallographic Database search of many other borane amine compounds. This anomaly was sufficiently troubling that we asked Tom Koetzle and Wim Klooster of the Brookhaven National Laboratories if they could obtain a neutron-diffraction structure of H_3BNH_3 (5). The results unambiguously show the presence of short H...H contacts (2.02 to 2.23 Å), but the most surprising aspect of this work was the demonstration that boron and nitrogen had been misassigned in the previous x-ray work, where the distinction between B and N is less marked than in n diffraction; such a misassignment of two light elements differing by two units in atomic number was surprising. With the corrected assignment, the shortest H...H contact now indeed corresponds to the expected N-H...H-B conformation (**6** with $Y = \text{B}$ and $X = \text{N}$) (5).

The dihydrogen bond seems to be general for interactions between hydrides YH with a hydridic hydrogen and classical hydrogen bond donor groups, such as NH or OH bonds. It has a marked structural preference and also influences physical properties. Just as nature uses the classical H bond in enzymatic catalysis, we now need to harness the dihydrogen bond to promote chemical reactivity and selectivity, for example, in chemical catalysis. This is an area that will challenge our still limited ability to design molecules to have useful and tunable catalytic properties.

References and Notes

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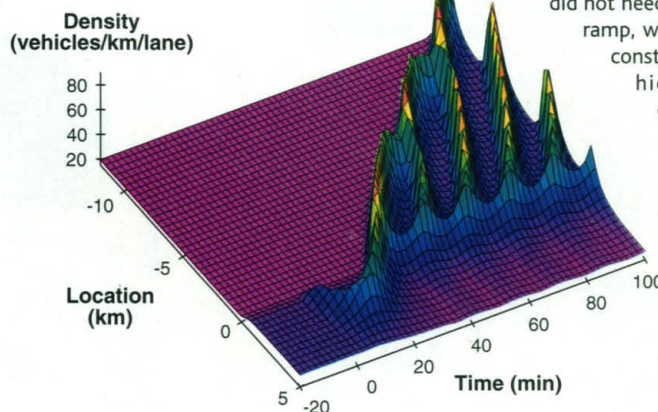
PERSPECTIVES: TRAFFIC THEORY

Jams, Waves, and Clusters

Dirk Helbing and Martin Treiber

Have you been suffering from traffic jams lately and asking yourself why freeways are not free ways anymore? Help may be on the way. There have been several recent advances in traffic theory, notably those that treat traffic like a fluid. Researchers at Seoul National University (1) have now offered an interpretation of a recently discovered state of congested traffic, called "synchronized" traffic (2). Their fluid-dynamic simulations could be a useful tool for an optimization of traffic flow on motorways.

When Nagel and Schreckenberg presented their cellular automaton model of traffic flow in 1992 (3), allowing for a more than real-time simulation of the entire road system of large cities, they probably did not anticipate the resulting flood of publications and the enthusiasm among scientists on the subject of traffic theory. By treating huge numbers of interacting vehicles similar to classical many-particle systems, physicists have recently contributed to a better understanding of traffic flow. The mathematical



Life in the slow lane. Formation of the recurring hump state (RH) on a freeway for the model and parameters used by Lee *et al.* (7). Because we used free rather than periodic boundary conditions, the inflow at the on-ramp located at 0 km did not need to be balanced by an off-ramp, which is more realistic. The constant ramp flow of 318 vehicles per hour and lane causes a higher vehicle density downstream of the ramp. Nevertheless, free flow pertains, until a short perturbation of the ramp flow occurs at time 0 min, which moves downstream in the beginning. However, with growing amplitude, the perturbation changes

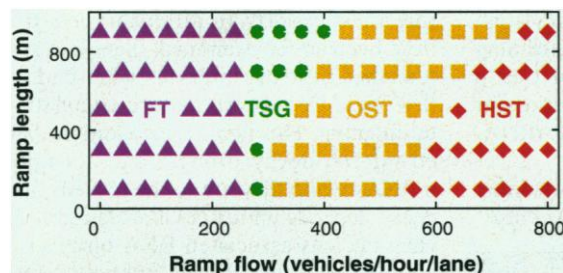
its propagation speed, reverses its direction, and finally induces another, bigger perturbation, when passing the ramp. This process repeats again and again, in this way generating the oscillating RH state. When passing the ramp, the perturbations continue their way upstream, until they merge with one of the humps that were born later.

tools that they use, stemming mainly from statistical physics and nonlinear dynamics, have proved their interdisciplinary value many times. This includes concepts reaching from self-organized criticality and phase transitions up to the kinetic theory of gases, fluids, and granular media.

In traffic, drivers try to maximize their own advantage (that is, their velocity, safe-

ty, and comfort) within the constraints imposed by physical limitations and traffic rules. Under certain conditions, their competitive, nonlinear interactions give rise to the formation of collective patterns of motion like traffic jams. The various observed phenomena on freeways are surprisingly rich: Apart from free traffic and extended traffic jams behind bottlenecks, there are

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On the highway. Phase diagram of the various traffic states that can occur close to an on-ramp in the presence of small perturbations in the ramp flow. We show the dependence of the traffic states on the ramp flow and the ramp length for a flow of 1800 vehicles per hour and lane on the freeway. For small ramp flows, free traffic (FT) survives. At higher inflows, two different kinds of RH states can build up, either triggered stop-and-go waves (TSG) or oscillatory synchronized traffic (OST). High ramp flows are associated with a homogeneous form of synchronized congested traffic (HST).

localized clusters (small moving jams) and stop-and-go waves. In addition, Kerner and Rehborn (2) have recently discovered a hysteretic phase transition from free traffic to a new form of congested traffic (mostly appearing close to on-ramps) that had not been identified in more than 40 years of traffic research, they say. Kerner and Rehborn call it “synchronized” traffic because of the synchronization of velocities among lanes. However, the more characteristic feature is its high flow in spite of the breakdown of velocity, which is in contrast to typical traffic jams. Downstream of the ramp, the breakdown of velocity eventually relaxes to free traffic in the course of the freeway. Another interesting property is the wide scattering of synchronized traffic states, when plotted in the flow-density plane, which differs from the quasi-linear density dependence of free traffic flow.

Lee *et al.* (1) have now suggested an explanation for this hysteretic phase transition. They simulated freeways, including on- and off-ramps, with a fluid-dynamic traffic model that is closely related to the Navier-Stokes equations for viscous, compressible fluids. However, it contains an additional relaxation term describing adaptation of average vehicle velocity to an equilibrium velocity, which monotonically decreases with growing density. In comparison with previous simulation studies, Lee *et al.* used another velocity-density relation and a considerably different set of parameters. With a temporary peak in the on-ramp flow, they managed to trigger a form of oscillating congested traffic that is propagating upstream, but pinned at the location of the ramp (see figure on previous page). They call it the “recurring hump” state (RH) and compare it with autocatalytic oscillators in chemistry. Free traffic would correspond to a point attractor and the oscillating traffic

state to a stable limit cycle. In terms of nonlinear dynamics, the transition corresponds to a Hopf bifurcation, but a subcritical one, because the critical ramp flow depends on the size of the perturbation.

Lee *et al.* point out that free traffic survives the assumed pulse-type perturbation of finite amplitude, if the ramp flow is below a certain critical value. However, once a RH state has formed, it is self-maintained until the ramp flow falls below another critical value that is smaller than the one for the transition from free traffic to the RH state. This proves the hysteretic nature of the transition. More-

over, Lee *et al.* could show the gradual spatial transition from the RH state to free flow downstream of the ramp. They also managed to reproduce the synchronization among neighboring freeway lanes as a result of lane changes. Therefore, they suggest that their model can describe the empirically observed first-order phase transition to synchronized traffic. The two-dimensional scattering of synchronized traffic states is understood as a result of the fact that the amplitude of the oscillating

traffic state depends on the ramp flow.

Although the interpretation of synchronized traffic by Lee *et al.* does not quantitatively agree with the observations, in various respects it comes pretty close to reality. Meanwhile, our recent work has offered a more complete explanation (4). Above all, the findings are also of great practical importance. A detailed analysis shows that there is a whole spectrum of different states that can form at ramps. Their occurrence decisively depends on the inflow as well as the ramp length (see figure on this page). This is relevant not only for an appropriate dimensioning of ramps, but also for an optimal on-ramp control.

Traffic theory is now more interesting than ever before. Recent advances have yielded a better understanding of traffic flow phenomena as well as realistic and fast simulation models. Scientists are now prepared to design on-line controls for efficient traffic optimization, calculate the environmental impact of congestion, and develop methods for traffic forecasts.

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PERSPECTIVES: MOLECULAR BIOLOGY

Nuclear Functions Charge Ahead

Anita K. Hopper

In eukaryotic cells, chromosomal genes are first transcribed into RNA as large precursors and processed into mature RNAs in the cell's nucleus. These mature RNAs are then exported out of the nuclear interior to the cytosol, where they direct protein synthesis. What prevents the transcripts from traversing the boundary between the nucleus and the cytosol before they are completely processed? The report by Lund and Dahlberg on page 2082 of this week's issue provides surprising answers to this question. By injecting test RNAs into *Xenopus* oocytes, Lund and Dahlberg show that a proofreading system located within the nucleus and an ordered pathway of pre-tRNA processing are responsible for exclusion of pre-tRNAs from the cytosol. The proofreading system monitors both the appropriate three-dimension-

al structure of tRNAs and the fidelity of the processing at the 5' and 3' ends of the RNAs. Only properly folded tRNAs with mature termini leave the nucleus.

How is this proofreading accomplished? Even though there was no previous evidence that the enzymes that load amino acids onto tRNAs (aminoacyl synthetases) function in the nuclear interior, the fact that they process only tRNAs with mature 3' termini (1) and that there are nuclear pools of these enzymes (2) led Lund and Dahlberg to propose that aminoacylation might be the proofreading step. Now they provide compelling evidence that, contrary to dogma, tRNAs are charged in the nucleus and that inhibition of aminoacylation retards tRNA export from the nucleus. Thus, nuclear tRNA aminoacylation is a proofreading mechanism which ensures that only properly folded tRNAs with mature ends are exported to the cytosol (see the figure).

Previous studies of tRNA processing in *Xenopus* oocytes indicated that removal of intervening sequences (introns) from pre-

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