# Quantum Molecular Virtual Laboratory

WHAT happens to water under high pressures and temperatures? Why does silicon carbide break where it does when strained? How does DNA interact with water?

Complete, accurate answers to these deceptively simple questions—and others like them—require knowing what is going on at the atomic level. This means one must account for the behavior of individual atoms and electrons in an entire system: how they move, how they chemically bind, and how those bonds form and break. Not an easy proposition, once one moves beyond a small number of simple atoms.

Computers have long been used to model material behavior, both on the large and small scales. Macroscopic-scale modeling applies statistical mechanics methods to the system as a whole, ignoring details about how each atom responds. Atomic-scale modeling applies the laws of quantum mechanics—fundamental physics equations that describe electrons—but because of the complex nature of the equations, these models can handle only a few atoms at a time.

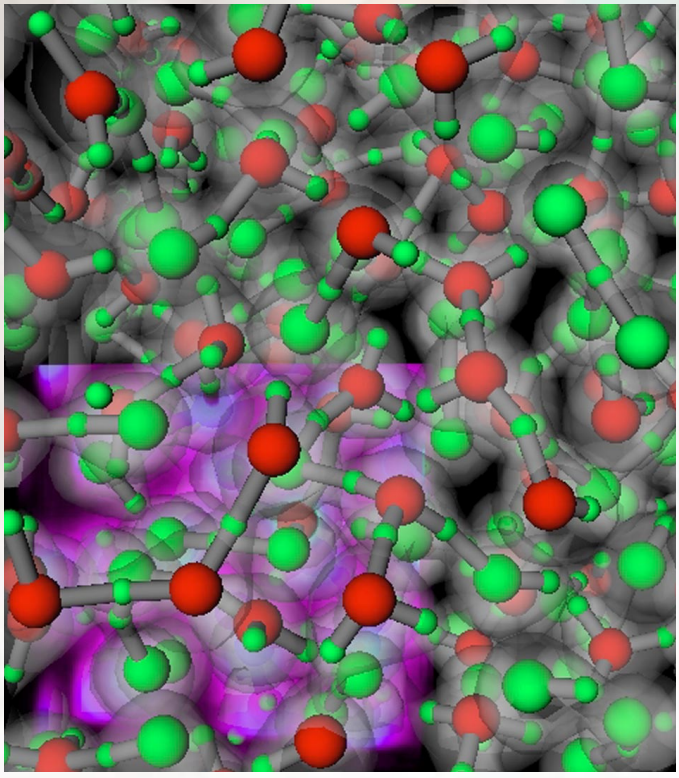

**Figure 1.** This quantum-level simulation of hydrogen fluoride–water mixtures at high temperatures and pressures took 15 days on the ASCI computer, on which trillions of operations per second were performed, to calculate one picosecond of the mixtures' atomic interactions.

Lawrence Livermore physicists Francois Gygi and Giulia Galli and their collaborators are using the computer power of the Department of Energy's (DOE's) Accelerated Strategic Computing Initiative (ASCI) and Gygi's JEEP code to push the limits of atomic-scale modeling of complex systems. ASCI, guided by the Office of Strategic Computing and Simulation under the DOE Assistant Secretary for Defense Programs, is developing capabilities to simulate nuclear weapons performance in lieu of nuclear testing. To do so requires computers of unprecedented computational power and speed, as well as simulation codes such as JEEP.

JEEP, which Gygi began developing at the Swiss Federal Institute of Technology about five years ago, uses quantum molecular dynamics (QMD) methods to simulate the behavior of materials at the microscopic level. "Unlike the macroscopic-scale codes, we make no assumptions in using JEEP," explains Gygi. "Using QMD, we input only absolutely known quantities into the code—that is, the identities of the atoms and the laws of quantum mechanics. Combining this approach with ASCI's computational power, we can examine material systems of hundreds of atoms and thousands of electrons extremely accurately."

With JEEP, the ASCI computer becomes a virtual laboratory, where scientists can follow the trajectories of atoms and study the forming and breaking of chemical bonds. This powerful combination can be used to predict physical properties of various materials, investigate properties not directly accessible through physical experiments, and interpret and complement physical experiments.

QMD simulations have a number of applications, from deepening our understanding of materials under extreme conditions—a vital issue for DOE's Stockpile Stewardship Program—to forming a better understanding of complex biological systems.

## Modeling the Impossible Experiment

The detonation of some high explosives produces hydrogen fluoride and water, both of which are hydrogen-bonded systems. Little is known about this mixture because hydrogen fluoride is toxic and corrosive, making experiments difficult.

Using the JEEP code on the ASCI computer, Galli, Gygi, and physicist Francis Ree conducted quantum-level simulations of hydrogen fluoride–water mixtures at high temperatures and pressures (Figure 1). These simulations were of unprecedented scale: a picosecond-long "peek" at the interactions of 600 atoms with 1,920 electrons required updating and computing 200 million unknowns. It took 15 days and the entire resources of ASCI's Sustained Stewardship Blue Pacific machine, with teraops (trillions of operations per second) calculational power, to simulate this one picosecond's worth of interactions.

The results provided a better understanding of high-explosive detonation products, revealing their molecular interactions and chemical reactions. The results also helped scientists better understand the equation of state of the mixture. The simulations indicated that hydronium fluoride and hydrogen difluoride anions are produced at high pressures, something that has been hypothesized but not yet observed.

## Stretch and Break

In another numerical experiment, Gygi and Galli simulated what would happen when a microscopic chunk of amorphous semiconductor (silicon carbide) is stretched past its breaking point (Figure 2).

"One of the advantages of computational simulations over experiment, in general, is that we can define chemical purity at 100 percent," explains Galli. "We can create the configuration that we want, apply a strain to the system, and let the code run. We watch what happens, what bonds break and where, and how the resulting microfracture relates to the chemical properties of the material."

These quantum simulations provided numbers relating to the elasticity and hardness of the material that could then be compared to results gathered from physical experiments. Galli notes that this was the first time hardness had been computed from first principles for a disordered alloy. "In the past," says Gygi, "it's only been computed for crystal or ordered structures, because disordered systems are much more complex."

They also discovered that the simulated semiconductor material broke at a silicon-rich "island" and were able to define the surface where the material cleaved. "Most of the surface atoms were silicon," says Galli. "In laboratory experiments with this material, physicists find precisely that, so we were pleasantly surprised when we saw it in our numerical experiment as well."

Galli and Gygi plan to continue these studies by simulating atomic clusters residing on other types of semiconducting surfaces as well.

## Delving into DNA

Their most recent work involves examining components of the familiar two-strand, double-helix DNA structure. Each strand of DNA consists of a "backbone" on which chemical bases attach. When the two strands are wound around each other in the familiar configuration, a base from one strand attaches to a base on the partner strand, forming base pairs that step up like ladder rungs (Figure 3).

Working in conjunction with Michael Levitt from Stanford University and Livermore's Eric Schwegler, Gygi and Galli are examining what happens to the DNA backbone in water, its natural medium. They plan to isolate a fragment of the DNA backbone and simulate how a molecule of dimethyl phosphate from that fragment interacts with water molecules. While the Livermore scientists use JEEP for the simulation, Levitt will be running a simulation code with his widely used model of this interaction. The numerical experiments at Livermore are expected to validate or invalidate some of the assumptions

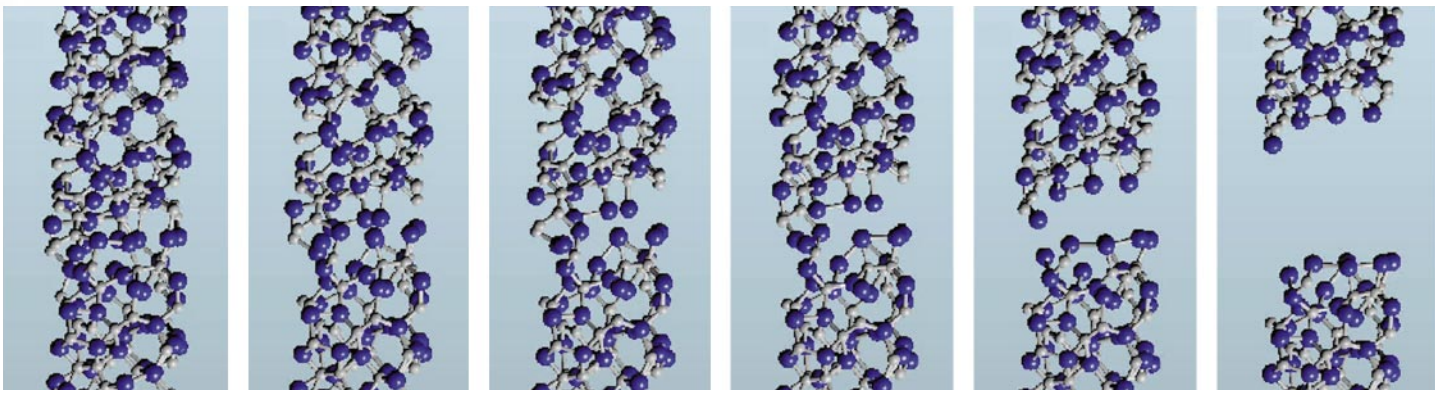

**Figure 2.** A chunk of silicon carbide, a disordered structure, was simulated being stretched to breaking to see which bonds break and how the resulting microfracture relates to its chemical properties.

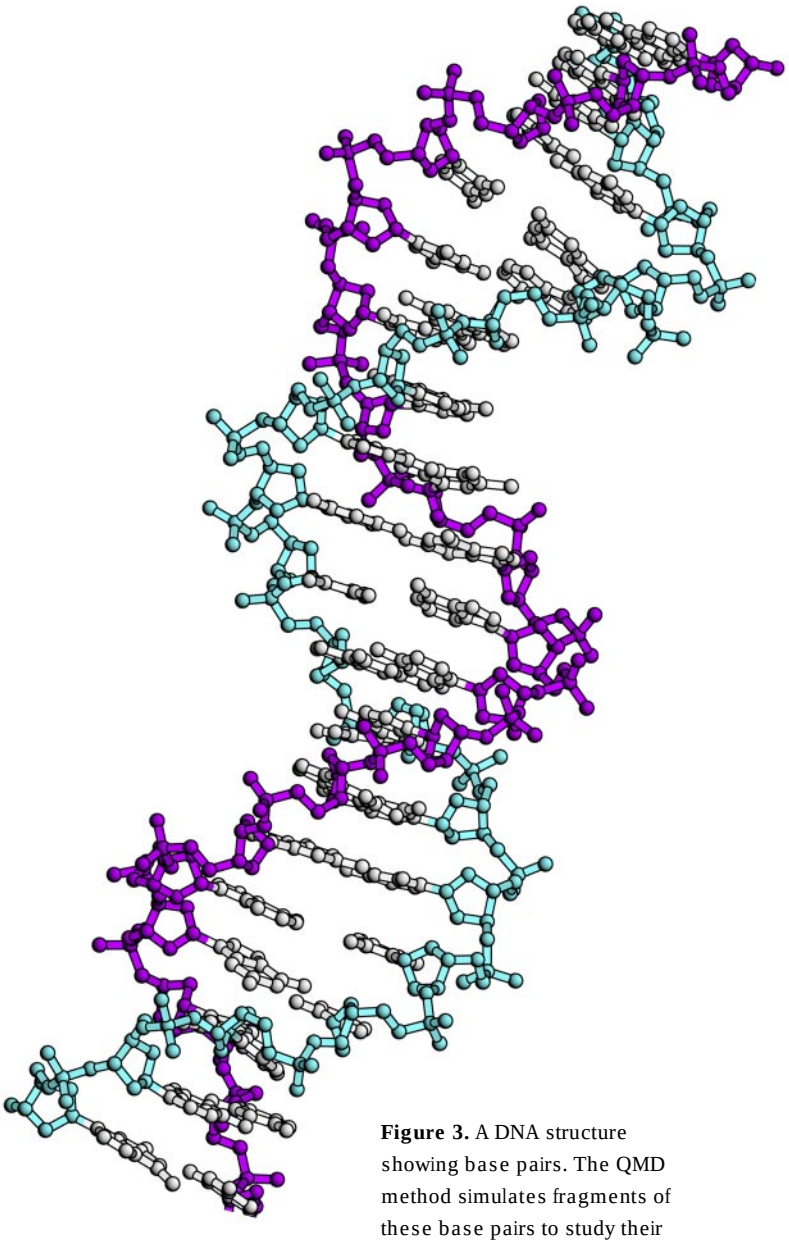

**Figure 3.** A DNA structure showing base pairs. The QMD method simulates fragments of these base pairs to study their molecular interactions and understand DNA binding and replication mechanisms.

made in standard models and serve to improve them. The results will also deepen understanding of this complex biological system. The work is being carried out within a Laboratory Directed Research and Development strategic initiative on computational biology led by Mike Colvin.

In another DNA experiment, Gygi, Colvin, Raymond Fellers, and Daniel Barsky are extracting a single DNA base pair to see how the complementary bases interact. They expect to better understand what causes DNA to bind and which molecular interactions are key to binding. On a larger scale, they hope to find out how binding mechanisms affect the replication of DNA.

At stake is understanding the fidelity of DNA replication. Sometimes, because of damage or mutation, a different molecule replaces one of the bases. The question then is, will the DNA successfully replicate itself? "Understanding this issue is a very long-range goal," Gygi notes. "For the short term, we hope to calculate the energy needed to separate a base pair and, through the results, discount certain scenarios of DNA binding."

"One key thing to keep in mind about all this work," adds Gygi, "is that the JEEP simulations do not provide the full picture. But they do provide key pieces to a puzzle, which allow us to look at yet other pieces and say whether those are a part of the same puzzle."

### Laboratory Is a Unique Environment

The Laboratory provides the requisite elements for performing QMD: top-notch physics, the biggest computational machines available, and state-of-the-art visualization tools to help view and interpret enormous amounts of data. "There are few places in the world where you can pull all this together," says Gygi. "We've been able to apply our methods to different problems and learn things that relate to other areas of research. The big machines with terascale computing power have made it possible to study more and more complex systems, more reliably and accurately. Finally, these big machines have made it possible to build a bridge between two worlds of simulation—the macroscopic-scale simulations using statistical mechanics and the atomic-scale simulations using quantum mechanics."

*—Ann Parker*

**Key Words:** Accelerated Strategic Computing Initiative (ASCI), computational biology, DNA, high explosives, JEEP, material behavior, quantum molecular dynamics (QMD), semiconductor.

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# AAA in the Sky for Satellites

JUST beyond Earth's upper atmosphere, huge numbers of satellites and related "space junk" orbit about the planet. Their numbers will continue to grow as new launch vehicles bring about more routine and lower-cost access to space. Forecasts show that during the next decade, between one and two thousand new satellites will be put in orbit. Over time, some of them inevitably will begin to fail and will need to be inspected, monitored, repaired, or removed.

Lawrence Livermore is developing a very maneuverable microsatellite that can operate as a service vehicle in space for ailing satellites. The tiny, 40-kilogram vehicle, dubbed MicroSat, will be the first truly agile, small satellite. Once deployed, it will perform close-up inspections to determine the health and operational status of other satellites in orbit (Figure 1). Because the MicroSat can get close to other satellites, it can use new types of diagnostic sensing techniques to collect data unattainable from the ground. Active vibration sensing, for example, can yield specific information on moving parts that can be used to evaluate and characterize vehicle wear and performance degradation remotely. Thermal imaging can reveal surface features invisible to the eye, including leaks and nonuniformities that may result from changes in thermal insulation or structural fatigue.

These on-orbit measurements will offer early detection of potential failures and insight into events that might limit the life of the satellite. Periodic checks could allow preventive or corrective measures and avoid unexpected system breakdowns that lead to service outages, as occurred in 1997 to a communications satellite supporting a large paging system. The Livermore MicroSat is being designed to perform autonomous docking with ailing satellites and could eventually fly missions to repair or retrieve them. A docking maneuver is shown in Figure 2.

The Livermore team of 15 engineers and technicians is led by physicist Arno Ledebuhr; engineer Joe Kordas is the deputy project leader. The MicroSat program is funded by the U.S. Air Force Research Laboratory and is a spin-off from the Clementine II Program, which consisted of an asteroid fly-by and impact experiment. That earlier project was discontinued in 1997 and redirected by the Air Force to a series of MicroSat Earth-orbit demonstrations.

The team is working toward a date in 2002 when one of its MicroSats will be flown on either the space shuttle or an expendable launch vehicle. If flown on the shuttle, the Livermore MicroSat will ride on a National Aeronautics and Space Administration *Spartan 251* "mothership carrier" spacecraft bus. The Livermore MicroSat will have to autonomously perform a series of complex tasks and conduct various close-in proximity maneuvers within a few meters of the *Spartan* carrier. It will collect stereo images and perform multiple autonomous dockings with the *Spartan*. Experiments

**Figure 1.** In this artist's rendering, a MicroSat gets a close look at a larger satellite. The goal is for the MicroSat to rendezvous with a satellite, inspect it, dock with it, service it, and verify its performance. It will look for signs of wear, including atomic oxygen and ultraviolet surface damage, micrometeoroid impacts, and debris cloud generation from leaks or other deterioration. These data can be stored on board or forwarded to ground control through an Ethernet connection.

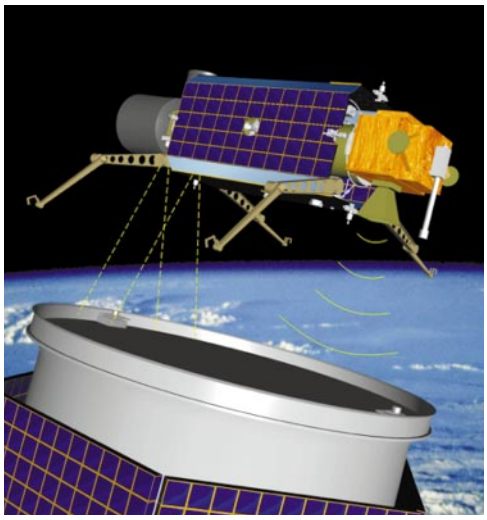
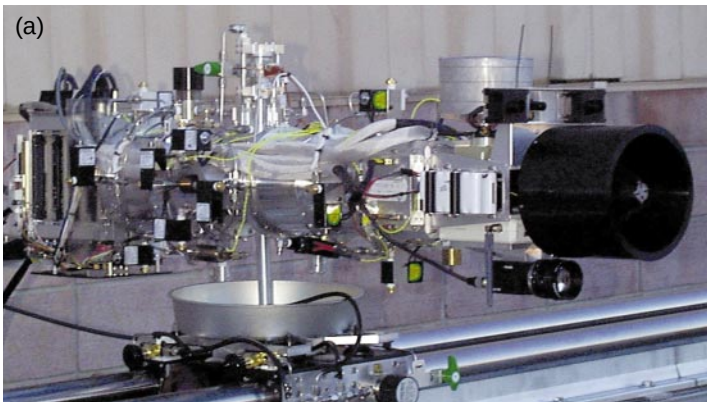


**Figure 2**. Active radar or lidar, augmented by stereo imaging, will be used for precision ranging during the final docking phase. Once docked, the MicroSat will be able to repair or replace subsystems, tow or push the satellite to a different orbit, and pull "space junk" out of orbit.



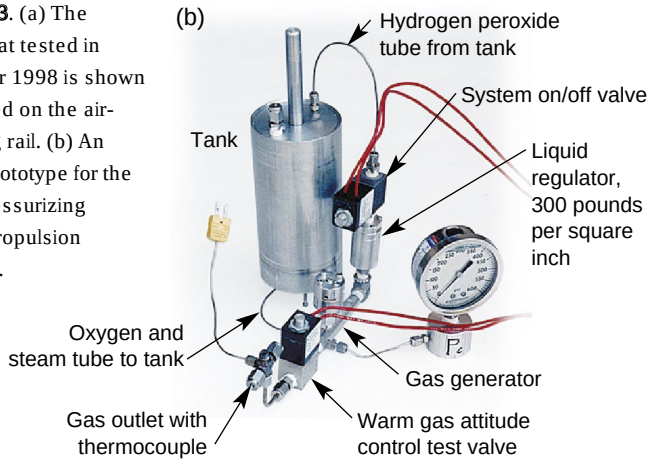




**Figure 3**. (a) The MicroSat tested in October 1998 is shown mounted on the air-bearing rail. (b) An early prototype for the self-pressurizing micropropulsion system.

will include the transfer of data and power between the two spacecraft. The Livermore MicroSat will then maneuver itself into its original deployment canister on board the *Spartan* mothership, which will be retrieved by the space shuttle and returned to Earth. Follow-on spacecraft experiments will examine autonomous docking onto a spinning satellite, propellant transfers, and towing experiments.

## Old Hardware Put to New Use

The first prototype MicroSat was constructed in 1997 with spare hardware collected during earlier program efforts. It was operated on a new dynamic air-bearing table that enabled extensive and repeated ground testing of its guidance, navigation, and control software (see *S&TR*, September 1998, pp. 24–26). The next prototype was based on the Clementine II asteroid-impact probe vehicle and contained the first liquid propellant propulsion system. This MicroSat design was augmented with additional support subsystems to provide stand-alone operation in orbit, including solar arrays for battery recharging, thermal management, micropower impulse radar for docking, stereo cameras for passive ranging and telepresence, and a global positioning system receiver. The third vehicle incorporated improvements in propulsion, electronics, and sensors. For future vehicles, the team wants to add grappling and robotic arms for manipulation during docking and servicing missions.

The test vehicles combine the team's unique designs, other Livermore developments, and commercial systems. To date, three prototype vehicles have been ground tested on the air-bearing table, and the two most recent models have been tested outside on an air-bearing rail.

## Darting about in Space

A critical aspect of the MicroSat design is its propulsion system, which must be able to move the vehicle about in orbit as well as control the satellite's attitude. There is no precedent for small, agile orbiting satellites with the large propulsion capability of the Livermore MicroSat designs. For maximum agility and range, the MicroSat must have the highest possible ratio of fuel capacity to overall mass. This goal is achieved by reducing the vehicle's dry weight and using miniaturized subsystems throughout.

Conventional spacecraft propulsion systems use high-pressure-fed toxic liquid fuels, but these systems cannot be miniaturized easily. Many small spacecraft use compressed gas such as nitrogen, which works well for attitude control but not

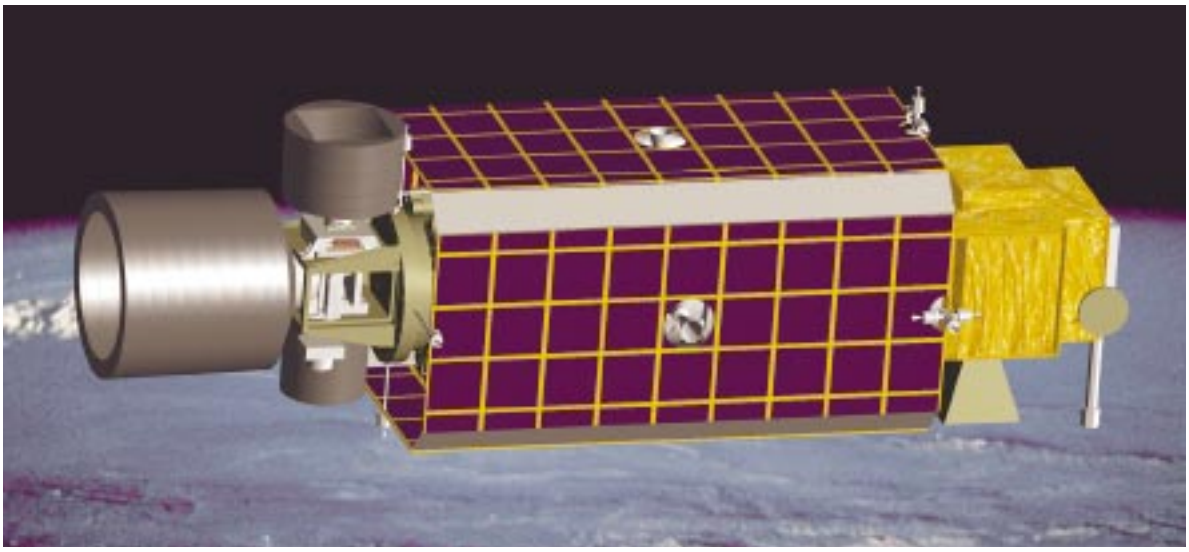


**Figure 4.** Artist's rendering of the MicroSat that will fly on the space shuttle.

for maneuvering. Compressed gas tanks also tend to be heavy. "Enabling agile maneuvering on a tiny scale requires fundamental advances," notes lead propulsion engineer John Whitehead.

Liquid can be stored more efficiently (that is, in lighter weight tanks), so MicroSat's innovative propulsion system relies on the concept of making gas as needed from liquid fuel. The system supplies tiny gas jets for vehicle attitude control and small precision maneuvers and fuels liquid thrusters for large orbital maneuvers.

Most rocket fuels are toxic, but Whitehead opted for nontoxic, high-concentration hydrogen peroxide ($H_2O_2$) to ease experimentation and development processes and thus reduce the cost of the project. Hydrogen peroxide was the first choice because of its proven track record. The U.S. space program used it in the past, and the Russians still fly their *Soyuz* vehicles with it.

For testing purposes, the Livermore team's first prototype MicroSats used compressed nitrogen ($N_2$) only. The next vehicle used $N_2$ for attitude control but added liquid $H_2O_2$ thrusters for directional maneuvering. The $N_2$ forced the $H_2O_2$ out of the liquid thrusters in a pressure-fed system.

The latest version, tested in October 1998, eliminated the $N_2$ system altogether, saving the weight of its relatively heavy storage tanks. A patented micropump designed by Whitehead is used to self-pressurize the liquid $H_2O_2$ tank, with oxygen and steam derived from the propellant itself. Shown in Figure 3, the system is lighter than its predecessors, although it still requires a higher-pressure liquid tank to operate. This self-pressurized system provides a constant system pressure as propellant is expended. It could be launched unpressurized or at low pressures, making launch safer as well.

The next step is to develop a slightly larger and more efficient pump that draws the liquid $H_2O_2$ out of its tank, making the satellite even more lightweight and agile. More of the system's total weight can be devoted to fuel and less to components.

Aside from the revolutionary propulsion system design, the Livermore MicroSat uses the latest generation of Power PC processors and compact PCI-format electronics. It also incorporates advanced active pixel sensors that, along with miniaturized laser ranging systems, will provide the necessary range and velocity data to allow autonomous docking by MicroSat. Figure 4 shows the team's vision for MicroSat's final design.

Ledebuhr says, "The MicroSat will move like a hummingbird darting around." Some day, near-Earth space may be dotted with these autonomous, hummingbirdlike MicroSats. They won't change flat tires, but they will help other satellites stay healthy.

*—Katie Walter*

**Reference**

"Testbeds Wring Out Technologies," *Aviation Week & Space Technology*, April 5, 1999, pp. 52–53.

**Key Words:** agile satellite, hydrogen peroxide propulsion, microsatellite (MicroSat).

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