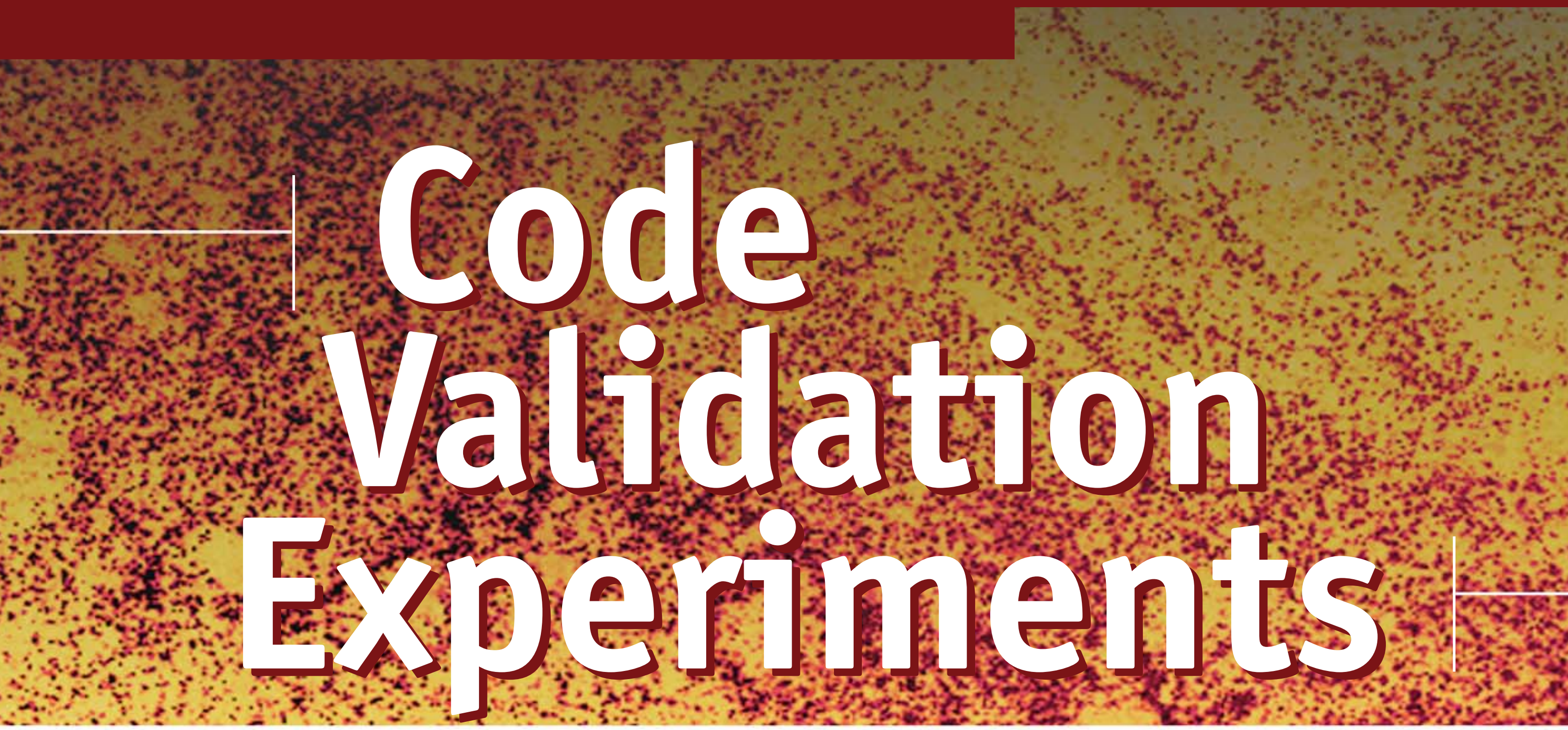


Code Validation Experiments

— a key to predictive science

by Brian Fishbine

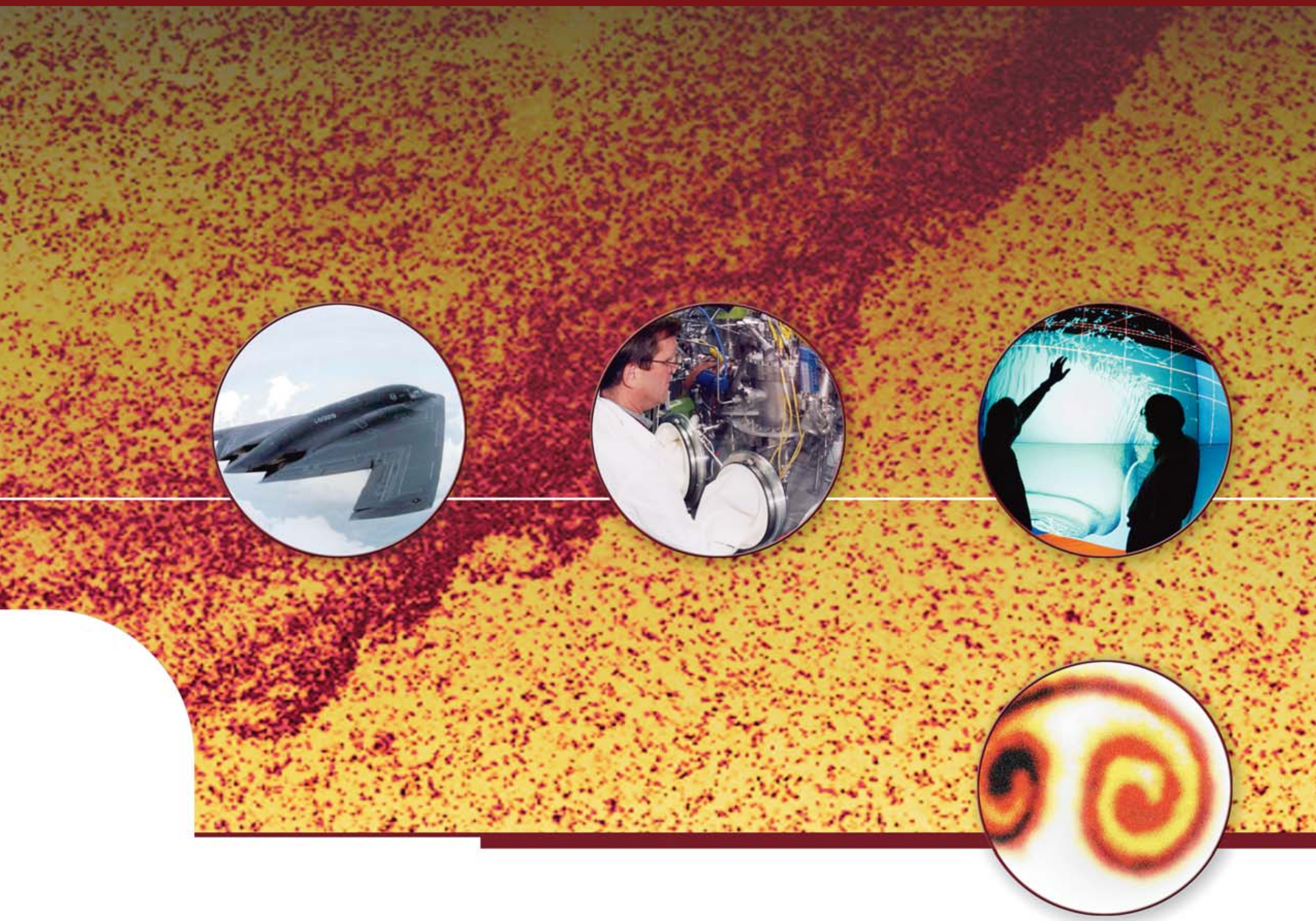
Small-scale laboratory experiments are helping to validate computer simulations of nuclear weapon performance.

The goal of stockpile stewardship—and Los Alamos' core mission—is to ensure the safety, reliability, and performance of the nuclear stockpile. The current ban on underground nuclear testing, however, severely limits the options for carrying out this mission. As a result, we now rely heavily on simulations produced by computer programs, or codes, to predict the performance of a nuclear weapon under various conditions.

Simulations provide far more diagnostic information than a nuclear test does. Using models of the physical processes that occur in a nuclear detonation, a computer can calculate variables such as temperature and pressure for any point in the calculational space of the simulated explosion with high spatial resolution—from the time the virtual bomb goes off (or before) to any time later.

New visualization tools can then present the huge volumes of information produced by a weapon simulation in ways scientists can quickly grasp. (A complete simulation produces nearly fifty times the information contained in the Library of Congress.) For example, one of the new Los Alamos PowerWalls—which each provides a 4- by 2-meter stereo display—can immerse weapon scientists in a full-color, three-dimensional movie of, say, the temperature field of a simulated thermonuclear fireball.

But these stunning displays pose a daunting question: do they show what will really happen? A simulation is only



as good as the equations, algorithms, and computer hardware that go into it, no matter how striking the display. If the computer models are wrong, inappropriate, or incorrectly implemented or executed, the simulation will be flawed—which is unacceptable for stockpile stewardship.

To help ensure that the predictions of weapon simulations are as accurate as possible, experimenters and code users at Los Alamos are using data from a variety of small-scale experiments to validate some of the physics models in the codes. The laboratory experiments discussed in this article focus on one of several fluid instabilities that have been studied by weapon scientists for decades. (Nearly sixty years ago, the Manhattan Project scientists who built the first atomic bomb realized that fluid instabilities could prevent a successful detonation.) However, these small-scale experiments occur at temperatures and pressures far removed from those in a nuclear weapon explosion and use materials quite different from those in nuclear devices. To fully validate a weapon code also requires the use of data from nuclear tests performed before the test ban went into effect as well as data from other experiments, as we discuss later in the article.

Richtmyer-Meshkov Instability

The fluid instability of primary interest in these small-scale experiments is the Richtmyer-Meshkov instability, which occurs when the interface between two fluids with different densities is accelerated by a shock wave

Presley Salaz

New visualization tools such as the Los Alamos PowerWalls help scientists grasp the huge volumes of information produced in a computer simulation of a nuclear explosion. The scientists here are viewing a three-dimensional simulation of a fluid instability. The code-validation experiments discussed in the article produce a two-dimensional version of a similar fluid instability.

striking the interface perpendicularly. The instability was first predicted in 1960 by R. D. Richtmyer, a Los Alamos theorist, and first experimentally observed in 1969 by E. E. Meshkov, a Russian experimentalist.

The instability develops whether the shock travels from a dense fluid to a less-dense fluid or vice versa. For flat or spherical interfaces, the instability causes slight disturbances at the interface to grow into large ripples that breach the interface and mix the fluids. The instability has been observed in inertial confinement fusion (ICF) experiments, in which intense laser or particle-beam pulses heat and compress small, layered metal spheres filled with deuterium and tritium in order to produce fusion reactions. It is also believed to occur in supernova explosions.

Only in recent years, however, have researchers been able to produce the Richtmyer-Meshkov instability in small-scale experiments that yield high-quality data, which is essential for good code validation. Some of these experiments have been performed at Los Alamos by Robert Benjamin and his research team. Related research has also been performed at other national labs, at several universities, and by private industry.

Some of the recent simulations of the Los Alamos experiments were done by Cindy Zoldi, who completed her Ph.D. in applied mathematics at the State University of New York at Stony Brook this past spring, then joined the technical staff at Los Alamos. Zoldi's graduate work involved validating the RAGE code, one of several unclassified codes used to improve physics models through comparison of code results with experimental data.

Gas Column Experiments

In these small-scale experiments, the Richtmyer-Meshkov instability is produced, along with other instabilities, when a planar shock wave propagating in air strikes a small column of sulfur hexafluoride gas, which is five times denser, or heavier, than air. The experiments are designed to produce results that are as two-dimensional (flat) as possible in order to validate the RAGE code in two dimensions. Three-dimensional validation efforts are possible in the future.

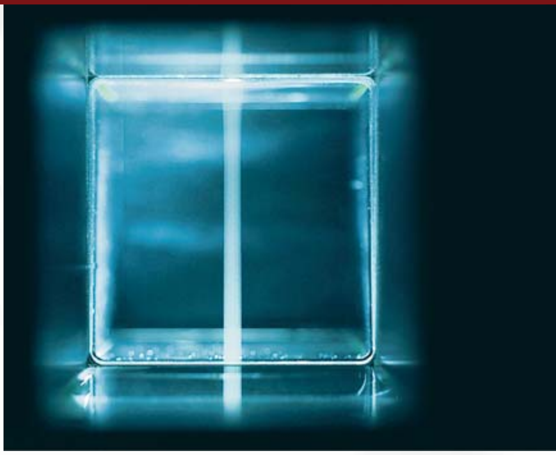
For these experiments the quantities of interest are the gas density and velocity. Seven sequential snapshots of the density show the shock wave first distorting the column of sulfur hexafluoride, then producing finer and finer swirling motion that eventually mixes the gases turbulently. The gas velocity late in the instability's evolution (750 microseconds after the shock wave has left the downstream edge of the column) is also determined from two successive high-resolution snapshots of the evolving column. The velocity is then used to determine the vorticity, a measure of the intensity of the gas swirling.

To measure the gas density and velocity, the experimenters uniformly mix microscopic glycol/water droplets with air and/or sulfur hexafluoride before piping the gas mixture(s) to the experimental chamber. The droplets, generated by a fog machine like those used in theaters for special effects, are about 0.5 micrometer in diameter. Because they're much larger than gas molecules, the droplets scatter light much more efficiently, enabling the gas density to be measured by photographing the brightness of the gas/droplet mixtures. By measuring how groups of the droplets move, the researchers can also produce maps of the gas velocity within and near the shocked gas column.

The gas column is formed by slowly and smoothly piping the dense sulfur hexafluoride through a circular nozzle into the air already present in the experimental chamber. By lighting up cross sections of the column with short laser pulses, the experimenters photographically record the column's density or velocity. Before each laser pulse slices through the gas column, it is spread into a horizontal, fan-shaped sheet about 1 millimeter thick.

The experimenters determine the gas velocity by measuring how far and in what direction groups of the glycol/water droplets move between two successive laser-pulse snapshots. Pattern-recognition software ensures that the velocity is determined for the same group of droplets in two successive frames. Los Alamos was the first to measure high-velocity flow in a shocked gas using this combination of "tracer particles" and pattern-recognition software. The technique was a breakthrough for shocked-gas studies and has greatly enhanced the quality and completeness of the code validation work discussed here.

The first section of the shock tube in which the shock wave is generated contains nitrogen pressurized to about three times atmospheric pressure. This section is separated by a polypropylene membrane from a second region of the shock tube that contains air (which is mostly nitrogen) at atmospheric pressure. Rupturing the membrane

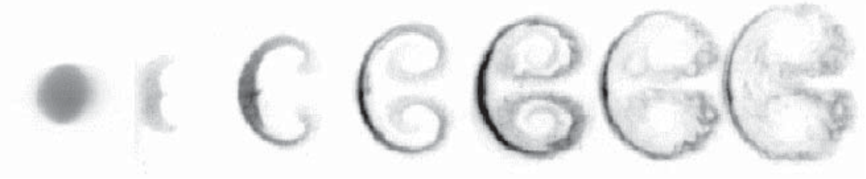


Richard Robinson

The gas column is formed by piping sulfur hexafluorlde, a gas five times denser than air, through a circular nozzle into ambient air. The column is actually twice the size shown in this photo.

Density Snapshots

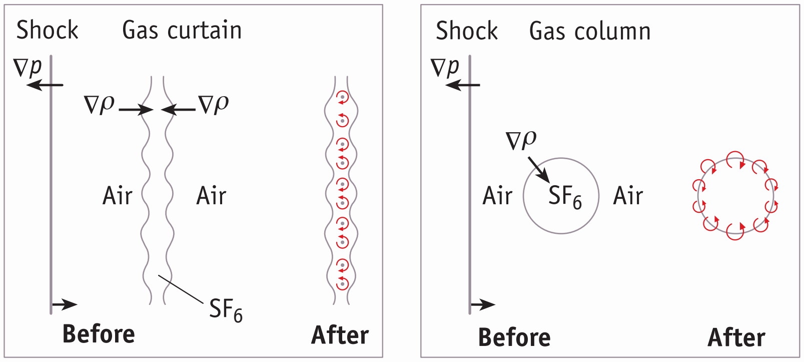
Experiment



Simulation

Comparison of the experimentally observed and simulated evolution of the shocked column's density. Because these images are negatives, regions of high gas density are darker than regions of low gas density. The initial conditions of the column are shown at the far left; its initial diameter is about 6 millimeters. The shock wave moves from left to right. Time also proceeds from left to right, with 140 microseconds between frames. Time is measured from the moment the shock wave has left the downstream edge of the column. The entire experiment is over in less than a thousandth of a second. Good agreement is seen in the larger-scale structure of the density snapshots. Differences in the smaller-scale structure are the subject of continuing research. Note the pair of large vortices on the downstream side of the shock-wave/column interaction. The core of one of these vortices is used as a reference point for comparing the experimentally observed and simulated velocities late in the instability's evolution.

Vorticity in Shocked-Gas Experiments



(a) (b)

Shocked-gas experiments before and after shock arrival. Vorticity, a measure of the intensity of gas swirling, is a key feature of the complex fluid flow produced by the Richtmyer-Meshkov instability (and other fluid instabilities). Vorticity is produced by the interaction of the incident shock wave's pressure gradient (∇p) with the density gradient ($\nabla \rho$) at the boundary between the sulfur hexafluoride (SF_6) and the surrounding air. The maximum vorticity is produced when the pressure gradient is perpendicular to the density gradient. The schematic compares the vorticity produced in shock-wave experiments with a curtain versus a column of gas. The first shocked-gas experiments of this type at Los Alamos used gas curtains. The directions of the incident shock wave's pressure gradient and velocity are shown by the oppositely directed arrows on the shock front. (a) For a gas curtain, the density gradient points into the curtain at each of its two interfaces. The vorticity distribution just after the shock wave strikes the curtain can be roughly approximated as a row of small, equally spaced vortices of equal size. (b) For the gas column, the density gradient points radially inward. The large vortices at the sides of the shocked column show that much larger values of vorticity are produced for a gas column, which more severely test a code's ability to model complex fluid flow.

abruptly releases the nitrogen into the second region, producing a shock wave with a speed of about 400 meters per second, or 900 miles per hour. Although polypropylene looks like the clear plastic used to wrap food, it has the unique property of shattering when ruptured, making it ideal for generating high-quality shocks.

After leaving the shock generator, the shock wave encounters the gas column formed within the experimental chamber. The chamber has windows through which the laser pulses pass and through which three cameras view the column's initial state and later distortion and breakup.

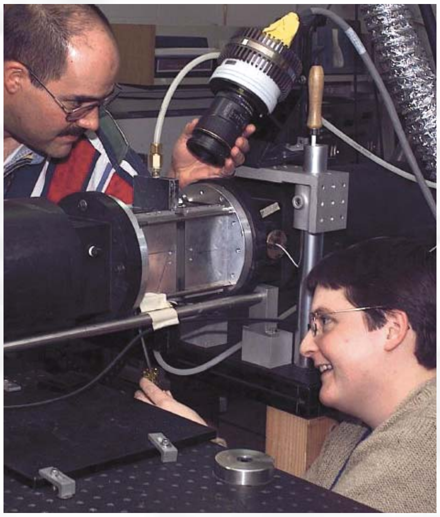
The experiment is fairly compact—the basic apparatus fits on a 6- by 2-meter "tabletop"; the gas column is about 6 millimeters in diameter and 7.5 centimeters tall. However, these small experiments produce big results, as the doctoral dissertations and publications flowing from the research confirm. In addition, four postdoctoral researchers who originally worked in Benjamin's research team were later hired at Los Alamos as technical staff members.

Collaboration is Key

But the validation work has not been easy. Once the experiments began to produce useful data, it took about two years to get the RAGE code results and the experimental data to agree quantitatively. The effort involved close collaboration between the code users and the experimenters—the key to good code validation, says Tim Trucano, a code validation expert at Sandia National Laboratories in Albuquerque, NM. Trucano is a member of the Validation and Verification Program for the Department of Energy's Advanced Simulation and Computing (ASC) program, which involves Los Alamos, Sandia, and Lawrence Livermore National Laboratories. The ASC program, formerly called the Accelerated Strategic Computing Initiative (ASCI), focuses on simulations for stockpile stewardship.

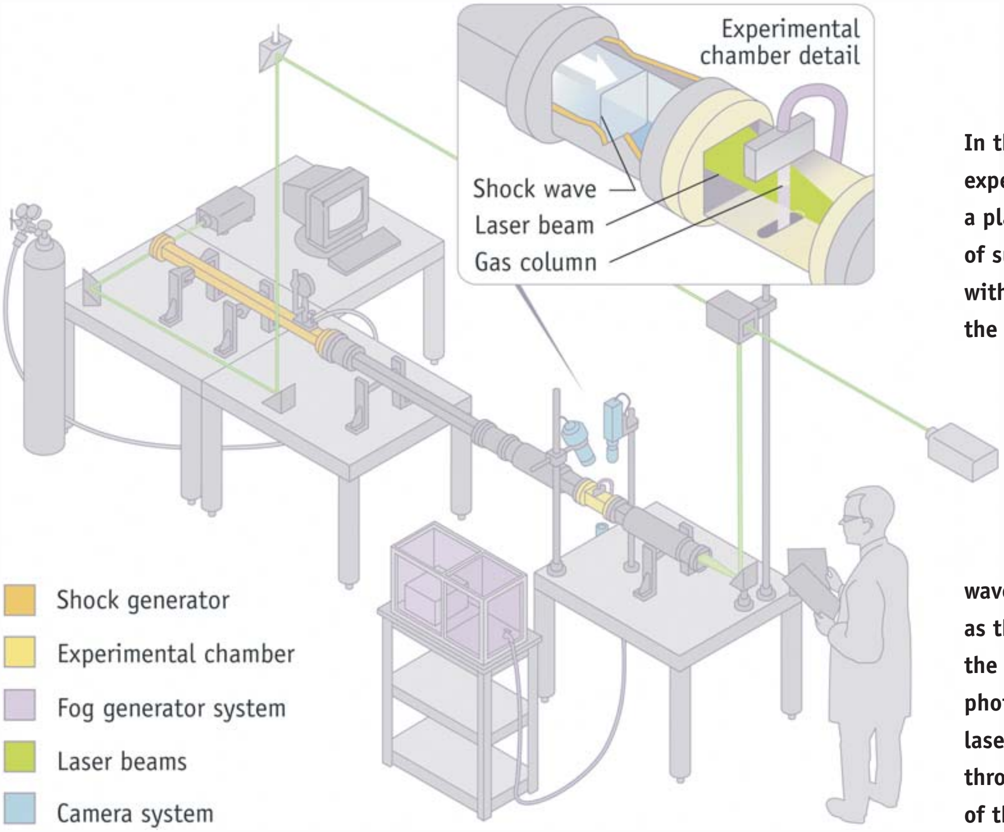
Initially, the simulation showed the shock wave distorting the column generally as seen in the early stages of the experimental shock-wave/column interaction. However, quantitative comparisons of the simulated and experimental results for the distorted column's outer dimensions as functions of time and for the velocity and vorticity fields at a single time were poor. In particular, the simulated peak velocities were about two times larger than the experimentally observed ones.

There were several sources of error. For one, Zoldi was able to obtain better agreement with the experiment by using an initial boundary between the sulfur hexafluoride and the surrounding air that was more diffuse than that indicated by initial measurements. Subsequent measurements confirmed that the boundary was indeed more diffuse. In addition, the velocity and vorticity comparisons improved when the experimenters (1) mixed the fog with both the sulfur hexafluoride and


John Flower

Los Alamos researchers Paul Rightley (left) and Kathy Prestridge (right) prepare to take shocked-gas data that can be used for code validation.

Shocked-Column Experiment



In the gas-column code-validation experiments, a shock generator produces a planar shock wave that strikes a column of sulfur hexafluoride gas formed in air within the experimental chamber. Before the gases are piped into the chamber, they can be separately mixed with a fog of microscopic glycol/water droplets to make them visible. Cross sections of the column's density are photographed before the shock wave arrives and at specific times later as the shock wave distorts and breaks up the column. The light source for these photos is a 1-millimeter-thick pulsed laser beam spread into a fan that slices through the gas column about one-third of the way down.

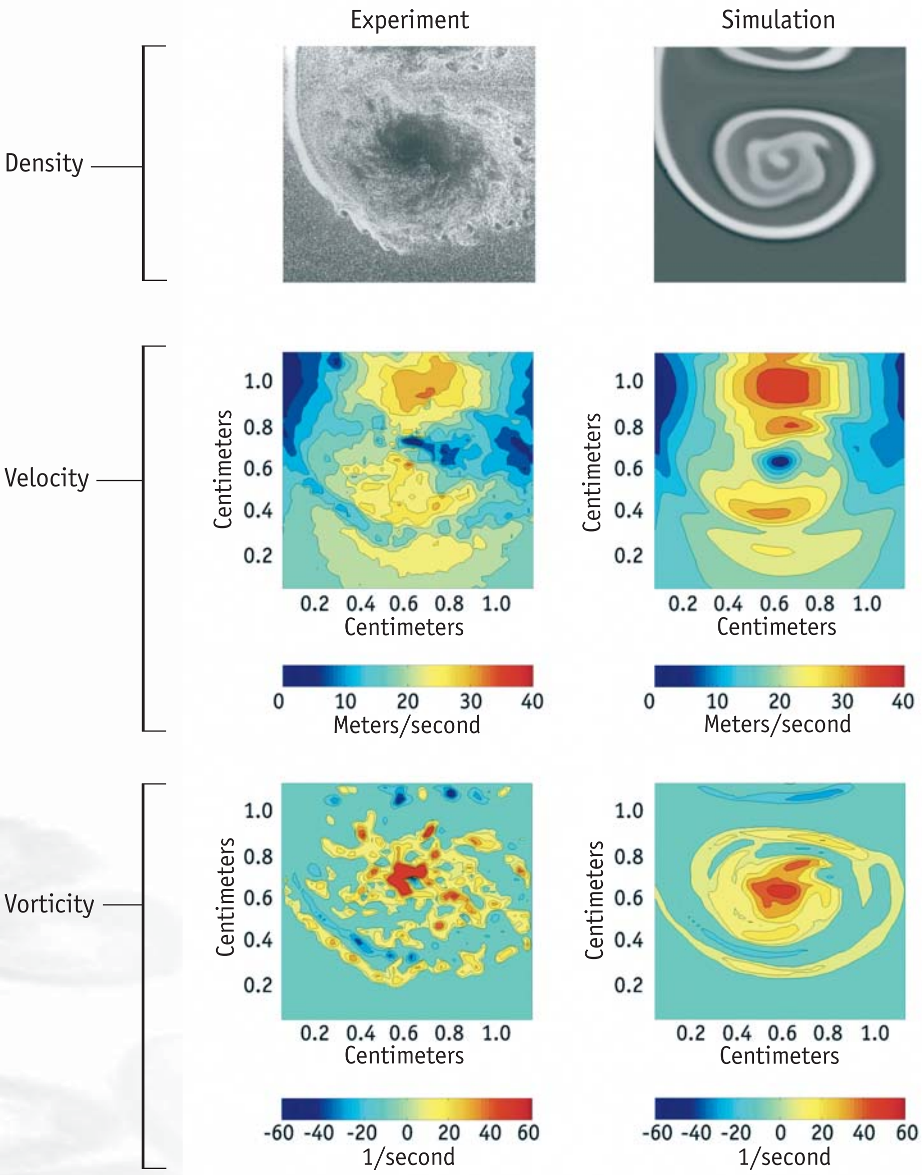
the air to obtain velocity data for both gases and (2) used a higher-resolution camera to take the photos used to measure the velocity.

There was also a problem with the way the predicted and experimentally observed velocities were initially compared. In addition to the large velocity produced by the shock wave's impact, the column receives a small velocity induced by the pair of large vortices generated in the shock wave's wake. The effect of this added velocity had not been taken into account. When it was, together with the other improvements, the experimental and simulated values for the fluid's peak velocity agreed to within 10–15 percent. The various fixes substantially improved the velocity comparison.

In Trucano's view, this work is a perfect example of the give and take between experimenters and code users that is required for good code validation. And the collaboration paid off with good agreement between the simulation and the experiment for the larger-scale structure. But at present the RAGE code cannot reproduce the later experimental phases when submillimeter ripples form that lead to turbulent gas mixing. The ripples are quite clear in the laser-pulse photos (see cover photo, for example) but not in the simulations.

A major purpose of code validation is in fact to determine the ranges of experimental parameters for which the code produces accurate results. (It's not mathematically, physically, or economically possible for a code to exactly reproduce the experimental

Experiment and Simulation Comparisons



The experimentally observed and simulated density, velocity, and vorticity for a shocked gas column 750 microseconds after the shock wave has left the downstream edge of the column. After two years of close collaboration between the experimenters and a code user, the experimental and simulated magnitudes of the peak velocities now agree to within 10–15 percent. The signs and magnitudes of the vorticity are also similar for the two cases. As seen in the close-ups of the density comparison, the simulated results reproduce the larger-scale structure of the experimentally observed results but not the smaller-scale structure.

results.) For this particular experiment the code is now valid for the larger-scale structure, although efforts are ongoing to reproduce the fluid's late-time smaller-scale behavior as well.

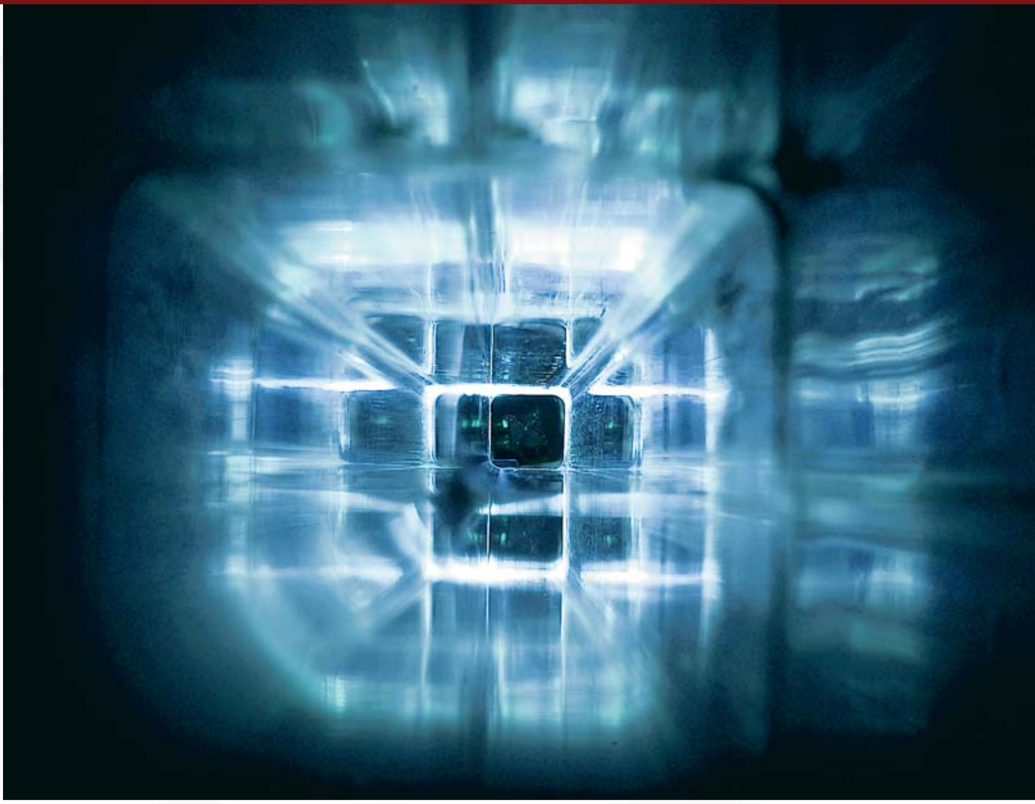
Although the agreement obtained thus far gives confidence in the code's ability to correctly model complex fluid flow, the validation technique itself can be made even more quantitative. Other Los Alamos researchers are using advanced mathematical tools—fractals, wavelets, and structure functions—to quantitatively compare the simulated and experimentally observed complexity of the turbulent fluid's late-time structure. Their research is at the forefront of the new science of code validation.

Regarding the importance of using experiments to validate codes, Los Alamos Director John Browne says, "Code-validation experiments are the foundation of predictive capability."

Other Validating Data

In fact, weapon code users at Los Alamos currently use data not only from small-scale experiments like Benjamin's but also from nuclear tests performed before the Comprehensive Test Ban Treaty went into effect and from a variety of large-scale experiments as well, including hydrotests, subcritical tests, and magnetic-compression and ICF experiments.

Hydrotests help code users interpret the results of some codes that simulate the implosion of a nuclear weapon. During implosion, shock waves produced by high explosives compress nuclear materials to supercritical mass. (The term hydrotest comes from the fact that, during implosion, the high pressures and temperatures generated by the high explosives cause metals and other materials to flow like liquids.) By imploding nonnuclear surrogate materials with properties similar to

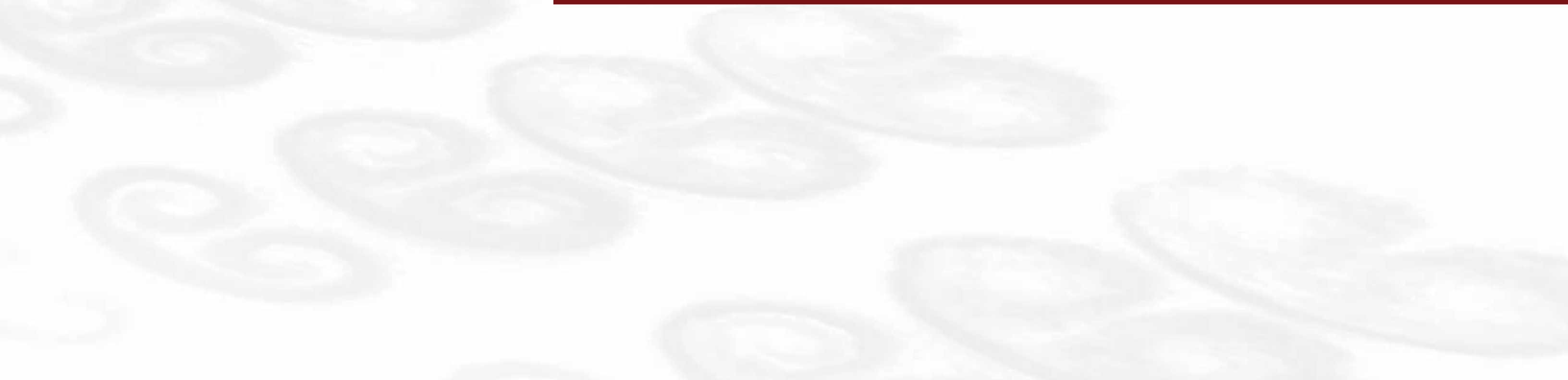

Richard Robinson

Internal reflections produced this kalaidoscopic image of the shock tube used in the shocked-gas experiments. The end of the tube, whose internal dimensions are 7.5 by 7.5 centimeters, is the small black square at the center.

The Researchers

Robert Benjamin received a B.S. in engineering physics from Cornell University and a Ph.D. in physics from M.I.T. Since joining the Lab in 1973, he has done x-ray and optical imaging for ICF experiments, developed diagnostics for pulsed magnetic-compression experiments, and conducted fluid-instability experiments. Benjamin received the 1994 Los Alamos Fellows Prize for outstanding research and became a Laboratory Fellow in 1997. He has three patents and over thirty publications.

Cindy Zoldi received a B.S. in electrical engineering from the University of Maine and an M.S. and Ph.D. in applied mathematics from the State University of New York at Stony Brook. She joined the Lab in 2002 as a technical staff member. A member of the Society for Industrial and Applied Mathematics, the American Physical Society, and the Association for Women in Mathematics, Zoldi has presented her research on fluid instabilities at various national and international conferences.



those of nuclear materials, hydrotests simulate weapon implosion without producing a nuclear explosion. In contrast, data on nuclear materials without implosion is obtained from subcritical tests performed at the Nevada Test Site.

At present, Los Alamos has two hydrotest facilities. PHERMEX, the Lab's hydrotest workhorse for nearly forty years, takes x-rays of implosion from a single direction at two times. When fully operational in 2004, the second facility, DARHT, will take x-rays of implosion from two perpendicular directions at up to four times.

More recently, protons instead of x-rays have also been used to image implosions. Proton radiography has the potential to take tens or hundreds of images per hydrotest, providing implosion movies and possibly three-dimensional images as well. Using protons produced by the 800-million-electronvolt accelerator at the Los Alamos Neutron Science Center, preliminary proton-radiography experiments are being used to test concepts for "advanced hydrotest imaging."

Ranging from small shocked-gas experiments like those in Benjamin's lab to large hydrotests, a wide variety of experiments are providing the data scientists need to validate the physical models in the weapon codes. John Browne puts the importance of code validation in a national perspective. In a statement to Congress this past June, he observed that a major component of the stockpile stewardship mission is "predictive science," which will allow the weapons complex "to evaluate how any issue in the stockpile, or any change that we might consider, will affect system safety, reliability, and performance." ■

Code Validation and Stockpile Stewardship

By Ray Juzaitis, Associate Director, Weapons Physics

The goal of stockpile stewardship is to ensure that the weapons in the enduring nuclear stockpile, both today and in the future, are safe and reliable and will perform as expected—including those weapons that may have undergone changes due to aging, refurbishment, or other required modification. To meet this goal, we must sustain our existing expertise in weapon physics, engineering, and manufacturing, as well as sustain the technologies and facilities that support our mission. To meet the challenge potentially posed by future changes in requirements, we must also explore and develop new expertise and new support capabilities.

Because stewardship activities must occur without nuclear testing, we now rely heavily on computers to simulate nuclear weapon performance. Indeed, some of the most powerful computers and computer programs in existence are currently used to assess, in astonishing detail, the performance of complete nuclear weapon systems.

But decisions about the stockpile based on simulations will be well founded only if the simulations' physical models are validated with experimental data. The accompanying article describes validation work at Los Alamos that draws on data from elegant and precise small-scale experiments with shocked gas columns. These experiments are helping us explore and understand hydrodynamic instabilities, which play a significant role in nuclear weapon performance. These experiments also provide an excellent example of the experimental science needed to validate the simulations upon which stockpile stewardship vitally depends.