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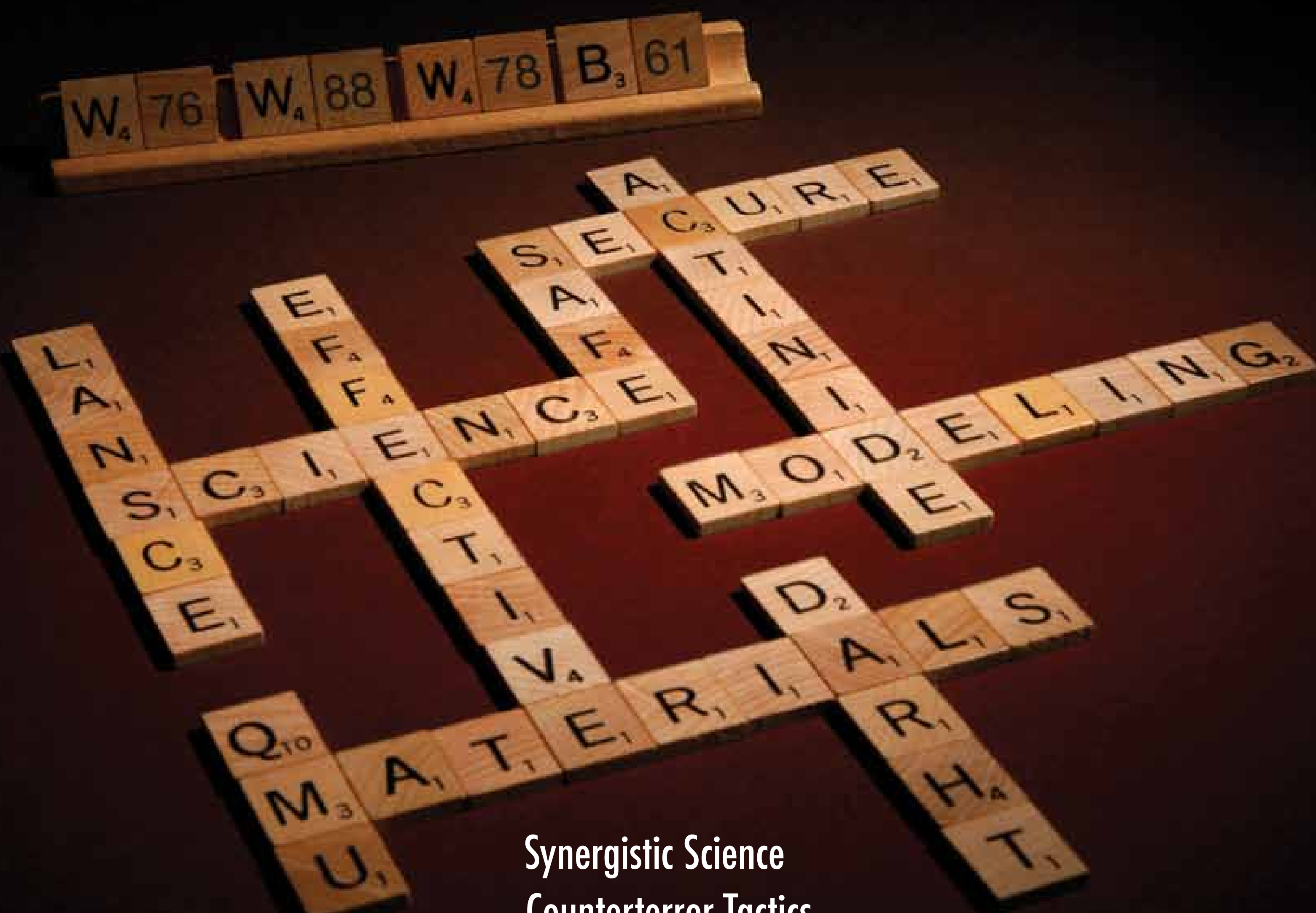

Synergistic Science
Counterterror Tactics
Hydrodynamic Chaotic Mixing

Los Alamos
NATIONAL LABORATORY
EST. 1943

About the Cover: Interdisciplinary, collaborative capabilities in science, technology, and engineering are some of Los Alamos National Laboratory's greatest assets. Read more in our cover story, *Synergistic Science*, about the future of the Lab's Weapons Program and how colleagues cross programmatic boundaries to create a safer, more secure world.

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Multidisciplinary Experts Tackle Our Toughest Challenges

Los Alamos National Laboratory leaders came together on stage to highlight their support of the institution's cross-disciplinary foundation and achievements.

Charles McMillan, principal associate director for Weapons Programs, and Terry Wallace, principal associate director for Science, Technology, and Engineering cohosted an all-employee meeting March 18 at the Lab. McMillan outlined the policy dynamics affecting the institution's future and emerging opportunities, while Wallace emphasized capabilities-based scientific strategies. From finances to signature facility development—the leaders' message reiterated that the Laboratory is well positioned for a productive future.

Highlighting the President's congressional budget request for a $5 billion nuclear weapons increase—one of the largest within the government—McMillan said proposed funds support the Lab's mission of ensuring the continued security and effectiveness of the nation's deterrent and nonproliferation.

In Prague last year, President Barack Obama announced his nuclear weapons disarmament agenda. "To seek the peace and security of a world without nuclear weapons. First, the United States will take concrete steps towards a world without nuclear weapons. To put an end to Cold War thinking, we will reduce the role of nuclear weapons in our national security strategy, and urge others to do the same. As long as these weapons exist, the United States will maintain a safe, secure and effective arsenal to deter any adversary, and guarantee that defense to our allies," said the President.

McMillan referred to Obama's speech, adding, "I can understand why there are those who have predicted the demise of the Weapons Program. Over the last several years, some have questioned the future of the national nuclear weapons program because there has been a vigorous discussion around the goal of "global zero." The Weapons Program will remain at the core of this Laboratory as long as this nation requires a nuclear deterrent. [We will] draw on the creativity of the entire Laboratory, bringing to bear our strongest teams to address the most challenging nuclear national security problems through experiment, modeling, simulation, design, engineering, and production."

Essential Connections

One of the Lab's greatest assets is the multidisciplinary approaches to tackling our complex challenges. Roadrunner, the record-breaking supercomputer provides codes for a variety of research, from explosion and materials simulations to climate change models; the Los Alamos Neutron Science Center provides data for weapons performance evaluation—and even cancer detection; The Dual-Axis Radiographic Hydrodynamic Test Facility—the world's most powerful flash x-ray—provides critical information to scientists. These are just a few examples of how the world-class scientific capabilities cross programmatic boundaries for the greater good.

Speaking about the Roadrunner example, McMillan said, "Without the work done by people from many different parts of the Laboratory, it would not be possible for the Weapons Program to begin benefiting from this new computing platform." He reminded attendees, "those connections are essential for the success of the Weapons Program."

Cohosts McMillan and Wallace present collaborative plan.

The Principal Associate Directorate Weapons Program (PADWP) budget is roughly divided by thirds: one third toward Los Alamos design physicists, engineers, and technicians working directly on stockpile issues. One third is spent on staff who provide crucial capabilities; such as materials experts, the technicians who fabricate parts, and the mathematicians and computer scientists who, McMillan said, make it possible to do the simulations we rely on in a world without nuclear testing.

The budget's latter third is drawn from the Principal Associate Director for Operations (PADOPS) that provides the complex facilities required for weapons research, including testing facilities, firing sites, and the infrastructure. "Without the capabilities associated with operations, the Weapons Program would rapidly grind to a halt," McMillan said. "It takes the creativity of the entire Laboratory to execute the Weapons Program."

The Future of Weapons

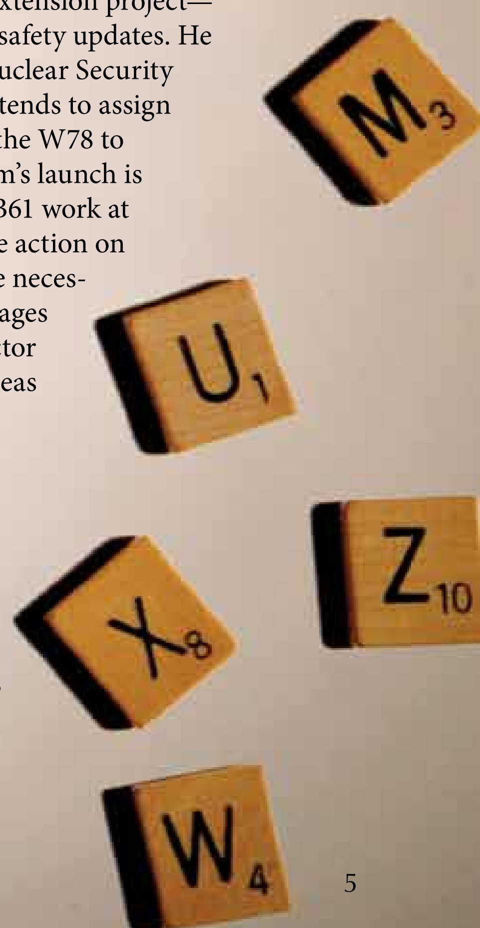
The program's future will be shaped by new policies, outlined in the Quadrennial Defense Review, Nuclear Posture Review (NPR), and the New Strategic Arms Reduction Treaty (START).

"These elements will place substantial expectations on the science, technology, and engineering (ST&E) capabilities at Los Alamos. As the stockpile has become smaller, the premium on confidence in the weapons has grown. I believe this trend will continue placing increasing demands on the ST&E supporting the stockpile," said McMillan. "Regardless of the detailed path forward, for the foreseeable future, we will continue to have stockpile responsibilities.

"It is understandable that some might think the Weapons Program would be holding a 'going out of business sale.' This is not going to happen. Even in a world with many fewer, or even no nuclear weapons, the skills of the Weapons Program would continue to make contributions to national security and international stability through an understanding of signs of weapons development or stockpile reconstitution. These are capabilities we exercise today with the Global Security Program."

McMillan discussed the formation of nuclear weapons assessment teams at Los Alamos and Lawrence Livermore National Laboratory that independently prepare baseline models for the other lab to follow. He also noted the Weapons Program is applying its unique strengths, new technologies, and newly acquired knowledge to the B61 life extension project—including nuclear package safety updates. He announced the National Nuclear Security Administration (NNSA) intends to assign the life extension work on the W78 to Livermore, and the program's launch is expected to coincide with B61 work at Los Alamos. "We must take action on the W78 and the W88…the necessity for work on these packages is clear," the associate director noted. "I want to see our ideas shape the future stockpile. We must be prepared with compelling concepts."

McMillan said although recent staffing trends and projects "have not been encouraging," the three major national laboratories urged federal officials and influential groups to consider the stockpile as a



McMillain said...

Why are we here?

To ensure the safety, security, and effectiveness of US nuclear deterrent and provide expertise in nuclear weapons ST&E that supports international stability

What will we do?

Apply the exceptional ST&E capabilities of Los Alamos to preserve the US nuclear deterrent

How will we do it?

Draw on the creativity of the entire Laboratory, bringing to bear our strongest teams to address the most challenging nuclear national security problems through experiment, modeling, simulation, design, engineering, and production

What is the environment in which we will do this work?

- The best people prepared for unforeseen challenges
- Safety and security as a solid foundation for all of our work
- Technical excellence coupled with timely delivery
- Balancing creative innovation with disciplined execution

deterrent, providing ST&E necessary to support the deterrent and the nuclear infrastructures requiring recapitalization.

"These efforts have borne fruit," McMillan said. "The resources appear promising.

"With the President's budget request…I no longer expect staffing in the Weapons Program to continue on a downward trend. Rather, I expect it to stabilize." He continued, "This will allow modest, very selective hiring across the Laboratory…to deliver on our near-term commitments while building the Laboratory staff that will ensure continuing expertise in the science and technology of nuclear weapons."

While the budget is being finalized, there is funding at Los Alamos for B61 extension, some science campaign increases, and the Chemistry and Metallurgy Research Replacement, according to McMillan. The Obama administration's $11.2 billion request for the NNSA represents a 13.4 percent increase for the agency from the previous fiscal year.

"[The proposed budget] represents an extraordinary vote of confidence by the administration," McMillan said. "Only by working together as a team can we succeed."

> We must deliver to create that future —there is real work to do.
>
> —Charles McMillan

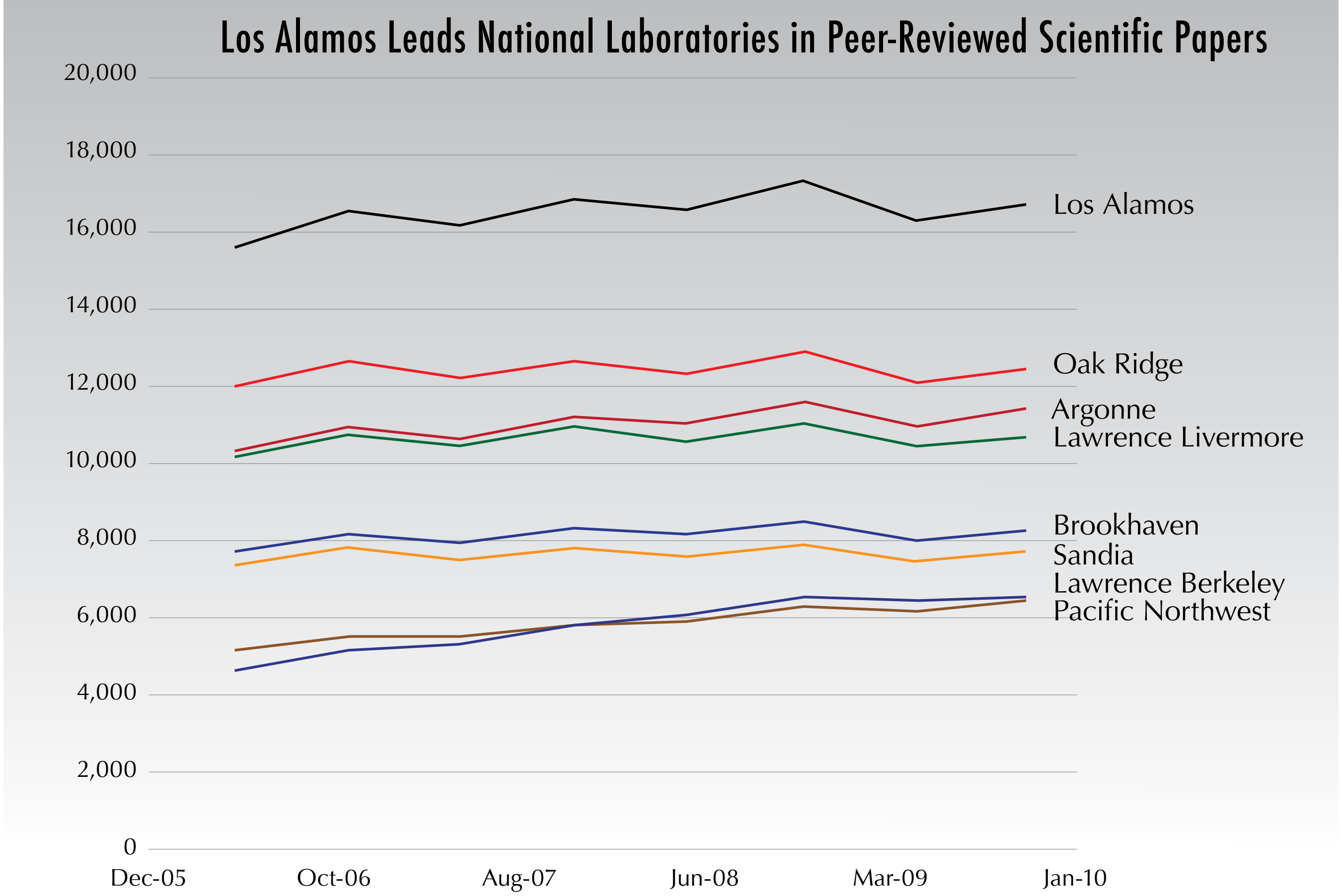
The Long Road Ahead

"I must sound a second note of caution as well—execution. There are those who look at the proposed changes to the budget and say, 'They can never use that much money effectively. They won't deliver,'" McMillan advised. "If we fail, the proposed uplift in the out-years will be at risk. I am working…to build execution plans that will ensure that Los Alamos is organized for successful execution."

Challenges lie ahead. McMillan emphasized how the Lab must demonstrate its credibility.

"If we are to be considered by others as best in class, we must bring outstanding ideas coupled with rock-solid delivery of product," said McMillan. "We must deliver on important work we have been asked to do for the nation. We must deliver to create that future—there is real work to do." *—Kirsten Fox*

Editor's Note: after McMillan's speech, two major nuclear policies were released. In early April, the Department of Defense released the NPR, a legislatively-mandated review establishing US nuclear policy. On April 8, President Obama, again in Prague, and Russian President Dmitry Medvedev signed a historic nuclear document—START—agreeing to reduce the nuclear stockpiles of both nations.

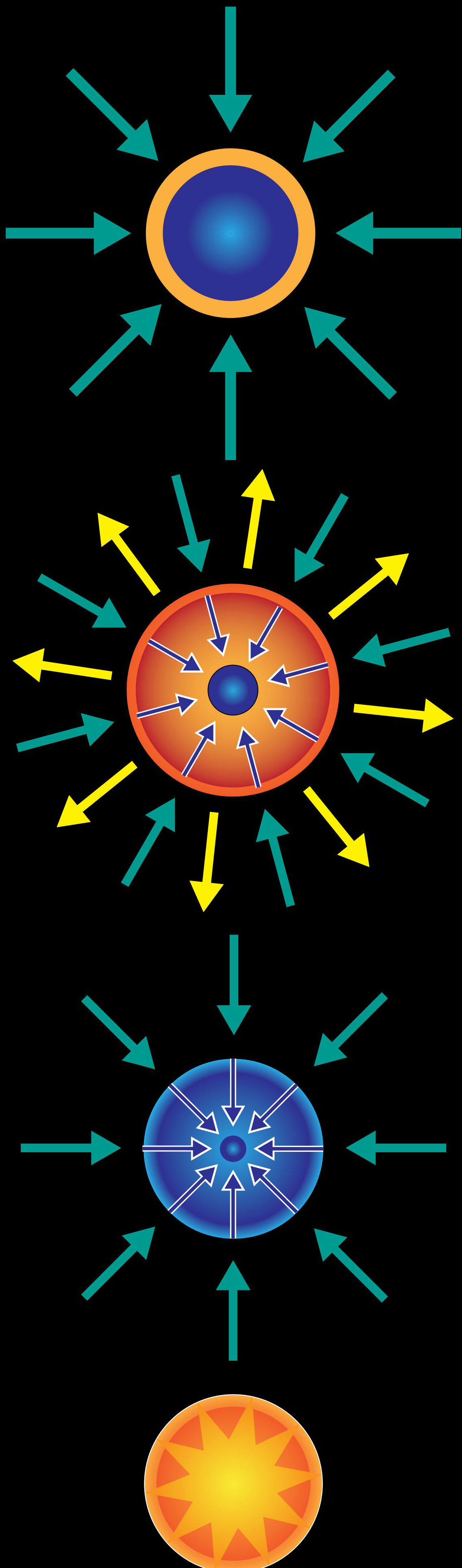


ISI Web of Knowledge data: All fields papers published May 2005–November 2009

Physics Papers and Citations (as of November 2, 2009)

Institution	Papers	Papers Ranking	Citations	Citations Ranking	Citations per Paper
LANL	6897	14	119,248	12	17.29
ANL	5235	29	95,749	19	18.29
ORNL	4122	52	63,823	41	15.48
BNL	4074	55	93,008	21	22.83
LLNL	3828	60	66,204	39	17.29
LBNL	2409	135	40,074	94	16.64
SNL	2112	168	30,993	135	14.67
PNNL	631	533	8,786	445	13.92

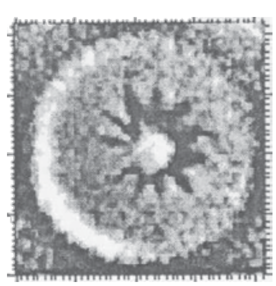
Data from the ISI Web of Knowledge Essential Science Indicators at http://www.isiknowledge.com/ESI.
Data updated as of November 2, 2009, to cover period January 1, 1999–August 31, 2009.



MODELING Chaotic Mixing

Moving interfaces between distinct fluids in a multifluid system are often unstable. Small perturbations at such interfaces grow as a result of nonlinear fluid-dynamic processes and evolve into chaotic (turbulent) mixing regions. Three major types of hydrodynamic instability play an important role in mix processes: (1) the Rayleigh-Taylor (RT) instability, occurring when a fluid pushes another fluid of higher density; (2) the Richtmyer-Meshkov (RM) instability, which takes place when a shock wave accelerates a perturbed interface between two fluids of different densities; and (3) the Kelvin-Helmholtz (KH) instability, which arises when a nonzero velocity discontinuity exists between the two fluids.

Figure 1. The stages of inertial-confinement fusion (*at left, from top*): (*1*) Laser beams or laser-produced x-rays rapidly heat the surface of the fusion target, forming a surrounding plasma envelope. (*2*) Fuel is compressed by the rocket-like blowoff of the hot surface material. (*3*) During the final part of the capsule implosion, the fuel core reaches 20 times the density of lead and ignites at 100,000,000˚C. (*4*) Thermonuclear burn spreads rapidly through the compressed fuel, yielding many times the input energy. The green arrows represent incident electromagnetic radiation; the yellow arrows represent blowoff; the blue arrows represent inwardly transported heat. The black and white image at left is an inertial-confinement fusion target, a cylindrical hohlraum target of deuterium-tritium, being compressed by the Nova Laser. This shot was done in 1995. The image shows the compression of the target at t = 2.61 ns, as well as the growth of RT instabilities.



Chaotic mixing is an important subject. Hydrodynamic instabilities occur in technological applications, such as inertial-confinement fusion (ICF) capsules (Figure 1), laser ablation, combustion, and chemical engineering. They also occur in natural physical phenomena ranging from astrophysical to micro scales, including supernova explosions, galaxy and cluster formations, atmospheric flows, and polymer surface structures. Our ability to understand and perhaps to control the chaotic mixing produced by unsteady hydrodynamic flow is important for industrial applications in laser micro machining and aeronautics. The role of hydrodynamic instabilities in initiating chaotic mixing has attracted the interest of leading physicists and mathematicians for many decades and has been the subject of extensive experimental, theoretical, and numerical investigations.

In this article, we review some of the ideas and methods that are being used to understand chaotic mixing. These range from relatively simple analytic models to large-scale numerical simulations. The emphasis is on verification of the results through mesh convergence studies and careful analysis of numerical algorithms as well as on validation through detailed comparison to experimental observations.

Basic Phenomena of Mixing Layers

Many complex phenomena are associated with the evolution of an unstable fluid interface, described here for the case of Rayleigh-Taylor instability. The macroscopic features of the mixing layer include its size and rate of growth and the size distribution of any coherent structures that may be present. Microscopic features refer to local concentration and temperature distributions and their effects on chemical reactions, such as combustion, that may be taking place in the mixing layer. Both macroscopic and microscopic properties must be accounted for to arrive at a thorough, and relevant, understanding of mixing layers.

It is helpful to organize a description of the evolution of the macroscopic properties of a mixing layer into a number of stages, as follows. Stage 1: Exponential growth of small-amplitude initial perturbations. Stage 2: Nonlinear growth resulting in the formation of coherent structures (bubbles) which penetrate into the surrounding fluid (Figure 2). Stage 3: Interactions among coherent structures that can lead to their amalgamation, breakup, and other features. Theoretical and analytic work has largely been focused on understanding some of these macroscopic properties. (See “Theory” section.) However, a full quantitative understanding of either the macroscopic or microscopic properties must ultimately rely on numerical simulations. (See “Numerical Simulations” section.) The FronTier simulation relates the microscopic properties of the mixing layer to their effects on chemical reactions, such as combustion, that may be taking place in the mixing layer.

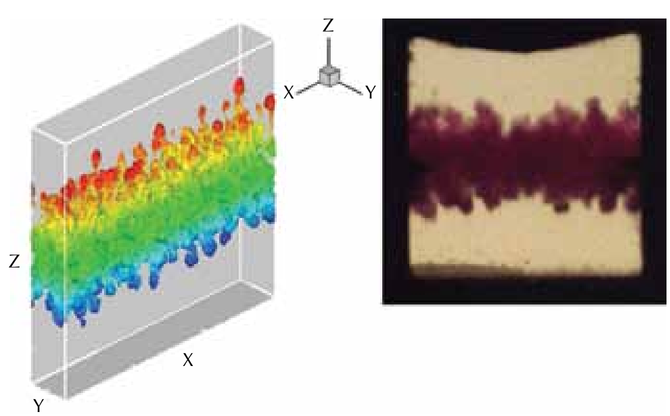


Figure 2. Left plot shows the tracked 3D RT instability simulation, which shows a sharp interface. The initial state was a gently wavy interface separating a high-density fluid (bottom) from a low-density one (top) (the density ratio is 1.89:1.0). Gravity (pointing up) then destabilizes the interface, producing the mixed regions shown. Unmixed regions are transparent. Red, yellow, green and blue show successively higher densities (Courtesey of the Front Tracking group at Stony Brook and LANL). Right is a photo copy of the seventh plate of experiment #112 of Smeeton-Youngs for the miscible mixing of NaI solution and pure water (the purple color is for visual effect, courtesy of D.L. Youngs).

Theory

Bubble growth rate

The speed of a single bubble of a light fluid rising in a cylindrical tube has been measured in experiments. For multiple bubbles, bubble merger models predict the penetration rate of fingers of light fluid into the heavy fluid. For RT mixing, it is observed that the bubbles increase in size through a process of bubble competition and merger. In this process, large bubbles are accelerated relative to the mean bubble motion, whereas small ones fall behind. That is, the smaller bubbles are removed from the interface of advancing bubbles, and the larger, more advanced bubbles expand to fill the resulting space. Sharp and Wheeler proposed a model to describe this process in 1961.[1] The model was refined by Glimm and Sharp in 1990[2] and 1997[3] to include the hydrodynamical accelerations (positive and negative) given to advanced and retarded bubbles due to their positions relative to the mean bubble penetration height. Such models were extended to three dimensions by Oron et al. in 2001[4] and independently by Cheng, Glimm, and Sharp (CGS) in 2002,[5] with improved predictions. The three-dimensional (3D) models predict not only the growth rate for the bubble (light fluid) interface, but also the bubble height-to-width ratio. For this quantity, the agreement of the CGS model with experimental data is quite good, as shown in table below.

Bubble Height-to-width Ratios in Experiments and Models

Cheng et al. (2002): Model	3
Oron et al. (2001): Model	1–1.5
Smeeton and Youngs (1987): Experiment	3.3
Dimonte and Schneider (1996): Experiment	2–4

The equations for bubble dynamics in this model are formulated using scaled variables, from which the Agt^2 growth law has been removed. This being the case, the self-similar (scale invariant), late-time solution appears as a fixed point.

For the case of RT mixing under constant acceleration (g), the bubble penetration height h_b satisfies the scaling law $h_b = \alpha_b A g t^2$, where $A = (\rho_s - \rho_b)/(\rho_s + \rho_b)$ is the Atwood number, t the time, $\rho_{s(b)}$ (s = spike = heavy fluid, b = bubble = light fluid) the fluid density in the spikes (bubbles), and α_b is called the bubble growth rate. In the bubble merger model, α_b is determined by four directly measurable quantities: (1) The mean merger rate $\omega = \langle 1/t'_m \rangle$, where t'_m is the time to merger for a pair of interacting bubbles, thus ω is also called the mean inverse time to merger. It is evaluated at the fixed point. (2) The maximum height separation (h'_m) between two neighbouring bubbles for instantaneous merger. (3) The speed of a single bubble c_b in a periodic array. (4) A geometrical factor k giving the increase in radius for a single merger event, slightly less than ½. Each of the preceding is expressed in scaled units. The fixed point formula for α_b is given by

$$\alpha_b = \frac{k}{4}\left(c_b + \frac{1+k}{2} h'_m \omega\right)\omega. \quad (1)$$

This equation has been verified by direct comparison to experimental data.[5] The above quantities are evaluated directly within a statistical model for the bubble dynamics.

Two quantities define this model: the bubble velocity and the bubble merger criteria. The bubble velocity is defined as the sum of a single (periodic array) bubble velocity and a bubble interaction term, the envelope velocity.[5] The bubble velocity as a sum of these two terms has been tested against simulation data. The criterion for bubble merger is defined to be the time at which the slower bubble starts to move backwards, using this two-term formula for the bubble velocity. Note that the bubble interaction term can have either sign, so that a zero total velocity is possible. The bubble merger criterion was shown to be an insensitive parameter in the model.

From these two inputs, ω and h'_m are determined. For example, for uniformly sized bubbles, $k = 0.414$, $\omega \sim 0.43$, $h'_m \sim 1.82$, taking $c_b = 0.532$ for hexagonal bubbles, then $\alpha_b \approx 0.048$. For non uniformly sized bubbles, α_b increases depending upon the size distribution. If the nonuniformly distributed bubbles have a distribution in radius with a variance of ~ (0–50)%, the scaling constant α_b for bubbles in 3D RT is in the range of ~ 0.05–0.06, in good agreement with experimental results ~ 0.06 ± 0.01.[6–9] The same formulas yield the bubble height-to-width ratio ~ 2.9–3.1 which, as we have noted, agrees with experimental data.

Mixing Layer Properties

Buoyancy drag models are based on a phenomenological equation describing the balance of inertial and drag forces acting on both bubbles and spikes that occur in mixing layers. The equation is applicable to both RT and RM flows, and describes both transient and asymptotic properties of the flow.

The basic equation in the buoyancy drag model[9–11] is

$$(\rho_i + k_i\rho_{i'})\frac{dV_i}{dt} = (\rho_i - \rho_{i'})g(t) - (-1)^i \frac{C_i\rho_{i'}V_i^2}{|h_i|}, \quad i = 1,2, \tag{2}$$

where the "added mass" coefficient k_i and the drag coefficient C_i are the model's phenomenological parameters, $i = 1 = b$ (bubble) and $i = 2 = s$ (spike), $V_i \equiv dh_i/dt$ is the velocity of the edge i of the mixing zone. The form of the drag force reflects the assumption that the fluid infinitely far upstream of the bubble or spike is stagnant. For given α_b, the growth rate of spikes (α_s) can be obtained by assuming a stationary center of mass of the mixing layer. The results are in good agreement with the linear electric motor (LEM) experiment data (Figure 3).[8]

Remarkably, it is possible to solve equation (2) analytically, thus obtaining an explicit expression for the edges of the mixing layer as function of time.[12] To leading orders in t, the result is

$$|h_i(t)| \approx \frac{1}{4a_i^2}Ag(t-t_0)^2 + \frac{\gamma_1}{a_i}(1+f_{i0})^{-1/2a_i^2}\sqrt{Ag|h_{i0}|}(t-t_0) + \frac{\gamma_1^2|h_{i0}|}{(1+f_{i0})^{1/a_i^2}}, \tag{3}$$

where

$a_i^2 \equiv ½\{1 + C_i[1-(-1)^i A]\}$,

$f_{i0} \equiv (1-a_i|V'_{i0}|)/(1 + a_i|V'_{i0}|)$,

$V'_i \equiv V_i/\sqrt{Ag|h_i|}$, and

$$\gamma_1 \equiv (1+f_{i0})^{\frac{1}{2a_1^2}}\left(1+\frac{2f_{i0}}{(1+f_{i0})(1-4a_1^2)}\right),$$

$h_{i0} = h_i(t = t_0)$ is the initial position of edge i of the mixing zone. Equation (3) displays for the first time the entire dynamical evolution of the trajectory of the RT mixing edges (for both early and late time) in terms of the physical parameters (A, C_i, k_i) and the initial conditions (Figure 4). It also reveals the

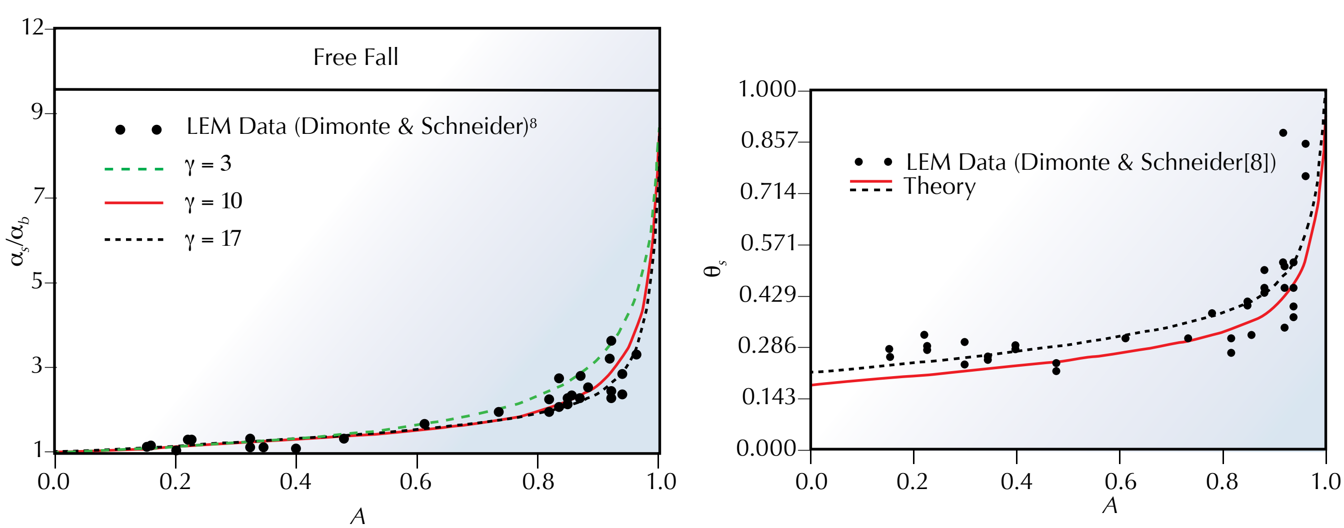


Figure 3. In the left plot, the ratio of α_s/α_b as a function of Atwood number A is shown for α_b ~ 0.05. The dashed, solid, and dotted lines, are respectively, for model parameter γ = 3, 10, 17. The solid dots represent data from LEM experiments. Right plot displays the power coefficient θ_s for RM mixing. The solid and dotted lines are predictions of the present model for α_b = 0.05 and for α_b = 0.06, respectively. The solid dots are data from LEM experiments.

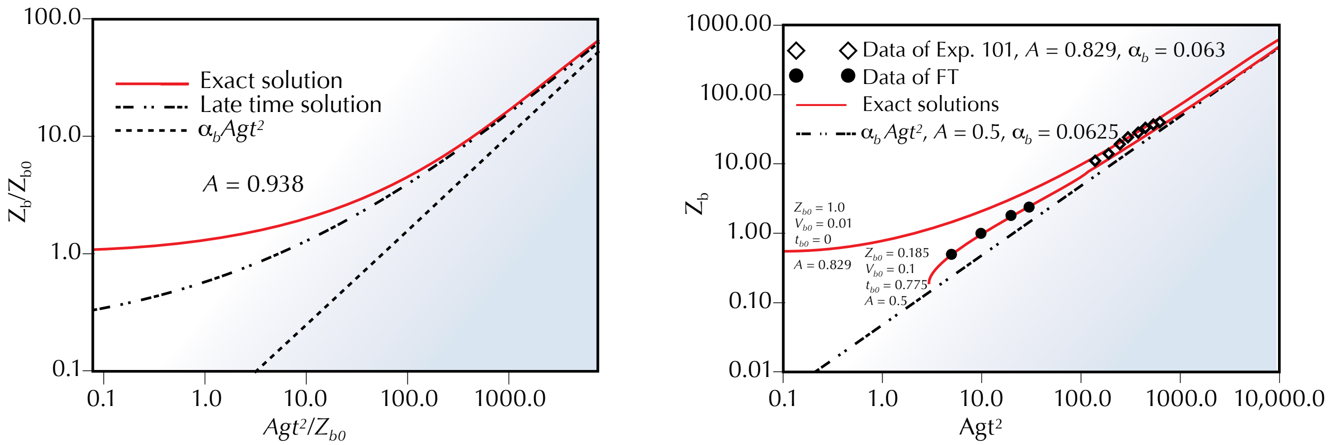


Figure 4. Left plot shows the entire dynamical evolution of the trajectory of the RT mixing bubble front for A = 0.938 (here $h_b = Z_b$). The solid line represents the exact solution, the dashed line denotes the late time asymptotic solution, and the dotted line gives the pure leading order asymptotic solution. Right plot presents the comparison of simulation data to the exact solution of the model equation on large scales. The solid curves provide a possible explanation for the curvature of the preasymptotic simulation data and for the straight line of the asymptotic experimental data. The pure leading order asymptotics are shown in the dash dot straight line.

dynamical transition of the system from an early (but still chaotically mixing) behavior to the late-time self-similarity regime. This solution thus provides a deeper understanding for the self-similarity assumed in the other models. It also shows that the corrections to the leading order expressions (~ Agt^2) for $|h_i|$ depend on the initial conditions. A significant difference between our model and related models appearing in the literature is in the treatment of the drag term in equation (2). In our model we have consistently used the ambient fluid density $\rho_{k'}$, as discussed by Landau, instead of the displacing fluid density ρ_k used in the work of others. Also, our expression gives A-dependent drag coefficients if the RT bubble mixing rate α_b is independent of the Atwood number A. These results are consistent with both experiments and numerical simulations.

The exact solution for RT mixing shows that the RT mixing layer grows exponentially at early times, then linearly during the intermediate stage with a dependence on initial conditions, and later reaches the self-similarity regime and grows as αAgt^2. The usual αAgt^2 solution is only a late-time self-similar solution. The real physical process indeed undergoes a dynamic transition from initial condition dependence to independence. The experimental data relate these variables in a nearly linear manner, and a fit to the slope determines α_b.

Applying the drag coefficients specified from the RT mixing growth rate to RM mixing ($g = \delta(t)$) gives an expression for the edges of the RM mixing layer at any time t,

$$|h_i(t)| = |h_{i0}|\left[1 + \frac{(1+2a_i^2)}{2|h_{i0}|}|V_{i0}|(t-t_0)\right]^{\frac{2}{1+2a_i^2}} . \qquad (4)$$

This solution shows that the exponents and coefficients in equation (4) are explicitly related to the drag coefficient, Atwood number, and initial conditions. For large t, the trajectory of the mixing front of fluid i has the asymptotic behavior

$$|h_i(t)| \sim |h_{i0}|^{1-(\theta_i)} |V_{i0}|^{\theta_i} \theta_i^{-\theta_i} (t-t_0)^{\theta_i} , \qquad (5)$$

where

$$\theta_i \equiv 2/(1+2a_i^2) = 1/\left\{1 + \frac{C_i[1-(-1)^i A]}{1+(-1)^i A + k_i[1-(-1)^i A]}\right\},$$

$$i = 1,2$$

are scaling model parameters for RM mixing similar to the growth rate α_i in RT mixing. These parameters can be measured in experiments. For A = 1, θ_s = 1. These results appear to agree with existing LEM and other experimental data (Figure 3).

We also see that unlike RT mixing, the dynamical evolution of the mixing layer in RM mixing always strongly depends on the initial conditions. These solutions provide the clearest explanation offered to date of the often-noted fact that RT mixing often (in the absence of long wavelengths) loses memory of its initial conditions, while RM mixing does not.

Numerical Simulations

It is well known that (Eulerian) finite-difference solutions of fluid equations with density discontinuities lead to substantial amounts of numerical mass diffusion. Three facts make mass diffusion particularly important in chaotic mixing simulations. First, the instability itself is driven by density differences, so that mass diffusion acts to mask the driving force of the instability. Second, the interface between the two fluids is unstable and its area increases very significantly throughout the simulation, thus allowing for enhanced numerical (or physical) mass diffusion in a 3D mixing context. Third, the solutions are computationally expensive and represent a balance between conflicting objectives, leading to gross under resolution and consequent substantial numerical mass diffusion. The two conflicting objectives are (1) statistical inclusion of a sufficient number of modes to allow the randomization of mode-mode interactions to have a chance to develop and (2) sufficient numerical resolution per mode to allow accurate simulations. In a typical 3D simulation, the bubbles grow in the z direction and are arranged in a planar array, with some 50×50 modes present initially in the x,y plane, each resolved with about 5×5 mesh cells. The numerical diffusion of a density jump will quickly spread to a width of three cells. Under such conditions, much of the density contrast is obliterated by the numerical integration of the equations. This unpleasant picture has been confirmed quantitatively in an analysis of such a typical simulation performed by Xiaolin Li at Stony Brook using a typical numerical method. The numerical mass diffusion reduced the density contrast by 50%, just about the amount by which the simulation underpredicted experimental results.

Having explained the problem, we describe an ideal solution, which is of course just what happens in the physical world. For immiscible fluids (such as oil and water), there is naturally a sharp boundary between the two fluids, even after stirring. More representative is the case of miscible fluids, which do not maintain a sharp boundary, such as coffee and cream. We are interested in the miscible case, but for extremely short time periods, so that they behave much as their immiscible cousins, the oil and water mixtures. For the short time of interest, there is a rapid transition region between the mostly coffee and the mostly cream regions. We locate the surface where the coffee-cream mixture stands at 50%, also known as the 50% iso-concentration surface.

This surface is called the interface, or front. It is a marker for the location of a sharp transition from coffee to cream. Specialized numerical methods are needed to achieve an acceptable approximation of this picture at the very early time, of well-stirred but not well-mixed coffee and cream. These methods all do something special at or near the location of this sharp transition region. The main goal of all such methods is to keep the transition region from coffee to cream as narrow as it would be in the early time for the well-stirred fluids we are describing. To keep the transition region narrow, it is necessary to eliminate numerical mass diffusion as we now explain.

Over the years people have developed high-resolution numerical methods specifically designed to avoid numerical mass diffusion. One of the methods, Front Tracking, developed by the Front Tracking group at Stony Brook and LANL, uses two grid systems. One is a regular grid, which stores the normal fluid variables throughout space. The other is a surface grid, defined on a moving surface (the "front"), which follows (tracks) the moving discontinuity.

Conventionally, difference operators are defined using stencils that may cross the tracked interface. When this occurs these difference stencils and operators are replaced. The state values on the remote side of the interface are replaced with extrapolated ghost-cell state values. In this way, the state values associated with the stencil are all taken from a single side of the tracked interface. This ghost-cell algorithm was introduced by Glimm, Marchesin, and McBryan in 1980[13] and has become widely used in other interface algorithms. This method has been improved through extensions to 3D and robust treatment of topology bifurcations. In a feature which is still experimental, the differencing of the front is completely conservative and replaces the ghost-cell algorithm. This algorithm has been tested extensively on purely mathematical surface deformation problems of interest to the computational interface community. It has been found to be the best of the methods compared. In comparisons, it has outperformed other methods (including level-set and volume-of-fluids methods).

As one continues to improve the strictly numerical aspects of the front-tracking algorithm, it has been realized that improving the physical modeling and solving equations that better represent physical reality are critical. Normally the simulations are conducted with idealized physics, omitting surface tension (for immiscible fluids), physical mass diffusion (for miscible fluids), viscosity, and compressibility. The tracked simulation results presented here include all four: surface tension, mass diffusion, viscosity, and compressibility. The first three have provided the leading order correction for idealized physics for most of the various experiments previously conducted.

As the numerics is of necessity not fully resolved, an important improvement to the simulation was to include subgrid-scale (turbulence) models for viscosity and diffusion. The result was a striking success: the simulations, now having both better physics and better numerics, finally agree with experiments (Figure 5).

It is worthwhile to point out that the agreement with experimental results also required improved modeling of initial conditions, such as the discussed long-wave-length perturbations ("noise") in some experiments and the width of the initial mass diffusion layer.

Furthermore, we would like to point it out that the simulation results of others disagree with experiments and with tracked simulations in the overall growth rate. These investigators find a growth rate half or less of the experimental value.

Comparison of tracked to untracked simulations clearly indicates that numerical mass diffusion in untracked simulations is a major contributor to the discrepancy. Numerical surface smoothing in the untracked simulations also plays a role in the discrepancy.

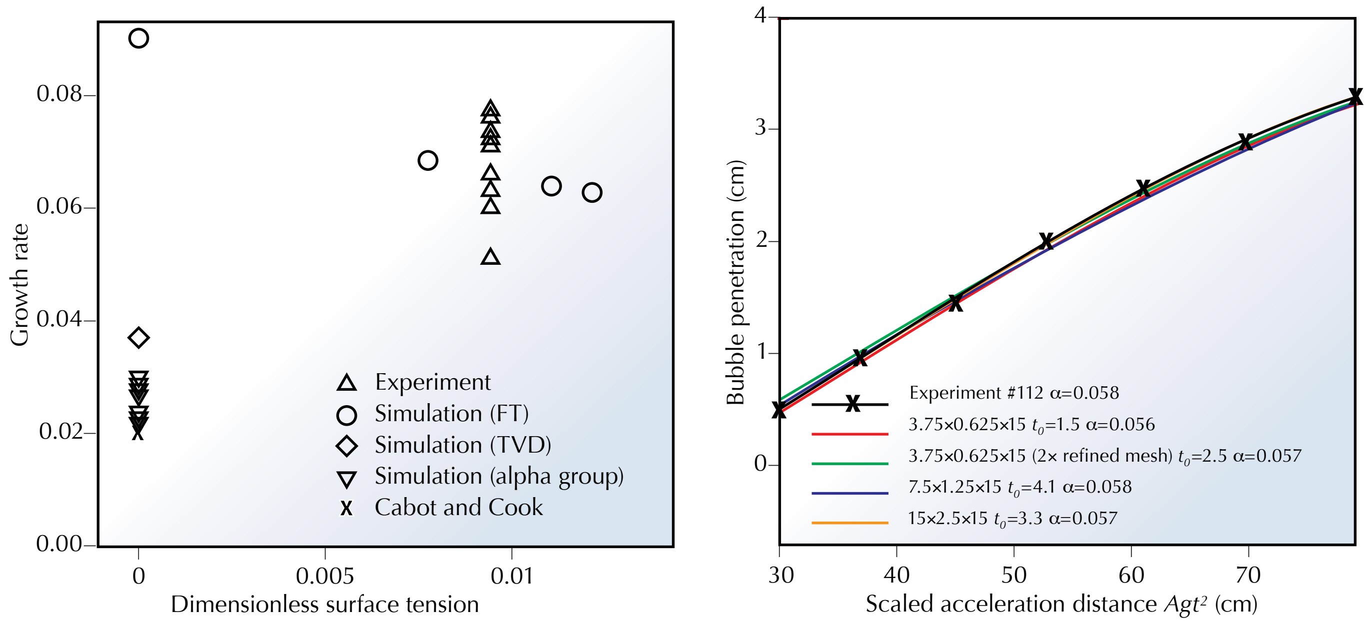


Figure 5. Left plot shows the RT growth rate α_b vs. dimensionless surface tension σ. Shown are all experimental values not using surfactants, several front tracking-simulations with varying levels of surface tension including one without use of surface tension, and several untracked simulations without use of surface tension. We note (a) the excellent agreement of the tracked simulations with experimental results, (b) the significant dependence of the tracked simulations on surface tension and (c) the discrepancy between the untracked simulations with experimental results, with tracked simulations, and with each other. Right plot displays the light fluid (bubble) penetration distance vs. an acceleration length scale, Agt^2. The crosses are the experimental data points and the other curves show several simulations at different levels of grid and statistical resolution. Here statistical resolution refers to the number of initial unstable modes in the simulation. The entry t_0 in the figure legend is a time offset, as the initial times of the experiment and the simulation were not designed to coincide. (Courtesy of the Front Tracking Group at Stony Brook University and LANL.)

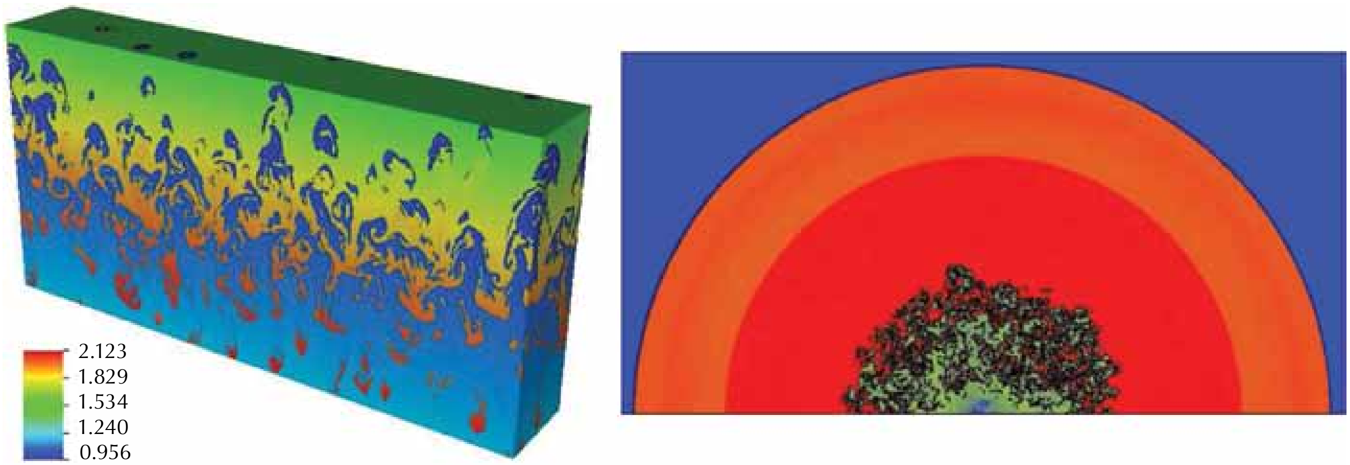


Figure 6. Left shows the density plot for the tracked 3D Rayleigh-Taylor simulation with experiment #112 of Smeeton-Youngs. Right plot shows late-time density for the circular Richtmyer-Meshkov fluid instability. A circular shock, initially at the outer region of the domain, has moved inward through a perturbed circular interface. Upon reaching the interface, it reflects as an outgoing circular shock wave. Upon recrossing the now strongly perturbed interface, the interface becomes extremely chaotic at late time in its appearance. (Courtesy of the Front Tracking Group at Stony Brook University and LANL.)

Figure 6 demonstrates the tracked 3D RT and 2D (circular) RM simulations performed by the Front Tracking group at Stony Brook and LANL; in these calculations, the numerical mass diffusion is very low.

Finally, for further comparison, we demonstrate the simulations for circular RM instabilities at late time, respectively, by Front Tracking (FronTier) and by untracked RAGE (Radiation Adaptive Grid Eulerian)[14] in Figure 7.

The results indicate that the mix structure in FronTier is more complex than in RAGE. For example, the FronTier interface breaks up into droplets whereas the interface in RAGE is smoothed by numerical mass diffusion. At reshock the fingers are heated to a much higher temperature in the FronTier simulation than the corresponding fingers in the RAGE simulation. The main cause for this is the thermal and mass diffusion at the interface in RAGE and the mixed cell hypothesis at a cell level in RAGE and most other computational

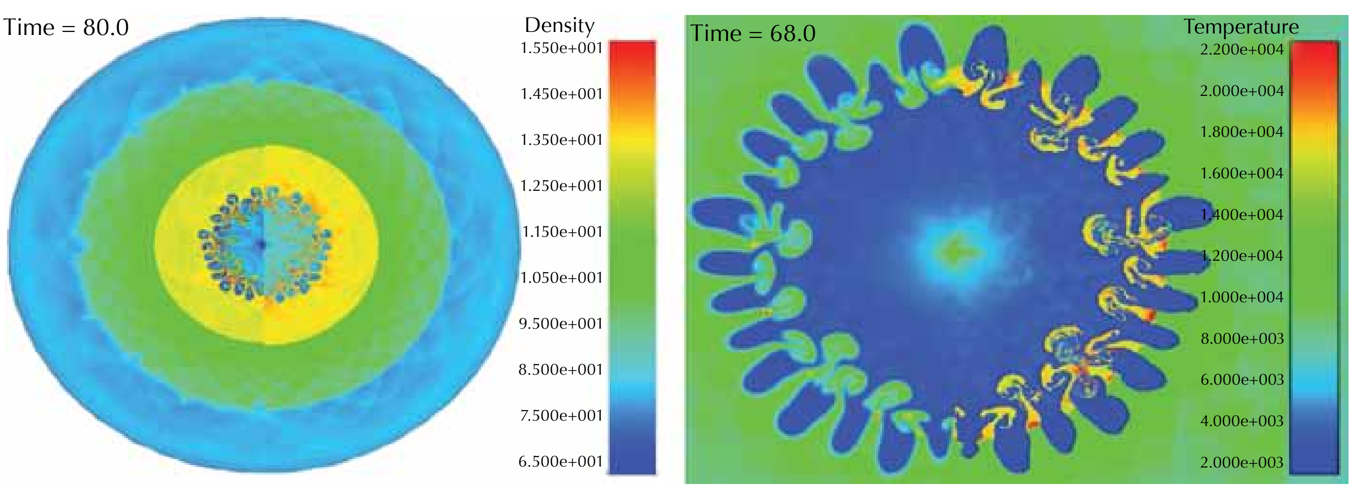


Figure 7. Left plot shows the density difference between the RAGE and FronTier simulations. Right plot shows the temperature difference between the RAGE and FronTier simulations. In each plot, the left side is from untracked RAGE simulations and the right side is from tracked FronTier simulations. (Courtesy of the Front Tracking Group at Stony Brook University and LANL.)

fluid dynamics codes. With front tracking, after shock FronTier continues to have a significantly higher maximum temperature.

Conclusions

In this paper, we have presented theoretical predictions for the Rayleigh-Taylor instability growth rate from the bubble merger model and the dynamical evolution of the mixing fronts (bubbles and spikes) for both the Rayleigh-Taylor and Richtmyer-Meshkov instabilities from the buoyancy drag models. All theoretical predictions have excellent agreement with experimental data. We have also demonstrated numerical simulations of the 3D Rayleigh-Taylor problem and the 2D circular Richtmyer-Meshkov problem with the Front Tracking code in which the numerical mass diffusion is very low. The simulation results from FronTier with an improved front-tracking algorithm and improved physics modeling (including surface tension, physical mass diffusion, viscosity, and compressibility) on the overall RT growth rate are in good agreement with the experimental data while simulations of others give a growth rate only half or less of the experimental value. Comparison of tracked to untracked simulations from RAGE indicates that numerical mass diffusion in untracked simulations is the primary cause for the discrepancy between simulations and experimental data. Clearly, the tracked simulation has outperformed other methods.

Despite successes, many important issues are still unresolved. These include the robust and reliable quantification of the instability evolution; the self-organization, randomness, and stochastic description of unsteady mixed flows; and most importantly, the error quantification of the simulations and the resolution of verification and validation. Glimm et al. observed that an interface between two fluids in a chaotic mixture scales as Δx^{-1} over the range of grids practical for 3D simulations today, and in the absence of regularization, such as by molecular or turbulent mass diffusion.[15,16] Since, for any numerical code, an elementary error estimate (L1 norm) is $\Delta x \times$ [Interface length or area], it was concluded that the overall error is O(1); in other words, the error is not convergent over this range of grid refinement. A nonconvergent error or a solution that converges to a code-dependent limit is a major problem for the goal of predictive simulation. Therefore, exploring the correct resolution for verification and validation and for various physical and numerical regularizations is extremely important.

As mentioned above, the regularized simulations must have physical (molecular and turbulent) transport in their correct proportions. For miscible flow, this is a balance between viscosity and mass diffusivity. The ratio of the two is the Schmidt number. Since the physical values of these transport coefficients are so small relative to most grid spacings, they really have no effect in most simulations, leading to the O(1) error estimate. The correct simulation increases the physical transport coefficients with turbulent ones. When this is done, the divergent estimate for the interface is broken and the O(1) estimate for the error is no longer true; in fact, convergence under mesh refinement is attained. Without turbulent transport terms, the results are ambiguous and even code dependent, so that verification and validation is not possible.

—Baolian Cheng

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Baolian Cheng

Since she joined the Lab in 1994, physicist Baolian Cheng has made significant contributions to the Stockpile Stewardship Program. Research covering pit aging, primary physics certifications, boost metrics, and chaotic mix has earned her a multitude of prestigious awards.

Cheng was awarded the Lab's Distinguished Performance Awards in 2005 and 2006. She garnered two Defense Programs Awards of Excellence from the National Nuclear Security Administration. Cheng won two Los Alamos Achievement Awards for outstanding work in primary metrics in 2007 and 2008.

Cheng works in the X Division's Theoretical Design Primary Physics Group. She earned her doctorate in theoretical astrophysics from University of Illinois at Urbana-Champaign in 1993. She is a graduate of the Lab's Theoretical Institute for Thermonuclear and Nuclear Studies, and has more than 60 refereed journal publications plus 60 invited talks.

Cheng is very active in scientific communities and weapon programs. She is a frequent referee for many peer-reviewed physics and defense-research journals, and has served on the Los Alamos Laboratory Directed Research and Development and Department of Energy review committees, to name a few.

Cheng has been praised by Los Alamos award committee members for her "unusual creativity and breakthroughs on the theoretical understanding of a nuclear device," and plays a "critical role in the Laboratory's primary physicist capabilities in maintaining the nation's stockpile."

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EXPLOSIVES SCHOOL Saves Lives

Hazard Expertise and Science Protect Soldiers

Los Alamos scientists are using their high explosives technical expertise to train US military personnel to recognize homemade explosives (HME) they might encounter while deployed abroad.

HMEs have become a primary threat for our troops because the required ingredients are readily available, inexpensive, and the information is widespread. Understanding and recognizing the hazards of their precursors and mixtures will better prepare military personnel for a wide variety of scenarios.

Personnel from all branches of the military attend an intensive three-day course at the Laboratory to learn how to detect, identify, and characterize a wide variety of improvised explosive compounds and their ingredients. Students also learn vital information about how these explosives are manufactured and employed.

"We're teaching these young men and women what to look for in order to help them separate the good guys from the bad guys," said Becky Olinger of the Lab's High Explosive Science and Technology Group. "Our military troops are seeing a lot of improvised explosives in Afghanistan, so we're teaching them how to use all their senses, coupled with state-of-the-art technology, in order to enhance their awareness of colors, textures, and odors typical of explosive materials or ingredients, as well as how to recognize human indicators that are common to bad guys who have handled these materials or ingredients."

One of the key tools used is the LANL-developed Emergency Response Explosives Field Guide (EREFG) that catalogs the spectrum of energetic materials and compounds and has been used by the Department of Defense and other government agencies for years.

"It's like an information highway with everything you want to know about high explosives—potential ingredients, sensitivity, performance, and how to recognize, identify, and safely handle these materials," said Olinger.

Laboratory experts show military personnel how to use commercially available colorimetric kits in the form of sprays or drops that indicate, for example, the presence of nitrates or peroxides—common ingredients in improvised explosives. They learn hands-on how to analyze samples with portable explosives detectors deployed in combat zones, such as the Ahura FirstDefender Raman infrared spectrometer.

"Suppose you come across a big pile of gray powder, like 25 pounds of unknown material. What do you do?" asked David Moore, of the Shock and Detonation Physics Group, talking to attentive US Marines learning how to take analysis samples.

"First, very carefully, take a really small sample," responded one of the Marines.

"Exactly," said Moore. "If it ignites, you don't want the whole pile to go up."

In addition to classroom and laboratory settings, trainees get hands-on training in the field where they witness a variety of both improvised and conventional explosives detonations so that they can experience the amount of energy available in the materials. Trainees also hone their field skills and test their situational awareness with several realistic mock scenarios set up by the Laboratory's Hazardous Devices Team.

The class evolves with the latest intelligence so that scientists stay current with the threats. LANL scientists are also working with the Department of Defense's Joint Improvised Explosive Device Defeat Organization to get feedback from the troops who have graduated from the class so that they can improve the course based on what the troops have learned in the field or add components that the troops find necessary for future classes. For example, when military personnel found a new device, scientists built a mock device for use in future classes.

The training started in October 2008 with a pilot course for senior military officers and progressed to include US Marine infantry, US Army explosive ordnance disposal (EOD), and reconnaissance personnel from many ranks. The program may expand to offer advanced training designed for EOD specialists on methods to neutralize improvised explosive devices.

"We learn a lot from many of the students, too," said Olinger. "The students provide valuable information to assist with our developing scenarios for future training and in helping us add even more valuable information to the EREFG database."

Scientists from Los Alamos National Laboratory's Chemistry, Dynamic and Energetic Materials, Emergency Operations, and International and Applied Technology divisions share their multidisciplinary expertise to protect military personnel.

—Becky Olinger and Kevin Roark

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Explosives school demonstration shot of a potassium perchlorate mixture.

COUNTERTERRORISM Tactics

Empower Employees to Safeguard Science for Global Security

Editorial by William M. Phillips, III

There is something amiss in the world currently. Several tragic and devastating terrorism attacks were allegedly linked to Islamist radical elements from multiple terrorist networks: the recent New York terror attempt by suspect Faisal Shahzad; admitted subway bomb plot suspects Najibullah Zazi and Zarein Ahmedzay, the latter of whom ranted in court about America's war against Islam; Abdulmutallab's failed attempt to blow up a Christmas-day US flight—he touted "jihad fantasies" online and had ties to al Qaeda; the successful suicide bomb attack in Afghanistan against CIA officers by double-agent Mohammed, a "top five jihadist" according to terrorism specialist Jarret Brachman. And these are just the attacks against Americans within the last few months.

Terror is the goal of many of these attacks, according to US government officials.

"I would say that that was intended to terrorize, absolutely," White House spokesman Robert Gibbs stated in recent briefing regarding Shahzad's failed Times Square attack. "And I would say that whoever did that would be categorized as a terrorist, yes."

And although attempts failed, terrorist networks are advanced and well funded.

"The jihadists are showing impressive counterintelligence ability," Reuel Marc Gerecht, a senior fellow at the Foundation for Defense of Democracies wrote in a recent newspaper editorial. Gerecht further noted, "Al Qaeda has revealed that it is capable of running sophisticated clandestine operations with sustained deception."

As the head of the counterintelligence program at a major US Department of Energy (DOE) nuclear weapons lab, I am frankly quite worried by Mr. Gerecht's astute and timely observations.

It would seem that as the so-called War on Terror drags on, our adversaries are becoming increasingly sophisticated and innovative. They are also demonstrating that the jihadists' activity is not monolithic and that it is as varied and diverse in tactics and philosophy as it is in the types of people who become jihadists.

Although in Arabic, jihad literally means struggle, the word is frequently associated with warfare in defense of Islamic territory and—more often, terrorism.

The times are past when we can say with unwavering confidence that the energy of the radicalized Islamist/jihadist movement will dissipate. Evidence does not support this. We would only be naïve fighters in the counterterrorism (CT) wars to think that our adversaries were any less intelligent than we are—or less committed to what they see as religious struggle. We have not seen a direct attack by the jihadists upon our energy resources or our nuclear weapons facilities—but if recent attempts serve as an example of heightened terrorist determination, it would be absurd for us to assume such attacks won't happen. Prudence and historical wisdom suggest that we need to put more intellectual, fiscal, CT, and counterintelligence (CI) resources into analyzing attack risks for our weapons infrastructures. As Gichin Funakoshi, the founder of Shotokan karate said, "Calamity springs from carelessness." We must not be careless in our understanding of the jihadists and/or preparedness to deal with them.

Al Qaeda has revealed that it is capable of running sophisticated clandestine operations with sustained deception.

William M. Phillips, III is the LANL Counterintelligence Program Director. The retired Central Intelligence Agency officer is an avid Japanese martial arts student.

It may not be as difficult as we may have once thought for a determined adversary to acquire a double agent with sensitive infrastructure access. How do we prevent this or harden our infrastructure to these types of penetrations?

One of the best ways of addressing this challenging and philosophically provocative issue is by strengthening the education of those working within the energy and nuclear weapons establishments about terrorism—and espionage—threats.

The success of the terrorist…is only limited by his or his organization's creativity, initiative, and commitment to cause. Al Qaeda has shown that it has all three of these attributes in disturbing quantities.

Protection from Within

The best way to educate people about risks, and therefore reduce them, is to apply traditional counterespionage operational techniques to the CT phenomena. One way to help is for weapons facilities to consider supporting a more robust CT component of existing counterintelligence programs and increasing awareness about employees' international connections.

The virulence of our terrorist adversaries is so great now that large institutions, and particularly those involved with nuclear weapons, might choose to consider making CI and CT an element of each employee's annual performance appraisal—separate from standard security training. This sensitivity training will enhance their core mission, whether it is engineering, science, or technology, thereby supporting the Lab as a whole and protecting facilities from attack.

"Deal with a dangerous situation while it is safe…eliminate what is vicious before it becomes destructive."

—Chinese Philosopher Lao Tzu

It is hard to convince people who are not from the CI, CT, and security disciplines that counterespionage awareness is crucial to better protect Lab programs, interests, and personnel.

At Los Alamos National Laboratory, we have had some success in increasing the awareness of employees. However, given the obvious increase in creativity of the terrorist adversary, it may be time to ratchet up the conversation.

We must remember that the success of the terrorist or espionage operative is only limited by his or his organization's creativity, initiative, and commitment to cause. Al Qaeda has shown that it has all three of these attributes in disturbing quantities.

Improving education about jihadists' methods is part of the psychological war that is occurring. The great Chinese tactician and philosopher Sun Tzu said that one goal in warfare is to "make your enemy think that your normal force is extraordinary and that extraordinary is normal," according to translations of his book, *Art of War*. It appears that we may be failing in this aspect of the conflict. Our adversaries, the jihadists with whom we are locked in a global conflict, appear to not believe that we can defeat them. So in one sense, we have failed.

Education of the community is a weapon, too. The tragic success of the recent deadly attack against our nation's external intelligence agency should give pause. We cannot, as Sun Tzu said, "rely on the likelihood of our enemy not coming, but on our readiness to receive him."

Make your enemy think that your normal force is extraordinary and that extraordinary is normal.
***—Sun Tzu,* The Art of War**

Finally, some might argue that the United States, as an imperial power, is on the decline as evidenced by the recent collapse of the stock market, and our seeming inability to permanently neutralize the terrorist adversary. These developments, in my view as an counterintelligence professional, will be exploited by the jihadists and foreign intelligence adversaries who may presume our nation is not paying attention. They will plan.

We have much work to do. —*William M. Phillips III*

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OPTIMAL Quantum CONTROL

Lasers Provide Safer Remote Explosives Detection

Suicide bombs, improvised explosive devices (IEDs), explosive-packed cars or trucks, land mines—these weapons kill or maim people around the world every day. In response, scientists are trying to develop ways to detect weapons from a safe distance before they can go off.

David Moore is one of those scientists. A Los Alamos laser spectroscopist, Moore is also an expert on remote explosives detection. He and several Los Alamos colleagues are currently collaborating with researchers at Princeton University to develop a new technique that uses carefully shaped ultrashort laser pulses to remotely detect trace amounts of explosive molecules. (Each pulse lasts for only 8 femtoseconds [fs], or 8 million billionths of a second.)

These molecules can be found in the vapor emitted by an explosive or in explosive particles in a fingerprint left on the surface of an explosive device by its builder. But it's not easy to detect the tiny amounts of explosive molecules present in these forms from a safe distance, in a reasonable amount of time,

David Moore's research that detects concealed threats has many applications, including airline passenger safety.

and despite other nearby molecules that can mask the targeted molecules' chemical signatures.

For example, the explosive particles hidden in a terrorist's fingerprint on the door of an explosive-laden car (or on the outside of an IED) typically have a density of about 1 milligram (mg) per square centimeter (cm).

A first-generation fingerprint—the first fingerprint put down after a bomb handler's finger or glove has been contaminated by explosive material—usually contains the largest amount of explosive material. In successive generations of fingerprints, the amount of explosive material decreases exponentially—but never quite goes to zero. As a result, there are always trace amounts of explosive molecules at the scene of such an impending crime. Los Alamos detection methods decipher vital clues.

Detection sensitivity may eventually make it possible to foil even the most fastidious bomb maker.

Recent studies suggest it would be desirable to be able to detect amounts of explosive material as small as small as 0.001 mg/cm^2 or so. Such a detection sensitivity may eventually make it possible to foil even the most fastidious bomb maker. Moreover, for safety, the instrument should detect the explosive molecules from a distance of at least 10 meters (m), although even much larger distances are clearly desirable.

Moore says all known instrumental methods have been studied for remotely detecting explosives, but none of them even comes close to meeting the task's demanding requirements. A promising approach, however, is to use laser beams to remotely detect explosive molecules through their interactions with light.

CARS Insurance

In particular, a type of laser-probe technique called coherent anti-Stokes Raman spectroscopy (CARS) could be a game-changer for remotely detecting explosives. (See sidebar on page 23 for a description of Raman spectroscopy and CARS.)

Last year, Israeli researchers obtained useful CARS spectra from a sample containing less than 1 mg of KNO_3 (an ingredient in gunpowder) and another sample containing less than 4 mg of RDX (an explosive) by firing a rapid succession of 30-fs laser pulses at the samples from a distance of 5 m. The researchers acquired CARS spectra good enough to positively identify these molecules in just 3 seconds.

To get the best results, the researchers intuitively adjusted, to some extent, the "shape" of the laser pulse—that is, how its amplitude varies with time. Improving on this approach, the Los Alamos/Princeton team uses automated closed-loop adaptive algorithms, as described below, to optimize pulse shape much more flexibly and accurately. The team's method also works despite the presence of contaminating molecules.

Such molecules are a serious problem for remotely detecting explosives. In a real setting, say, on a street in Kandahar, extraneous molecules will be "embedded" with the targeted molecules, making it harder to detect the targeted ones. Moreover, in a real setting—unlike a controlled laboratory setting—it's not possible to know in advance what contaminating molecules could be present. However, quantum control, coupled with automatic pulse shaping, will allow the team to enhance detection of the targeted molecules even when unknown contaminating molecules are present.

Taking Quantum Control

When the first laser was successfully operated in 1960, scientists immediately thought to use it to control the behavior of atoms and molecules at the most basic level, where quantum mechanics rules. Now called quantum control, this dream has become reality in the last decade or so.

In quantum control, a molecule's structure, vibrations, or rotations are controlled by the electric field of light, which pushes on the molecule's electrons. Because laser pulses can now be produced with durations comparable to the periods of natural molecular vibrations and rotations (about 30 fs), a molecule's electrons can now be nudged by light pressure on comparable time scales. This makes it possible to adjust these vibrations and rotations *as they occur* to produce desired effects.

In fact, extremely precise adjustments of these vibrations and rotations are now possible—because the shape of an ultrashort laser pulse can now be very precisely controlled. This means that a molecule's electrons can be nudged in just the right way at just the right time to enhance particular types of molecular motion while suppressing other types.

Quantum control can also be used to increase the yield of a chemical reaction or to produce a reaction not otherwise possible, but using it to manipulate molecular motion is particularly relevant to explosives detection because each Raman line—a narrow peak in intensity in a molecule's Raman fingerprint—is associated with a specific molecular vibration or rotation. The Los Alamos/Princeton team uses quantum control to excite molecular vibrations so that the constructive or destructive interferences of the vibrations enhance certain Raman lines of a particular type of molecule (e.g., explosive molecules) while suppressing certain Raman lines of the other types of molecules that also happen to be present.

Finding the Right Shape

In theory, the pulse shape needed to produce a certain molecular effect through quantum control can be calculated from the Schrödinger wave equation—which governs the quantum-mechanical behavior of subatomic, atomic, and molecular systems. But appropriate forms of the wave equation are too complicated to be solved on existing supercomputers. However, *experiments*, rather than calculations, can be used to find the right shape.

In this case, the researcher starts with a particular shape, measures how effectively the shape produces the desired experimental result, and then adjusts the shape to produce a better result. This is the "closed-loop" aspect of optimal quantum control.

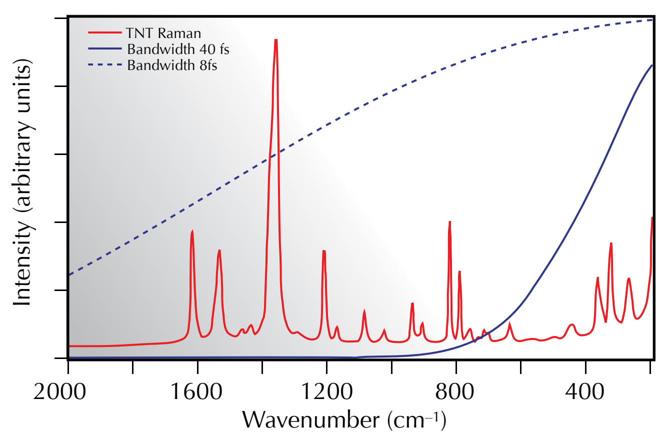
But what shape should the researcher start with? And how should the shape be changed to produce better results? As mentioned, intuition has been used with some success—to systematically vary the peak intensity or the times between the pulses in a series of pulses, but automated-optimization approaches are better yet.

To implement an automated approach, the researcher first defines a "fitness function," which measures how well a particular shape produces the desired result. As the experiment is repeated, a computer algorithm decides after each repetition how to adjust the shape so the value of the fitness function increases for the next repetition. After many repetitions, the fitness function approaches a maximum value as the pulse converges to its optimum shape.

In initial experiments, the team defined a fitness function that would maintain the peak intensities of the Raman lines of the explosive molecule of interest and minimize the peak intensities of the other molecules present, while simultaneously maintaining the relative peak heights of the Raman lines of the explosive molecule. The main problem encountered in these experiments was in defining the fitness function. In the end, a fitness function that performed reasonably well was found by trial and error.

A Pulse with Potential

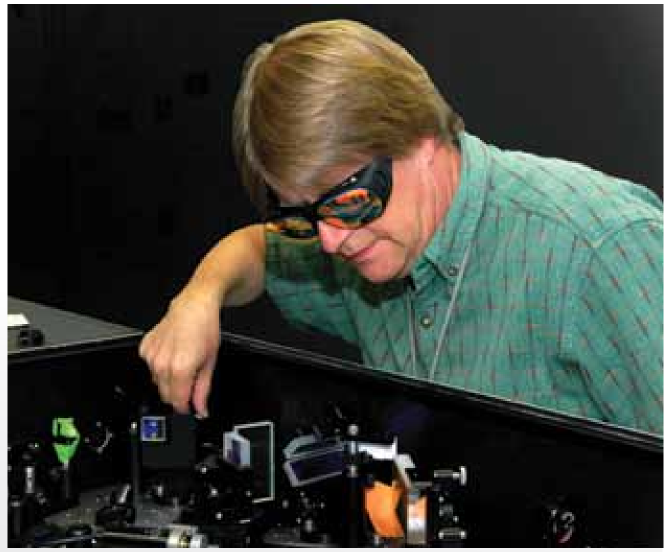
The team also focused on producing laser pulses with the most potential for remotely detecting explosive molecules. These days, 30-fs laser pulses are fairly common. But to use CARS to detect explosive molecules, the ultrashort laser pulse should also have a



The spectral bandwidth of laser pulses with a narrow bandwidth (8 fs) and a wide bandwidth (40 fs) compared with the Raman fingerprint of a molecule of TNT. The wide-bandwidth pulse covers most of the Raman lines in the fingerprint region and can therefore excite most of the vibrational modes associated with those lines, which is why the wide-bandwidth pulse has more potential for identifying an explosive molecule in the presence of contaminating molecules.

Moore Receives LANL's Fellows Prize

Los Alamos scientist David S. Moore recently received the Laboratory's 2009 Fellows Prize for Outstanding Leadership in Science or Engineering.



Moore was selected by some of the Lab's most esteemed scientists. The committee selected Moore for "his inspirational technical leadership in the fields of shock physics and the science of explosives detection." According to the prize committee, Moore is a nationally recognized leader in explosives detection and "is an exemplary citizen to the Laboratory, to the international scientific community, and to the nation." He was also praised for his mentoring skills.

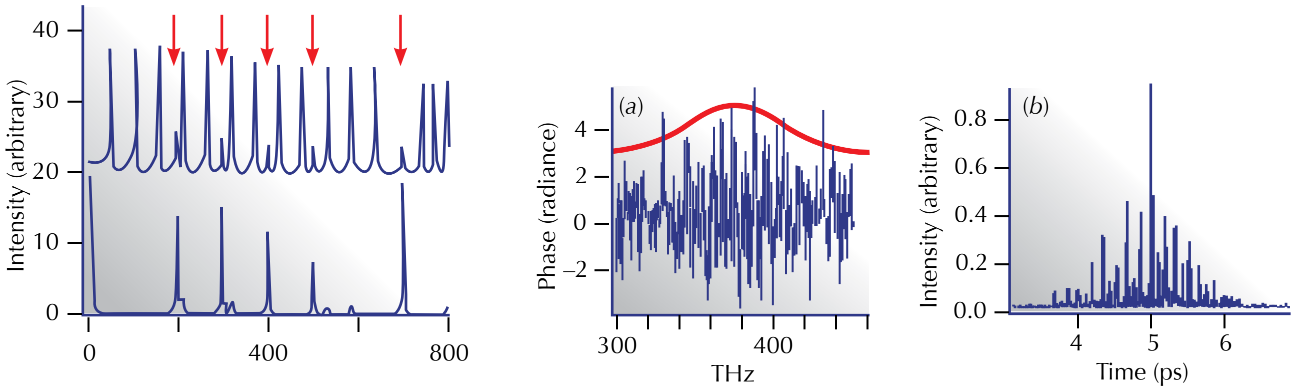
In 2004, Moore received the prestigious American Physical Society Fellowship for "breakthroughs in the use of nonlinear optical and ultrafast spectroscopies used to understand the behavior of molecules under shock compression." He holds four patents and authored more than 130 publications and five book chapters. Moore, educated at the University of Utah and the University of Wisconsin, was also an Alexander von Humboldt Foundation fellow in Germany.

large spread of wavelengths—also called bandwidth—so the pulse can excite most of the Raman lines of the explosive molecules of interest.

In the presence of contaminating molecules, a wide-bandwidth pulse has more potential for detecting explosive molecules than a narrow-bandwidth pulse does—because a wide-bandwidth pulse can be adjusted to enhance more of an explosive molecule's Raman lines while suppressing the Raman lines of other molecules that are present.

To produce a suitable wide-bandwidth pulse, the team first focuses a 30-fs laser pulse in argon gas to produce a plasma channel. As the pulse passes through the channel, the channel's electric-field-dependent index of refraction increases the bandwidth of the pulse. However, the channel simultaneously smears out the pulse's frequency components in time, which increases the pulse length to typically several hundred femtoseconds. To correct for this effect, the pulse is then passed through a pulse shaper, which realigns the frequency components in time—the pulse is now said to have zero phase—and reduces the pulse length to 8 fs. At this point, the pulse length is at its theoretical minimum for the pulse's increased bandwidth.

Such a pulse is ideal for performing optimal quantum-control experiments. For one thing, a pulse length of 8 fs is short enough to excite the Raman lines of interest. (Several hundred femtoseconds is much too long.) For another, using a pulse with zero phase



(*Left*) Computer simulation showing that pulse shaping can enhance selected vibrational peaks in an artificial molecule. The upper spectrum was excited by an unshaped pulse. The lower spectrum was excited by a pulse shape optimized by an adaptive genetic algorithm to enhance the five peaks marked by the arrows. (*Right*) The frequency-dependent phase (*a*) and time-dependent intensity (*b*) of the simulated optimized pulse used to produce the lower spectrum at left.

ensures that the optimizing algorithm can find the best pulse shape efficiently.

Results to Date

The team first began exploring optimal quantum control with computer simulations that used an adaptive genetic algorithm to optimize the shape of a pulse to selectively excite five vibrations in an artificial molecule.

The team then went on to optimize the shape of a time-compressed 8-fs laser pulse in actual experiments. The goal was to enhance the detection of liquid nitromethane, an explosive chemical, mixed with two other liquid chemicals—toluene and acetone—as contaminants. The encouraging results of these experiments are shown in the figure below.

The Future of Explosives Detection?

Detecting explosive devices from a safe distance before they can go off is hard because only trace quantities of explosive molecules will be available for detection—in explosive vapor or the bomb maker's fingerprints. The explosive molecules must also be accurately identified despite the presence of other molecules. Existing detection methods come nowhere near the mark, but optimal quantum control methods, combined with nonlinear spectroscopies such as CARS, could one day be totally on target. —*Brian Fishbine*

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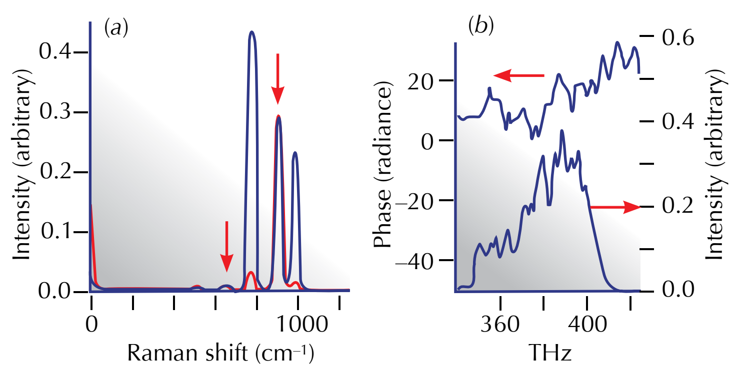
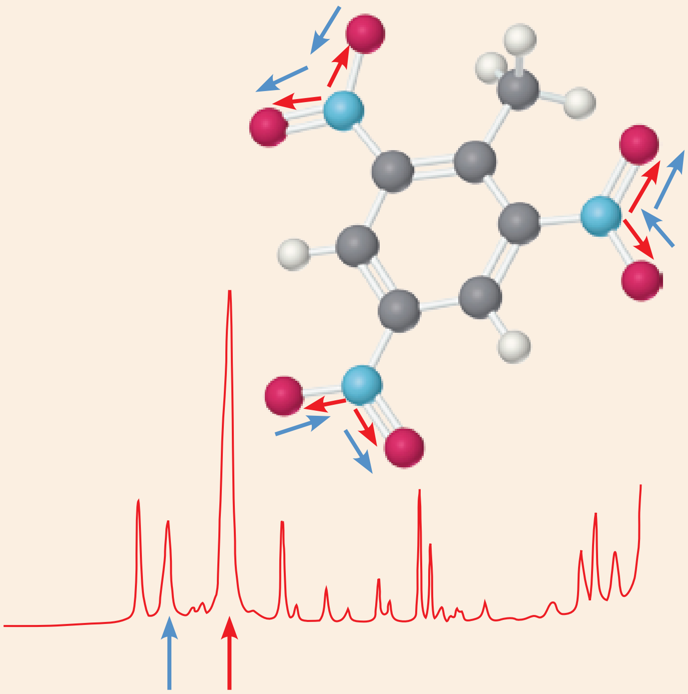
(*a*) CARS spectra for a 1:1:1 volumetric mixture of toluene, acetone, and nitromethane. The arrows mark the nitromethane peaks of interest. The black dotted curve is the Raman spectrum produced by the unshaped pulse. The solid red curve is the spectrum produced by the optimally shaped pulse shown in (*b*). Together with the nitromethane line near 900 cm^{-1}, the two lines on either side of it—produced by chemicals other than nitromethane—largely dominated the spectrum produced by the unshaped pulse. The shaped pulse greatly suppressed the two major lines on either side of the nitromethane line, showing the potential of optimal quantum control to identify targeted molecules in the presence of contaminating molecules.



Using Raman Spectroscopy to Lift Molecular Fingerprints

The way a molecule interacts with light is largely determined by how the atoms composing it go together. For example, a molecule's atoms are bound together, usually in pairs, by electrostatic forces acting like tiny springs. Each atom can vibrate along a spring's axis at a frequency determined by the spring's strength and the masses of the atoms at each of the spring's ends. Other vibrational modes are also possible. Sometimes, a molecule can rotate around the principal axes of its reference frame at frequencies determined by its atoms and their placement.

When a molecule absorbs or emits a photon from, say, a laser beam, the amplitudes of various molecular vibrations or rotations can increase or decrease, respectively. The transfer of light energy to—or from—a molecule that produces a change in the intensities of its vibrations or rotations can be observed by measuring how the molecule absorbs light or how the wavelength of incident laser light changes during scattering.



In this ball-and-stick model of TNT, the blue arrows indicate oppositely directed motion (antisymmetric vibration) of the two oxygen atoms (red balls) centered on a nitrogen atom (blue ball). Red arrows indicate motion in the same direction (symmetric vibration) of the same two oxygen atoms. Hydrogen atoms are white; carbon atoms are gray.

This second measurement method is based on the Raman effect, in which the scattered light's wavelength becomes longer when the molecule's vibrational or rotational energy increases and shorter when that energy decreases. The wavelength change is also known as Raman shift. Chandrasekhara Venkata Raman, an Indian scientist, first measured the effect in 1928 and received the Nobel Prize for his work in 1930.

Raman used filtered sunlight to perform his experiments, but laser light is better because it is more intense and has a very narrow bandwidth. Higher intensity decreases the time required to measure a Raman spectrum; narrow bandwidth makes it easier to detect the very slight changes in wavelength caused by changes in molecular vibrations or rotations.

A plot of a sample's absorption as a function of wavelength provides a unique fingerprint for each type of molecule. Although infrared absorption is commonly used to identify molecules, detection methods based on this type of spectroscopy are harder to implement at adequate stand-off distances than laser-based methods are. For this and other reasons, Raman spectroscopy—which can also make use of similar molecular fingerprints—is currently one of the most promising types of laser probing for remotely detecting explosive molecules.

But ordinary Raman scattering is very weak. Its cross section—the ratio of the scattered to the incident light—is 14 to 15 orders of magnitude smaller than those of absorption or fluorescence. However, the Raman cross section can be greatly enhanced by driving the scattering coherently (i.e., in phase) using one laser to excite the Raman lines and a second laser to drive the scattering coherent at the difference frequency between the two lasers.

One of these coherent methods—coherent anti-Stokes Raman scattering or CARS—combines two photons at the excitation frequency with one photon at the Raman-shift frequency to produce a coherent beam at the anti-Stokes, or blue-shifted (higher-frequency) wavelength.

CARS can be extremely sensitive because its cross section depends on the product of the square of the excitation-laser intensity, the intensity of the Raman-shift laser, and the square of the concentration of the molecules to be detected. Also, the scattered signal is coherent and emitted in a narrow beam—like a laser—which makes detection much easier, especially from a distance.

JOSEPH MARTZ

Stanford University William J. Perry Fellow in International Security
Center for International Security and Cooperation

Joseph C. Martz

The Nuclear Weapons Complex as **Deterrent**

Challenges and Issues

In February of 2007, former Secretary of Defense Bill Perry joined former Secretaries of State George Shultz and Henry Kissinger and Senator Sam Nunn in calling for a recommitment to achieving a world without nuclear weapons. Their *Wall Street Journal* editorial received wide exposure and discussion, continuing with President Barack Obama's April 2009 speech in Prague in which he endorsed this goal. The recently released Nuclear Posture Review (NPR) embraces these ideas. The NPR balances several important issues and concerns in a reasonable and responsible way. It recognizes the diminished role that nuclear weapons can play in a 21st century environment in the protection of vital US national security interests, while recognizing that nuclear deterrence can and should continue for both the US and our international security partners. Los Alamos National Laboratory and Stanford University have played a role in these developments, and the implications for the future of the national laboratories and the nuclear weapons complex are profound.

With this backdrop, I was asked in the Spring of 2009 if I wished to serve as the inaugural William J. Perry Fellow in International Security at Stanford University. After 27 years at LANL, this would be my first lengthy assignment away from Los Alamos. My prior work in plutonium and pit science, my work with the enhanced surveillance campaign, and my recent work with X Division and the reliable replacement warhead design competition provided a firm foundation in the technical aspects of nuclear weapons and deterrence. The goal of this fellowship was to bring this technical perspective to a more policy-focused environment, expanding upon the knowledge at Stanford's Center for International Security and Cooperation (CISAC) to connect the social and physical sciences addressing national security. For the first Perry fellow, there was a strong desire to focus on technical elements and means to achieve the vision laid out by "the four horseman" as the senior diplomats have become known. How might nuclear policy, the nuclear stockpile, and the nuclear complex itself be configured to preserve the benefits of deterrence in an environment of further stockpile reductions?

CISAC's distinguished history in the area of nuclear deterrence and policy began in 1983, with several former laboratory directors including Sig Hecker of Los Alamos (current CISAC co-director) and Mike May of Livermore, current faculty members plus prominent officials, including former Secretary of State Condoleezza Rice. CISAC research on foreign nuclear weapons programs is world class. John Wilson Lewis and Xue Litai's treatise on Chinese nuclear development *China Builds the Bomb* and David Holloway's *Stalin and the Bomb* are considered by many the most comprehensive studies of their kind. Other CISAC faculty have written extensively in the areas of nuclear policy, nuclear weapon accidents, and nuclear war planning and effects.

An example of the impacts of this work is the interaction between CISAC and North Korea. Lewis, invited to North Korea, asked Hecker to accompany him in 2003, resulting in Hecker's annual diplomatic return trips. Hecker physically held samples of North Korean plutonium on his first visit, an effort his hosts indicated was to demonstrate "the viability of their deterrent." This exchange became a "Track Two" dialogue with North Korea and is among the most significant discussions between the United States and North Korea in the last two decades.

With the presence of Perry and his associates at CISAC—aided by George Shultz and former Stanford Linear Accelerator Director Sid Drell at the nearby Hoover Institution—Stanford research is turning toward issues raised by the vision of a world without nuclear weapons. Given the close connection between CISAC and the national labs, it was natural for CISAC to reach out to the labs to bring current-generation expertise in nuclear weapons to this area.

In the 1984 book, *The Abolition*, Jonathan Schell said, "The capacity for retaliation would consist less and less of the possession of weapons and more and more of the capacity for rebuilding them, until, at the level of zero, that capacity would be all."

Will a capability-based deterrent be seen as provocative to the international community? How might those countries that have US nuclear assurances feel about this strategy? What is the impact of this strategy on arms control and nonproliferation? Answers to these questions are complex.

My own interests in this area are long-standing. The idea that the nuclear weapons complex—including the national laboratories—serves as a component of the deterrent by simultaneously preserving security while reducing the nuclear stockpile appeals to me. In *A World Without Nuclear Weapons: End-State Issues*, Schultz stated,

> "We have to change our way of thinking about nuclear deterrence. [We need] ideas including stretching out time for decision making during a nuclear crisis and relying increasingly on an ability to reconstitute nuclear forces as a safer form of nuclear deterrence."

The "ability to reconstitute nuclear forces" as a form of deterrence is not new. Ted Gold and Rich Wagner wrote in 1990 about this idea in *Long Shadows and Virtual Swords: Managing Defense Resources in the Changing Security Environment.*

The weapons complex as a deterrent component poses many highly technical questions, many of which are the core of my research. Key questions include the timing and capacity of the nuclear weapons complex for reconstitution and the survivability and redundancy of the complex—especially the vulnerability of a capability-based deterrent to a first strike. In addition, military deterrence issues must be addressed—particularly the reconstitution of delivery systems and platforms.

Other critical questions are in the area of international relations, perceptions, and the reaction of both allies and adversaries to these ideas. Will a capability-based deterrent be seen as provocative to the international community? How might those countries that have US nuclear assurances feel about this strategy? What is the impact of this strategy on arms control and nonproliferation? Answers to these questions are complex and nuanced, and I've just begun addressing a subset of them with the help of colleauges. Let's examine the need for agility in the nuclear weapons complex as an enabler of a capability-based deterrent.

In evaluating the idea of a capability-based deterrent, it's essential to understand that this capability does not stand on its own, at least not initially or for the foreseeable future. A companion (smaller) deployed nuclear arsenal works hand in hand with the capability to preserve security. The vast majority of threats can be met with a much smaller number of nuclear weapons.

Historically, most of the weapons in the stockpile were designed to deter the Soviet Union. A shift in US strategy beginning in 1970 resulted in the removal of most tactical nuclear weapons and adoption of a deterrent—rather than warfighting—role. Since arms control agreements have been reached, both Russian and US stockpiles have decreased dramatically. How far can the strategic balance be extended? Recent negotiations with the Russians resulted in the New START (Strategic Arms Reduction Treaty) treaty which limits the total deployed stockpile to 1550 warheads, though the NPR makes clear that further reductions are possible.

Closely related to this discussion are the hedge and backup nuclear forces—weapons that are retained in the event of a breakout by Russian (or possibly, Chinese) forces, or the discovery of a technological surprise in US weapons. This stockpile situation is well suited to a discussion of a capability-based weapons complex. Agility of the complex becomes key in preserving an effective deterrent, embraced by recent policies. The NPR report stated:

> "Second, implementation of the Stockpile Stewardship Program and the nuclear infrastructure investments recommended in the NPR will allow the United States to shift away from retaining large numbers of non-deployed warheads as a hedge against technical or geopolitical surprise, allowing major reductions in the nuclear stockpile. These investments are essential to facilitating reductions while sustaining deterrence under New START and beyond."
> —2010 *Nuclear Posture Review Report*, Page 30

William J. Perry and Joseph C.Martz

In essence, we must be able to reconstitute a nuclear force more rapidly than a credible threat might arise. What type of threat might require the reconstitution of a nuclear force beyond the smaller stockpile envisioned? It's hard to construct scenarios in which potentially rogue states such as North Korea or Iran will require a rearming and Cold-War type response. Essentially, the two prior scenarios of an expansionist China or a recidivist Russia are the only credible threats for substantial rearmament. Thus, if the US can respond by reconstituting more rapidly than these threats could manifest, then the complex itself will serve a deterrent role. Response timing and reconstitution capacity are prominent in my research. On this point, the NPR report has limited detail:

> "New production facilities will be sized to support the requirements of the Stockpile Stewardship Program mandated by Congress and to meet the multiple requirements of dismantling warheads and eliminating material no longer needed for defense purposes, conducting technical surveillance, implementing life

extension plans, and supporting naval requirements. *Some modest capacity will be put in place to surge production in the event of significant geopolitical 'surprise.'*" [Ed.: author's emphasis]
—2010 *Nuclear Posture Review Report*, Page 42

An equally important issue in the establishment of the weapons complex as a greater component of deterrence is the confidence this brings to our leaders and those of our allies as well as the precedent and tone it establishes for the international community. As the NPR report stated:

"Today, the reassurance mission remains, but the deterrence challenge is fundamentally different. While we must maintain stable deterrence with major nuclear powers, the likelihood of major nuclear war has declined significantly; thus far fewer nuclear weapons are needed to meet our traditional deterrence and reassurance goals…Moreover, our most pressing security challenge at present is preventing nuclear proliferation and nuclear terrorism, for which a nuclear force of thousands of weapons has little relevance."
—2010 *Nuclear Posture Review Report*, Page 45

Gaining global transparency is an essential element in nuclear materials

The combination of a greater reliance on deterrence and the need to reduce proliferation (i.e., control nuclear materials and technologies) requires improved transparency by all parties. Transparency will assure allies that our capabilities are robust while deterring potential challengers. Gaining global transparency is an essential element in nuclear materials management. Timing is critical, as the US begins to design replacements for two large nuclear facilities (LANL's Chemistry and Metallurgy Research Replacement and Y-12's Uranium Processing Facility). Now is an ideal moment to consider transparency.

2010 has quickly become a year of historic developments and relevance regarding nuclear weapons, national policy, and international developments. Not since the end of the Cold War has so much attention been focused on the role of nuclear weapons in national security, including proliferation and terrorism concerns. A renewed commitment to reinvest in our nuclear weapons complex is an essential strategy component. Partnerships between Los Alamos and key centers such as CISAC ensure that policy makers are well informed.

Perhaps the most gratifying element of my time at Stanford has been the widespread recognition of the important contributions of Los Alamos and the rest of the national security complex to meet the evolving national security needs. My colleagues at LANL should feel very proud that their work is highly regarded well outside the boundaries of the Lab.

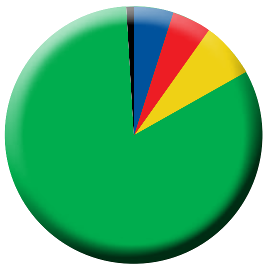
—Joseph C. Martz

PERFORMANCE SNAPSHOT

The Performance Snapshot gives our external customers data on how the weapons programs are performing in three critical areas: Level 1 and Level 2 programmatic milestones, safety, and security.

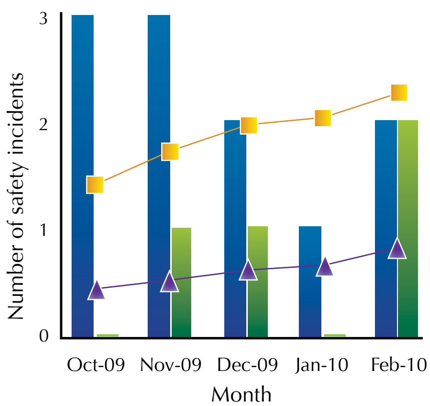
Level 1 and 2 Milestones

FY10 Quarter 2



Level 1 (L1) milestones—very substantive, multiyear, supposed to involve many, if not all, sites

Level 2 (L2) milestones—support achievement of L1 goals, annual milestones are reported to NNSA program management on a quarterly basis. Progress on milestones is entered into the Milestone Reporting Tool.



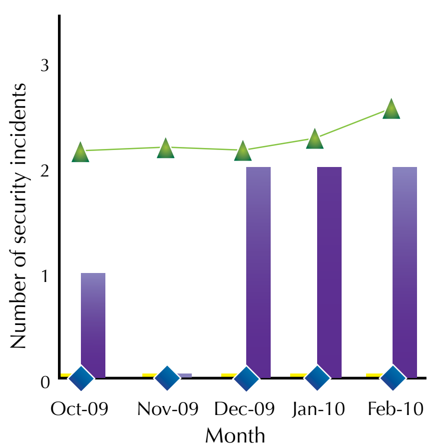
Safety Trends

October 2009 through February 2010

Total reportable cases (TRC)—those that result in any of the following: death, days away from work, restricted work or transfer to another job, or medical treatment beyond first aid or loss of consciousness

Days away from work, restricted work activity, or transfer (DART) to another job as a result of safety incidents

TRC 12-month cumulative*
DART 12-month cumulative*
TRC incidents per month
DART incidents per month
*per 200,000 productive hours



Security Trends

October 2009 through February 2010

Incidents of security concern (IOSCs) are categorized based on DOE's Impact Measurement Index (IMI) table (*below*). The IMI roughly reflects an assessment of an incident's potential to cause serious damage to national, DOE, or LANL security operations, resources, or workers or degrade or place at risk safeguards and security interests or operations.

IMI-1 & -2 normalized 12-month cumulative*
IMI-3 & -4 normalized 12-month cumulative*
IMI-1 & -2 incidents per month
IMI-3 & -4 incidents per month
*per 200,000 productive hours

Categories of IOSCs

(DOE M 470.4-1, Section N)

IMI-1 Actions, inactions, or events that pose the most serious threats to national security interests and/or critical DOE assets, create serious security situations, or could result in deaths in the workforce or general public.

IMI-2 Actions, inactions, or events that pose threats to national security interests and/or critical DOE assets or that potentially create dangerous situations.

IMI-3 Actions, inactions, or events that pose threats to DOE security interests or that potentially degrade the overall effectiveness of DOE's safeguards and security protection programs.

IMI-4 Actions, inactions, or events that could pose threats to DOE by adversely impacting the ability of organizations to protect DOE safeguards and security interests.

William**Parsons**

Many people believe J. Robert Oppenheimer built the first two atomic bombs—if not by his own two hands, then at least by his sheer intellectual brilliance. However, the task of actually building the world's first nuclear weapons and taking them into combat fell to an obscure Navy Captain who called Fort Sumner home, William S. (Deak) Parsons. A graduate of the US Naval Academy and the Naval Postgraduate School, Parsons was the preeminent ordnance engineer in the United States military. Recognizing that the wartime Los Alamos Laboratory needed an ordnance engineering expert, Manhattan Project Commanding General Leslie Groves did not hesitate in assigning this skilled naval officer to the Laboratory.

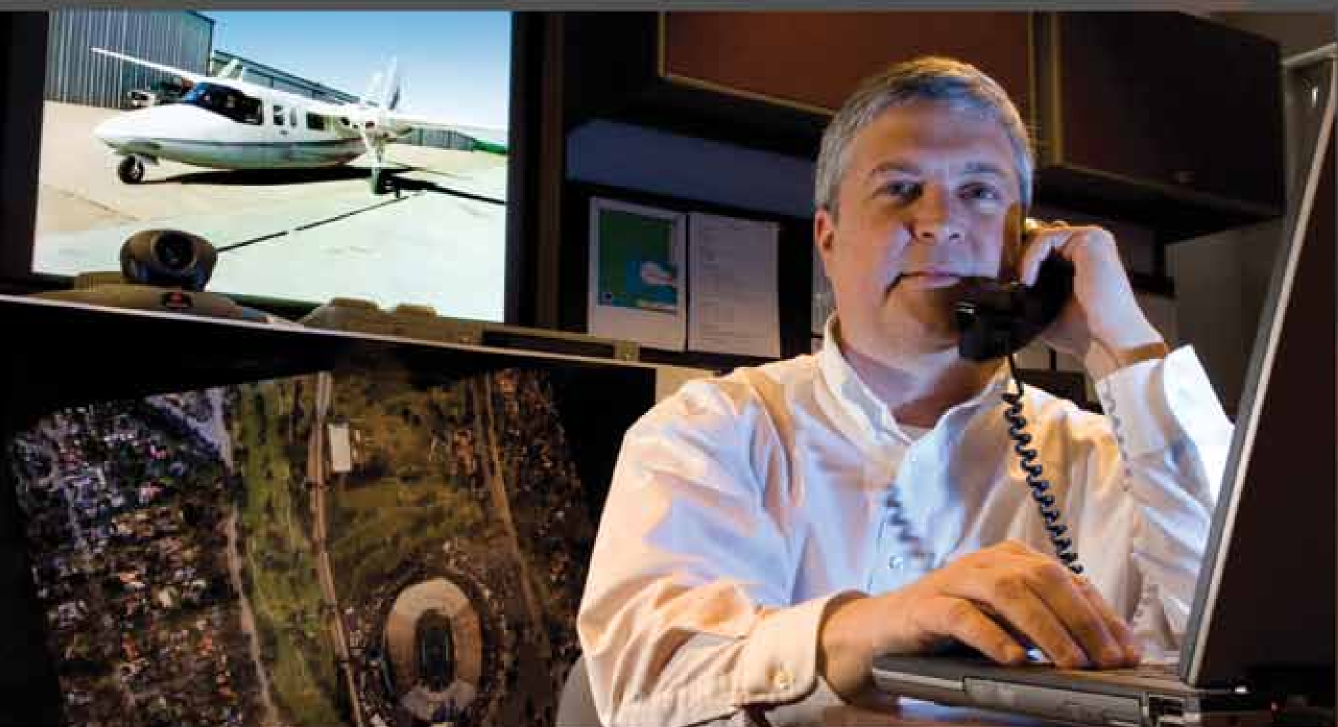
Parsons came to Los Alamos in June 1943 from the Navy's Dahlgren Proving Ground, where he had overseen the development of the proximity fuse and the use of radar fire-control systems for shipboard guns. His role in the development of the proximity fuse included a combat assignment in the South Pacific against enemy Japanese aircraft. At Los Alamos, Parsons' first task was to create the Ordnance Engineering Division (E) Division. As E Division Leader, Parsons had direct responsibility for the interior ballistics work on the uranium gun device, Little Boy; as well as the development of special high explosives for the implosion gadget, Fat Man. In addition to his technical leadership, Parsons was consulted on the use of tactical nuclear weapons and contributed to postwar nuclear posture planning.

Highly respected by leaders and scientists alike, Parsons served as Laboratory associate director beginning in the summer of 1944. Although there was no official "second in charge" of the Lab, Parsons was the undisputed leader in Oppenheimer's absence. Parsons' role at Los Alamos was so important that Oppenheimer commented, "I have always understood your position here as including responsibility and authority for the determination of the actual components of the weapon…It has not been my intention to take the direct responsibility for this determination myself; I have neither the qualifications for, nor the intention of, doing so in the future."

In August 1945, as head of the Laboratory's Project Alberta, Parsons assumed command for the combat use of the Little Boy and Fat Man. Flying aboard the Enola Gay on the Hiroshima strike mission, Parsons armed Little Boy by inserting the gun powder into the bomb's firing system. Parsons was awarded the nation's Silver Star, Distinguished Service Medal, and Legion of Merit awards for his wartime work at Los Alamos and his courage in flying the first atomic combat mission. After leaving the Laboratory in 1945, Parsons continued to play a leading role in nuclear affairs serving as deputy task force commander for Technical Direction for Operation Crossroads in 1946 and again for Operation Sandstone in 1948.

Although Parson's wartime work and role in developing the atomic bomb were extraordinary, the Navy promoted Parsons to the rank of commodore—a lower rank than he deserved according to many. It was not until 1948 that he achieved the higher rank of rear admiral and an assignment commensurate with his role in nuclear affairs—deputy and assistant chief of the Navy Bureau of Ordnance. Shortly after this appointment, Parsons died unexpectedly of a heart attack on December 5, 1953. Naval officer Frederick Ashworth, Parsons' deputy, eulogized, "There is no one more responsible for getting this bomb out of the Laboratory and into some form useful for combat operations than Captain Parsons, by his plain genius in the ordnance business."

—Roger Meade



The EPA recently deployed Los Alamos' ASPECT technology to BP's massive oil spill. ASPECT (Airborne Spectral Photometric Environmental Collection Technology), aboard a twin-engine aircraft, collected air-sampling data and photo documentation for immediate environmental evaluation. The technology, deployed to numerous emergencies, helped responders image, map, identify, and quantify chemical vapors and plumes. It also collected data to protect citizens at major events attractive to terrorists. The one-of-a-kind technology provides critical information via infrared mapping, spectrometers and Global Positioning Systems. The full assessment, including data collection and LANL analysis, takes less than 15 minutes.