Sandia RESEARCH

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When you ABSOLUTELY POSITIVELY have to get it right

engineering sciences

Sandia National Laboratories

Exceptional service in the national interest

Sandia National Laboratories

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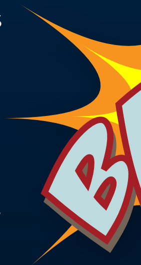

To request additional copies or to subscribe, contact:
Zachariah Harris
CTO Programs Office
Sandia National Laboratories
P.O. Box 5800, MS 0359
Albuquerque, NM 87185-0359
Voice: (505) 845-8729
Email: zrharri@sandia.gov

www.sandia.gov

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Credits:

CTO Office: Robert W. Leland, Julia Phillips, Chris Miller

Internal, Digital & Executive
Communications Manager: Valerie Smith

Editor:
Nancy Salem
(505) 844-2739, mnsalem@sandia.gov

Writing:
Neal Singer, Sue Major Holmes,
Patti Koning, Nancy Salem

Photography:
Randy J. Montoya

Design:
Michael Vittitow

ON THE COVER

Sandia Labs mechanical engineer Ryan Schultz adjusts a microphone for an acoustic test on a B61-12 system. The unit is surrounded by banks of speakers that expose it to an acoustic field. The sound pressure reaches 131 decibles, similar to a jet engine. "It is very exciting to experience first-hand the challenges of direct field acoustic testing on a large scale," Schultz says.

(Photo by Randy Montoya)

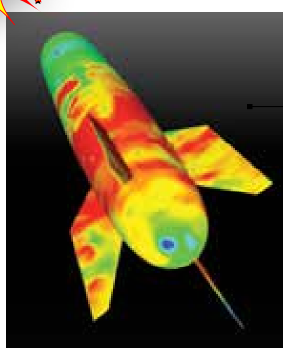

Table of Contents

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RELIABLE PREDICTABLE FUNDAMENTAL

Engineering Sciences is deeply embedded in the DNA of Sandia National Laboratories. Since its formation, Sandia has defined and executed the unique role of a national lab with an engineering mission and a heritage of bringing deep scientific and technical depth to solve the nation's most challenging national security problems. The foundational roles that Engineering Sciences play in the execution of Sandia's support of the national nuclear deterrent are exemplified in the lab's current engagement in full-scale engineering development of three simultaneous weapon modernization programs, which requires the design and development of hundreds of highly specialized components with extremely high reliability specifications. We have applied this expertise in high-reliability engineering based on robust scientific discovery and technical advances to the design and development of integrated systems for a broad array of critical national security applications.

Sandia's Engineering Sciences Research Foundation focuses the lab's engineering disciplines and diverse business needs to realize integrated solutions. It provides leadership and stewardship across the lab's technical capabilities in solid mechanics, structural dynamics, thermal science, fluid mechanics, aerodynamics, electromagnetics and reactive processes including combustion, energetics and fire. Achieving excellence across the broad range of engineering disciplines depends on cross-cutting advances in computational techniques, experimental capabilities and our ability to integrate the knowledge to enable high-confidence decision making. Combining computational and experimental simulation lets researchers improve designs, analyze performance margins and assess the safety and reliability of components and full systems.

In this issue of Sandia Research, you will see how Sandia continues to push the limits of engineering through the development of sophisticated predictive capabilities. As seen in the cover story, this requires the integration of physics discovery using advanced diagnostics and experimentation, physics model development, and advanced computational tools and methods that are validated and applied to support critical design decisions and product qualification. Another story looks into the quest by a team of Sandia researchers to ensure the accuracy of the computations relative to actual experimental data. As the team's manager says, the work is fundamental to the lab's technical foundation and the fulfillment of its unique national security mission.

Other stories take you inside the challenges facing Sandia's engineers to understand the shock to the components of a B61 nuclear weapon when ejected from an aircraft; the dynamic tools being used to study the physics of detonation and the materials used for homemade terrorist bombs; and a look into the future of Engineering Sciences as Sandia researchers and engineers strive to engineer materials for specific purposes with built-in reliability. And you will meet some of the nation's amazing scientists and engineers who are conducting this remarkable and critically important work.

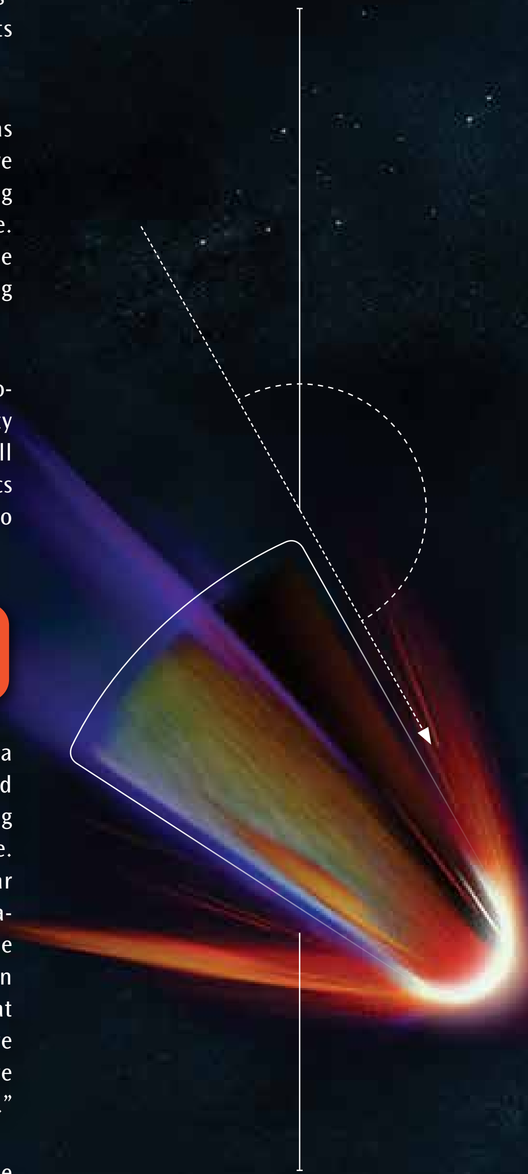
Justine Johannes
Director
Engineering Sciences Center

A space vehicle hurtles toward Earth carrying a nuclear weapon and closing in on a barrier that will test it in countless ways. Standing guard is the atmosphere, gaseous layers 60 miles above the planet that keep objects from pummeling it to pieces.

Some are uncontrolled celestial or space debris, such as small meteoroids or pieces of old satellites. Others are controlled technology like a space vehicle, re-entering the atmosphere from a mission on a navigated course. Objects on a random trajectory break up or disintegrate when they hit the massive forces of atmospheric drag and aerodynamic heating.

The same fate awaits controlled spacecraft. But technological advances have made re-entry and extreme-velocity flight less damaging to payloads and electronics. Still scientists need to know if the latest weapons, electronics and other systems are tough and reliable enough to withstand re-entry and other kinds of transport.

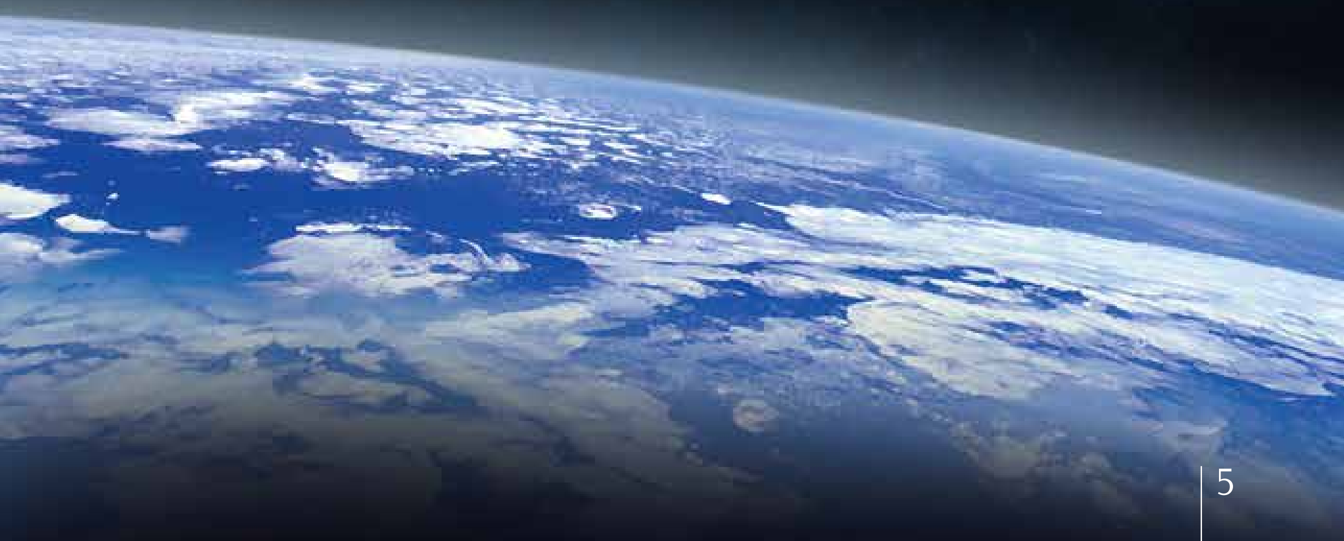
GOOD TO GO



By Nancy Salem

The Engineering Sciences Research Foundation at Sandia Labs is advancing the use of experimental ground and flight testing along with computational modeling and simulation to better predict system performance. “We’re worried about the electronics and non-nuclear components of a weapon surviving the harsh vibration environments as the vehicle comes back into the atmosphere,” says Todd Simmermacher, a manager in analytical structural dynamics. “It’s very similar to what you see in the movie Apollo 13 when the astronauts are coming back and get jostled around, but 10 times more harsh. The concern is it will shake apart the electronics.”

Aerosciences manager Jeff Payne says engineers simulate re-entry and other transport environments to evaluate



The world can be a rough and tumble place for the sensitive materials and electronics in weapons and other complex engineered systems. It takes skilled experimental testing with a big dose of computer modeling to be sure they will survive the ride.

components and determine if they will survive. The work covers a range of vibration environments including transportation, launch and re-entry. Historically the bulk vibration data were gathered by flight and ground testing. "We measure how a weapon system responds to the flight environments and replicate that response on a shaker to collect data under tightly controlled conditions," Payne says. "The flight data measure the performance of the vehicle in a particular re-entry setting, but there is uncertainty in our knowledge of the exact atmosphere, speed and temperature, and there are challenges relaying that data to the ground during flight."

Building a complete picture

The challenges produce uncertainties in the flight data that cannot be eliminated. The re-entry conditions the ground tests replicate can be tightly controlled but cannot fully reproduce the flight environment. "Modeling and simulation can be used to reproduce flight environments, but care must be taken to ensure the physics models are accurate," Payne says.

Modeling fills the gaps by simulating a larger variety of the flight conditions the vehicle could experience than can be explored through tests. "Typically on a flight test there are a limited number of trajectories that are flown," Simmermacher says. "We want to expand that and cover its full operating envelope." Modeling and simulation also improve and complement testing by designing better tests and providing a detailed understanding of observed phenomena during testing.

The essential trio of flight testing, ground testing and modeling and simulation together build the most complete picture of a system and how it performs. "We use the strengths of each to solve complex problems," Payne says. "The more complex the system, the more integrated the approach has to be. No one tool will provide you with everything you need. If a ground test can't get the environment right, we go to modeling. Sometimes the ground test is a high representation of the flight test and we don't have to rely on the modeling."

The Engineering Sciences Research Foundation has its roots in the nation's nuclear weapons program. The level of computational and experimental expertise was a natural outgrowth of the need for greater amounts and precision of data after underground nuclear testing ended in 1992. U.S. Department of Energy investments in high-performance computers helped boost Sandia's computational expertise.

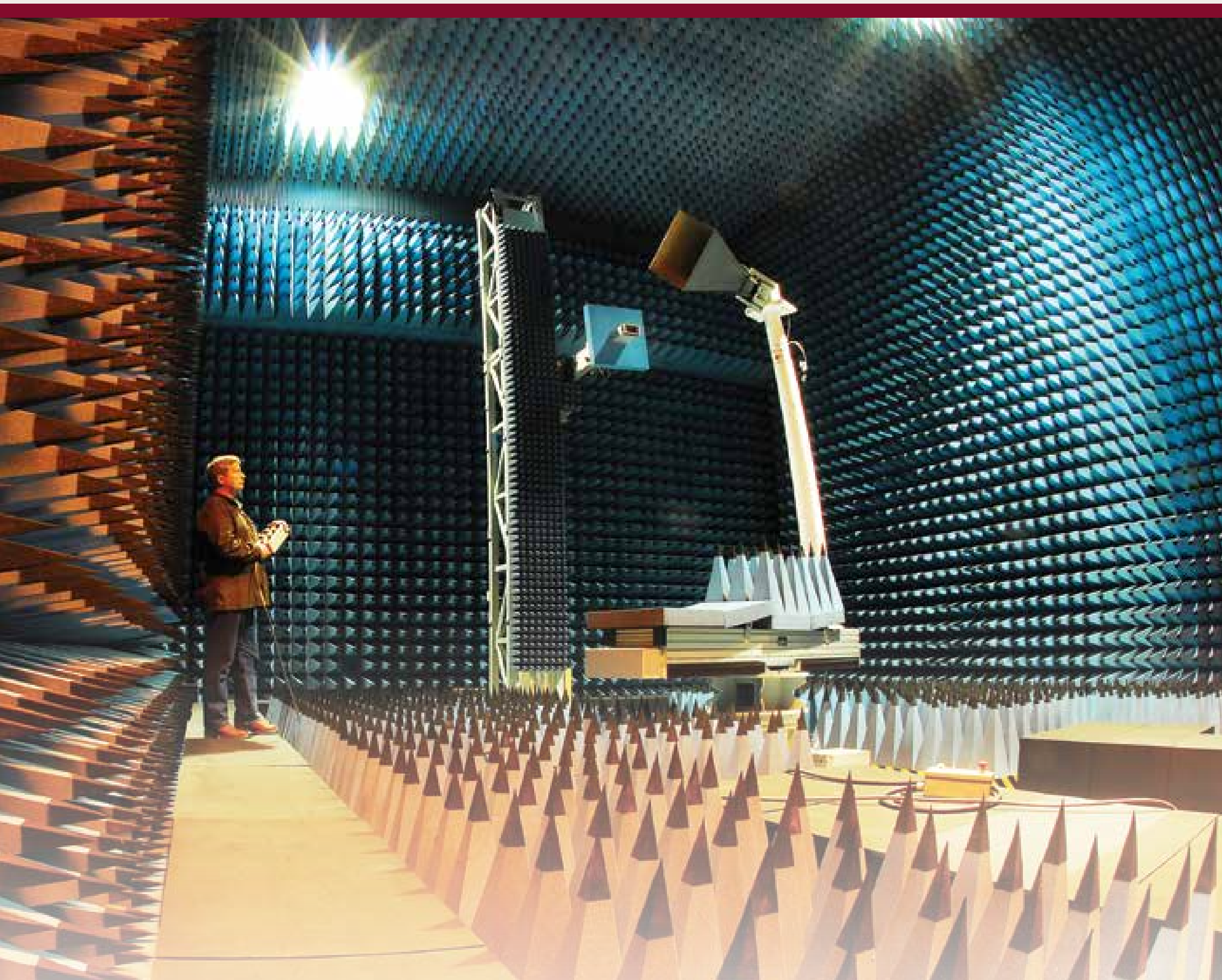
Researchers in engineering sciences are deeply involved in programs to modernize the nuclear stockpile. Their work is critical to Sandia's national security and nuclear weapons missions. "Being able to simulate these environments and better understand performance of the system and also better explore the design space is extremely important and hasn't been done in the past," Simmermacher says.

The harsh realm of re-entry

Ballistic weapons are shot high into the atmosphere and come down fast. "Very high, very fast," Payne says. "It's a severe environment." The vehicle carrying the weapon heats up from frictional loading as it re-enters the atmosphere. Aerodynamic or compressible fluid loads on the outside produce large rigid body accelerations and produce harsh random vibration. The random vibration loading is produced through a coupled fluid/thermal/structural process. "It's complex, coupled phenomena where fluid dynamic and thermal loadings drive the structural response," Payne says.

The flight vehicles must be designed to complex specifications to ensure performance. Because the precise re-entry environment cannot be fully reproduced in ground testing or controlled in flight, researchers use computational modeling to get the loading and thermal condition of the vehicle correct and propagate

Technologists Curt Tenorio, left, and Jessie Fowler install instrumentation on a B61-12 unit for a vibration and shaker-shock test. It will be subjected to the amount of vibration and shock it would experience in a lifetime of transportation and aircraft captive carry environments.



Engineer Ward Patitz checks out the anechoic chamber at Sandia's Facility for Antenna and RCS Measurement, or FARM, where weapon components undergo radar cross-section tests.

those loads through the structure down to the component or subcomponents of interest.

Captive carry: point A to point B

Vibration also can wreak havoc when a weapon is carried in the bay of an airplane. As the aircraft prepares for weapon release, the bomb bay doors open, letting the external flow field enter the bay. Turbulent air flows over the top of the weapon cavity and produces broadband acoustical noise that produces random loads. "Resonant tones form in the cavity, putting additional unsteady load onto the test unit," Payne says. "Getting that environment right with both the broadband acoustical noise and standing waves is difficult with a full-scale unit, so we rely more heavily on flight testing and modeling and simulation."

To ensure the accuracy of the models that predict the loading, subscale experimental data can be used to validate the modeling and give researchers a better understanding of the physics inside the cavity. "Flight testing and modeling move ahead in parallel and work together to push forward our predictive capabilities," Payne says.

Anatomy of a test

The experimental process moves from basic to complex starting with simple models of the aircraft. A rectangular cavity is tested in a wind tunnel to understand the unsteady surface loading and low field features. These data are compared to the modeling and simulation predictions until researchers are confident they can anticipate its behavior. Complexity is added to the cavity geometry so it more closely represents a real bomb bay, with ramps and finer details within.

Engineers then experiment with a surrogate weapon in the cavity and develop a fluid and structural

MEET

Katya Casper

Katya Casper was interested in engineering from an early age. At 7, the Tennessee native dreamed of designing the first rover to visit Pluto. She took flying lessons at age 17 in exchange for working at the flight school's front desk. Passion for flight drove a change in her undergraduate major at North Carolina State University from computer to aerospace engineering, where she led a senior design team in building a turbojet powered aircraft. Casper, who enjoys rock climbing, mountain biking, skiing and ultimate Frisbee, is passionate and excited about her work at Sandia. "It's really satisfying when a complex setup produces meaningful results, especially when it's something nobody's done before," she says.

STATS

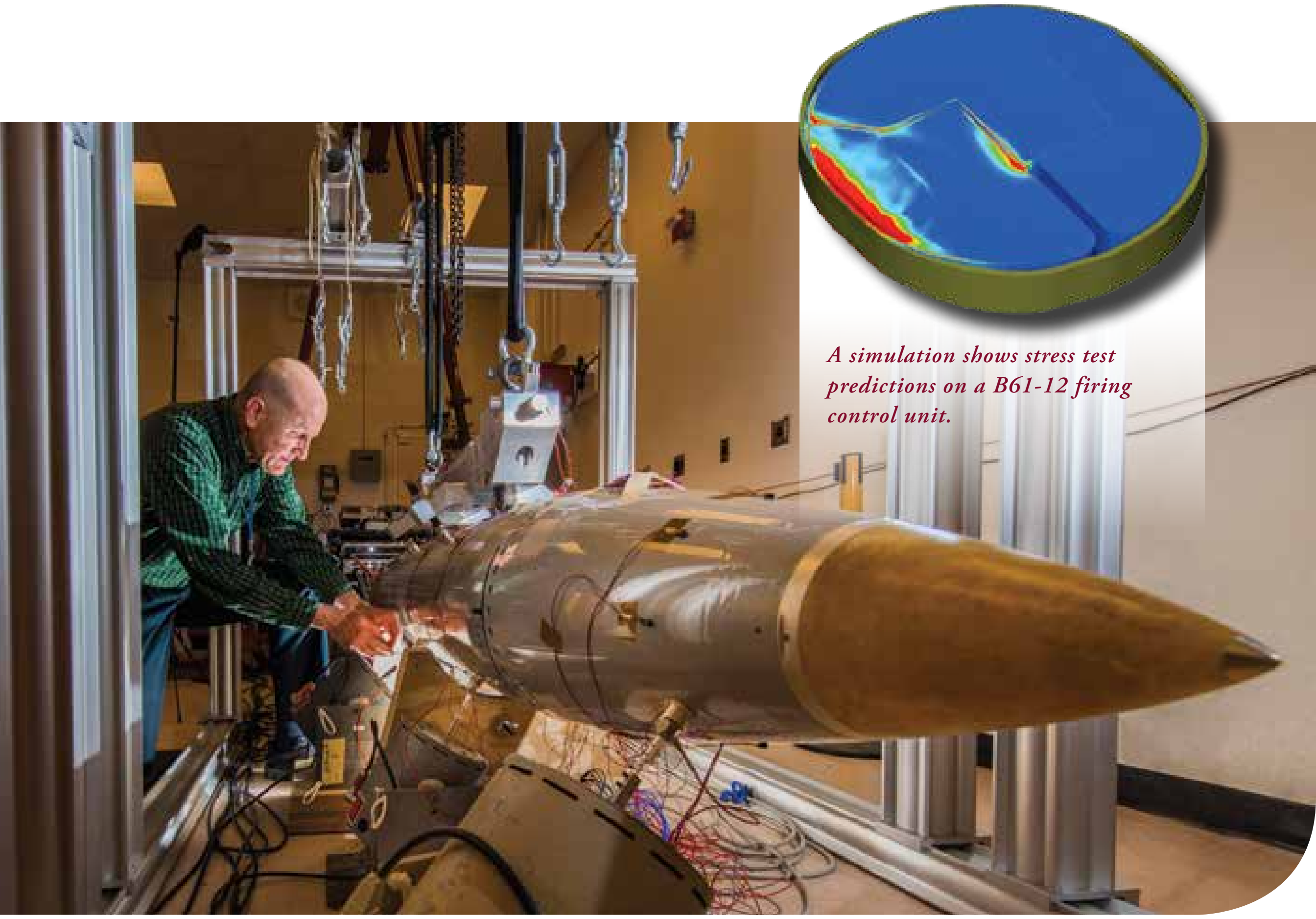
- Bachelor of Science in aerospace engineering from North Carolina State University.
- Master of Science and Ph.D. in aeronautics and astronautics from Purdue University.
- Casper interned at NASA, Boeing, Purdue and Sandia while completing her doctoral work.
- Works in Sandia's Aerosciences Department studying experimental fluid mechanics. The wind tunnels she uses allow her to conduct experiments at speeds as high as Mach 14.

dynamics model. "This building block approach ensures both the loading and structural response are accurately predicted," Payne says. "The final step is to compare the modeling and simulation predictions to operational flight test data."

The work is important because modeling and simulation improve ground and flight testing through better-designed experiments. With both re-entry and captive carry it provides a glimpse into what the environment will look like before a flight test. Engineers can advance life extension programs for nuclear weapons such as the B61 by designing and replacing limited-life components more efficiently. "With modeling and simulation we can provide the environments those components will see earlier in the process and do a better job of designing to those environments," Simmermacher says.

Ensure mission success

Payne, Simmermacher and their colleagues develop specifications for engineers in other areas of the labs that design and build components and systems. On Nov. 17, 2011, Sandia's Integrated Systems Program did the first test flight of the Advanced Hypersonic Weapon (AHW), which was launched from the lab's Kauai Test Facility. A Sandia-designed booster system launched the AHW glide vehicle and deployed it on the desired flight trajectory. The test demonstrated the viability of the boost-glide approach to long-range atmospheric flight and data collection on a variety of advanced technology subsystems.



A simulation shows stress test predictions on a B61-12 firing control unit.

Structural dynamics engineer Randy Mayes sets up a B61-12 test that seeks to replicate the combined acoustics and vibration inputs in aircraft captive carry. The goal is a better laboratory test of captive carry environments. Test results provide parameters for modeling and simulation.

Simmermacher says Sandia engineers built and analyzed the rocket superstructure around the third-stage motor, which launched the AHW, and results were used to develop control systems and assess flight worthiness.

"The purpose of our work is to ensure mission success by making sure the structures can all withstand the environments they will see during launch, release and subsequent re-entry," Simmermacher says. "The biggest thing we learn every time we do this type of program is the importance of having test data and analysis. They help each other. Trying to match the model to the test data, you learn a lot about your model, your test and the full system, the hardware and how it behaves."

Engineering Sciences touches programs across Sandia, from defense systems such as satellite payloads, hypersonic vehicles and rail guns to energy systems including engine efficiency and wind turbine performance, and homeland security interests like aircraft safety and improvised explosives. The foundation's expertise includes solid mechanics, structural dynamics, combustion, thermal science, fluid mechanics, aerodynamics, energetics, electromagnetics and electrical sciences, and shock physics.

Other organizations recognize Sandia's computational expertise and have adopted the lab's computer codes. "Engineering Science is constantly improving its tools and capabilities to provide deeper insight into the behavior of the systems and components that we design and are responsible for," Payne says. "Through a combination of operational testing, computer simulation and experimentation, the Engineering Sciences Research Foundation is pushing the forefront of the technology used for designing and qualifying nuclear weapons. While Sandia's engineering sciences capability began and remains grounded in the nuclear weapons program, it has come to permeate every mission space of the laboratory." ■

Mechanical engineer Sean Kearney studies jet flames with laser diagnostics to make temperature and soot measurements of the heat release from a fire onto a weapon system. "We want to understand how much heat gets transferred from the fire to the weapon," he says.

BY PATTI KONING

THERE ARE ALL KINDS OF EXPLOSIONS, SOME GOOD, SOME BAD. AND EACH HAS A COMPLEX MECHANISM. SCIENTISTS ARE USING DYNAMIC TOOLS TO STUDY THE PHYSICS OF DETONATION AND SHED MORE LIGHT ON MATERIALS SUCH AS THOSE FOUND IN A HOMEMADE TERRORIST BOMB.

To most people the time between ignition and explosion seems instantaneous, but not to mechanical engineer Marcia Cooper. She's made a career out of understanding what happens to materials in the tiny window between shock and chemical reaction.

"We are working toward a fundamental understanding of how energetic materials respond to a stimulus," she says. "This is especially crucial for what we call 'non-ideal explosives' — often used for industrial applications or even to make homemade terrorist explosives — that have a long and complex detonation wave structure. We can't use our understanding of ideal explosives to predict how these materials behave. In a sense, we are starting from scratch."

Cooper runs Sandia's Light Gas Gun Facility at the Explosive Components Facility and a unique diagnostic, the optically recording velocity interferometer system (ORVIS), which is an important variant of the more familiar velocity interferometer system for any reflector (VISAR), both of which were invented at Sandia. Although other researchers at Sandia and elsewhere have used ORVIS sporadically, Cooper is just the third owner of the system at the labs. Douglas Bloomquist and Stephen Sheffield, who created the ORVIS diagnostic, were the first, followed by Wayne Trott, who mentored Cooper. Building on the accomplishments of her predecessors, she has advanced ORVIS' diagnostic capabilities along with mesoscale model development.

ORVIS works by reflecting laser light off a moving surface. In the Gas Gun Facility, projectile impact onto an explosive generates a shock or detonation wave that accelerates the material surface. As the impact or shock interaction with the measurement surface occurs, light is reflected to up to three interferometers, which allows researchers to see movement in very high resolution. With the ORVIS diagnostic, light beams from the interferometers are collected optically onto ultra-high-speed cameras. Those data can be used to provide an essentially continuous record of variations in velocity on a moving surface in both space and time — something no other diagnostic tool can do.

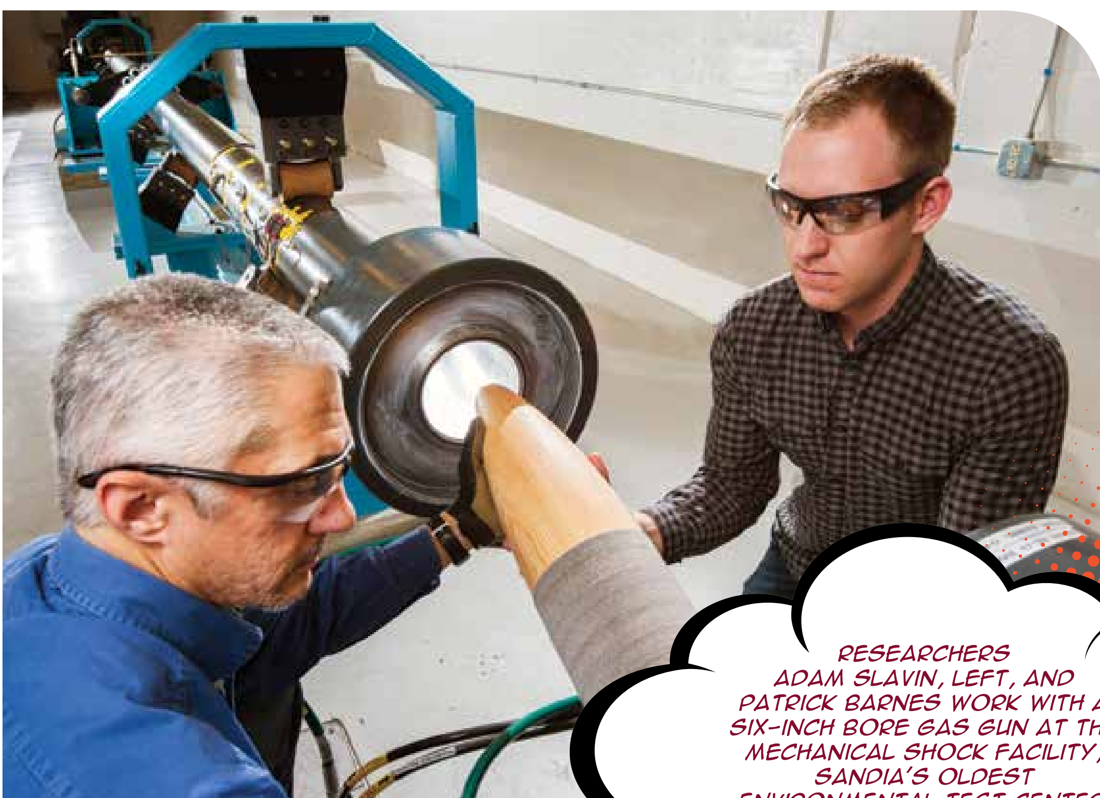
The stars aligned

Initially, ORVIS was designed to capture data from a single focused laser spot on the material under study. Trott implemented a line-imaging capability and, with Cooper, developed that further into a surface-imaging capability and the ability to collect data simultaneously from multiple laser sources.

"Wayne and Marcia were the perfect match to transform the capabilities of ORVIS. The stars aligned, in a sense," says senior manager Jaime Moya. "Marcia overlapped with Wayne at the end of his career, and working together, they advanced the capabilities of ORVIS to enable experiments that are advancing our knowledge base on explosives to the very forefront."

Mesoscale modeling is important because it allows researchers to study how a material reacts to shock at a granular level, which drives the reaction. It's the difference between seeing a sandbox as a box versus a collection of grains of sand, each with individual characteristics and physical relationships to one another that can affect how the collection responds to shock.

"If you collect data from a single point, you have to make assumptions about how the rest of the material behaves. ORVIS can now collect data from a whole region of a moving surface, so it's a much better,



RESEARCHERS ADAM SLAVIN, LEFT, AND PATRICK BARNES WORK WITH A SIX-INCH BORE GAS GUN AT THE MECHANICAL SHOCK FACILITY, SANDIA'S OLDEST ENVIRONMENTAL TEST CENTER.

MEET

Marcia Cooper

Growing up in Kentucky, Marcia Cooper had no doubt she would one day pursue a career as a mechanical engineer. Her father, a mechanical engineer and former Air Force pilot, built and flew model sailplanes and drove and worked on sports cars. Her grandfather restored antique cars. "They were always doing mechanical things, and it rubbed off on me," Cooper says.

Her thesis at the California Institute of Technology focused on gas-phase detonation, a topic that led to an interest in joining Sandia's research and testing in energetic materials. Sandia hired her to work in Energetic Material Dynamic & Reactive Science. Cooper's most interesting projects have included joint work with NASA's Jet Propulsion Laboratory on propellant burning behavior in accident scenarios during rocket launches and their impact to the environment. More recently, Cooper carried on Sandia's research in diagnostic advancement of the Optically Recording Velocity Interferometer System, or ORVIS, used to measure particle velocity histories in shock wave experiments on condensed-phase explosives.

Cooper is passing her passion for mechanical engineering to her 2 ½-year-old son. A recent lesson showed how a lever can make it easier to lift up a vehicle spare tire.

STATS

- Bachelor of Science in mechanical engineering from Purdue University.
- Ph.D. and Master of Science in mechanical engineering from the California Institute of Technology.
- Still early in her career, Cooper has authored or co-authored numerous publications, including refereed journal articles, refereed conference proceedings, conference papers and presentations, and technical reports.

more accurate description of what the material is undergoing," says Cooper. "With this capability, ORVIS provides the experimental data to validate mesoscale models."

Detonability of non-ideal explosives

More recently, Cooper has turned ORVIS' rich diagnostic capability toward non-ideal explosives like ANFO (ammonium nitrate/fuel oil) and potassium chlorate and sugar. With the threat of terrorists using non-ideal explosives in homemade weapons, there is a strong push to gain a better understanding of the detonability of these materials.

"We looked at the mechanical response and mixing in these materials and how they cause the onset of a chemical reaction that ultimately can lead to detonation," Cooper says. "Our experiments with the Gas Gun Facility and ORVIS fed into a larger effort, which is still underway, to assess the material characteristics, with the ultimate goal of creating predictive models."

She says non-ideal explosives have a distributed reaction zone, which means that the chemical processes that lead to detonation occur in multiple steps and the process is more susceptible to environmental changes. "It's a complicated problem. Our experiments focused on mixing, which is a small piece of a very complicated system of how the material reacts to shock," she says.

Cooper's role at Sandia is somewhat unusual in that her work supports a variety of topics in direct support of Sandia's national security mission and for a broad range of customers. For oil-services companies, she characterized explosives used for drilling deep holes to ensure that they could perform reliably under extreme high pressure and temperature. On another project for the Department of Defense, she characterized shock properties of materials in sympathetic detonation conditions.

Cooper also couples ORVIS to benchtop experiments on explosives and inert materials. “While most people associate ORVIS with the Gas Gun Facility, ORVIS is completely separate,” she explains. “We are moving to modern techniques that can be done on a smaller scale and with less consumables.”

Cooper’s work, says her manager Leanna Minier, is advancing the understanding of the physics underlying detonation. “People like Marcia are asking the tough questions and finding new ways to study detonation, which is pretty hard because detonation, by its very nature, means everything that was there suddenly goes away, including your diagnostic,” she says. “Developing diagnostics that allow us to see reactions on the mesoscale takes a lot of creativity. The quest is for a predictive model that can define the material properties you need for the performance you want. Marcia is driving us down that path.” ■

what’s next

ENGINEERING TURNS UPSIDE DOWN, INSIDE OUT TO GET THE BIG ANSWERS

A typical engineering problem might be to simulate what happens when a hurricane hits a turbine designed for a 30 mph wind. Sandia National Laboratories wants to flip it around: Design a wind turbine to operate safely and at peak performance across all the conditions it could face in a lifespan.

Producing the best design for a range of operating conditions will require a fundamental understanding of uncertainties and variability in materials, better algorithms for computer modeling and improved ability to model across multiscales and multiphysics, aided by more powerful computers, says David Womble, a computational simulation senior manager. The payoff could be huge.

One aspect of computational design is to put material exactly where it’s needed. Simulation modeling sciences manager Ted Blacker says that’s “topology

By Sue Major Holmes

optimization.” Instead of coming up with a design and analyzing how it will perform, the needed shape can be calculated to handle the expected loads. Then emerging production methods such as additive manufacturing — as in 3-D printing — can build the very general shapes, essentially laying down material only where it’s needed. It is similar to how nature adds strength to a tree by thickening a branch to manage more stress, he says.

The future also could bring materials engineered for specific purposes. Sandia has begun a laboratory research challenge to move from analyzing failure to engineering materials reliability, including understanding what causes degradation and breakdown. Since performance varies greatly over time, predictions will require experiments and modeling that account for materials’ intrinsic variability.

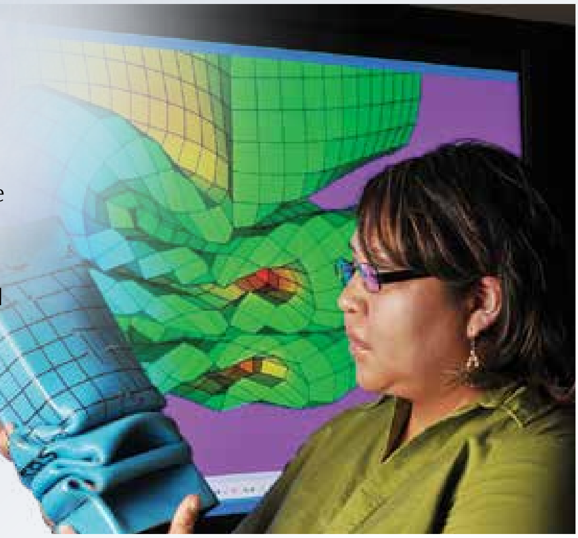
Engineers use large, high-fidelity codes that couple some properties, such as thermal and mechanical properties. For example, they simulate nuclear weapons systems to determine the response to various environments, such as crash, fire or lightning strike.

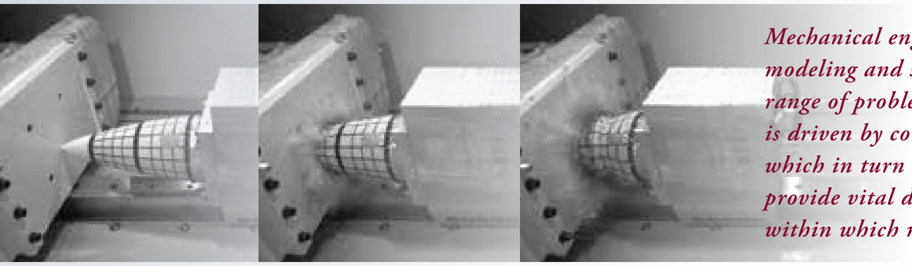
Such calculations today lack integrated multiscale and multiphysics capabilities. Defects in materials make a difference at the molecular scale, but at larger scales the codes must average the variables since it’s impossible to model everything in molecules. So engineers need to understand physics at different scales to predict physical phenomena accurately. And while they can’t see atoms, they can run experiments at the grain scale to refine computer codes and models to predict behavior.

Creating sophisticated codes is not easy. Fractures, for example, begin at the molecular scale and eventually become visible cracks. They don’t happen the same way twice, and models must capture this seemingly random behavior. “We don’t have good physical models for the fracture process to understand the physics to do the problems we want to do,” Womble says. “We need to know more than the fact something fails; we want to know how it fails.”

Tomorrow’s engineers will require new types of computers already on the horizon, new codes and algorithms that run on those machines and new models that capture the physics. And with future computers expected to be hundreds to thousands of times more powerful, “we want to use that computing power to solve new and innovative problems,” Womble says.

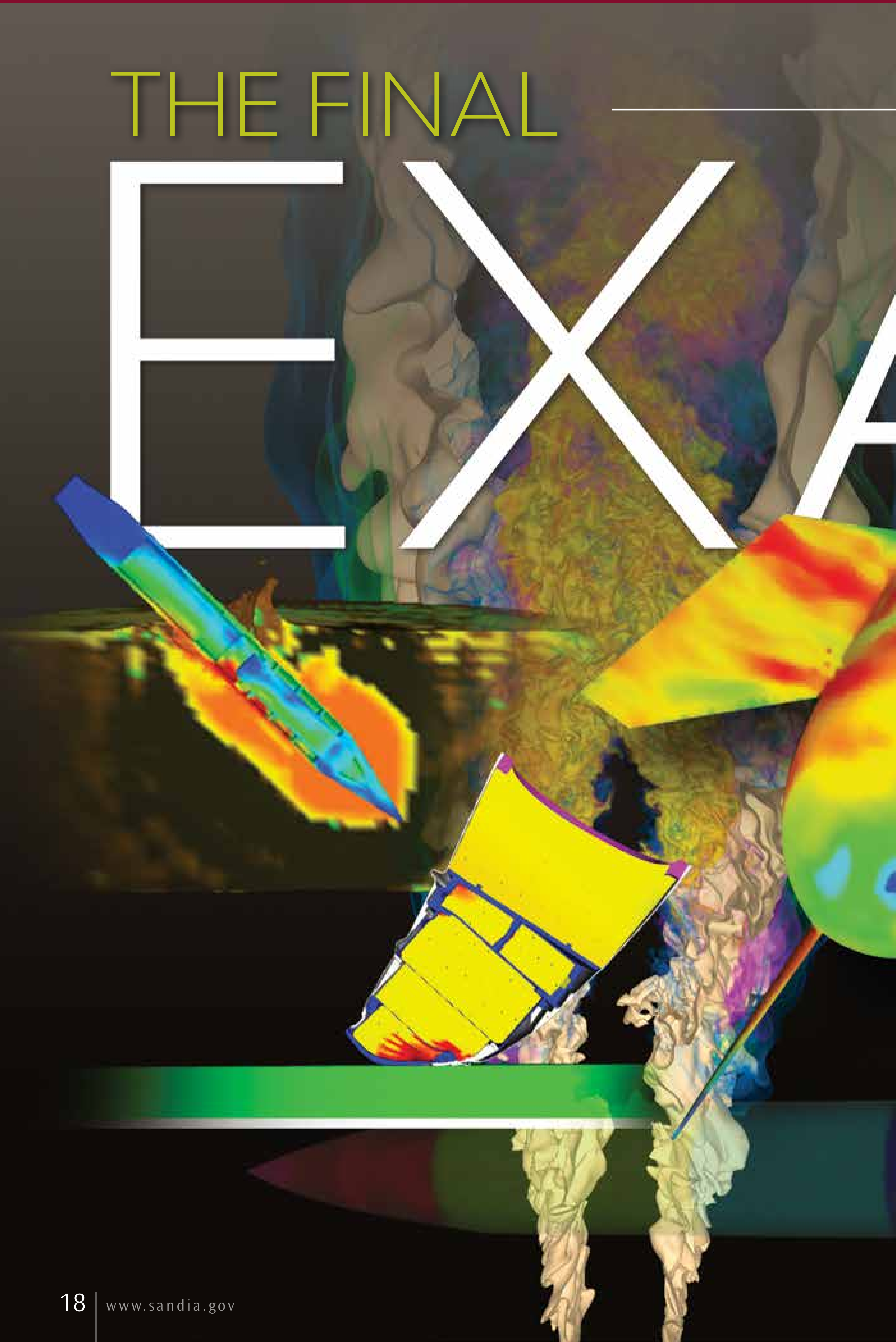
“There is lot of research being done, lots of progress being made in how to use the capabilities in engineering practice,” he says. “I see significant differences in how we’ll do engineering work in the next decade.”





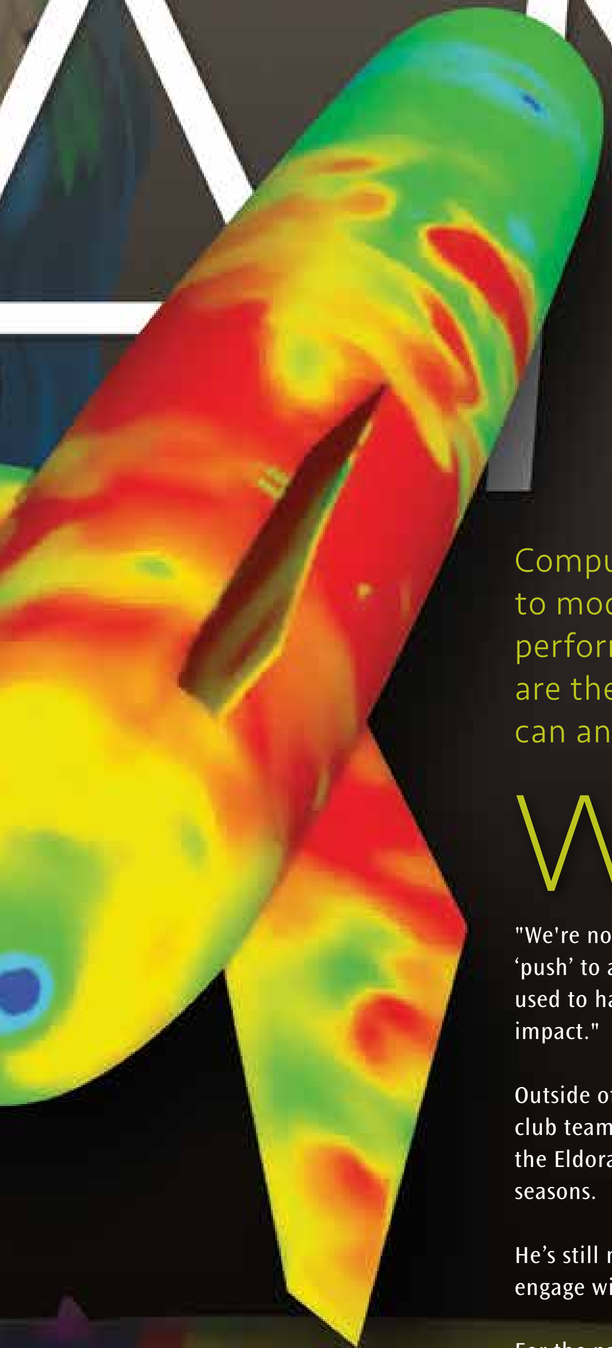
Mechanical engineer Jhana Gearhart uses modeling and simulation to study a wide range of problems. Modern engineering is driven by computational simulations, which in turn depend on experiments to provide vital data and validate the range within which models can be used reliably.

THE FINAL EX



By Neal Singer

AM



Computer simulations are increasingly used to model real-world systems from weapon performance to space flight. But how accurate are they, really? A team of Sandia researchers can answer that high-stakes question.

Walt Witkowski manages a team of Sandia researchers who determine shades of inaccuracies that might invalidate computer simulations.

"We're not widely known," Witkowski says, "but we're changing from a 'push' to a 'pull' technology. That is, people are coming to us now; we used to have to tell them they should come. We're starting to make an impact."

Outside of work Witkowski is widely known indeed. He coached soccer club teams to more than 15 New Mexico championships and motivated the Eldorado High School boys' soccer team to four state titles in nine seasons.

He's still motivating, says his Sandia colleague Rich Hills. "Walt helps us engage with other groups throughout the labs."

For the past two years Witkowski has led efforts to assess the accuracy of computations relative to experimental data at Sandia. He says the work of his group, Verification and Validation, Uncertainty Quantification and Credibility Processes, "is not sexy, but it's about our technical foundation. If the foundation's not good, you know what happens to the house."

Sandia's expertise in computational simulations played a key role in helping NASA determine the cause of the 2003 space shuttle Columbia disaster. Using supercomputer simulations and experimental materials characterization data, Sandia showed that the most probable cause of the accident was damage to the shuttle's wing from foam debris.

Toward more realistic simulations

Witkowski's 14-person team assesses the accuracy of computational simulations. It leads to changes that strengthen the simulation's relation to experimental reality. His department supports a variety of Sandia work, from nuclear weapon quantification and design to social modeling and windmill design.

"We form a team including the modeler," he says. "We can't do it on our own, but we can help him or her be more effective."

Simulations can be overly deterministic, he says. "Each produces a single result that approximates reality, but they can predict only so well. Material properties vary, and so do individual units formed on a production line. Even weather has variability that affects something flying through the air.

"If we were going to model breaking through this table," he says, putting his hand on the desk in front of him, "we don't know exactly how to quantify the uncertainties because the wood parameters vary from here to here." He moves his hand a short distance. "Simulations typically insert a value for density, but density is really random. So even though we know the velocity of a penetrator, the depth it will go through the wood is variable because the properties of the wood vary. So our group characterizes the range of possible outcomes for the model, using model sampling and other sophisticated schemes."

That subtle analysis is a long way from Robert Goddard's seat-of-the-pants experimental rocket launches with his band of high-school-educated helpers on the plains outside Roswell in the 1930s. There the simple question was, will it fly? Here the stakes riding on accuracy are far higher.

"Not only do we list all the physics phenomena we're trying to mimic in a model," says Witkowski, "we even assess the adequacy of the mathematical model representing the physics, and its implementation in a code. There's an obvious question of adequacy in going from the smooth curves of math theory to discretized, yes-no computer processes."

Daunting task to test the codes

The group must also establish that codes work as expected for user applications. "Sierra [a major Sandia code] has verification algorithms that test many features of the code, but not all of them. We try to determine which sections relevant to the simulation are not tested, and then add tests to cover those features. Because new features are added daily and their usage changes, that's a daunting task."

The modified simulation ideally is then validated with experimental data.

MEET

Joe Bishop

Outside Sandia, Joe Bishop takes the road less traveled. He lives on about a half-section of land in the mountains east of Albuquerque near the rural community of Estancia. He has horses, chickens, dogs, cats, even goats until recently, and says his weekends are devoted to such pursuits as building barns, putting up barbed-wire fences and dodging rattlesnakes.

Bishop works on five Sandia projects, including a major multi-disciplinary research effort called Predicting Performance Margins, aimed at filling in gaps in the fundamental understanding of material variability. Bishop is researching the question: "What is material variability and how is the complexity and richness of the microscale manifested at the macroscale?"

He's also on Sandia's team within the Center for Subsurface Energy Security, a collaboration between the labs and the University of Texas Austin, and one of several Energy Frontier Research Centers funded by the Department of Energy. The project studies how to put carbon dioxide underground to ease global warming due to greenhouse gas emissions. "Most of the scientists I work with are in geosciences. The story of me working on this project is funny because my school background is aerospace. The two fields are at opposite ends of science and engineering." Bishop is there because his skill in fracture mechanics and computational modeling applies not only to aerospace and mechanical engineering but to the field of geophysics.

STATS

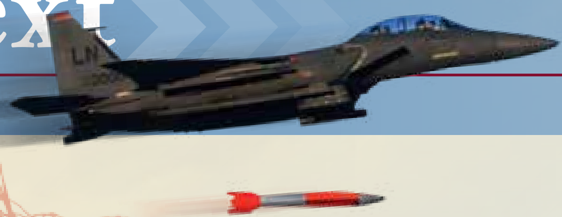
- Bachelor of Science, Master of Science and Ph.D. in aerospace engineering from Texas A&M University.
- Bishop spent eight years, from 1996 to 2004, in the Powertrain Division of General Motors Corp. before joining Sandia in engineering sciences.

"We're not telling people how to do their job better. We're trying to offer unified processes and tools to help facilitate their work. The problem," says Witkowski, "is that we have so few people and there are so many different applications."

The group, which plays a national leadership role through its involvement in professional societies, had its origins about 12 years ago in the Accelerated Strategic Computing Initiative (ASCI). Former manager Martin Pilch says the ASCI focus was high-performance computing that would fill the gap caused by ending underground nuclear tests. The group was expected to advance verification, validation and uncertainty quantification to ensure the credibility of high-consequence predictions using the advanced codes for nuclear weapon applications.

"Today," Pilch says, "the focus is broad deployment of methodology to the full spectrum of applications, although methodology development still continues." ■

what's next



By Sue Major Holmes

INVERSE MATH HOLDS THE KEY

Sandia is using an inverse method to understand how weapon components respond to forces such as shock or vibration when it's not possible to directly measure those forces.

The Environments Engineering and Program and Test Integration department creates environments to test weapon systems and components developed throughout the laboratories. Traditionally, engineers have fielded an instrumented test unit to gain data to define environmental requirements. However, that approach only can measure response data at a limited number of points, and any future design changes could invalidate the results.

There are significant advantages to using analytical models to complement the testing program. Still, while engineers routinely measure the internal responses of a test unit, it's often impractical to measure the input forces. However, identifying the true input forces is critical to a successful analytical modeling effort, and the solution lies in the inverse method to derive input forces.

One example of such a problem is the shock environment associated with a B61 nuclear weapon ejected from an aircraft. "We don't directly measure the forces that are being input into the bomb during ejection tests," says manager Scott Klenke. "But it's critically important for us to understand how the bomb's internal components respond to the various input forces. Because we don't directly measure these input forces, and generally measure a limited number of component responses during our tests, the inverse approach really helps us in determining what those input forces are to the weapon."

The inverse approach uses the results of modal test measurements or analytical models to construct the transfer function matrix, a mathematical relation between inputs and outputs, to estimate the forces. It's a useful technique for a variety of problems where test conditions can't be measured directly, says Klenke.

A modal test, a mechanical test designed to measure a structure's response to vibration, is typically conducted using instrumented hammers or small shakers to input forces on the test item while accelerometers measure its response. In the case of a B61, modal tests were conducted at input points where the weapon is held by the aircraft ejection rack and at the rack piston ejection points. Engineers take internal measurements while forces are input on the test item, then use the data to generate the transfer function matrix for the inverse problem, Klenke says.

Using this matrix and the original measured component responses from ejection tests, the inverse method estimates the input forces. Researchers then use those forces in a model to predict responses at other points on the weapon that weren't measured, Klenke says.

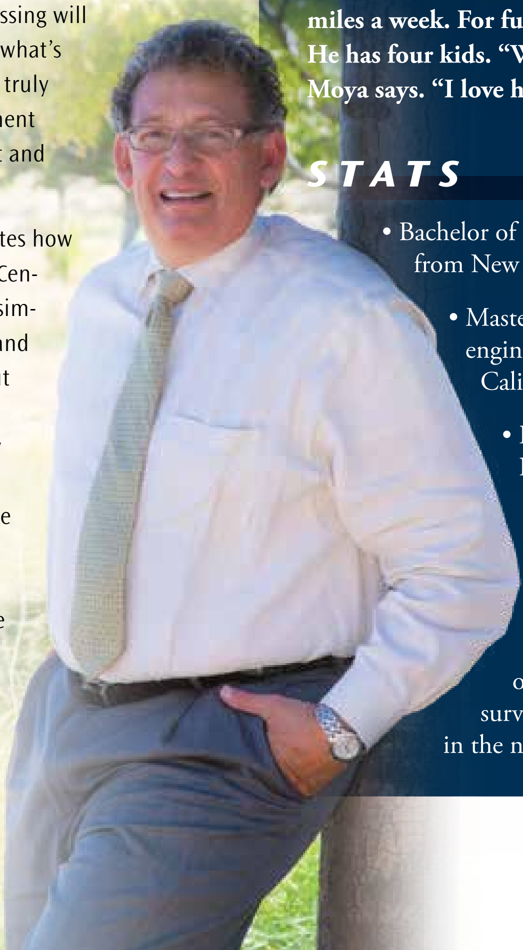
Predicting component responses at locations that weren't measured allows researchers to develop environments and get good representations of what environments components must survive for development and qualification — ensuring components' safety and effectiveness, he says.

The technique of inverse problems has been around for years, but Klenke said improvements in computer modeling and processing will "give us more confidence that what's coming out of our models will truly provide us with better component specifications for development and qualification testing."

The technique also demonstrates how Sandia's Engineering Sciences Center couples experimental and simulation techniques to understand how a system performs without measuring every conceivable point. "This is a good capability that we're pushing forward in terms of improvements," Klenke says. "Improving our modeling capabilities, improving our approaches to testing and how we apply and utilize experimental models to bridge that gap are really important research areas that allow us to produce a better result." ■

MEET

Jaime Moya



Jaime Moya's dad was a rocket man. He worked at White Sands Missile Range in southern New Mexico taking high-speed photos of missiles, aircraft and other vehicles that get thrust from a rocket engine. "His job sparked my interest in propulsion and defense-related activities," Moya says. "By the time I was in high school I knew that's what I wanted to do." Moya is from El Paso, Texas, where he still has family and sits on the Engineering Advisory Board at the University of Texas at El Paso. In college Moya studied mechanical engineering with an emphasis on thermal fluids. Professors steered him to Sandia Labs 30 years ago. "I thought 'This is it. This is the place,'" he says. Moya helped start the lab's Fire Science and Technology Group and the Thermal Test Complex, a state-of-the-art fire science research center. He later worked in experimental validation. Moya joined the Explosive Technologies organization seven years ago. "I'm still doing the things I liked to do as a kid," he says.

Moya commutes to work by bike, logging about 100 miles a week. For fun he and his wife play bridge. He has four kids. "We get together often as a family," Moya says. "I love hanging around with them."

STATS

- Bachelor of Science in mechanical engineering from New Mexico State University.
- Master of Science in mechanical engineering from the University of California Berkeley.
- Received the 2005 Engineering Professional Achievement Award from the Hispanic Engineering National Achievement Award Corporations, or HENAAC.
- As a senior manager his key responsibilities include oversight of the design, production and surveillance of explosive components in the nuclear weapons stockpile.

Sandia
RESEARCH

Sandia National Laboratories
P.O. Box 5800, MS 0359
Albuquerque, NM 87185-0359

LOOKING BACK

Look under the hood of any car on the road today and you'll see fingerprints of the Combustion Research Facility (CRF). Its scientists have been instrumental in unlocking the secrets of combustion and making automotive engines better.

The 1970s energy crisis spurred Sandia researchers to use tools developed for nuclear weapons to study combustion. Their goal was more efficient and cleaner conversion of fuels to energy. Automotive engineers at that time did not have access to lasers and supercomputers.

In 1973, Sandia researchers Dan Hartley, Ron Hill and Taz Bramlette proposed a combustion research program to the Atomic Energy Commission, predecessor to the U.S. Department of Energy. Eight years later the CRF opened its doors as one of Sandia's first user facilities and welcomed research partners from industry and academia.

Thousands of scientists from all over the world have visited the CRF to collaborate on advanced laser diagnostics, combustion chemistry, reacting flows, engine combustion and other fields. The center has doubled in size with a wing of 16 labs added in 1999 and the Combustion Research Computation and Visualization building in 2010.

Today CRF is the anchor of Sandia's Livermore Valley Open Campus, a partnership with Lawrence Livermore National Laboratory to create a space for collaborative work.

— Patti Koning

Researchers at Sandia's Combustion Research Facility were part of an international team that detected a new class of compounds, called enols, previously unknown in flames. The breakthrough could lead to soot reduction, fewer pollutants and improved fuel cells.