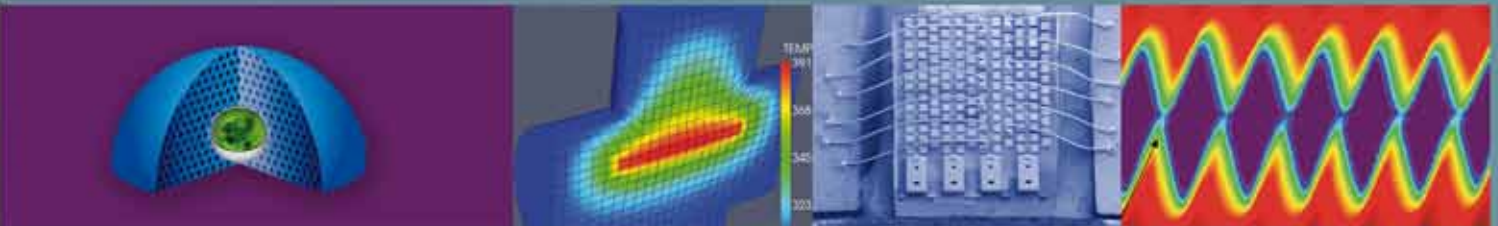




# RISK, CHALLENGE *and* REWARD in LDRD





**From the Vice President of  
Science, Technology, and  
Engineering and  
Chief Technology Officer**

**J. Stephen Rottler**

As authorized by Congress, the Laboratory Directed Research and Development (LDRD) program at Sandia National Laboratories (SNL) is crucial to maintaining the vitality of our Labs in mission-critical science and engineering (S&E) disciplines. As SNL's sole discretionary R&D program, LDRD enables our technical staff to pursue innovative, high-risk and potentially high-value research and development (R&D) for a range of difficult S&E challenges facing our nation. This brochure communicates some experiences of our LDRD principal investigators and their staff in managing technical risk within their LDRD projects. These examples demonstrate not only that we are working at the forefront of S&E, but also that we are seeking and achieving scientific advances and technological breakthroughs despite the technical risks encountered in our LDRD endeavors.

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# Risk, Challenge and Reward in LDRD

## INTRODUCTION

Like all creative human activity, scientific research is a risky endeavor. When one poses a scientific hypothesis, intrinsic to that process is the risk that the hypothesis may be incorrect or ill-founded, or that the proposed technical methodology is inadequate. And as a hypothesis or a technology moves farther away from established norms, the risk becomes even greater. As a consequence, a “creative leap” is often necessary to boldly venture into unknown territory, rather than simply taking a small evolutionary step.

## The LDRD Program

The LDRD program at the DOE/NNSA National Laboratories funds projects at the leading-edge of scientific and engineering research, where the hypothetical and/or technical unknowns tend to be either more numerous or more tenuous. Hence, the associated risk tends to be significant. Specifically mandated by 1991 Congressional legislation [1], the program directs a percentage of national laboratory budgets to employee-suggested proposals, selected based on merit, through a rigorous, peer-reviewed competition. LDRD investments are made in a fashion that addresses the emerging and future requirements of national security, including nuclear security, energy security, homeland security, and scientific discovery and innovation. LDRD program-funded research is therefore challenged to be leading-edge in its search for novel technical solutions to daunting national security challenges.

## Defining High-Risk Research

The 2008 ARISE (Advancing Research in Science and Engineering) Report of the American Academy of Arts and Sciences [2] outlined the following qualities of high-risk scientific research. It “has the potential to disrupt conventional thinking and to transform our understanding of the world, by 1. demonstrating the potential to generate deep change in concepts; 2. producing new tools or instruments allowing the entire

community to extend its reach; 3. creating new subfields of science; or 4. bringing together different scientific subfields to make discoveries otherwise impossible.”

## Taking on Challenges

Quantifying technical risk in terms of success-failure probabilities is extremely difficult, and perhaps inappropriate for leading-edge R&D. One way of identifying and, to some extent, measuring technical risk is through the identification of the associated science and technology challenge represented by the ambition embodied in the research objectives. Sandia uses the following scales of increasing ambition to evaluate the challenging nature of LDRD proposals:

### Science Challenge

- No change in existing scientific framework or field
- Incremental increase within existing scientific framework or field
- Significant advance in an existing scientific framework or field
- Creation of a new scientific framework or field

### Technology Challenge

- No change to existing product/technology
- Incremental refinement or customization of an existing product/technology
- Significant improvement of a product/technology
- First ever product/technology of its kind

While most LDRD projects focus on either a science or engineering challenge, many projects include ambitious objectives to advance both technology and scientific knowledge. A defining characteristic of high-risk research should be the pursuit of game-changing science or technology. The challenges inherent in such high-risk research are manifested in a number of ways identified by LDRD investigators. Sometimes fundamental laws of nature that may not have been previously encountered or understood present obstacles to achieving the research

objectives. For example, combinations of processes, components, or materials may be incompatible, or models or processes that are valid in a certain size range fail when applied to a different (smaller or larger) scale. Rarely, investigators discover instances in which previously accepted outcomes have either been misconstrued or misunderstood by other researchers.

## Managing Technical Risks

Risk management in leading-edge research can encompass several possible strategies, including:

1. The research plan may include investigating several alternate technical approaches, either simultaneously or as “fall-back” options.
2. A team may include external collaboration, engaging other research groups with unique and complementary expertise.
3. A project plan may include a time-delimited period in which to demonstrate specific milestones or successful risk mitigation.

Technical risk management strategies must generally balance the need for focused plans to achieve research objectives with the need to flexibly respond to unanticipated outcomes, whether encountered as obstacles, or serendipitous findings that open up new opportunities in a different direction [3].

## Unexpected Outcomes and “Failures”

Stakeholders may logically inquire, “If what LDRD funds is high-risk, then where are the failures?” Hence, a key issue for program managers is to remain cognizant of the diversity of consequences that may be associated with risky R&D. This can be a quite complicated task. Researchers willing to undertake high-risk research are frequently tenacious about their approach, and therefore, averse to “giving up” an approach that may not be returning desired results. Undoubtedly, local project failures do occur, but such local failures do not necessarily lead to a global project failure. Rather, it is quite common for experiments and technologies to return either negative or ambiguous answers, and if risk-mitigation has been part of the research plan, these outcomes can stimulate creativity and redirect the research more toward its goal.

Other than successful attainment of a project’s stated goals, other constructive outcomes can

result from encountering and managing technical risks. Periodic reporting and reviews are built into the program to discover and monitor such outcomes. For example, scaling back project goals and accomplishing results of lesser consequence, nonetheless will move knowledge forward. And although there are instances in which a project does, in the end, disprove its initial overall hypothesis or invalidates a given application of its methodology, even those instances advance the scientific frontier, and hence to view those outcomes as failures is really to adopt an erroneous view of the nature of science. The ARISE report emphasizes that frequently there is enormous value in “fortuitous findings not related to the main objective of the research program.” Such findings, including “failures,” can be significantly important in advancing scientific knowledge.

## Rewards of High-Risk Research

Technical risk management strategies are likely to succeed when bolstered by the ingenuity and persistence of the researchers in pursuing their objectives. Indeed, as a result, some projects achieve “unanticipated success.” Many ambitious LDRD projects do achieve the originally stated goals, and sometimes accomplish even more than initially planned. Even if not fully successful, projects with audacious objectives can have tremendous impact, transforming our understanding of the world with new discoveries, and producing new technologies to make our nation more secure.

In this publication, we examine 12 LDRD projects at Sandia, funded over the fiscal years 2006 through 2008, to better understand how they exhibit one or more of the aforementioned criteria for high-risk research, the challenges they faced, the obstacles they encountered, the risk management strategies they employed, and ultimately, the scientific and technical advances they achieved. These histories reveal pertinent characteristics of high-risk scientific investigators — creativity, tenacity, and the willingness to confront risks and failures of various types. Our goal is to demonstrate ways in which LDRD-funded research creatively confronts and mitigates technical risk. ■

# Taking on Technical Challenges

## Thriving on Scientific Hurdles

Proposing to demonstrate that a long-held view of possibility in classical (aerodynamic) physics may be incomplete is clearly to take on a rather large challenge and therefore to incur a large risk. When a project also proposes to embody this theoretical transformation within an actual functioning physical device, the risk incurred is magnified. Such was the case in the LDRD project headed by James “Red” Jones, who proposed to develop an inexpensive, small-caliber guided bullet system for use by U.S. ground forces, designing a system in which no spin-stabilization is imparted to the bullet. That this was an inordinately risky engineering feat is underscored by the opinion — widely held in the applied physics community — that such a feat was “impossible,” violating fundamental ideas in projectile aerodynamics. Hence, Jones’ attempt to secure funding for the notion from the defense-research community fell on fallow ground. This type of research classically demonstrates a hypothesis that perches the project’s investigators at a precarious edge, which, often, others have eschewed because conventional wisdom has declared a particular direction to be fruitless, or as in this case, “impossible.”

This project’s solution, according to Jones, was to exploit “a different side of physics” to take advantage of physical principles that were not generally being considered and pursue a solution to stabilizing a non-spinning bullet, as well as to guiding that projectile after its accelerated emergence from a rifle

barrel. The project examined several aspects of the problem, including aerodynamics, navigation, and controls. However, since it was not funded sufficiently to study all aspects of the issue, research activities were logically focused by the principal investigator (PI) onto the most important guidance component, the actuator. In these studies, additional risk derived from the fact that in order to model outcomes, the available computational codes were designed for modeling larger structures and therefore has to be scaled-down for this



Track of test projectile

project’s modeling initiatives, which necessarily would guide experimentation. “Any time you scale-down, unexpected things can happen,” Jones observed in commenting on the dangers of

extrapolating outside of realms in which actual data exist. “Understanding your solution space is part of research,” he trenchantly emphasizes.

Interestingly, as the research progressed, observers who had initially deemed the project’s goals “impossible” began to regard it as perhaps more feasible. However, the project’s course was hardly without bumps or potholes. “This was a hard problem,” Jones emphasizes, but “if it were easy, it wouldn’t be fun,” he clarifies, displaying the attitudinal disposition of the researcher who thrives on challenge, a requisite characteristic for someone who chooses to engage in high-risk research.

Jones also emphasizes that risk mitigation in such circumstances involves due diligence that both precedes and accompanies the

course of a project. Judicious elaboration of milestones during project formulation is the first step, but even if a disparity exists in the project's progress with respect to those milestones, careful allocation of resources during the project's course can mean that shifts in direction become possible, particularly if such shifts are accompanied by increases in knowledge. Ultimately, such knowledge acquisition, a significant forward movement of the boundaries of scientific uncertainty determine whether a project's staff have been, in Jones' view, "good custodians of taxpayer dollars."

Ultimately, the project outcomes proved to be quite close to the originally proposed concept, despite the "huge engineering challenges" that remain. But the PI and other observers of the project seem clear in their assessment that

*" . . . if it were easy, it wouldn't be fun,"*

without the risk, one cannot surmount the hurdles, make the type of progress that this project appears to have realized, in this case, a demonstration that a physics hurdle deemed "impossible" was actually only very difficult to overcome. Surmounting this large difficulty rewarded the project team with the feasibility demonstration of an inexpensive, small-caliber guided bullet, fulfilling Jones' prediction that pursuing a risky alternative physics pathway would be worthwhile. But it was also one that required an investigator willing to assume that risk of proposing to challenge dogmatic thinking and rigid adherence to accepted methodology. Historically, such a trait appears to be essential to individuals in science and engineering who have made transformative discoveries.■

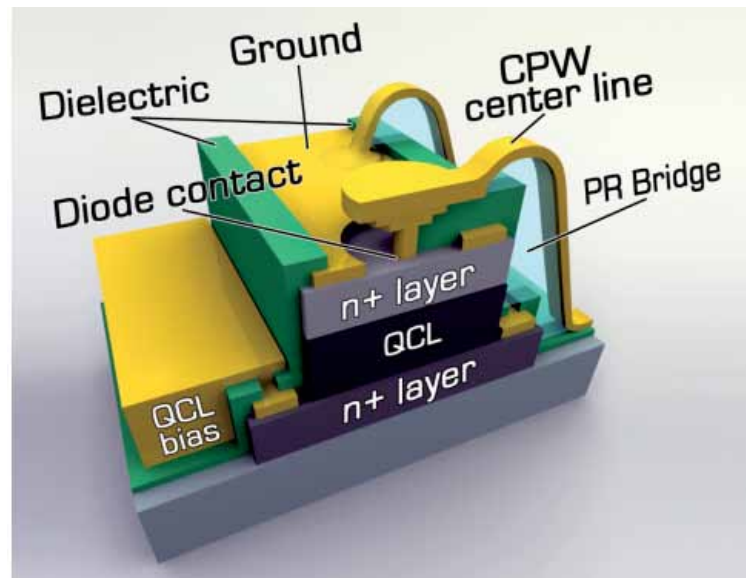
## Persistence and Creativity

Falling between microwaves and infrared, the terahertz region of the spectrum of electromagnetic radiation has been difficult to tame in terms of its potential uses in threat-detection and secure communication, in one respect, because the extant devices for generating, transmitting, and receiving (transceivers) the frequencies above 1 THz have been large, fragile, and/or expensive. Taking the risk to design and engineer a completely monolithically integrated, compact, all solid-state, single-chip THz transceiver, with the potential for imaging objects behind visibly opaque materials, high-spatial-resolution radar applications, and secure high-bandwidth communication links, clearly could have high payoff for Sandia and NNSA. However, it was a significant risk because of the contrast between what existed and what this LDRD project proposed to accomplish — essentially a quantum leap from unwieldy bulky systems to widely adaptable, mass-producible THz transceivers. To successfully create a fully integrated transceiver required plunging into unknown territory to couple the THz laser and detector in a way that had never been considered or demonstrated before.

Sometimes, however, risk, although identified beforehand, still manifests in a fashion whereby its management poses an enormous challenge for a PI. During his initial proposal process, Mike Wanke recognized that his choice to propose the design and engineering of a terahertz transceiver, with a diode located in the core of a quantum cascade laser (QCL), was the most challenging — and by far the riskiest — of other lower-risk alternatives, which would, by themselves, represent significant advances in the field of solid-state terahertz devices. Hence, right from the project's inception, Wanke had concerns that the danger in proposing the "home run," the highest-risk alternative, might

be viewed as too daunting, thereby jeopardizing his chance for funding. What if he were being injudicious in proposing something so risky? Perhaps a lower-risk version of the proposal would stand a better chance at funding; and perhaps not, if it were assessed as not risky enough, not proposing a large enough potential advance in the field. It would appear that this “balancing act” might be a common one for LDRD proposal writers.

While framing the riskiest of the alternatives in his LDRD proposal, Wanke had nonetheless automatically formulated alternative possible research paths by carefully considering his options, and the relative risks entailed in each. The project would involve physical process development and engineering that had never been accomplished before, together with the development of a novel modeling capability. Even with three years, the risk of not succeeding was high, and there were other still-operant research programs whose outcomes were important to the success of this Grand Challenge LDRD, and which, therefore, drew some of the PI’s time and energy during this project’s onset year. Additionally, an obvious rate-limiting process was the growth and processing of crystals that had the ability to lase at the desired frequency (>1 THz). Already, at the start of the project, a delay was anticipated due to the movement of research space and equipment into new facilities. But when key crystal-growth equipment took nearly a year longer to come back on-line after a variety of unanticipated events, and new procedures to improve safety delayed the onset of operations in a new clean room, the bold, risky, integration part of the project was forced to a standstill, the only available laser material, a few crystals grown a week before the initiation of moving.



**Technical drawing of the elements of the THz transceiver**

Wanke pursued several avenues in an attempt to obtain suitable experimental material and processing for QCL development, mostly with limited success. Ultimately he was able to collaborate with the University of Massachusetts, Lowell, to obtain more active material, with Spire Corporation and European colleagues to process some bare lasers, and with Jet Propulsion laboratory to obtain high-frequency Schottky diode, that allowed the researchers to obtain experience with how the components worked together even if they were not on the same chip. “I had to use a lot of my connections in the outside world to get us working lasers so we could rearrange and at least attack some of our milestones,” Wanke explains about his dilemma.

Fortunate that he had a few sample to work with that did actively lase, Wanke was compelled to carefully use these as substrates for learning to combine the QCL and diode. “Without the ability to process integrated lasers and diode from scratch for a while, we used other techniques not located in the cleanroom



to remove small amounts of materials on the top of existing lasers, and redeposit diodes into the holes,” Wanke recalls, which even in the absence of successful Schottky diode fabrication, taught the team valuable lessons. For obvious reasons, the project failed to meet its second-year milestones. While the external review board was impressed by what was salvaged, the board and internal management were understandably pessimistic about completing all milestones, and requested a new plan with an extremely tight focus given the limited time remaining.

Certain aspects of the project were cancelled, a decision was made to reduce the effort on the “home-run”, highest risk path, and a go/no-go date was set to terminate the project if there was no significant progress beforehand. But the tide was turning for the better. They received excellent laser material at the beginning of the year before another unexpected event shut down growth again. Close to their own deadline, as the chip fabrication was nearly complete, the chip shattered. With no time to start again it was glued together to finish the fabrication steps. Remarkably the devices worked. The experience gained regarding crystal processing during the second year, allowed the project to continue. The success during that period was clearly a result of the way the team dealt with the unforeseen, uncontrollable setbacks during that second year — “a failed year in milestone terms, but hugely successful in terms of team building and learning,” Wanke offers in retrospect.

The team successfully demonstrated the fall-back plan, namely a QCL into a rectangular

waveguide, and with a new crystal wafer grown at the halfway point of the final year, re-engineered the entire process. With three months remaining, the riskiest proposed outcome — the diode and QCL on a single chip — was brought to fruition. The management of this very risky project demonstrates not only the management of risk through parallel path planning, but also the persistence and creative aspects of the LDRD investigator and team. In the face of what probably seemed like insurmountable challenges at the time, Wanke and his team persisted in trying whatever alternative avenues were available, and ultimately refused to give in to the calendar as it ticked away their opportunity to actualize their scientific vision.■

“a  
*failed year in milestone terms, but hugely successful in terms of team building . . .*”

## High Risk — High Reward

**B**y all external measures — publications, the genesis of new companies and new capabilities, Sandia's effort in fiber laser technology has provoked transformative results in three ways, first from the perspective of the physical science (laser optics) itself and second from the perspectives of two engineering areas, optical engineering and thermal-dissipation (heat transfer) engineering. With respect to the physics itself, high-powered lasers have always suffered from inefficiency. Powered by electrical energy, the transformation to optical energy (light or electromagnetic radiation) has hovered around the 5% level or below, that is, over 90% of the electricity used to power traditional high-powered lasers has ended up as heat. As a corollary, these instruments have required elaborate water-based cooling systems to draw away this “waste heat,” rendering them large, bulky and difficult to transport.

The idea itself — that optical fibers, themselves, passive carriers of light, could be made into active lasing light-emitters — was not new, but there appeared to be fundamental limits on the power that could be generated from such fiber lasers. This was a result of the fact that as the fiber's core of rare-earth material was increased in mass to make more atoms available for the activation process that subsequently produced coherent light emission, the “quality” of the emitted light became degraded, the fundamental mode, the desired light becoming “tainted” by undesirable light modes. The upside was that energy transformation efficiency appeared to be far higher than for conventional lasers. Sandia scientists therefore approached a fundamental problem in laser optics, whose success promised to transform the view of what was possible in the optics realm of fiber lasers. But over and above the infusion of transformative knowledge into the field, the results would also provide a

new tool, in this case, a high-power laser of significantly higher efficiency and portability, promising, for example, the extension of capabilities for the military in sensing and free-air communications, and to the atmospheric sciences community in a number of different contexts. The risk of undertaking the project was reasonably obvious, given that no one had yet discovered a way to increase the power of fiber lasers without corrupting beam quality. Sandia's mode-filtering or “bend-loss” technique, a story in itself (a collaboration with the Naval Research Laboratory) was able to remove the undesirable light-emission modes from the beam, leaving a high-powered, high-quality laser beam. That this was a transformative outcome is well-illustrated not only by the technology's receipt of an R&D100 Award, but by its being named the most enabling technology of 2007 by R&D Magazine.



**Photograph of prototype novel heat exchanger design**

But the story of high-risk, high-reward does not end with those awards, for as the team worked with higher-power beams, they began to encounter “waste-heat” problems, based on the fact that even at the higher efficiencies (nearly 40%), significant quantities of heat had to be removed from the device. But regressing to water-cooling would represent a loss of portability. Hence, led by its second PI, Jeff Koplrow, the project embarked on an endeavor to improve the design of air-cooling systems

that would enable the instrument to remain air cooled and portable.

Citing risk-intolerance as a guarantee of failure, that is “failure to accomplish anything of significance,” Koplow was particularly focused on the unique role of Sandia’s Grand Challenges in bringing together individuals willing to engage in risky research, which could, potentially, reveal as much from encountered roadblocks as from unimpeded successes. “There is not nearly enough respect paid to negative results,” Koplow asserted, their value in dollars-and-cents terms potentially large, when those results serve to direct other researchers away from consuming resources following fruitless research avenues.

This brings into focus the larger question of the role of national laboratories. For Koplow opines that private industry risk has become severely limited by quarterly reports, and that federally funded university research may approach risky, leading-edge projects, but only on a generally small scale. In each of these circumstances, risk therefore becomes delimited; in the corporate arena, for example, innovation is in a sense, centrally planned, management always with one eye focused on the financial bottom line, while the other encourages scientific discovery. Since the scope of risk is lowered, so is the scope of the potential reward. If these observations have validity, the importance of risk in larger-scale projects funded by national laboratory LDRD or LDRD-like programs means even that much more to the society at large. For in the face of global-scale challenges, only global-scale solutions will be adequate.

Exemplifying this scenario was a new task on air cooling added during the final year of this

project. Once the key technological innovation of mode-filtering had broken through prior power-output ceilings for fiber lasers, the remaining question was how much could power be increased. But when it became apparent that further power scale-up was limited largely by the ability to air-cool the system, this constituted a roadblock, a “local failure.” It offered the option to either “declare victory and move on” with the significant, power increases already achieved, or else a creative opportunity to address what had already been characterized by the Defense Advanced Research Projects Agency (DARPA) as a technology (air-cooling) “unchanged over the past 40 years.” The decision to pursue this challenge was clearly, a risk in and of itself, particularly given that, as illustrated by the R&D awards, the project had achieved its original goals. And in this case, beyond fiber laser cooling, lay the promise of supervening limitations encountered in many

*“Risk intolerance is a guarantee of failure to accomplish anything of significance.”*

other areas of air cooling, most notably in processor-chip technologies, where clock-speed increases have been more limited by the inability to remove heat from

computers than by any other factor. Hence, the fiber-laser team pursued a new design in air-cooling, and has patented this design, a prototype of which has so far lived up to initial predictions.

Koplow credits LDRD for allowing him to take this double risk, first the pursuit of an engineering design task unanticipated in the original proposal, and second, with a reasonably high chance of “coming-up empty.” In the end, however, those risks paid-off in grand style. Already having greatly impacted the laser industry through the viability demonstration of single-mode, high-power fiber-laser technology, this project now stands poised to impact numerous industries whose growth is constrained by inadequate thermal-dissipation capability.■

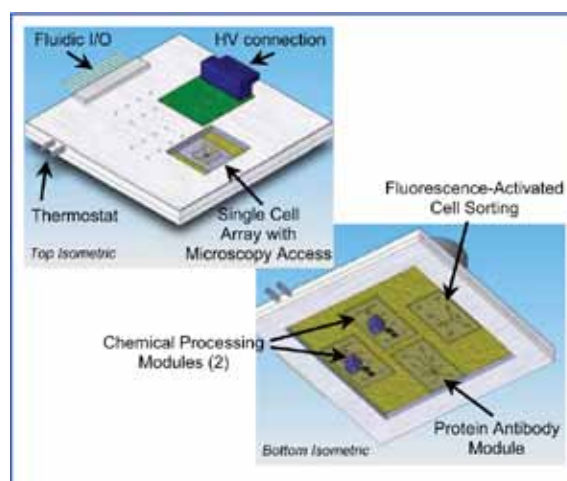
# Managing Technical Risks

## Striking a Balance

The Microscale Immune System Laboratory (MISL) Grand Challenge LDRD Project took a multifaceted approach to transforming the potential for performing cell biology research, more specifically, for culling data about signal transduction in cellular responses. In a sense, the outcomes of this project have opened up the very real possibility of creating a new subfield of cell biology research.

The fact that the immune system was the object of the project's inquiry is almost tangential to its ultimate discoveries. Macrophage cells, a type of white blood cells (WBCs), were the target of investigation because they form the first line of defense against invading pathogens, and a great deal is already known about the specific aspects of the signals exchanged among the various types of WBCs. However, given the available degree of sophistication in the research tools, such studies are necessarily statistical in nature, that is, the molecular decoding mechanisms to immunochemical (cytokine & chemokine, "hormone-like") signals are necessarily derived from a population of responding WBCs. The tools developed within MISL allowed the researchers to observe responses in single responding WBCs. Furthermore, and to the point about transformative science, those observations revealed new details about molecular mechanisms of cellular responses in signal transduction that could not have been discerned from the lower-resolution of population-derived responses. Hence, it is not an overstatement to pose that the increased resolution available through the observation of individual cells is poised to open a new subfield within cell biology, that of single-cell studies, complementing the already extant subfield of cell-population research with anticipated impact well beyond infectious diseases.

The challenge in pursuing such research is evident from the observation that it creates a tool enabling biological measurements that no one had heretofore been able to accomplish. Project principal investigator, Anup Singh quickly recognized that situation. "I learned about it (managing risk) on the fly; thankfully Glenn Kubiak (the Project Manager) was there to help implement a risk management process, Singh observed, in reflecting on his PI role of such a large and diverse project. Singh adds,



**Microfluidic platform schematic**

"we need to teach investigators how to assess and mitigate risk," indicating that he would wish to see some formal training, perhaps a workshop, put into place and offered as a prerequisite to submitting an LDRD proposal.

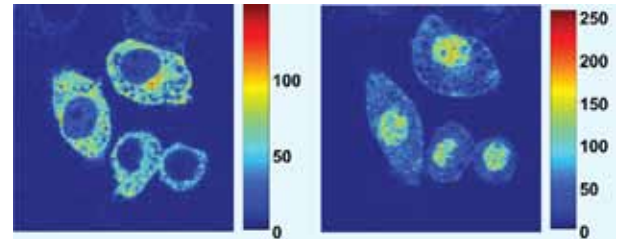
*"we need to teach investigators how to assess and mitigate risk"*

Singh described his pursuit of a graded approach to risk management in the MISL project. Key questions for Singh were quantifying risk and scaling relative risks, such that it would be easier to decide which risks demanded that investigators prioritize their mitigation. Technical staff were asked to identify key goals, and also, within their

implementation plan, to identify risks on a relative scale, with a mitigation timeline. He made it clear that the goal of the request was far more than a theoretical exercise; should risk fail to decrease, the investigators would be required to shift their activities to a backup plan, a “plan B.” For areas of highest risk, a formal plan B was required; for lower-risk project activities, Singh requested that individuals be aware of the risks and consider what possible backup plans might be appropriate. Risk was formally and periodically evaluated on a 3-month basis. Singh reviewed each backup, and if he were in any instance, unconvinced of the plan’s validity or feasibility, he constructed his own Plan B. He viewed this approach as necessary in light of what he characterized as the tenacity–Plan B balance. In other words, staff — energized by the excitement of pursuing solutions to unknowns in science — are generally reluctant to give up on an approach, frequently exhibiting tenacity of pursuit. While this “just give me a few more weeks” attitude is admirable, it is also precarious, unless risk mitigation is factored into the balance: tenacity in the face of undiminished risk can easily have a negative impact on the progress of a project whose funding is severely time-delimited.

With a project the size and breadth of MISL, there were three focus areas, namely biology, engineering (largely microfluidics), and computational modeling, and the team leader for each area was directly responsible for risk management and backup plans in his/her area. In certain instances of very high risk, Singh encouraged multiple technical staff to submit different approaches toward the same project goal, with the determining operational factor in adjudicating among them, the ability to lower risk over a finite time interval (6–9 months). In one key instance in the engineering area, three approaches were submitted, and 6 months later, only one of the three had lowered risk; solely this approach was allowed to move forward.

In retrospect, Singh, like Koplow (page 10), perceives several cultural issues in LDRD proposal submission. The first is an overall



**Hyperspectral images of immune system macrophages**

resistance to deeply consider risk mitigation. But even more germane is an almost opposite attitude, investigators believing that they may need to partially disguise a proposal’s risk to obtain funding, the perception being that the program does require that a proposal be risky in order to merit funding consideration; but not too risky. “PIs are being made risk-averse,” he believes. Hence, Singh sees a tendency to disguise risk, instead of meeting it head-on. He suggests that every proposal should be able to articulate a plan B, and perhaps even a Plan C, and therefore, that funding should be contingent not just on high-risk, but rather on risk with risk-mitigation strategies in place. This means, as a corollary, that success should be adjudicated not solely on a project’s meeting 100% of its milestones, but rather on some combination of milestones-met and risk-mitigated by way of alternate strategies implemented.

As the accomplishments of MISL indicate, proposing risky research that inquires deeply into unknown territory can produce immense returns, provided that risks are carefully managed with backup plans in place. This combination of risk with premeditated mitigation strategies appears to be the ideal in LDRD proposal and project management, and indeed needs to be encouraged in any possible fashion.■

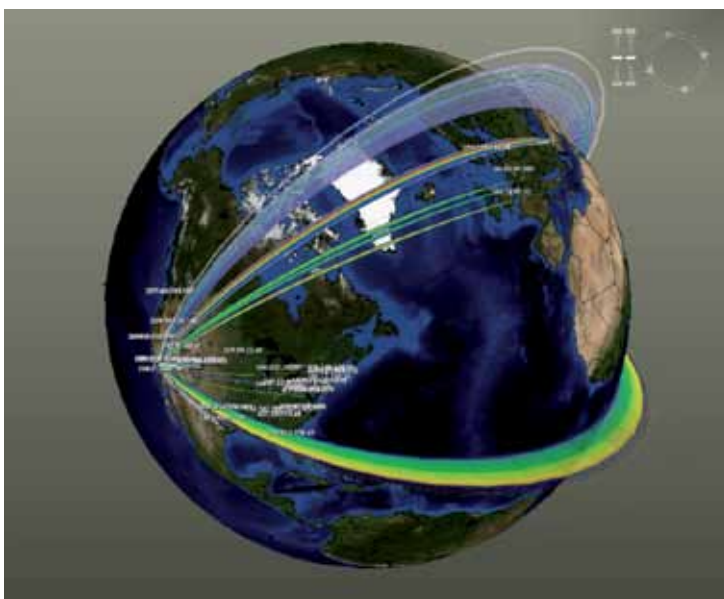
## An Option to Fail

Philip Kegelmeyer's Network Discovery LDRD Grand Challenge project falls under the rubric of a research effort that has the potential to develop a transformative capability in national security, in this case, for the US intelligence analyst community's incredibly difficult job of discovering or characterizing covert adversaries. It addresses computational science that is so non-obvious to an average person, that even the conceptualization of this project's research has an aura of risk surrounding it. Framing the hypothesis and an approach toward a solution represented a creative leap, and an obviously risky one — namely, that our most formidable adversaries are networks of people and computers whose interactions are so subtle that to discover them requires an ingenious piecing-together of incredibly disparate intelligence data, culled from large volumes, much of which might prove irrelevant. The idea of devising a methodology to accomplish that end seems incredibly daunting.

To actually carry it out requires the type of project structuring that original PI Bruce Hendrickson, Kegelmeyer, and the project team built into the research, as well as adaptability and ingenuity.

Citing novel National Institutes of Health (NIH) funding requirements for clinical studies, Kegelmeyer offered commentary about the importance of publishing negative results that was very much consonant with that of Troy Olsson (page 28), his overarching view capturing the notion that being friends to risk is a crucial aspect of the LDRD program. He was able to put a positive spin on the notion of LDRD as a "sandbox," a normally derogatory metaphor used by program critics to describe

the program as funding something akin to children playing with toys. But in Kegelmeyer's interpretation, the metaphor connotes sandbox as protected environment, where failures within program-funded research have less impact on Sandia as a whole (a view that, despite their disparate research areas, is also shared with Olsson). For this project, as an immensely risky incursion into an largely unstudied computational research space demanded that the investigators feel that they had the option to fail — either to prove that what they were



**Representation of global cross-talk among computers**

attempting was undoable, or at the least, that some of their assumptions about what was conceivable might have to be modified or abandoned. This acceptance of failure as possibility helps define the project's riskiness.

Kegelmeyer described a multifaceted risk-mitigation strategy in this project to develop analytical tools for revealing and analyzing adversarial cyber networks, developing an informatics capability that had not heretofore existed. He began by taking care to categorize two main categories of risk: First would be the failure to generate intelligent analyses of target networks; second would be the generation of useful analyses that might nonetheless be

unusable by intelligence analysts, the project's major target audience, either because the tools generated might be too complicated or awkward, or else, might fail to gain their trust.

The project managed risk along several lines. First, a distinct human factors team, was assembled, led by a cultural anthropologist who studied the cognitive psychology of the intelligence community, in order to attempt to elicit a set of requirements from that community that would serve as a benchmark against which to assess the direction of tool development. This part of the project's inquiry assembled sets of use cases for the informatics developers, such that they might be better directed in answering a particular need in a fashion useful to the eventual community of users.

Next, at the end of each project year, the team assembled a prototype of the informatics accomplishments to that date into one coherent package, to confirm that the existing developmental algorithms had utility before continuing development. Additionally, human factors feedback was solicited with respect to the user interface at that year-end prototyping. Active intelligence analysts were recruited for this purpose, and compensated for the time during which they elaborated details of their specific challenges and addressed use-cases to test the prototypes.

Finally, as an ongoing risk-management strategy, the project team interfaced with in-house experts in both the areas of cyber security and technological surprise, even to the extent of engaging a formal liaison to these experts, such that they would attend weekly team meetings.

The project did, nonetheless, encounter several types of local failure during its course that compelled a response in terms of redirection and resource allocation. For example, part of the original project proposal was to leverage Sandia's significant experience at quantifying uncertainty (in the nuclear weapons arena) to address issues of uncertainty regarding noise and randomness in the cybersecurity data. However, the team found that the elicitation process for uncertainty did not produce useful feedback, as it did for other project aspects. The human factors team

*“Risk*

*mitigation strategies*


*revealed productive and unproductive*

*research paths.”*

discovered that how analysts think about uncertainty appears to be both situation- and individual-specific. Consequently, in the face of the apparent elusiveness of general principles of uncertainty, the team decided

to move resources away from a search for such generalizations, instead, generating a series of small case studies in this area and used them to fuel a workshop dedicated to selecting two of the most promising ideas for full attention. Kegelmeyer was aware of the difficulty of this problem and its risk of failure, as was Bruce Hendrickson, the project's proposer and original PI, when he first submitted the proposal. Realistically, the project team operated under the premise that despite the change in project course with respect to uncertainty quantification, even incremental advances matter for such a difficult problem.

“Did we lay down enough groundwork so that future studies will be able to use our results?” Kegelmeyer poses about the project's outcomes, concerned that he is unable to quantify an answer to his own question because of the difficulty of measuring “how much insight” one has generated in an intelligence analyst. But it seems clear from the attention paid to risk assessment and management that the



project's success appears to have resulted from setting into operation risk mitigation strategies adequate to reveal productive and unproductive research paths. And these strategies synergized with the team's willingness to declare "local failures" for project initiatives that appeared fruitless, while reinvesting resources into those that did appear to bear fruit.

Project outcomes have been diverse and impactful. For example, identification and documentation of significant user-interface issues were rectified. The feedback on both the interface and underlying analytics generated improvements, which in turn, resulted in the unexpected adoption for program use of both the first and second prototypes. The team completed parallel implementations of two basic tensor algorithms (PARAFAC and Tucker).

In essence, the Network Grand Challenge is creating a unique capability to answer currently unanswerable questions, a capability that should ultimately be applicable beyond the field intelligence arena to any problem in which the data is so complex or so voluminous as to defy its effective use. Its demonstrated analytical capabilities had already attracted significant external funding for follow-on work, from a variety of government and military sponsors. Furthermore, the project's capabilities are already being directly applied to Sandia's operational efforts in defending its own cyber security. ■

## Leveraging Strategic Partnerships

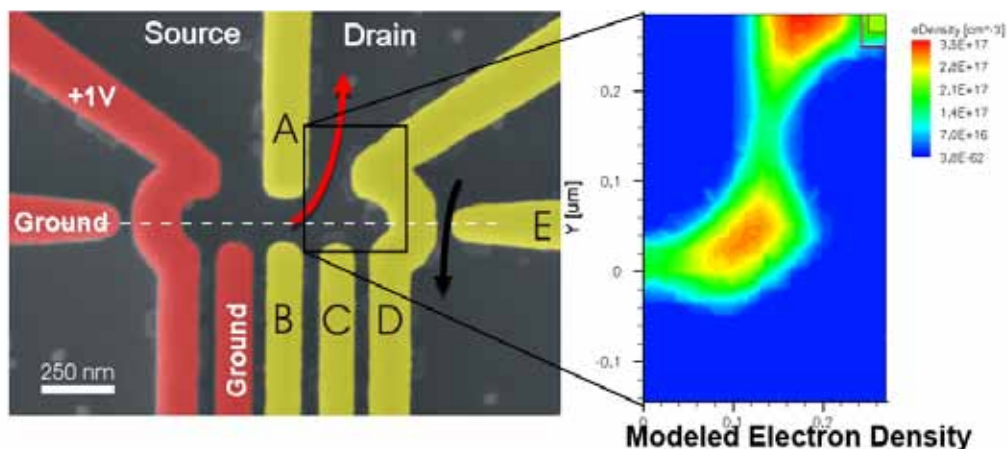
Quantum computing is widely viewed as a transformative technology and has been under serious consideration for over twenty-five years. For example, renowned physicist, Richard Feynman in his presentation at the First Conference on the Physics of Computation, in 1981, opined that it would likely be impossible to readily simulate aspects of quantum systems on a classical computer. Feynman proposed a model for a quantum computer (QC) that would be able to simulate quantum systems. Since that time, problems such as those in cryptography and several other areas have been proposed as far more amenable to solution by quantum computers, by comparison to their relative intractability on classical computers.

Problematically however, it appears easier to postulate the characteristics and potentialities of quantum computers than to actually engineer the physical elements — quantum bits (qubits) — required to construct one. Although several demonstrations have been made with fewer than 10 qubits, to create qubits that are appropriate for larger systems greater than 10 qubits — that is, low-error qubits — is a daunting challenge. Large-scale QC might require greater than 100,000 qubits which will require many leaps in technology including identifying the best material with which to actually build qubits. Given this track record, it is natural to view any project as rather risky that proposes to build qubits that are appropriate for a small quantum circuit. Several groups, worldwide, are attempting this feat, one of them based on this Grand Challenge LDRD project at Sandia. It is no stretch to venture that the first group to build low-error silicon qubits will have created a technology that will be radically transformative for the ways in which computational challenges are approached, as well as greatly enlarging the physics community's understanding of both theoretical and practical manipulation of quantum systems.



This challenge lies at a quite precarious edge of an already counterintuitive scientific subfield (quantum theory), wherein surprises seem never to cease astonishing even its most studied practitioners. Risk is almost woven into any project that seeks to enlarge the boundaries of the field, but is especially evident in projects like this one that propose to manipulate and control quantum systems.

teams, such that a reconfiguration was possible at many points, since communication with groups pursuing the alternatives was frequent and fairly liberal. For example, the Sandia team is pursuing the fabrication of a silicon quantum dot using metal-oxide-semiconductor technology, with the aim of electrostatically gating a single electron at the oxide-silicon interface. This approach contains the risk of increased sensitivity to defects in the oxide layer.



**Scanning electron micrograph of a silicon quantum dot with modeled electron density profile**

Clearly articulating his operational strategy of “building-in robustness” and mitigating risk by constructing a “technical plan with options,” LDRD PI, Malcolm Carroll recognizes that his team’s approach in designing physical qubits in silicon as something no one has ever done before, and that they are attempting it in a seriously compressed timeframe. But Carroll is also clear about his overarching risk-mitigation strategy — one involving the investment of 10 to 15% of the project’s budget in the identification of two research paths being pursued by other groups, internationally, whose outcomes can be rapidly adapted to the baseline path being pursued by the Sandia team. Carroll maintains, that through pursuing a primary path that complements the other paths, “we have been able to be more successful through directly contributing to the other leading groups while providing a way to rapidly adopt the other approaches if needed.”

Other teams internationally are examining single donors in silicon as qubits. The Sandia team proposed a parallel hybrid approach that uses single donor atoms incorporated within the crystal to confine electrons away from the oxide but uses the quantum dots to mediate certain qubit functions. The Sandia team’s donor qubit effort also benefits from the learning and infrastructure that the team is developing directly through the quantum dot research at the oxide-silicon interface. The other groups internationally have reciprocally benefitted from the results the Sandia’s quantum dot approach has provided through its research.

He describes the project’s primary path as set up in parallel with those of two other international

Meanwhile, a third group pursuing an alternative approach using a depletion mode SiGe alloy-based metal insulator field effect transistor (MISFET) is collecting results that are valuable to Carroll’s group because Sandia’s enhancement mode metal oxide semiconductor field effect transistor (MOSFET) design can

be transitioned to the replacement of silicon dioxide with an enhancement mode MISFET using SiGe as the insulator. Hence, enhanced ability to transition into this parallel path, should it prove more beneficial to project outcome, clearly mitigates risk in a very tangible fashion. According to Carroll, the project was structured in this parallel-path fashion from the outset.

The risk to this project-management structure is one of a very different genre — distraction, should too much focus be directed onto the

*“ . . . a balance between  
collaboration and  
competition”  
(as an approach to  
risk mitigation)*

alternative methodologies. But Carroll feels comfortable with the 10 to 15% project-time allocation for this purpose. Striking a balance between collaboration and competition can also be somewhat delicate, when using this approach to risk mitigation. He perceives another risk connected with the timeframe itself, which he characterizes as “going from zero to world-class in three years.”

Carroll found it valuable to meet weekly with the heads of each subproject team. For example, one such team is involved in designing a classic electronic circuitry to interface with and support the quantum circuitry, another team with modeling the functioning of the qubit-circuit interface. Carroll also commends the role of Grand Challenge project’s external advisory board (EAB), one whose “tough love” helped the project to address risk and sustain contact with the community of relevant research. “At the beginning, I doubted the value of the EAB

especially considering how much preparation and cost it requires,” he admits. Encountering some surprises, the project nonetheless met every first and second-year milestone.

To date, the project has developed the first disorder-free quantum dot behavior, one of the first MOSFET charge-sensed quantum dots and second-generation devices are in progress to achieve single-electron occupation, including experiments that have grown and are testing silicon-germanium MISFETs. Individual cryogenic circuit elements for the quantum-classical computing interface have been designed, fabricated and tested at the requisite low temperature of 4 K, including current-amplifier and comparators. Computational modeling of the disorder-free double quantum dot — which will provide ongoing design guidance — has proceeded apace, and significant advancements in the development of quantum circuits that perform error-corrected memory have also ensued.

Carroll views the LDRD program as the only way this research could possibly occur at Sandia. It is worthwhile noting that this project draws from prior, smaller LDRD investments in QC, projects without whose innovations the current Grand Challenge would have been unlikely if not untenable. Such sequential LDRD investments reflect Sandia’s commitment to this technology, whose applications not only in theoretical physics, but also in several areas of national security, would be remarkable. A successful project might create the possibility of a machine that could actually approach the types of problems that can only be solved by quantum computing, a giant step forward. To entertain risk for such a significant payoff lies at the core intent of the legislation that created the LDRD Program.■

# Encountering the Unexpected

## An Unanticipated Risk

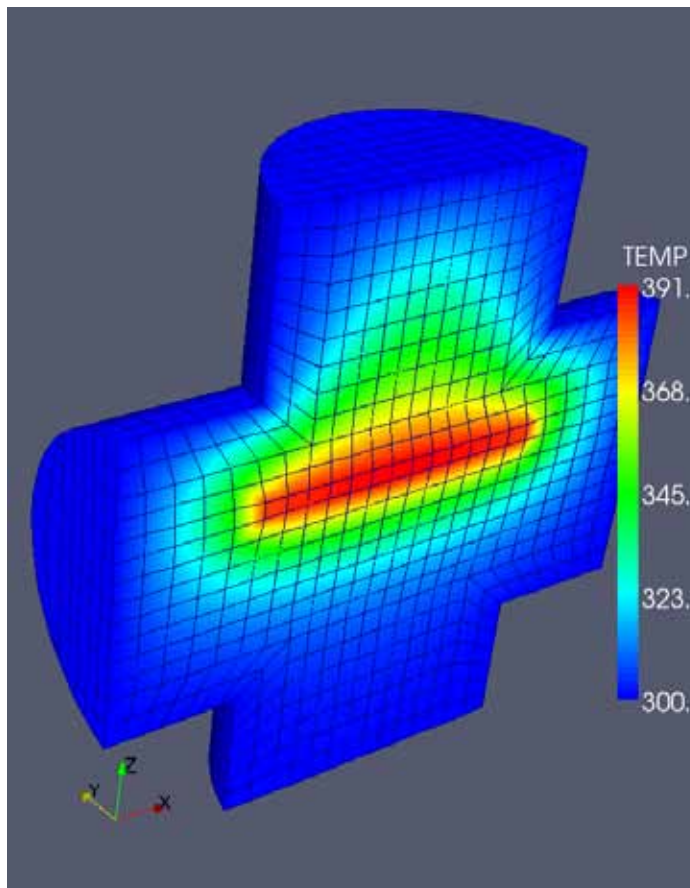
“**P**roving the negative” is necessary for scientific progress, but is “never as satisfying,” according to Randy Creighton, whose most-recent LDRD experience more-or-less placed him into that position. Creighton’s proposed LDRD project offered the prospect of transformative science and engineering from two perspectives. First, it would build on a set of prior research findings that claimed to demonstrate electricity production via catalytic reactions on a surface, in the absence of an electrolyte solution. Second, by creating such devices at the nanoscale, the research could engineer transformative devices, which through such chemistry, would be capable of culling electrical power from locally available environmental sources. This would, first, enable the military to more-efficiently run field operations, making such operation less dependent upon energy-delivery supply lines. Ultimately, such devices might offer electricity to regions of the planet that are still sufficiently underdeveloped to lack it. In both the scientific and the engineering senses, the transformative

potential of this work was obvious, and its risks also clearly significant.

However, in proposing to design and fabricate nanodiodes that could sustain this chemical-to-electrical energy transformation, Creighton encountered a risk that would have been genuinely difficult to predict in advance. Highly touted and publicized work by respected academic chemists — a set of prior research findings — began to exhibit flaws when employed as the underpinning of this LDRD project, leaving Creighton and his team in a position of having to investigate potential flaws in the work of others to attempt to pinpoint the reasons why their own proposed work was encountering what appeared to be insurmountable obstacles.

Creighton compares his experience to the cold fusion scenario, the similarity being that in

fundamental science arenas, what appears to be seminal research can sometimes fail to sustain its anticipated value when subjected to subsequent scrutiny. “We started at point A, and our world collapsed under us,” he candidly observes.



Calculated temperature profile of nanodiode heater

At issue were the results of research in surface chemistry by respected academic chemists, who had both proponents and skeptics. And although Creighton describes himself as “neutral,” he did assume a risk of trusting the veracity of results published in a peer-reviewed journal, which suggested that solid-state catalytic diodes could sustain, via precious-metal-catalytic oxidation of a substrate, a steady-state electrical current in the absence of electrolyte. While previous researchers had studied this effect, such “chemicurrents” had been observed only transiently and at elevated temperatures. But if — as suggested by the breakthrough research — such steady-state currents were possible at a reasonable efficiency, then Creighton’s pursuit of a lower-temperature version of the effect (while retaining efficiency and adequate current density), might well represent a solution to the need for local, environmentally fueled power sources.

After disappointing attempts to replicate the underpinning research, and additional publications by the academic researchers that appeared to imply that they had initially overestimated their efficiencies, Creighton directly consulted with a member of that academic team, who seemed to be steadfast about the initially published efficiencies.

“I did not set out to engage in controversy,” Creighton maintains, but it appears that circumstances surrounding the project’s inability to replicate its underpinning research essentially compelled his movement in that direction, in order to explain the reasons for his project’s lack of progress. Creighton has since pursued investigative science to support his hypothesis that the reported efficiencies are an artifact, the currents generated by a thermoelectric voltage source within the device, rather than as a result of surface catalysis as the primary electron source. In addition to computer modeling of the temperature profile within the device, a

complete physical and chemical model was constructed, a feat for which Sandia is uniquely equipped. These investigations appear to have verified Creighton’s artifact hypothesis, with significant impact on the field, in terms of illuminating future research, directing researchers away from dead-end research paths. And despite the change in course mediated by the unexpected disconfirmation of published research, the project did produce tangible outcomes such as marked improvements in procedures for diode fabrication.

*“illuminating future research, directing researchers away from dead-end research paths”*

“Unfortunately, you’re going to have failures . . . so having a tolerance for risk is very important,” Creighton emphasizes. Despite the “failure” of his project to accomplish initially proffered outcomes, it seems evident that the follow-on effort seeking to either confirm or disconfirm the prior published research is absolutely critical for further progress in this research arena. It would appear logical to assume that a high-risk research program such as LDRD should, at least on occasion, play a role in such fundamental inquiry of disconfirmation. In one sense, this project presents another example of a significant result, in this case, the ability to clarify essential aspects of fundamental concepts in a key research area from Sandia’s and the nation’s perspective — that of energy-security.■

## Snapshot of the Scientific Process

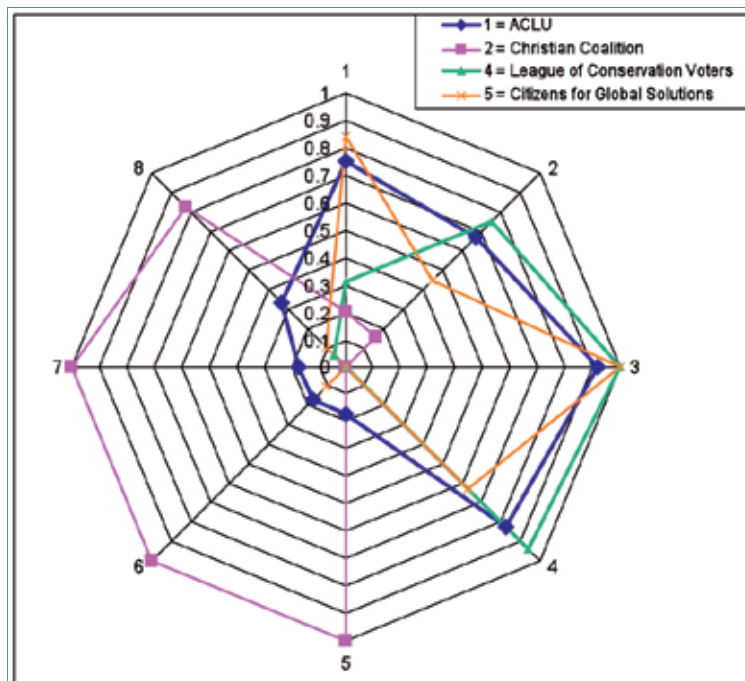
This project represented an initiative to push the limits on the analysis of text for the purpose of extracting insights about ideologies and their shifting natures, specifically as a predictive tool for national security. The premise of this research — should it succeed — was that developing such an ability would hold great predictive potential. If the intelligence community could deduce, from missives, statements, or other prose, that a given adversary's ideology had shifted from a

grammar and syntax play a key role, the attempt would be to employ so-called “bag of words” techniques in which syntax is lost, and word frequencies and proximities become the primary data sources. Project PI, Ann Speed, and the project team recognized the high-risk nature of the work from the project's inception. Unfortunately, the task of determining ideologies, and shifts in ideology from text in this way proved even harder than the team had surmised. It was clear, by the end of the project's first year that progress had been small. However, it was not clear whether the difficulty was due to the bag of words approach, the text

samples (and amounts) being used, or the classification techniques being used. Additionally, while generally understood as a set of beliefs that govern action in the world, the concept of “ideology” is rather difficult to pin down more precisely, particularly as it pertains to the operational link between a theoretical ideology and its manifestation in the behavior of an individual or group.

Thus, in the second year, the team utilized a different text corpus (speeches from the U.S. Senate as compared with translations of text from jihad groups in the Middle East) and applied more sophisticated classification techniques to the problem. Despite these changes, and despite trying multiple supervised and unsupervised classification techniques, performance did not improve.

“Now we have a better understanding what works and what doesn't,” Speed comments on the project's findings. “While subsequent work for the Air Force yielded better results using self-organizing maps as the method of classification, it is clear from this research that bag of words techniques for getting at



**Spider plot of the ratings of speakers from various special interest groups predicated on analysis of texts, an attempt to derive independent measures of “ideology.”**

more neutral to a more-hostile posture toward the US, for example, then that warning shot would be incredibly useful for the defense community's protective activities.

The project embarked on an analysis of text for the purpose of identifying ideologies and shifts in ideology, utilizing statistical text analysis tools. This meant that rather than using natural-language techniques, in which

something as ephemeral as ideology may not be the strongest approach,” Speed observes.

One result is that she is definitive in her support for the idea that “failures” are important when applying well-researched techniques to datasets that are outside the scope of their original conceptualization in hopes of developing operationally relevant knowledge. In this instance, it entails risk to attempt to apply reasonably well-understood cognitive science techniques to national security areas important to Sandia, which may be rather disparate from the arenas in which such techniques had been previously developed and utilized. As a corollary, Speed

*“Now we have a better understanding of what works and what doesn’t.”*

believes that there should be a greater role for national laboratories in performing high-risk research, given that academics tend to be driven by a “publish-or perish” ethic and that corporations, in competition with one another and responsible to shareholders, cannot readily afford to take such risks. “When you see published results, they’re a snapshot of the scientific process, during which nondiscovery plays a huge and repeated role,” Speed offers, in discussing the role of failures in research, particularly research in fields such as cognitive science that are relatively immature at Sandia by comparison to other Laboratories’ initiatives such as microsystem engineering, in which a deep and broad expertise has been cultivated over time.

She also sees a catch-22 implicit in the LDRD program investing in projects whose outcomes may not position their investigators

for either external or LDRD follow-on funding — specifically that researchers are encouraged to take risks in their research, but if that research fails to reach its goals, the researcher is at greater risk for being unable to secure funding to continue the work. She views this as another aspect of the risky nature of investments that probe into novel fields in which the Laboratories may not yet have assembled a critical mass of expertise. Perhaps in funding these areas, she argues, an awareness of the higher probability of failure requires that negative results do not equate with failure, but rather with disconfirmation of research pathways — illuminating the notion that unless research parameters can be adjusted, in this instance by applying different classifier techniques, it will be largely fruitless to follow these paths again. It requires such initiatives to delve into the underpinning factors that may have gone awry, ranging from experimental design to inapplicability or insufficient maturity of experimental approach. Since, as pointed out by others, it has become unfashionable and difficult to publish negative results, how that translates into subsequent funding for investigators entrapped in this catch-22 is a very real dilemma for someone in Speed’s situation.

Most importantly, her experience, like that of Randy Creighton (p. 19) indicates that — in addition to local failures that provoke course corrections — there are, indeed, more-global failures in LDRD projects, if failure is construed as an inability to meet milestones because of the disconfirmation of a research path. However, to view such events as failures for the scientific process runs counter to the spirit of science, in which, as Creighton also points out, an hypothesis disconfirmed through solid experimental design can be as valuable to further work in a field as a set of milestones accomplished. In this instance, the conclusion for the cognitive sciences national security research community was that to pursue this highly risky research path might require

several alterations to satisfy the technique's statistical nature, perhaps a combination of techniques, and certainly a better operational understanding of the somewhat poorly defined concept of "ideology." Investigators would need to carefully factor-in those key parameters before embarking on such a path. This clarifying information for both Sandia and the broader community represents a genuine form of progress, in the sense of guiding future attempts at such endeavors.■

## An Absolute Necessity

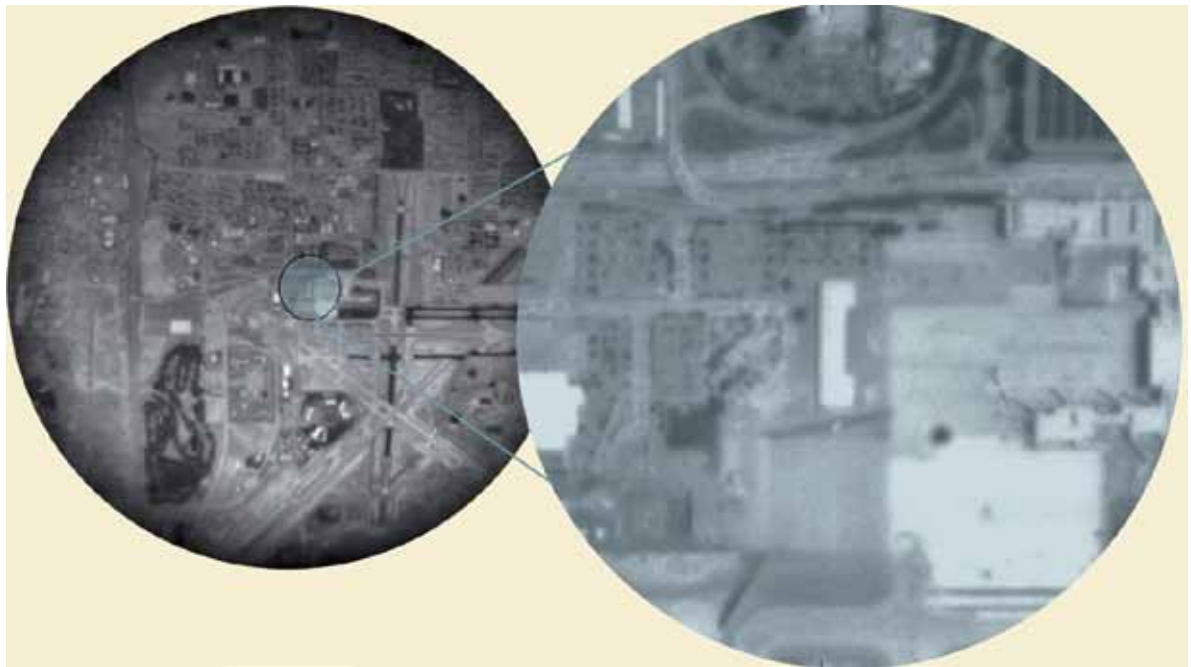
While one view of LDRD-sponsored research is its uniqueness in investigating a no-man's land such as quantum computing, where very little is scientifically established (see p. 16), there is another more-pragmatic view, expressed by LDRD PI, David Wick, that perceives LDRD projects as "necessary evils" in funding work that is simply too risky for sponsorship by other funding agencies. LDRD, in this view assumes a developmental risk, that by funding more-risky proof-of-principle research, ultimately brings Sandia business that builds on project outcomes. Wick fully understands that, aside from LDRD's funding of the basic research to which other agencies and customers are risk-averse, a large part of LDRD's value is its funding of projects within the context of the broadly diverse sets of expertise represented in a national laboratory setting, particularly one like Sandia, with its deep history of problem-solving engineering.

*"can't get customers to buy-in until a concept is developed to a certain maturity level."*

Wick's LDRD proposal and research was motivated by a clearly perceived, mission-related need, that of the military's (and DARPA's) search for improved variable field-of-view optics for both weaponry and night-vision goggles. Wick's solution was non-mechanical, in the sense of eschewing traditional lens elements that would move with respect to each other, as in the optical zoom of certain cameras (the 100 mm to 300 mm elongation of a long telephoto camera lens exemplifies this traditional solution). Problematically, these traditional optical solutions tend to be overly large and heavy, requiring significant power to move the lenses.

Instead, Wick and colleague Brett Bagwell turned to liquid crystal adaptive lenses, in which liquid crystal molecules within a transparent chamber are reoriented by applying a voltage across the lens, thus

In one sense, the outcome of the LDRD project could be termed a failure, in that a fully functional adaptive prototype was not the ultimate outcome: the system produced at the end of LDRD funding was too long and



**Image illustrating the zoom feature, the right-hand image, a magnification of the circled area of the wider-field left-hand image.**

changing the index of refraction and focal length of the lens. This high-risk approach seemed attractive to prospective customers, none of whom, however, had basic-research funding for such high-risk research; hence, the LDRD proposal.

Wick mitigated risk in the project by initially making certain compromises between a fully adaptive system and a conventional optical one. Rather than “shooting for the moon,” he and Bagwell were able to demonstrate how the incorporation of adaptive lenses would improve parameters, by producing a fully functional lighter-weight system requiring less power. One of the most important outcomes of the LDRD project was the investigation of other types of adaptive lenses, which Wick believes will lead to further breakthroughs in active imaging.

large for the intended application in night vision goggles. While a solution to the size problem is not yet imminent, the research did succeed in demonstrating proof of principle for a significant improvement in imaging for unmanned aerial vehicles (UAVs), where a somewhat larger size would be tolerable, to a sufficient extent that the concept brought forth two years of follow-on support from an external customer.

“LDRD is an absolute necessity,” Wick, in the end, admits, because one “can’t get customers to buy-in until a project is developed to a certain maturity level.” He reflects how much more convincing it is to be able to show those customers “a demo rather than a PowerPoint.” ■

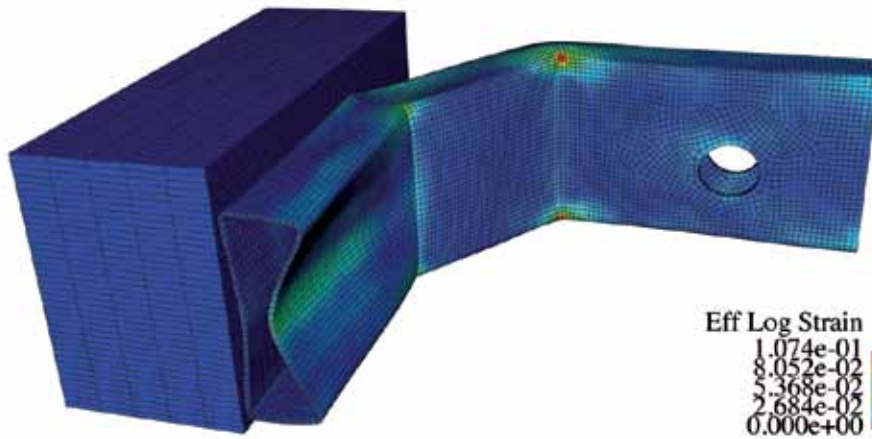


# Reaping the Reward

## A Major Course Adjustment

Taking responsibility for a project almost in midstream can be a daunting proposition, particularly when the new PI was not originally part of the project team. Fortunately for Ben Spencer, the project — modeling weld failure in materials — fell within the general sphere of his expertise. Nonetheless, the direction pursued in the project’s initial year had dead-ended without significant progress, so there was an inherently enhanced risk in agreeing to lead the project for its remaining two years of funding and pursuing a different tack in addressing the challenge.

The project’s original technical risk fell within the category of attempting to generate a new tool allowing the entire community to extend its reach. In this instance, the new tool would constitute a new capability in structural engineering — a novel multigrid method of modeling structural welds, so that, within the same model, the overall coarser structure of the material and a finer representation of the detail of a weld or welds could be simultaneously studied



Mesh model of different structures modeled in the project

and modeled to provide an engineer with the most comprehensive ability to make predictions about both failure probabilities and potential rectification strategies. In an era of aging infrastructure, such a capability is crucial for the

Nation’s infrastructure security.

That original path to this project envisioned two separate but interacting models, a global model of the material that would receive input from a finer-scale model of a weld. When applied to sample problems, this approach appeared to work satisfactorily for “well-behaved” welds, but was unsuccessful for the anisotropic behaviors that precede weld failures. Upon assuming the role of principal investigator, Spencer decided to try a new approach that transferred data between the coarse and fine meshes using an adaptation of techniques used in multigrid equation solvers. This method does not lose information critical for the modeling of failure in the fine mesh. The original approach gained computational efficiency by storing data from the fine mesh and only periodically evaluating that fine-scale model. The new approach evaluates the fine-scale model at every time step, but much larger simulation time steps can be taken because the time step is governed by the size of the coarse mesh rather than that of the fine

mesh. The approach gains computational efficiency through the latter strategy, while also retaining all of the higher-resolution information from the fine mesh.

Equally critical in a attempting to achieve the goals set for a three-year project in only two years was a mechanism to ensure agile software development. The

team decided to include the project in their organization’s “scrum” operational model, which the organization had found to be an efficient way of dealing with customer requests

for code development or modification. The team operated in three-week developmental cycles, with — on a rotating basis — one team member assigned to manage and prioritize requests. There were some of these cycles during which the LDRD project, treated as any other “customer,” did not rate top priority, and others in which it dominated in the prioritization mix. Either way, Spencer believes that “the ‘scrum’ operational mechanism prevented “piecemeal code shuffling,” and provided a more-intensive and better-directed assault on each project, including the LDRD project that he had inherited midstream.

Implications for the LDRD project included the challenge of nonlinear staff-resource utilization. On the other hand, Spencer reflects, LDRD allowed the team to try out new and

*“the outcomes achieved went beyond the originally stated goals”*

riskier ideas than it would have normally attempted in its work for other customers, and ultimately, in his view, the outcomes achieved went beyond the project’s originally stated goals. The end result turned out to be technical ability that will not only provide a reliable way to model weld-failure situations, but also do so in a more computationally efficient fashion. As a consequence, structural engineering adds to its “toolbox” of capabilities, a quite novel and powerful method for protecting infrastructure resources. That the risks were transcended is testament to the value of organizational teamwork and the willingness of technical staff like Spencer and his colleagues to face the risk of attempting new solutions in the face of roadblocks to success.■

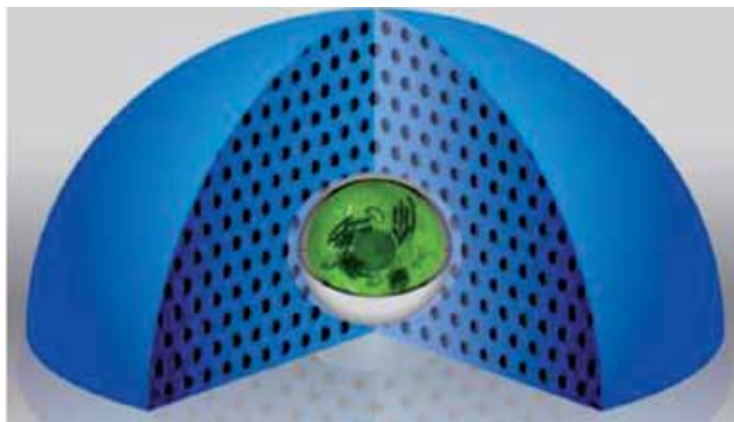
## A Serendipitous Discovery

Adopting the posture that research is “only a failure if no usable data” arises from it, Sandia LDRD researcher and University of New Mexico Distinguished Professor, Jeff Brinker, views LDRD project risk in the context of the more-global sphere of scientific knowledge, rather than solely in the narrower terms of project milestones. “Whatever outcome you get might be more interesting than the initial idea,” Brinker opines, and his seminal research in the field of novel extracellular environments is quite consonant with one of the characteristics of high-risk research, namely the serendipitous discoveries that can often occur when a scientist carries out investigations at a leading-edge, where the probability of an anticipated result is low, but as Brinker opines, the probability of finding out something interesting can be quite high. “You’d have to fall over yourself to not find something interesting,” Brinker frames it.

Brinker regards LDRD as a key mechanism to pursue truly leading-edge science, supporting ideas that have never been pursued before. But he also perceives it as flexible with respect to mitigating risk, allowing creative responses to mid-stream “failures,” what Brinker terms “corrections in direction.” In his own case, he perceives himself as having taken a major risk to have turned his novel materials research toward life science, mandating him to engage new communities of researchers without the benefit of a deep background in biology.

In the bodies of plants and animals, living cells tend to reside in a variety of environments, some chamber-like, as per the cellulose wall of plant cells, and the maze-like corridors of lymph-nodes, where white blood cells “hang-out” when not circulating in blood or crawling toward bacteria in tissues. Each of these chambers constitutes

a biological microenvironment, and each is specialized as a dynamic, actively remodeled locale that predispose certain types of signaling and signal reception and response. Since microenvironment is known to affect cellular responses, a logical “what-if” question posed but never thoroughly investigated is the following: “what if we could create artificial microenvironments for living cells? How could we thereby modulate and exploit their behaviors?”



**Nanostructured glass matrix that provides complete physical and chemical isolation of cells**

Aside from what might be envisioned as futuristic applications, implicit in pursuing the answer to these questions is the risk of conducting research in unknown territory. This activity, unique in biochemistry research clearly stands poised at the brink of a novel subfield of science, that of creating environments to

*“You’d have to fall over yourself to not find something interesting.”*

tease desired behaviors from living cells. Such research is manna for Jeff Brinker, who has always thrived on the unknown, his many incursions into the science of novel materials

having generated over twenty patents during his career.

In this instance, Brinker began with the hypothesis — a somewhat naïve one, by his own admission — that he could use novel microenvironments to manipulate cellular behavior. But a single-celled bacterium proved “smarter” than its investigator by actively reshaping and modifying its environment.

To a scientist like Brinker, this behavior was hardly a failed initiative, but rather represented an even more interesting fundamental challenge for investigation, a serendipitous discovery that mandated inquiry into its mechanisms and manifestations, which have paid off in medically relevant discoveries.

Ultimately, his project results have potentially redefined a phenomenon in the pathogenesis of bacterial diseases

known as quorum sensing, whereby the assumption is made that a critical population of bacteria (a so-called “quorum”) must be present to initiate virulence in bacteria such as multiply resistant staphylococcus aureus (MRSA), the cause of many dangerous and lethal hospital-acquired infections. Brinker’s results, suggesting that a single bacterial cell may be able to genetically reprogram itself to pathological virulence portends a potential shift in the medical-microbiological community’s approach to combating such infections. His research team has also begun to approach strategies to block the bacterial cell’s genetic reprogramming, molecular therapies more-specific than the usually administered antibiotics that tend to kill extremely important and beneficial digestive system bacteria along with the pathogenic ones (and which by acting

as a selective force in bacterial evolution have ultimately led to bacteria resistant to nearly all known antibiotic drugs). Thus, the findings from Brinker's high risk LDRD research show promise for addressing both a scientific frontier and Sandia's bioprotection mission in advancing the understanding of both microorganisms and the human cells that they sometimes attack.■

## Phenomenal Expertise

With the possible exception of DARPA whose defense-oriented work led, somewhat fortuitously, to civilian GPS devices, Troy Olsson perceives the research investment in the intelligence community — where his work has applicability — to be focused predominately in the short term, six months to one year, with little interest in longer-term investments. In light of this observation, he is firm in his disagreement with the premise that the type of research funded by LDRD would ultimately be pursued elsewhere, seeing little evidence that such would be the case in his research arena.

In discussing risk and its management, Olsson also reflects on what he perceives as a reluctance to report failures, a trend he sees as quite different from the scientific research of fifty years ago, when researchers were, in Olsson's view, more apt to publish both their failures and their successes. In that vein, he perceives an importance to "being upfront" about technical risks with whatever agency is funding his research; were he to accomplish a more-limited set of originally stated objectives as a consequence of that risk, at least his sponsors would have been forewarned to a certain extent.

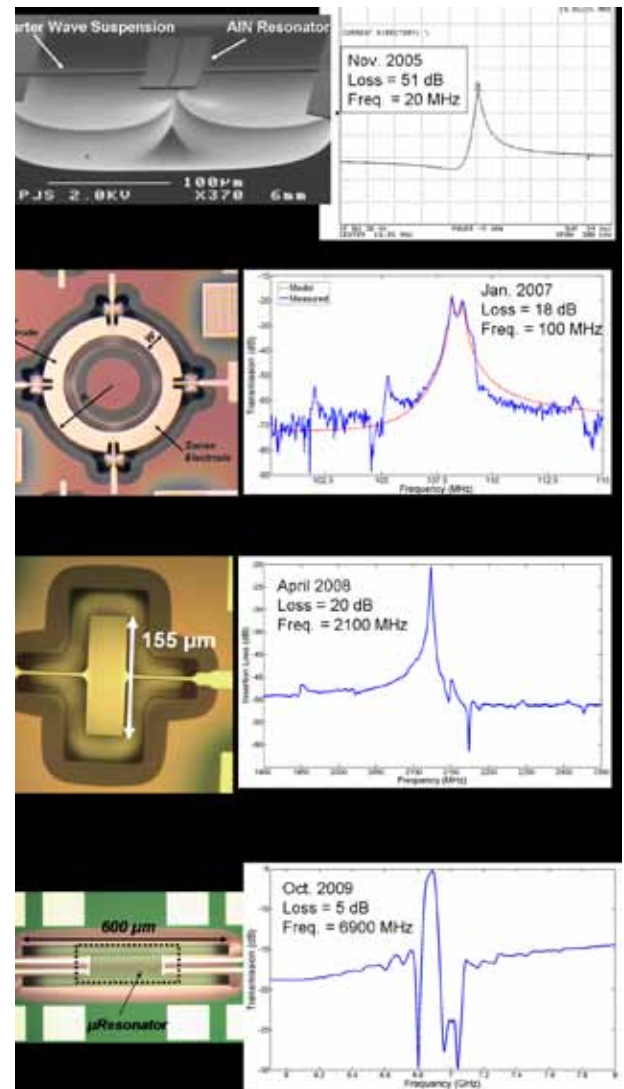
Olsson's LDRD effort proposed the development of methods for fabricating microresonators with low impedance and high-Q, from 10 MHz to 2 GHz. With the number of high-Q components in traditional radios limited by size constraints, this project has opened-up possibilities for new transceiver architectures that derive performance and security advantages from numerous miniature high-Q microelectromechanical system (MEMS) components that can be incorporated into such novel architectures as banks of high-Q MEMS filters and resonators. Miniature MEMS oscillators that are immune to vibration and shock and are

less than 2  $\mu\text{m}$  thick have also been designed and characterized and shock tested at >10000 G. MEMS resonators offer several advantages over traditional filtering approaches, such as smaller size, lower power consumption, and most importantly, integration with complementary metal oxide semiconductor (CMOS) circuitry. In traditional radio architectures, the number of high-Q filter and oscillator elements is limited by board space and interconnects. By incorporating MEMS resonators directly on top of standard CMOS, many high-Q resonators are now available to the radio designer without a size or cost penalty. This enables new radio architectures having desirable properties for military applications, such as very fast frequency hopping rates, low power consumption, and very small size. Such characteristics are also beneficial for crucial military radio characteristics such as low probability of intercept (LPI) and low probability of detect (LPD). Additionally, MEMS resonator-based radios should be more high-G shock tolerant, enabling radios in weapons and explosives.

In civilian applications, the use of MEMS resonators in RF circuits allows for highly integrated, low-power, frequency-agile radios. These radios can improve communications in an urban environment with frequency-selective fading. The transmitter could transmit a signal on several channels and the receiver could select the best channel. This could be communicated back to the transmitter and the radio could dwell there until the channel conditions change. This, in conjunction with other radio architecture changes, would make a robust, high-throughput radio in difficult urban conditions.

Olsson's LDRD proposal was preceded by preliminary investigations to demonstrate not only feasibility, but also applicability, that is, that the idea's value to its target community was worthwhile enough to merit further LDRD investment for development. With the value of a small footprint multispectral analyzer affirmed, Olsson had a plan for the technology's realization,

but lacked the materials and the technology to develop it. Initially, the project's dual focus on shock-hardening and gigahertz filter development was turned more toward the latter aspect, when Olsson's colleagues, his "sounding-boards" at



**Progressive improvements in microresonator design and performance from 2005 through 2009.**

Sandia, apprised him of the large interest in gigahertz filters.

But the fabrication required a novel process, which did not behave as expected, and this material-process development turned out, as he had predicted, to be a major failure risk.

This required a stepping back and re-analysis, examining the material by scanning electron microscopy and revisiting the device modeling. This local “failure” amounted solely to a temporary roadblock, as the team was able to retool the device-fabrication process, which included both etching and metal-sputtering. “We couldn’t have done it without MESA (Sandia’s Microsystems and Engineering Sciences Applications facility),” Olsson emphasizes. “It’s phenomenal to have expertise in the staff that support this [processing] equipment.”

Olsson’s sounding-boards at Sandia turned out to be prescient, given the follow-on funding that this work has received from Rockwell Collins and DARPA. More significant, however, is his commentary about his willingness to go forward with the risks that he knew were implicit in the project, and which did, indeed, manifest during fabrication. “I would never sign-up to do this for a WFO customer,” Olsson admits, his reasoning being that “failing at an LDRD project does not stain Sandia’s reputation.” With a customer, if I tell them I can deliver, I’m 100% sure.” These admissions clearly reaffirm his perception of the risk entailed in this project, the notion that failure was a definite possibility, and that it was only LDRD’s mission to fund such risky research that allowed him to propose it.

Meanwhile, in the midst of his WFO work, Olsson keeps his ears open for what he characterizes as “seeds for future LDRD proposals,” listening to the “dream technologies” of coworkers and customers. His desire to translate the realm of the imaginable to the realm of the possible continues to fuel his initiatives toward science and engineering at the leading edge.

“When this project began, it was an incredible risk to think that MEMS resonators could be scaled to GHz frequencies with impedances that were low enough to match to standard RF circuitry,” Olsson recalled. Sandia has now scaled MEMS resonator technology to 2.1

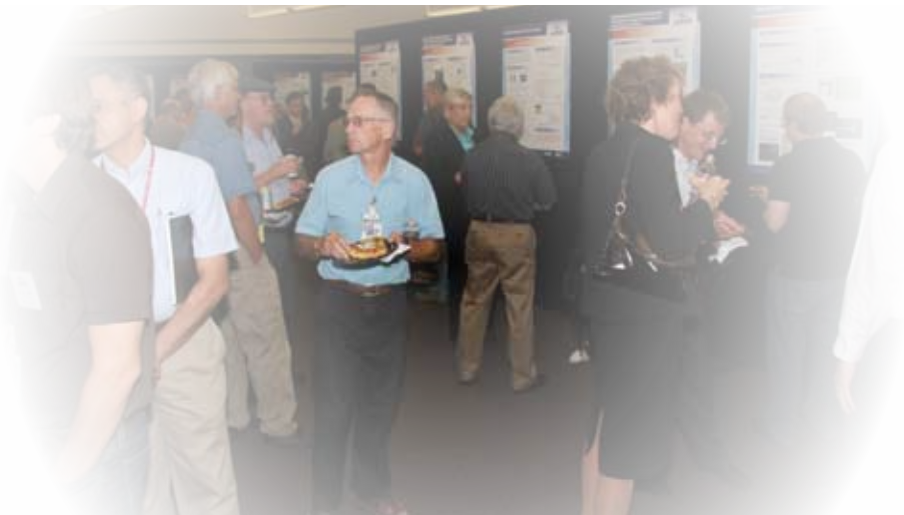
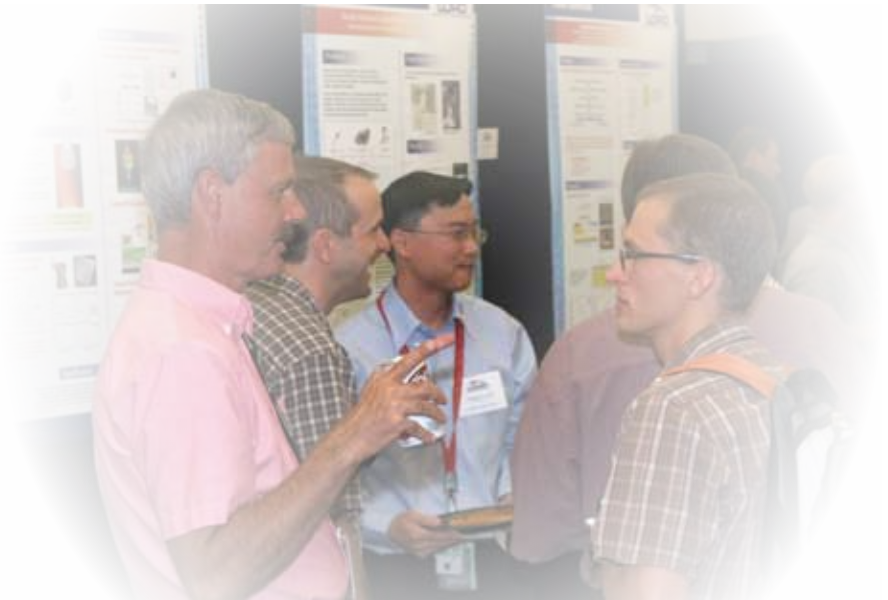
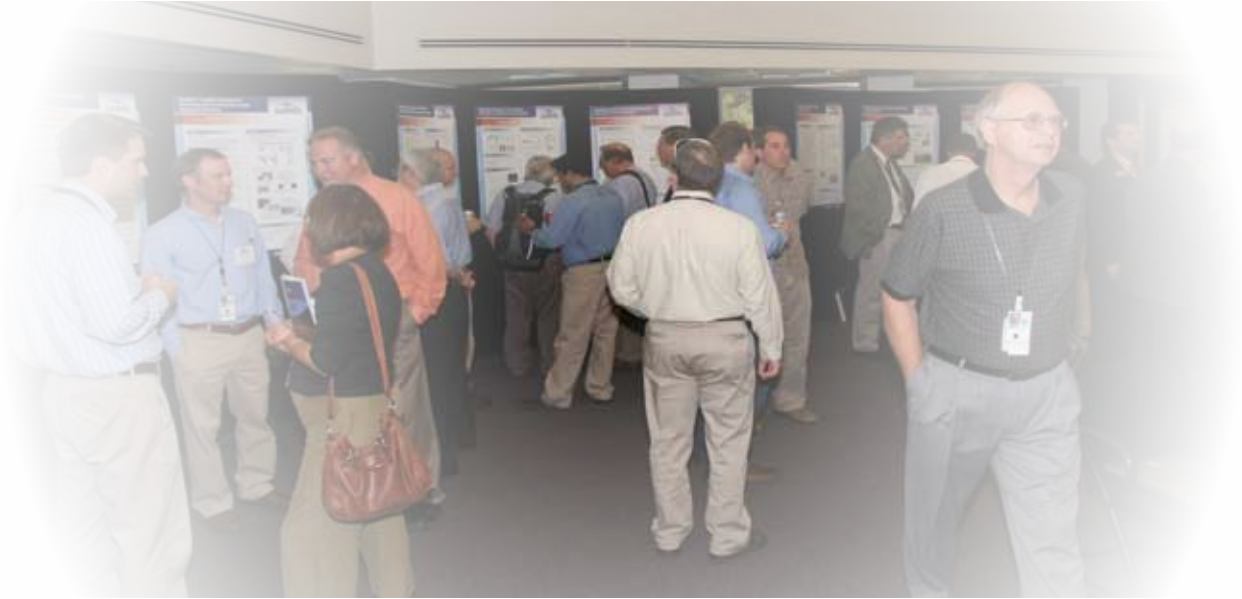
GHz (even higher in a follow-on project) with impedances that can be easily matched to antennas or RF circuits. “Because of our ability to scale resonator frequency while maintaining high-Q and low impedance, our filters now out-perform even surface acoustic wave filters while occupying one one-hundredth the area.” Olsson remarks.■

*“to translate the realm of the imaginable to the realm of the possible”*

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