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**Title:** Laboratory Directed Research & Development: Investing in the future of Los Alamos Objectives and Strategic Planning

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**LABORATORY DIRECTED RESEARCH & DEVELOPMENT:  
INVESTING IN THE FUTURE OF LOS ALAMOS OBJECTIVES  
AND STRATEGIC PLANNING**

**(LA-UR-11- )**

*William Priedhorsky*

*Laboratory Directed Research & Development Program Office*

*Los Alamos National Laboratory*

Presentation at LANS Functional Management Review of LANL LDRD Program

Los Alamos NM

August 17, 2011

**ABSTRACT**

LDRD is a program that invests in the future of Los Alamos by funding competitive, cutting edge work. Its objectives are to build technical capabilities and explore new mission solutions. LDRD funds projects across the breadth of the Laboratory, and is selected by peer review, using panels that draw from the breadth of the Lab. Projects more often than not benefit multiple missions. The Grand Challenges for the biggest projects, Directed Research, address the Laboratory's missions of Nuclear, Energy, and Global Security. Grand Challenges are updated annually. Some represent well-developed Lab strategy and attract a healthy number of proposals, while others require a clearer strategy and better Lab-wide participation.

We discuss the detail of the selection process. Service on LDRD committees is a unique opportunity to understand the breadth of science and technology at the Laboratory. We have evidence that the LDRD process successfully incorporates the strategic priorities of the divisions, and that peer review identifies the most successful projects, based on their eventual outcomes. Annual project appraisals ensure the quality, performance, relevance, and leadership of LDRD work. On the average, LDRD projects are rated Excellent to Outstanding. A few projects are managed technically by LANL Centers; these projects are consistently ranked highly by external reviews. LDRD postdoc projects (PRDs) attract a cadre of young researchers of high and increasing quality. A new Early Career program component invests in scientific leadership on the part of our newest staff members. LDRD researchers are distributed across the career ladder. Quantitative metrics of LDRD outcomes, such as R&D 100 awards, publications, patents, citations, follow-on funding, and external collaborators, show that the program has great success in building capability and exploring new missions solutions.

*This work was carried out under the auspices of the National Nuclear Security Administration of the U.S. Department of Energy at Los Alamos National Laboratory under Contract No. DE-AC52-06NA25396.*





## Laboratory Directed Research & Development: Investing in the future of Los Alamos Objectives and Strategic Planning

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W. Friedhorsky  
LDRD Program Director  
Los Alamos National Laboratory  
August 16, 2011

## Innovation for our Nation

LDRD is a competitive program by which Congress authorizes the Laboratory to invest up to 8% of its budget in research that is highly innovative and vital to our national interests.



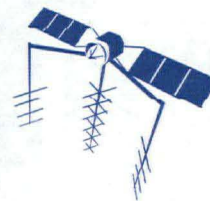
**ENERGY SECURITY**

**NUCLEAR SECURITY**

**GLOBAL SECURITY**



**SCIENTIFIC DISCOVERY**





## LDRD is Defined by Legislative Mandate and DOE Order

- The objectives of the LDRD program are to—
  - maintain the scientific and technical vitality of the laboratories;
  - enhance the laboratories' ability to address future DOE/NNSA missions;
  - foster creativity and stimulate exploration of forefront science and technology;
  - serve as a proving ground for new concepts in research and development; and
  - high-risk, potentially high-value research and development
 (DOE Order 413.2b)
- In other words, build capability and explore new mission solutions
- Hence the objectives of this Functional Management Assessment:
 

**Assess our technical quality and mission impact**

## Other Aspects of LDRD from Federal Guidance

- LDRD is not program development: "LDRD means research and development work of a creative and innovative nature ... for the purpose of maintaining the vitality of the laboratory in defense-related scientific disciplines." (Defense Authorization Act, 1991)
- LDRD funds cannot mix with program funds: "LDRD funds may not be used to: (1) Substitute for or increase funding for any tasks for which a specific limitation has been established by Congress or the Department, or for any specific tasks that are funded by DOE or other users of the laboratory; (2) fund projects that will require the addition of non-LDRD funds to accomplish the technical goals of the LDRD project, except as provided by legislation" (DOE Order 413.2b)
- LDRD PIs must be "permanent" staff: "the director of a laboratory or center involved [shall] form an internal review mechanism for determining which employee-suggested projects merit funding." (Energy Act, 1977)



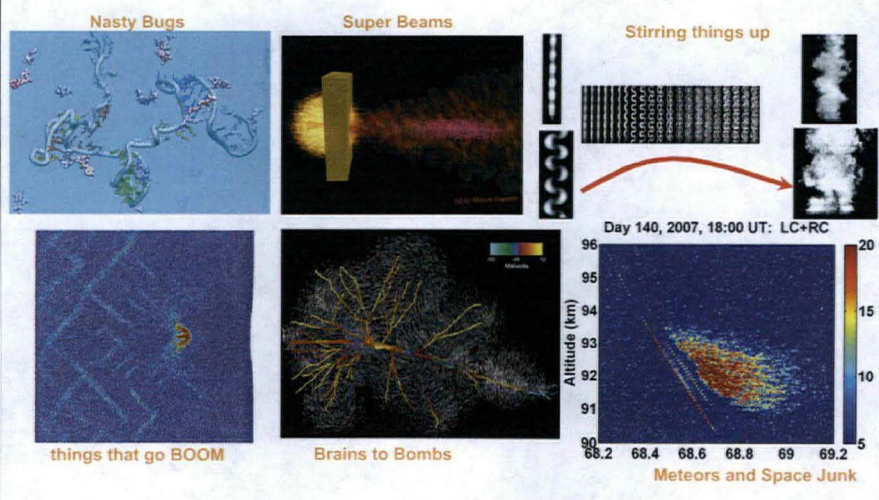
## LDRD Supports laboratory missions

Every LDRD project has a clear connection to one or more Laboratory mission.



## A few selected highlights

Technical breadth ... exciting spin-offs

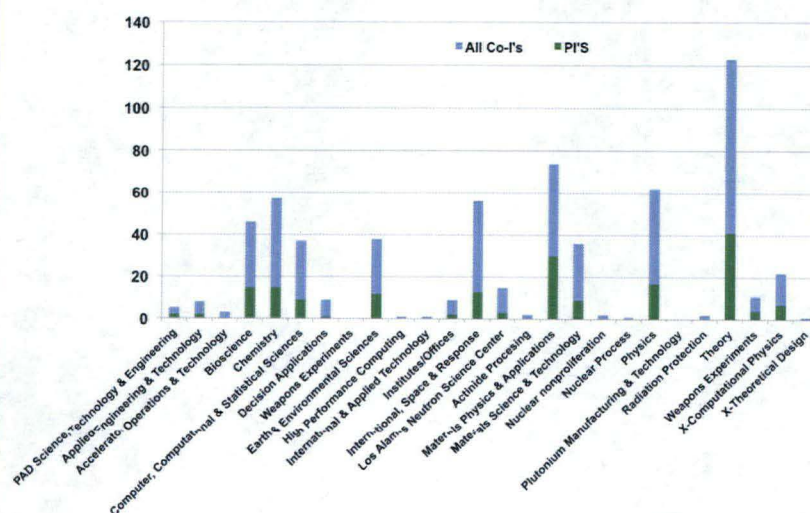




## LDRD selects for excellence

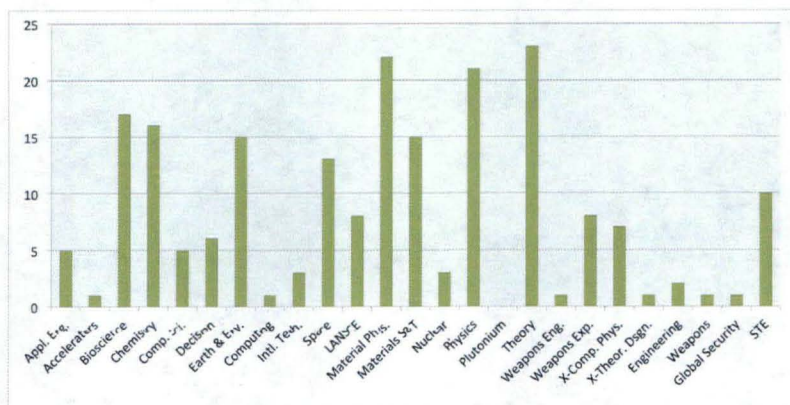
- Selection processes follow best practices established by NSF and NIH
- Senior Laboratory leadership sets S&T priorities
- LDRD opens a fair and open competition for ideas across the breadth of the Laboratory
- Line managers and staff across the Laboratory's technical divisions participate
- LDRD managers often serve on Federal agency proposal selections

## LDRD is executed across the breadth of the Lab





## An open market for ideas, driven by mission



Technical staff across the Laboratory serve on selection panels.

## Structure of the LDRD program

- **Directed Research (DR), \$79.6M**
  - Projects with a multidisciplinary approach to hard problems
- **Exploratory Research (ER), \$44.1M**
  - Basic and applied research projects directly from the staff
- **Postdoctoral Research & Development (PRD), \$9.2M**
  - Innovative projects to attract highly sought-after postdoctoral fellows
- **Early Career \$4M**
  - Developing emerging scientific leadership
- **Reserve, \$5.2M**
  - Flexibility to address emerging mission opportunities

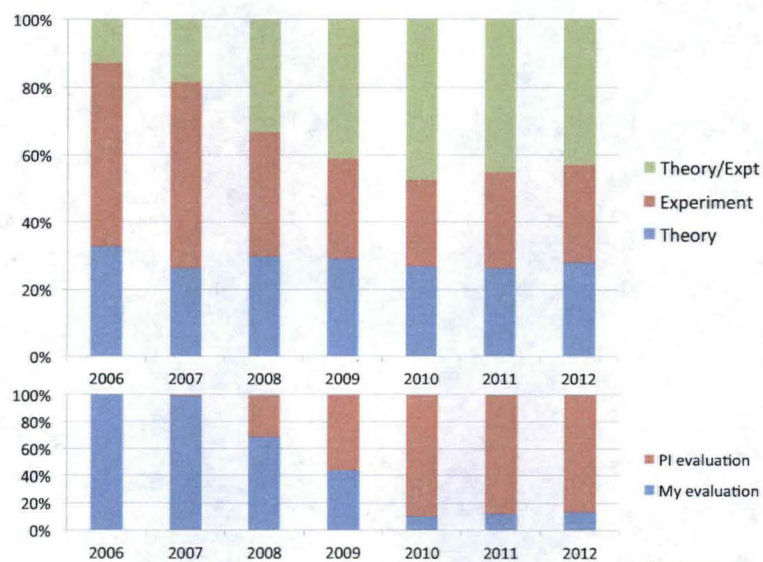
FY12 total \$142.1M



## Outcomes by Component

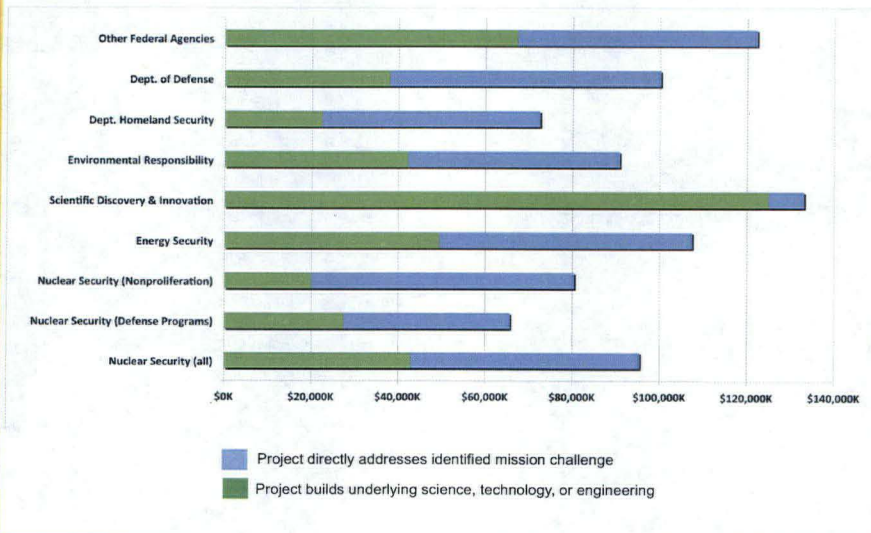
LDRD Component	2010 budget (mid-year)	2009 publications	Follow-on funding for 2009 projects
DR (regular)	52.2%	35.5%	54%
DR (centers)	4.4%	12.3%	
ER (regular)	31.0%	33.4%	39%
ER (reserve)	3.5%	0.2%	
Postdoctoral (PRD)	7.8%	18.5%	7%
Early Career	1.1%	—	—

## Experiment/Theory Balance

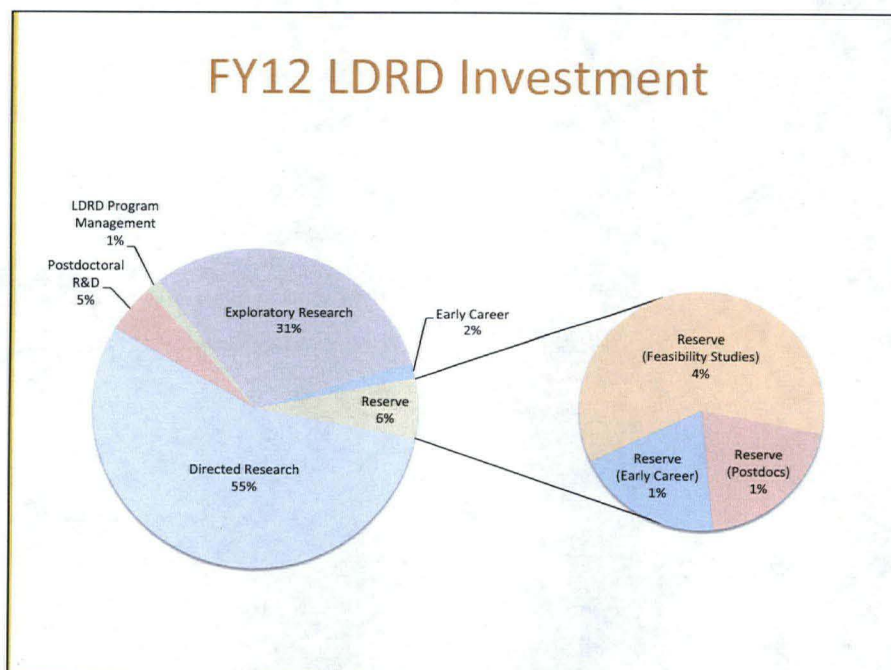




## FY12 Impact on DOE Missions



## FY12 LDRD Investment

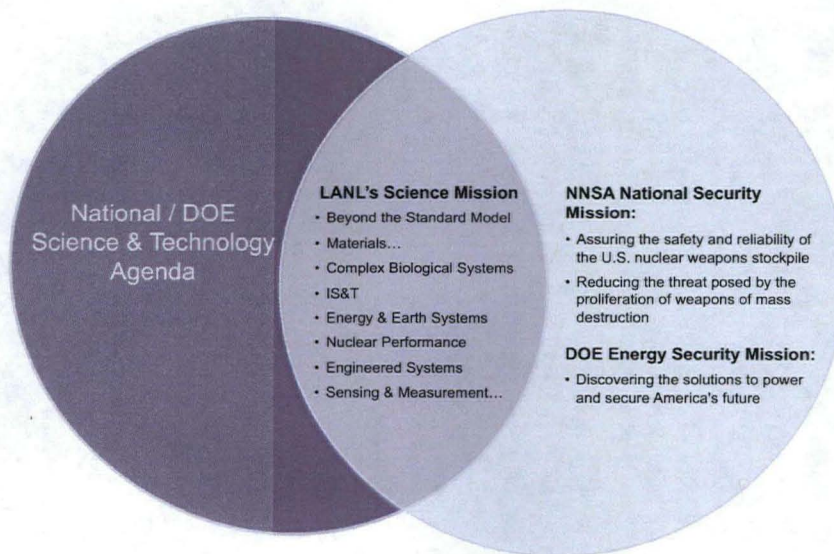




## Directed Research Grand Challenges

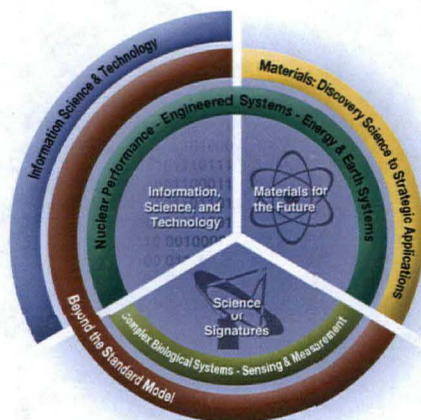
Directed Research Grand Challenges	Mission Impact
Beyond the Standard Model	Sensitive instrumentation and tools to manipulate massive data volumes, in support of national security missions
Materials: Discovery Science to Strategic Applications	Energy sources, efficiency and storage; sensing for threat reduction; materials underpinnings of stockpile security
Complex Biological Systems	Energy, national security, health and the environment
Information Science and Technology	Overarching capability supporting all Laboratory missions
Earth and Energy Systems	Energy and climate security
Nuclear Performance	Stockpile safety, surety and reliability
Sensing and Measurement Science for Global Security	Nuclear weapons of mass destruction, space situational awareness, global environmental treaty monitoring and emerging threats
Engineered Systems	Systems-level solutions for all missions

## Why these Grand Challenges?



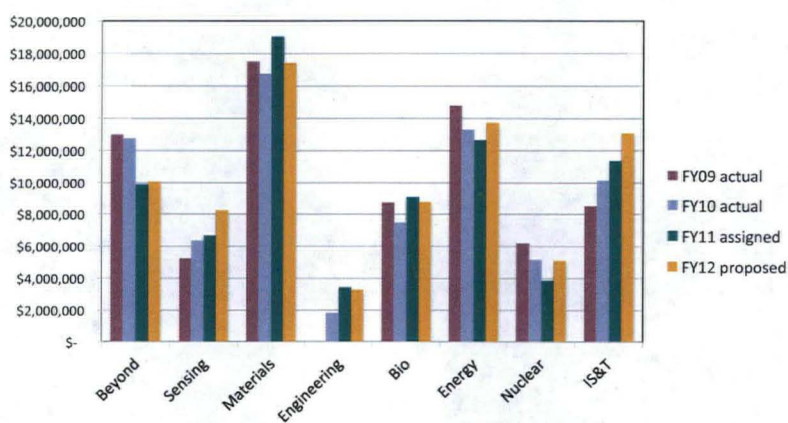


## Grand Challenges articulate Laboratory S&T strategy



Priorities within the Grand Challenges are informed by national R&D priorities, such as those of the Office of Science.

## Investment in Grand Challenges



Investment in the Grand Challenges FY09-12



## Coordinators work Lab-wide to update Grand Challenges annually



Drawing on Lab strategies, e.g. materials

## Grand Challenges Articulated in Strategic Investment Plan

### FY12 LDRD Strategic Investment Plan

W. Priedhorsky, F. Alexander, C. Barnes, S. Buelow, H. Hahn, D. Haynes, E. McKigney, A. Perelson, D. Rej, J. Sarrao  
version 3 January 2011\*

Laboratory Directed Research and Development (LDRD) at Los Alamos is the basis for science and technology excellence for the Laboratory, and builds capabilities for future mission challenges. This document sets out science and technology investment priorities for FY12 LDRD/Directed Research (DR) new starts. It behooves LDRD/DR proposers to clearly explain how their proposed R&D supports these S&T priorities, and will impact one or more Los Alamos missions.

*Open door for innovation:* That said, the LDRD process remains open to extraordinary, transformative initiatives in any area that supports the Laboratory mission, broadly interpreted. (Pre)proposals should reference the Grand Challenge that most closely applies, and make the case for their special scientific and strategic importance if they go significantly beyond the priorities of this plan.

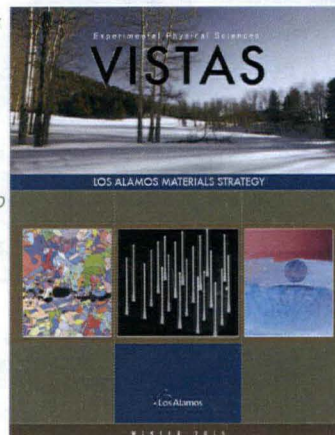


## Materials Grand Challenge draws on carefully developed Lab strategy

*"Central to the Grand Challenge in Materials is the vision of controlled functionality through discovery and application of fundamental materials properties and materials synthesis and fabrication techniques, reaching from the molecular level, through nano- to microscopic scales, to bulk material."*

Three central themes:

- Defects and Interfaces
- Extreme Environments
- Emergent Phenomena



## Sample Project: Extreme Environments Materials Grand Challenge

**Defects and Interfaces thrust:** the mechanistic multi-scale understanding and control of inhomogeneities, intrinsic and engineered, across all appropriate length and time scales that govern materials functionality



Simulation



Experiment



A sapphire flyer plate incident on copper, leading to material porosity and damage.

**Project:** Isolating the Influence of Kinetic and Spatial Effects on Dynamic Damage Evolution

D. Dennis-Koller (WX-9) PI,  
E. Cerreta (MST-8), Co-PI

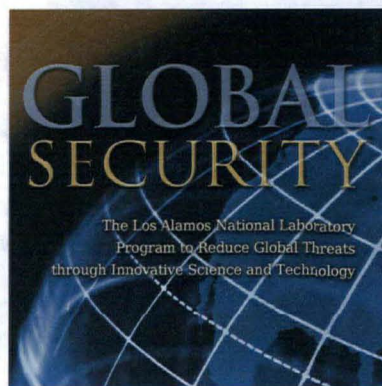


## Sensing and Measurement G.C. articulates mission challenges

*Definition: Develop sensing and measurement science to facilitate accurate and robust analysis and interpretation of national security threats.*

### Four FY12 priorities:

- Nuclear Threats
- Space Situational Awareness
- Treaty Monitoring & Verification
- Counterterrorism and Warfighter Support



## Sample Project: Space Situational Awareness Sensing and Measurement Grand Challenge

### Space Situational Awareness thrust:

- Understanding, assessing, quantifying, and predicting natural and man-made threats to the U.S. space infrastructure
- Signature science and exploitation for identification, analysis, assessment, tracking, and visualization of space systems and associated infrastructure
- New measurement science for exquisite visualization, characterization, and assessment of the space environment and space objects

**Project:** Combining point-measurements in space with a novel data-assimilative model (DREAM) to enable accurate estimates of the natural and artificial trapped energetic particle environment anywhere in near-Earth space.



### Beta-Version of Real-Time Data Assimilation

**Project:** DREAM - A Dynamic Radiation Environment Assimilation Model to Understand Acceleration, Transport, and Losses in Natural and HANE-Produced Radiation Belts

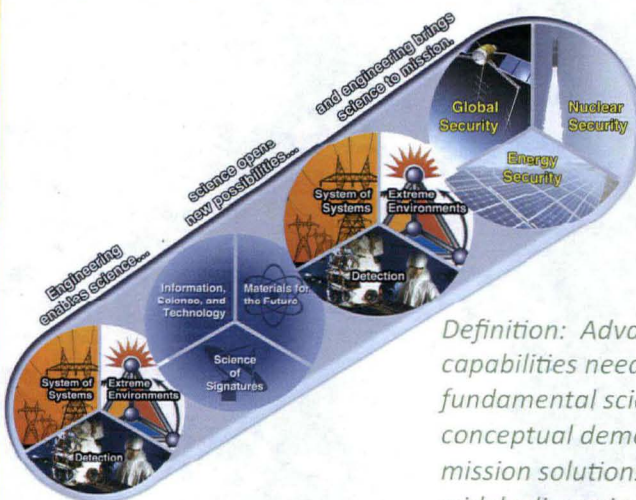
Geoff Reeves (ISR-1), PI



## LDRD is a metric of technical health

- **DR: Sensing & Measurement for Global Security**
  - FY10: 14 (2 funded) pre-proposals of 94 total (6 finalists)
  - FY11: 12 (2) pre-proposals of 78 total (3 finalists)
  - FY12: 8 (1) pre-proposals of 93 total (2 finalists)
- **ER: Measurement Science, Instrumentation, & Diagnostics**
  - FY11 27 (3) proposals
  - FY12 41 (4) proposals
- **Special Science of Signatures Reserve FY11**
  - 58 (8) proposals
  - More than materials in extremes (47)!

## Engineering Grand Challenge: Capability need clear, but LDRD approach?



*Definition: Advance the capabilities needed to move from fundamental science concepts and conceptual demonstrations to mission solutions that can be widely disseminated and applied*



### Sample project: Detection, measurement, characterization and attribution Engineered Systems Grand Challenge

**Thrust:** ...engineered infrastructure for detection, measurement, characterization, and attribution, including nuclear, chemical, and biological problems. Engineering contributions to these solutions include e.g. sensor networks, small satellites, and compact accelerators.

Wind power currently costs twice as much as electricity generated by burning coal. Anticipating turbine failure is key to increasing turbine efficiency.



**Project:** Intelligent Wind Turbines  
Curtt Ammerman (AET-1), PI



### Engineering Challenge Still Not Gelled

- ER category attracts numerous proposals
- DR: *Engineered Systems*
  - *Quantity up*
  - *Success rate down*

	Pre-proposals	Full Proposals	Projects
FY10	5	2	1
FY11	4	2	1
FY12	16!	4	0

- Are LDRD criteria and processes right for engineering projects?
- Are we attracting the best from our creative engineers?
- How do we identify innovation for an engineering project?

*Your advice welcomed*



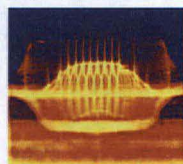
## Nuclear Performance Grand Challenge

*Definition: ...radically change the present manner in which experimental data, combined with theory, modeling, and simulation, are used to inform stockpile decisions.*

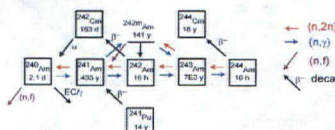
### Five FY12 thrusts:

- Scientific basis for surrogacy and scaling
- Boost (nonlinear fusion/fission interaction)
- Prediction and control of materials properties and behavior
- Evaluation of foreign threats and technological surprise
- Advanced physics models

Strong proposals, 2 selected, turnaround from disappointing FY11 response



**Ejecta and Richtmyer-Meshkov instability in explosively-driven metal**



**LDRD measurements and theory reduced uncertainties from >20% to <5%**

### Fruits of past LDRD:

Proton Radiography  
Americium cross-sections for diagnostics

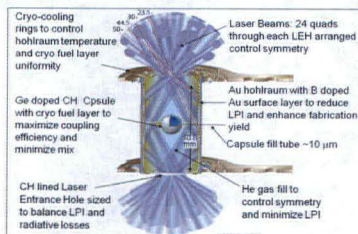
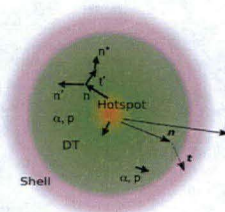
## Sample project: Co-mingled physics (boost) Nuclear Performance Grand Challenge

**Thrust:** Providing understanding of the complicated co-mingled physics of *boost*, and learning how to get the right answer for the right reasons.

One of the most challenging problems in high-energy-density physics is the calculation of turbulent mixing in compressible and converging flows with thermonuclear (TN) energy release, as in Inertial Confinement Fusion (ICF) capsules.

**Project:** Hydrodynamical Mix Studies at the National Ignition Facility (U)

M. Steinkamp (XCP-2), PI



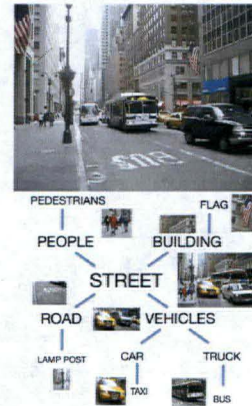


## Information Science and Technology Grand Challenge has matured rapidly

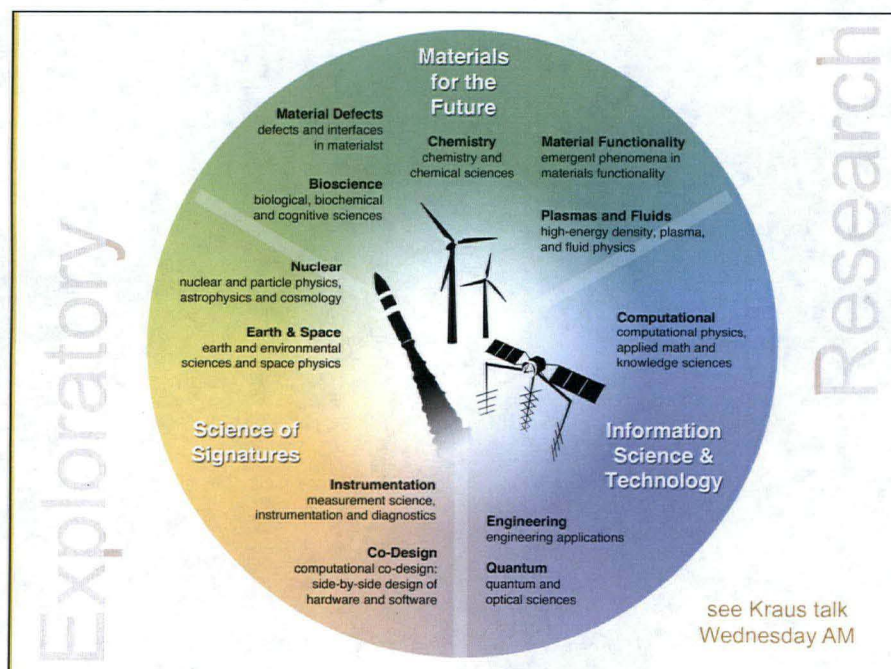
*Definition: ...the development of breakthrough mathematics, computer science, and underlying technologies required to extract information, knowledge, and insight from data.*

### Three FY12 Priorities:

- **Intelligent Data Acquisition, Management, and Analysis**
  - Knowledge extraction, Automated discovery, Interactive analysis, Active learning, Distributed computing, Anomaly detection, Data mining, Data lifecycle management, Compressive sensing, Semi-supervised learning, Smart Sensors
- **Computational Co-Design**
- **Quantum Information Science**



FY12 new start: Hierarchical Sparse Models for Robust Analysis of Video Data  
S. Brumby (ISR-2), PI





## ER Categories

ER Technical Categories contribute to current and future missions in global, energy, and nuclear security.

- Biological, Biochemical & Cognitive Sciences (BBC)
- Chemistry & Chemical Sciences (CHEM)
- Computational Physics, Applied Math & Knowledge Sciences (CAK)
- Defects & Interfaces in Materials (DIM)
- Earth & Environmental Sciences & Space Physics (EES)
- Emergent Phenomena in Materials Functionality (EPM)
- Engineering Applications (ENG)
- High-energy Density, Plasma & Fluid Dynamics (HPF)
- Measurement Science, Instrumentation & Diagnostics (MID)
- Nuclear & Particle Physics, Astrophysics & Cosmology (NPAC)
- Quantum & Optical Science (QOS)



**Laboratory Directed Research & Development:**  
**Investing in the future of Los Alamos**  
**Selection & Appraisals, Metrics & Outcomes,**  
**Reserve & Early Career**

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W. Friedhorsky  
LDRD Program Director  
Los Alamos National Laboratory  
August 16, 2011



## DR Selection Process

- Two-phase proposal process
  - Phase one: call for pre-proposals
  - Phase two: directed call for full proposals
- Science Advisory Board and Strategy Team help make proposal selections
- Recommendations are made to the Laboratory Director for final selection
- DR projects are funded at \$1.5M-\$2.0M/year for 3 years

## Standardized Scoring

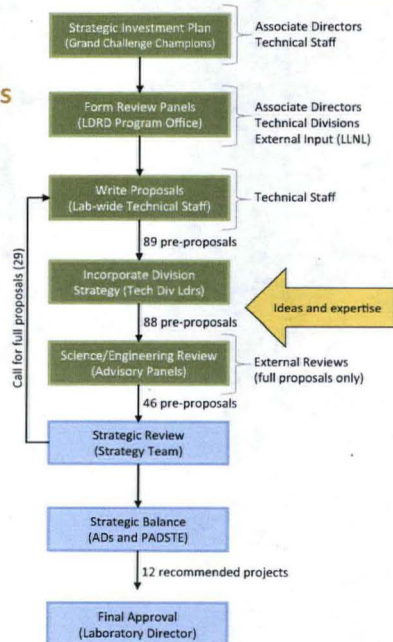
- Benefits of standardized scoring
  - Proposals from multiple subcommittees can be compared on fairer grounds
  - Proposals received out-of-cycle (Reserve) can be compared to proposals received in annual cycle
  - More ethically robust
- A 1-5 scale with clearly defined standards was established for FY11



## Proposal Scoring Table

Score	Overall	Innovation - 30%	Impact on mission and/or technical field 25%
5.0	Outstanding in all respects, failure to support would be a technical and/or strategic mistake. Essentially a perfect proposal.	Proposal articulates a fundamental intellectual advance and/or a fundamentally new approach to expanding our knowledge or understanding.	Potential for revolutionary impact on mission, a technical field, and/or a method/approach.
4.5	Excellent with only minor technical or strategic weaknesses, deserves highest priority for support. Some lack of detail acceptable.	Highly innovative, conceptually intriguing, surprising in its insight. "I wish I'd thought of that."	Potential for major impact on mission and technical field, with broad and important applications. Targets an important advance. Likely to place LANL at the forefront of the field and lead to publication in leading multidisciplinary journals (Science, Nature).
4.0	High quality in nearly all respects, should be supported if at all possible. Identifiable, though non-critical weaknesses may be present.	Innovation major if not stunning. Clearly differentiation of proposed work from past work in the field.	Addresses important problems for mission and technical field. Impact should be important. Potential to publish in leading multidisciplinary journals, likelihood of publication in leading journals in the field such as Phys. Rev. or JACS.
3.5	Very good proposal with important objectives. Proposal may concentrate on technique rather than underlying issues.	Work may need to be distinguished more clearly from previous efforts. Innovation less than striking, with some tendency towards incremental progress.	Potential impact clear but limited. Clear differentiation from previous or competing work may be unconvincing. Only modest potential for publication in leading journals.
3.0	Good proposal that is definitely worthy of support, even given other demands on discretionary Laboratory resources. Scores significantly below are probably not worthy of LDRD. Exposition may lack significant details.	Identifiable innovation, but transformational aspects do not stand out. Largely incremental in expected outcome.	Identifiable impact on mission or field. Exploration of mission solutions or development of capabilities would have a significant impact on LANL programs. Potential for publication in specialized journals.
2.0	Lacking in one or more critical aspects. Innovation and/or impact may be weak or poorly represented. Team or approach does not appear to appreciate challenges involved. Key issues not addressed. Lacks appreciation for major challenges.		Note: Assessment of impact may be downgraded if likelihood of success is low. Potential for publication applies for unclassified work only.
1.0	Serious deficiencies that render the proposal uninteresting (innovation and/or impact) or implausible (team or approach)		

## FY11 DR Selection Process





## Mitigating conflict of interest

- Conflict of interest (COI) is the biggest risk to the credibility of the LDRD proposal review process
- Definition of COI:
  - “COI occurs when an LDRD reviewer has a substantive connection to a proposal or to its author(s), a connection that could generate the perception or the reality that a review panel chair or member might evaluate the proposal on criteria other than those explicitly used in the LDRD process”
- LDRD policy requires declaration of all potential COI

*Conflict can be mitigated, not eliminated*

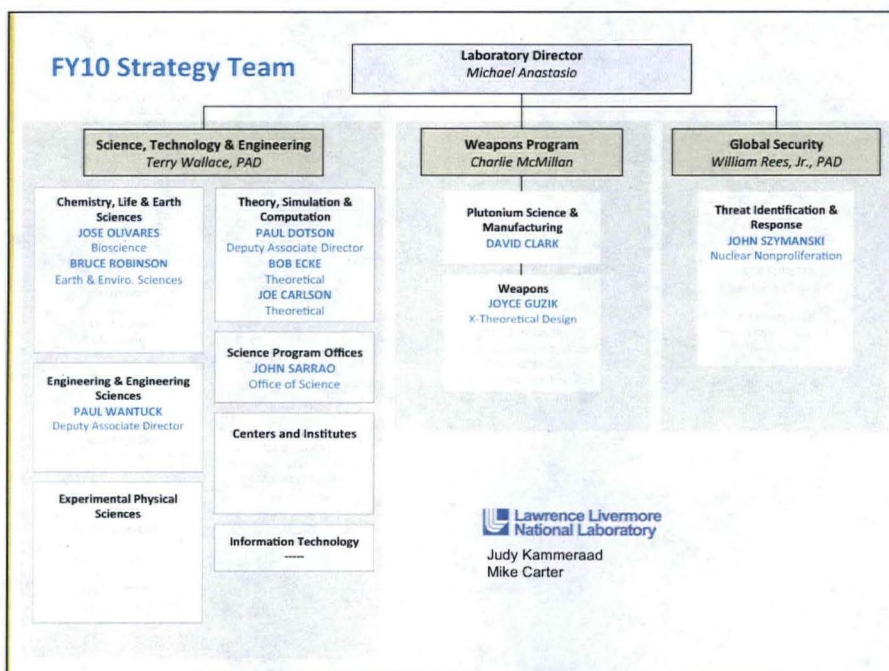
## Scientific/Engineering Advisory Panel

- Correspond to the Grand Challenges
  - One chair and up to 12 members who are at the forefront of their fields
- Conduct preliminary screening and assessment of (pre)proposals according to the following criteria:
  - Innovation and creativity
  - Potential mission impact
  - Viability of the proposed research approach
  - Qualifications of the team and credibility of team leadership

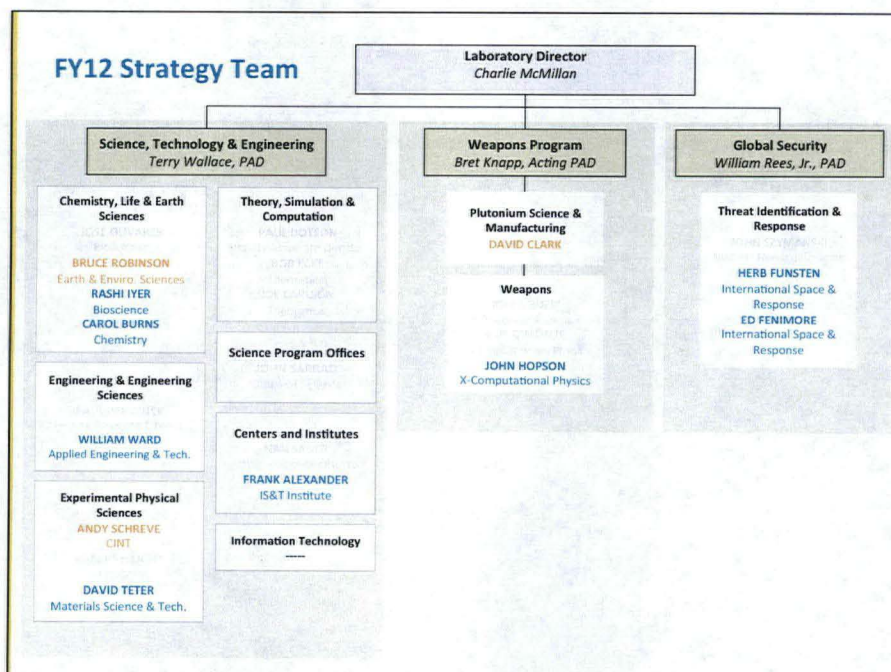


## Strategy Team

- Comprised of 12-13 technical staff who have a broad an integrative view of the Laboratory
- Assesses (pre)proposals based on their potential impact on strategically important issues for the Laboratory
- Emphasizes transformative research









## Where are they now?

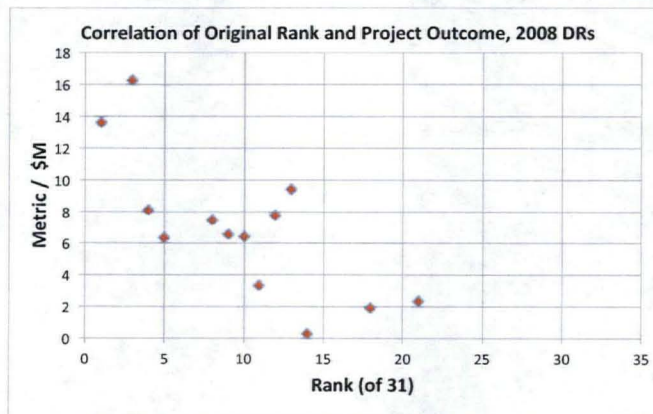
### FY02-04 Strategy Team Members

#### Highlights of their current responsibilities

**Dana Berkeland**, Program Manager at federal agency  
**Tanmoy Bhattacharya**  
**Greg Boebinger**, Director, National High Magnetic Field Lab  
**David Clark**, Director, Seaborg Institute  
**Harry Crissman**, Lab Fellow, retired  
**Maya Gokhale**, Computer Scientist, LLNL  
**Wu-Chun Feng**, Director, Synergy Laboratory, Virginia Tech  
**Michael Fisk**, Cybersecurity Technical Lead, LANL  
**Hans Frauenfelder**, Senior Lab Fellow  
**Herb Funsten**, Chief Scientist, ISR, LANL  
**David Funk**, WX Division Leader, LANL  
**Salman Habib**, in transition to ANL  
**David Janecky**, Deputy Group Leader, Environment Stewardship, LANL  
**Mikkel Johnson**, Lab Fellow, retired  
**Paul Johnson**, Lab Fellow, Acoustical Society of America Fellow  
**Sallie Keller-McNulty**, Dean of Engineering, Rice University  
**Hui Li**, American Physical Society Fellow  
**Tracy Light**, Space and Remote Sensing Team Leader, ISR, LANL

**Ferenc Mezei**, Hungarian Academy of Sciences and Academia Europaea  
**Albert Migliori**, Director, Seaborg Institute  
**Jeremy Mitchell**  
**James Morel**  
**Chris Morris**, Lab Fellow  
**William Parkinson**  
**Alan Perelson**, Lab Fellow  
**William Priedhorsky**, Director, LDRD, LANL  
**Art Ramirez**  
**Gary Resnick**, Bioscience Division Leader, LANL  
**John Sarrao**, Program Director, Office of Sciences  
**Nan Sauer**, Acting Associate Director, CLES, LANL  
**Andrew Shreve**, former acting Director, CINT, LANL  
**Karl Staudhammer**  
**Tom Terwilliger**, Lab Fellow, Biosecurity Center Leader  
**Les Thode**, Lab Fellow, retired  
**Frans Trouw**  
**David Vieira**

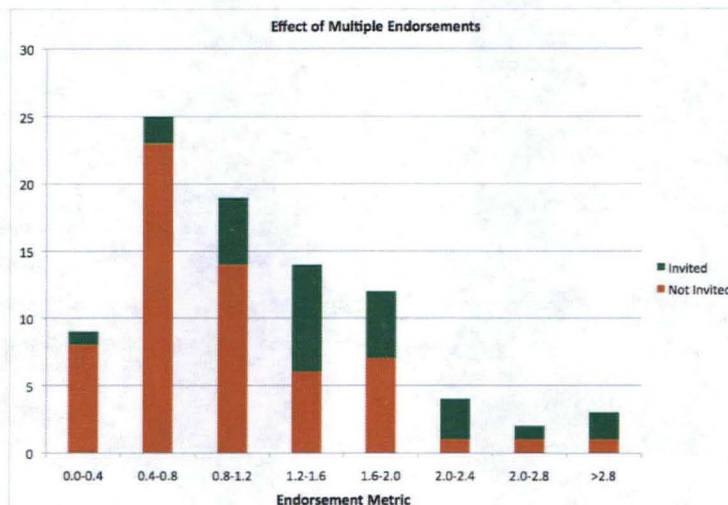
## How good a predictor is peer review?




- Metric is:
  - 2/3 fame (article = 1 pt, class. rept.= 1 pt, conf. proceeding = 0.5 pt, citation = 0.1 pt)
  - 1/3 fortune (follow-on project = 1 pt, major award = 1 pt, invention = 1 pt)
- Based on FY08 DR selections by a 33-person Strategy Team, no SAPs



### Imprint of division strategy: FY12 DR pre-proposals



### External Reviews and Feedback

- The final outcome of the review process is written feedback to the proposers
- A qualitative assessment is entered in 
- Feedback to FY11 DR proposals 100% complete
- Goal of obtaining external reviewers for at least 90% of proposals was almost met
  - Obtained external reviewers for 26/29 proposals (one of the three was classified, one confused by transfer from Computational Co-Design)



## Sample feedback on FY12 proposals

### Strategy Team feedback on funded proposal

The goal of this project is to use a combination of experimental and theoretical approaches to move towards the implementation of electrochemical processes for the reduction of  $N_2$  into  $NH_3$ , and for storing energy in chemical bonds of  $NH_3$ .

This is a strong proposal with a high potential payoff. The proposal makes a compelling case that our existing storage technologies are simply not up to the task, and that a liquid-fuel based system, with its high energy density and (in this case) easy transportability, could offer a transformative solution. They believe this fuel could/should be liquid ammonia generated electrochemically from  $N_2$  and  $H_2O$ . To recover the energy, the  $NH_3$  can be passed through a fuel cell to regenerate  $N_2$  and  $H_2O$ , or even burned in a properly designed internal combustion engine. Currently, however, the best known ways to generate the  $NH_3$  are not efficient enough for this application. They propose to improve the efficiency of its catalytic generation by developing solid proton-conducting electrolyte materials and nitrogen-reducing electrocatalytic materials. They will develop an improved scientific understanding of the key surface processes and the kinetics of the proton diffusion through the electrolyte material.

The large potential payoff is clear, and the credentials in their respective areas of some of the team-members are impressive. Both internal and external reviews were uniformly positive, and indicated that some aspects of the proposal, such as proton-conducting solids are potential game-changers. The proposal was viewed as too risky for industry and therefore well-suited for LANL. The work is clearly innovative, with the opportunity to position LANL for important future roles in energy storage.

## Sample feedback on FY12 proposals

### Strategy Team feedback on unfunded proposal

The impact of an accurate temperature measurement technique in extreme environments is apparent, especially in the context of MaRIE. The proposal is not especially innovative or creative; existing techniques will be tested and calibrated. The proposal feels like a science experiment to more completely understand the various temperature measurement techniques in extreme environments. There does not appear to be much engineering.

Here are some areas that would help clarify the proposal:

1. It would be nice to have a discussion of surface temperature versus bulk temperature in terms of the temperature measurement the various techniques provide in various environments and in terms of what is important to MaRIE.
2. A discussion of the anticipated causes for inaccuracies in each of the measurement techniques would be helpful. Are all three techniques needed? Maybe just two techniques should be evaluated.
3. What is the technical readiness level (TRL) for each of the techniques? What TRL is needed for each of the three questions you plan to tackle? What TRL is available to you currently? What equipment will be needed for the measurement techniques and the testing? What is existing and what needs to be found or procured?
4. A more thorough discussion of the experimental sample and their preparation and why those samples are the best choice for the tests is needed.
5. Although it was not explicitly stated, the early experiments appear to be stable and in environments that span extreme and not extreme. Are conventional temperature techniques (thermocouple, RTD, etc.) going to be used as a means of validation in these environments?
6. The final demonstration requires you to understand the physical phenomena. Will this understanding be material dependent? If so then what materials will you be focusing on and what makes them a good surrogate for future tests? How reliable do you hope to make your predictions,  $\pm 10\%$ ? What is considered success?



## Reserve: Responding to opportunity

- Top priority for Reserve funds
  - Intended to recruit ideas, staff, organizations and missions that do not have a history of LDRD success and lack competitiveness
  - Guided by strategic priorities articulated by senior laboratory management
  - Often attract first-time LDRD proposers (10 of 27 funded Reserve proposals were first-time LDRD PIs in FY10)
  - Reserve projects often result in internal/external follow-on funding (50% of Reserve PIs funded in FY10 resulted received competitive funding next cycle)

## FY11 Reserve increased \$6M mid-FY11

- Rational: Reinforce and respond to strategically critical areas
- Reserve investment is driven by mission needs for innovation in:
  - Materials in extreme conditions
  - Sensing and measurement
  - Sustainable energy
  - Computational Co-design
- Aligned with priorities set forth in the FY11 Strategic Investment Plan



## Special Reserve Calls

- Science and technology to probe and understand materials in extreme conditions (\$3.0 M)
  - 47 proposals, 9 funded
- Science of Signatures (\$1.5M)
  - 93 proposals, 8 funded
- Sustainable energy using LANL as a test bed (\$0.6M)
  - 17 proposals, 8 funded
- Computational Co-design (\$1.2M)
  - 8 proposals, 2 funded at DR scale

## Annual Project Appraisals

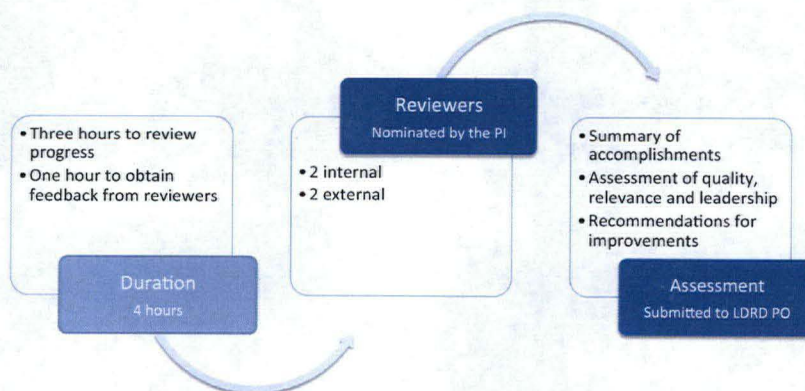
- Objective is to assess progress and provide peer input to help PIs maintain high quality work
- In addition to formal project appraisals, LDRD program managers conduct regular project visits
  - 90 minutes
  - In the PI's lab or office



## Formal DR Project Appraisals

- DR projects appraised annually
- Annual appraisals, with once in three years an intensive evaluation by internal and external reviewers
  - Organized by PIs according to guidance provided by the LDRD Program Director (P.D.)
  - Agenda and committee approved by LDRD P.D.
  - Committee membership not rubberstamped – frequent questions from P.D.

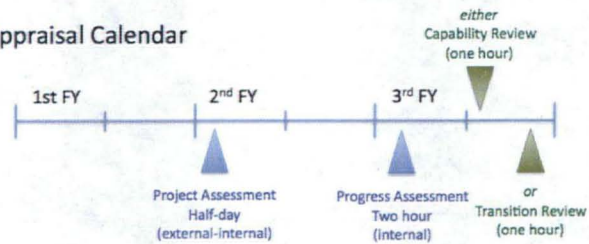
## Formal DR Project Appraisals



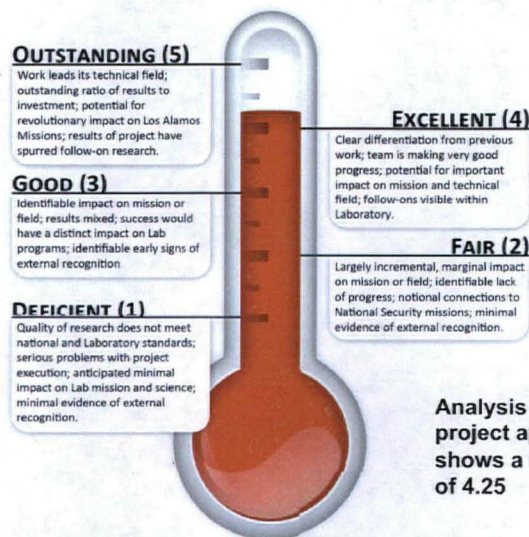


## Appraisal Calendar

### Appraisal Calendar



DR project appraisals average “excellent” to “outstanding” in external appraisals



Analysis of FY10 project appraisals shows a mean rating of 4.25



## DR Appraisal Highlights



Pat Unkefer, PI

**Distributed Metabolic Regulation: The key to Synthetic Biology for Carbon Renewal**

"The quality of work performed is excellent, which should lead to numerous publications describing both the technology developed as well as the science performed."

**Appraisal Committee:**

Srinivas Iyer – LANL

Samuel Kaplan – University of Texas

Robert London – NIEHS

Gary Resnick - LANL



## DR Appraisal Highlights



Mike Nastasi, PI

**Enhance Radiation Damage Resistance via Manipulation of the Properties of Nanoscale**

"In addition to the high-impact publications, the discoveries of interfaces as catalyst for vacancy-interstitial recombination are well received by national and international peers."

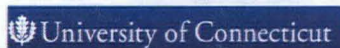
**Appraisal Committee:**

Hanchen Huang, University of Connecticut

Bob Averback, University of Illinois

Turab Lookman, LANL

Kurt Sickafus, LANL

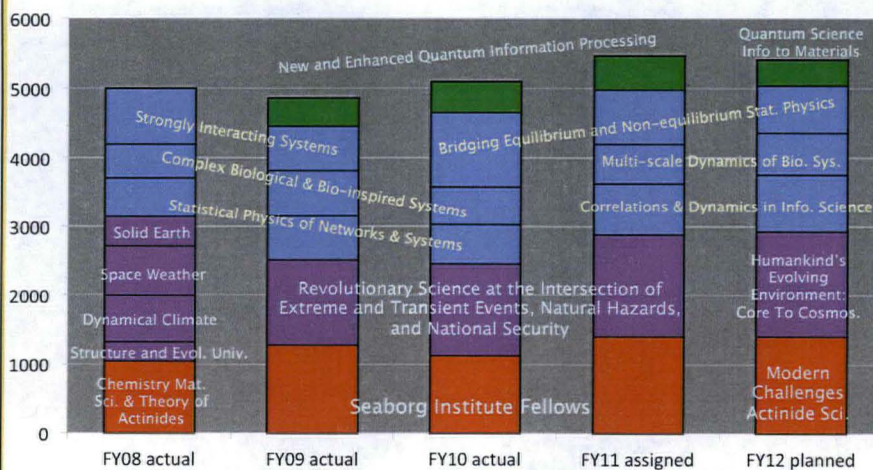




## Centers-led LDRD projects

- Technical projects of an integrated nature, typically postdoc and student-rich, that are most efficiently executed by a scientific Center
  - Seaborg Institute
  - Institute for Geophysics and Planetary Physics
  - Center for Non-linear Studies
- LDRD not used for operating expenses of Centers

## Investment in Centers-led projects





## FY11 review of Seaborg Institute

- **Committee**

- Darleane Hoffman, Lawrence Berkeley National Laboratory
- Al Sattelberger, Argonne National Laboratory
- Bruce Birsten, University of Tennessee, Knoxville
- Kerri Bloebaum, Lawrence Livermore National Laboratory
- Eric Bauer (Chair), Los Alamos National Laboratory, MPA-CMMS

- **Review highlights**

“The talks by the three Seaborg Postdoctoral Fellows at the review were excellent.”

“The funding model (50% for actinide research through Seaborg program/50% other) was an excellent model that should be retained...”

“Overall, the review committee thought that the Seaborg Institute Postdoctoral Program was outstanding. It remains an exceptional strategic investment of LANL LDRD resources towards actinide science...”

“The Seaborg Postdoctoral Fellowship Program is well aligned with the Plutonium Science and Research Strategy, in particular, with its goal of increasing workforce strength in actinide science.”

## FY11 review of Institute for Geophysics and Planetary Physics

- **Committee**

- |   |  |
|---|--|
| – Michael Liemohn, University of Michigan               | – Brian McPherson, University of Utah                  |
| – Greg Taylor, University of New Mexico                 | – Donald Wuebbles, University of Illinois              |
| – Carol Anne Oleyson, Florida State University          | – George Fuller, University of California, San Diego   |
| – Katrin Heilmann, Argonne National Laboratory          | – John Bradley, Lawrence Livermore National Laboratory |
| – Richard Aster, NIM Institute of Mining and Technology |  |

- **Review highlights**

“The quality of research supported by IGPP is comparable to or exceeds other top-notch programs for science funding in the nation, such as corresponding NSF or NASA programs.”

“By the strategic investment of modest funds, IGPP has initiated and promoted research in areas that later received major funding from NSF, NASA, DOE, or other funding agencies.”

“University connections built through IGPP notably prime the pipeline for bringing outstanding postdoctoral researchers and staff to Los Alamos.”

“IGPP is “clarifying” or confirming some critical components of the national R&D agenda and also serves as a flexible funding mechanism for advancing small-scale, but potentially pivotal, novel or exploratory research that may be difficult to support with other mechanisms.”



## FY11 review of Center for Nonlinear Studies

- **Committee**

- Nicholas Bigelow, University of Rochester
- Susan Coppersmith, University of Wisconsin
- Pierre Meystre, University of Arizona
- Thomas Witten, University of Chicago

- **Review Highlights**

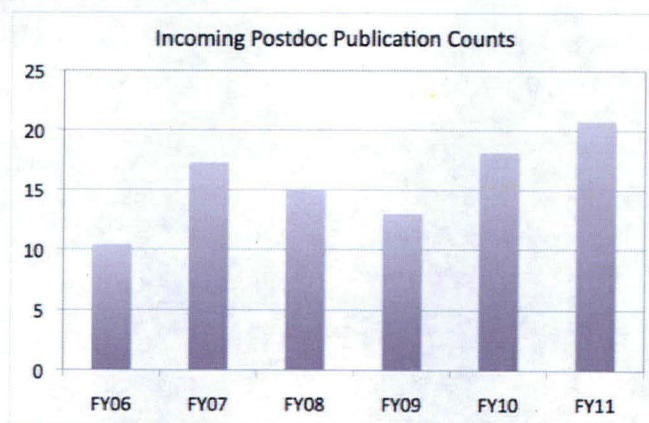
"CNLS has maintained a strong track record of developing postdocs into successful recruits to the permanent staff or winners of sought-after academic posts."

"CNLS activities are very valuable; they enable the Laboratory to be more nimble in taking advantage of new research opportunities of relevance to Laboratory priorities..."

"The 'Bridging' program has done an excellent job of maintaining external visibility while simultaneously enhancing programs of national strategic interest..."

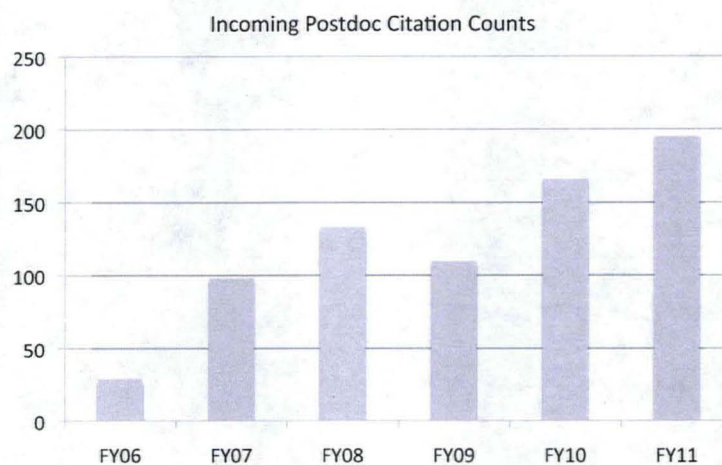
## LDRD postdocs: great and getting better

The quality of LDRD postdocs reveals a clear upward trend, evidenced by the high numbers of publications and citations at the time of hire.





## Another metric of quality



## Early Career Component

- Offers a special opportunity to develop scientific leadership on the part of entering scientists and engineers
- Eligibility limited to two year since staff member hire; 10 years after highest degree
- Two-year projects at \$225/yr; two calls per year
- Proposers limited to submitting one proposal per call, and a lifetime limit of two EC submissions
- Targeting 20% success rate (vs. 10% in most LDRD)
- Projects selected by peer-reviewed competition
- AD rankings an important input, strongly guided by focus on building future Laboratory leaders
- Division endorsements required for limited-term appointments, confirming the proposer will make a long-term contribution to the Laboratory



## Appraisal criteria focuses on leadership development.

- **Qualifications of PI and Team (50% weight)**
  - How well qualified are the proposing team and especially the PI to conduct a successful project, based on evidence of past technical accomplishment and leadership?
- **Innovation, and Creativity (20%)**
  - To what extent is the proposed project a major intellectual advance that would bring fundamentally new approaches to understanding?
- **Institutional Impact (20%)**
  - What impact would the project have on its technical field and/or the Laboratory's mission? What lasting benefit will it deliver to the Laboratory's human capital and the PI's career?
- **Research Approach (10%)**
  - How well conceived and organized is the proposed activity?

### Early Career proposals come from the breadth of the Laboratory

Round 1	Directorate	Submitted Proposals	Selected Proposals	Division
	ADE	2	1	Applied Engineering & Technology
	CLES	16	2	Bio Sciences
	EPS	17	2	Materials Physics AND Physics
	TIR	8	1	Intelligence & Space Research
	TSC	4		
	<b>Total</b>	<b>47</b>	<b>6</b>	
				Project Start Date: Nov. 1, 2010 (for FY 11) Project Success Rate: 13%
Round 2	Directorate	Submitted Proposals	Selected Proposals	Division
	ADE	2		
	CLES	13	3	Chemistry, Bio Science, AND Earth & Environmental Sciences
	EPS	6	2	Physics, AND Materials Science Technology
	TIR	2		
	TSC	7		
	<b>Total</b>	<b>30</b>	<b>5</b>	
				Project Start Date: April 1, 2011 Project Success Rate: 17%



## Early Career proposals come from the breadth of the Laboratory

Round 3	Directorate	Submitted Proposals	Selected Proposals (In Progress)	Division
	ADE	1		AOT
	ADW	3		WX, XCP
	CLES	4		B, C, EES
	EPS	9		MPA, MST, P
	TIR	5		D, ISR
	TSC	5		CCS, T
	<b>TOTAL</b>	<b>27</b>	<b>6</b>	

Start Date: October 3, 2011 (goal)  
Target success rate: 22%

## Early Career topics span all fields

### A sampling:

- Low-Frequency Acoustic Interferometry for Probing the Stratosphere.
- Exploiting Non-Innocent Ligands in Catalysis: New Base Metal Catalysts for the Reduction of Carbon Dioxide
- Solar Energetic Particles Entry and Trapping in the Magnetosphere: Filling a Major Space Weather Gap
- Non-Precious Metal Cathode Catalysts for Lithium-Air Batteries
- Combined Correlated NMR-electromagnetic Spectroscopy and Imaging
- Multi-Source Energy Harvesting for Remote Power Applications
- Rational or Irrational Design? A Synergistic Approach to Evolving an Industrially Important Enzyme

*No projects yet completed – results still out*



## LDRD is essential for recruitment and early career development



**Chris Fryer:** LDRD funding is the glue that allows me to leverage my programmatic work and tie it to my astrophysics research. This more public research then feeds back into the program, both by helping me take discoveries in academia and integrate them into the program as well as helping me attract great scientists to LANL.



**Dana Dattelbaum:** Several people from LLNL and the DoD labs have come up to me and wondered how we were able to engage in great basic research in areas that overlap/impact weapons program science. Bill's efforts to align LDRD with programs has clearly helped LANL in this regard. It has also enabled us to hire post-docs that can be focused on fundamental science.



**Dan Hooks:** Project Leader for High Explosives in NNSA Science Campaign 2, Team Leader in Shock and Detonation Physics (WX-9), and active researcher in crystallization and characterization of organic molecular materials. Dan came to the lab as a post-doc in 2000 and still remembers the LDRD charge code for that project.



**Malcolm Andrews,** National Security Fellow and EO Lawrence recipient LDRD has afforded me opportunities explore new realms of turbulence and fundamental problems, transitioning into new opportunities with programmatic impact and facilitating my career. I've also had opportunity to work with post-docs across multiple disciplines.

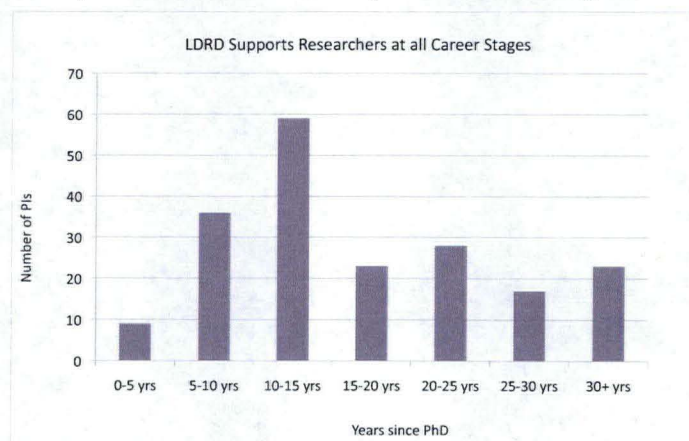


**Tim Germann:** The LDRD program has greatly benefitted my career path at LANL, providing the intellectual freedom and flexibility to explore new (and often risky) ideas. I started as a postdoctoral fellow and progressed into leadership roles. I'm currently leading a DR project that has pushed the spatio-temporal frontiers of peta-scale atomistic simulations further into the experimental regime.

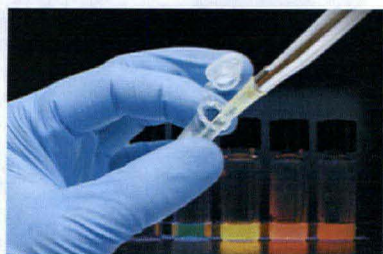


## Diversity of LDRD researchers

From early career to senior scientist, LDRD supports a diverse pool of the Laboratory's best and brightest



## NanoCluster Beacons



Team: Hsin-Chih (Tim) Yeh, James Werner, Jaswinder Sharma, and Jennifer Martinez

- NanoCluster Beacons are collections of silver atoms designed to illuminate when bound to nucleic acids, such as the DNA of specific pathogens.
- These beacons can be used to probe for diseases that threaten humans by identifying the nucleic acid targets that represent a person's full genome, and allow for personalized medication.
- They can also be used in quantitative biology applications, such as counting individual molecules inside a cell.





Team: Jaqueline Kiplinger and  
Thibault Cantat

## Th-ING

- A novel method known as Th-ING (Thorium Is Now Green), has been developed to circumvent the hazards and cost issues of conventional methods to produce a new thorium chloride reagent,  $\text{ThCl}_4(\text{DME})_2$ .
- This cost-effective, safe, "green," and scalable method will revolutionize the use of thorium in nonaqueous thorium chemistry and materials science.
- This method also stands to play a crucial role in creating one of the world's future sustainable energy sources.

## LDRD publications remain a large fraction of the Laboratory output

Peer-Reviewed Publications			
	CY07	CY08	CY09
LANL Pubs	1928	1780	1743
LDRD Supported	401	452	376
% due to LDRD	21%	25%	22%

**LDRD supports approximately 23% of the Laboratory's total publications (3-year average).**



## Top-cited papers are dominated by LDRD work

Citations			
	CY07	CY08	CY09
LANL Citations	20550	13830	7075
LDRD Supported	7796	4756	2652
% due to LDRD	38%	34%	37%
Top 50 Most Highly Cited Publications			
LDRD Supported	50%	42%	44%

## Follow-on Funding: One of several metrics

Projects active in FY10 played an important part on the path to \$98M of externally funded R&D.



"Genomes to Behavior: Predicting Bacterial Response by Constrained Network Interpolation" (\$11M)



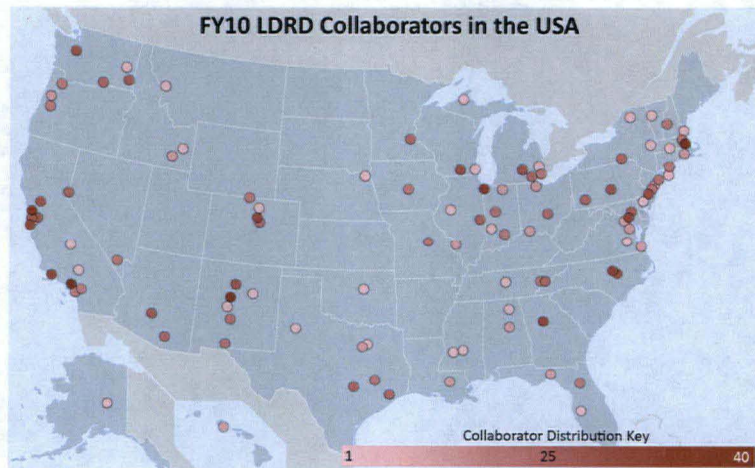
"Foundations for Practical Pattern Recognition Systems" (3M)



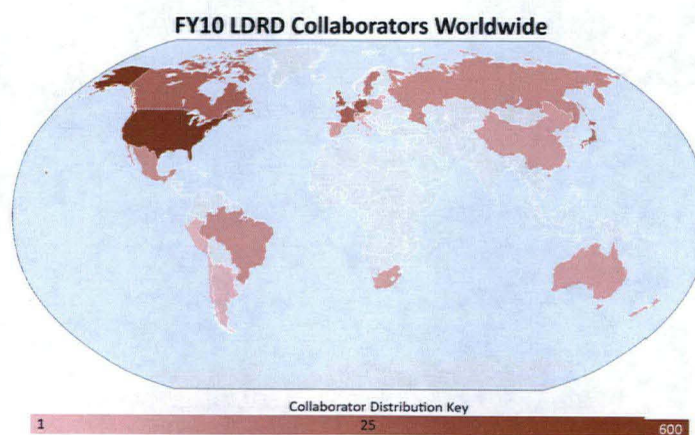
"Hot Spot Physics and Chemistry in Energetic Materials Initiation" (\$ 2.5M)



## LDRD enables external collaborations



## LDRD enables external collaborations





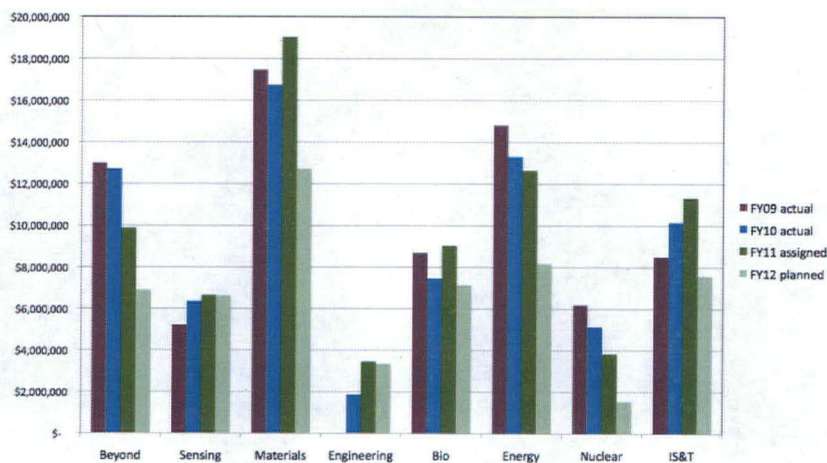
## Backup Slides

### LDRD builds multi-disciplinary teams

- We have evidence that partnered proposals increase their chances of funding by about 40%
  - In FY07-FY10, 448 pre-proposals were submitted
  - Of the 70 selected for funding, more than 50% partnered across principal directorates, while only 34% of the unfunded proposals were partnered



## Update on strategy: What we learn from proposals



### FY10 Metrics Summary

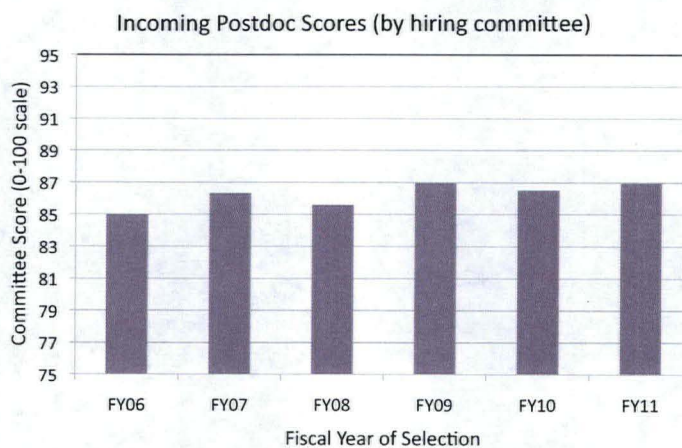
- Excellent
- Satisfactory
- Improvement sought

Metric	Evidence
LDRD work is of high technical quality and impact	<ul style="list-style-type: none"> <li>● Peer-reviewed publications remain a large fraction of Laboratory output (25%) <ul style="list-style-type: none"> <li>- LDRD supports approximately 23% (3-year average)</li> </ul> </li> <li>● Patents and disclosures remain a large fraction of Laboratory output (25%) <ul style="list-style-type: none"> <li>- LDRD supports approximately 30% (3-year average)</li> </ul> </li> <li>● Top-cited papers are dominated by LDRD work <ul style="list-style-type: none"> <li>- LDRD supports more than 45% (3-year average)</li> </ul> </li> <li>● Quantitative appraisal scores for ongoing projects show a pattern of excellence <ul style="list-style-type: none"> <li>- Independent project appraisal scores average outstanding to excellent</li> </ul> </li> <li>● Citation counts show that LDRD makes a major contribution to Laboratory technical output <ul style="list-style-type: none"> <li>- LDRD supports 37% of the Laboratory's total (3-year total)</li> </ul> </li> </ul>
LDRD is essential to the Laboratory's ability to deliver mission solutions	<ul style="list-style-type: none"> <li>● Success stories show clear path from LDRD investment to major mission impacts</li> <li>● Funded follow-on projects show LDRD prepares the Laboratory to meet national needs <ul style="list-style-type: none"> <li>- Active projects resulted in approximately \$89M in external funding</li> </ul> </li> <li>○ Proposals and briefings tracked by the program development mentor program show sponsor engagement <ul style="list-style-type: none"> <li>- Considering returning direct program engagement to line management</li> </ul> </li> </ul>
LDRD builds the Laboratory's human capital	<ul style="list-style-type: none"> <li>● Number of postdocs supported by LDRD provides a strong pool for future Laboratory needs <ul style="list-style-type: none"> <li>- LDRD supports approximately 60% of Laboratory postdocs (4-year average)</li> </ul> </li> <li>● LDRD supports researchers at all career stages, from postdocs to senior staff <ul style="list-style-type: none"> <li>- Analysis of PI career stages revealed LDRD is supporting a desirable cross section of the Laboratory population</li> </ul> </li> <li>● LDRD supports numerous and substantive national and international collaborations that reinforce internal capabilities <ul style="list-style-type: none"> <li>- LDRD researchers established 735 collaborations worldwide</li> </ul> </li> </ul>
LDRD is a major factor behind the Laboratory's technical reputation	<ul style="list-style-type: none"> <li>● LDRD work contributes significantly to awards such as R&amp;D 100, Lab and Society Fellows, and others</li> <li>● Journal covers based on LDRD work show a prominent national impact (FY11+)</li> </ul>



## We hire high-quality postdocs

- The quality of LDRD postdocs reveals a clear upward trend, evidenced by the high numbers of publications and citations at the time of hire.



## LDRD supports a large fraction of the Laboratory's patents and disclosures

Patents				
	FY07	FY08	FY09	FY10
LANL Patents	49	28	52	56
LDRD Supported	22	8	12	12
% due to LDRD	45%	29%	23%	21%

Disclosures				
	FY07	FY08	FY09	FY10
LANL Disclosures	166	116	110	116
LDRD Supported	49	36	38	16
% due to LDRD	29%	31%	38%	21%



## Project Appraisals

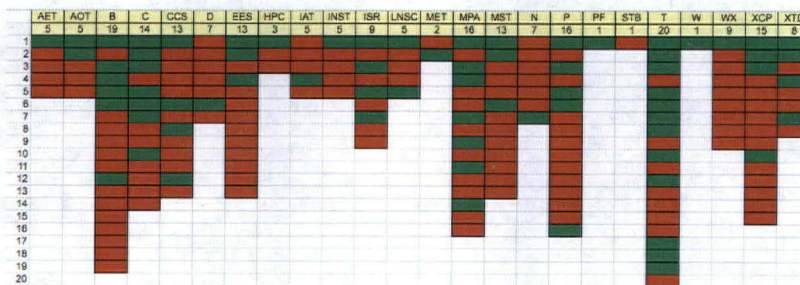
- The LDRD Program Office conducts an appraisal of every ongoing project it intends to fund in the next fiscal year.

## DR Appraisal Criteria

	<b>Quality</b> Are the science and technology results of high quality compared to national and international peers?	<b>Performance (Project Execution)</b> Is the project making good progress against its milestones? Is it well-conceived and executed?	<b>Relevance</b> Is the project continuing to support the strategic directions of the Laboratory?	<b>Leadership</b> Are the results of the project defining R&D directions for the broader community?
<b>Outstanding</b>	Work leads its technical field. Pioneering a fundamental intellectual advance and/or a fundamentally new approach to expanding our knowledge.	Outstanding ratio of results to investment. Project is actively managed to address difficulties and respond to new opportunities.	Potential for revolutionary impact on Los Alamos missions or technical fields essential to Los Alamos missions.	Results of project have spurred follow-on research at other facilities and impacted national agenda; prizes & fellowships.
<b>Excellent</b>	Clear differentiation from all previous work. Likely to place Los Alamos at the lead nationally or among DOE peers.	Team is making very good progress and delivering a breadth of results.	Potential for important impact on mission and technical field, with broad and important applications.	Follow-ons visible within Laboratory; invited talks and steering committee roles.
<b>Good</b>	Perhaps incremental in expected outcome. Identifiable impact on mission or field.	Results mixed, but some distinct successes. Overall, a good Laboratory investment.	Success would have a distinct impact on Lab programs.	Identifiable early signs of external recognition.
<b>Fair but lacking in one or more critical aspects</b>	Largely incrementally, marginal impact on mission or field. Publications few and low-impact. Inadequate understanding of peer standing.	Identifiable lack of progress. Team or approach does not appear to appreciate key issues. Teaming and communications issues.	Notional connections to National Security missions. Inadequate connections to stakeholders and national community.	Minimal evidence of external recognition.
<b>Deficient</b>	Quality of research does not meet national and Laboratory standards.	Serious problems with project execution.	Anticipated minimal impact on Lab mission and science.	Minimal evidence of external recognition.

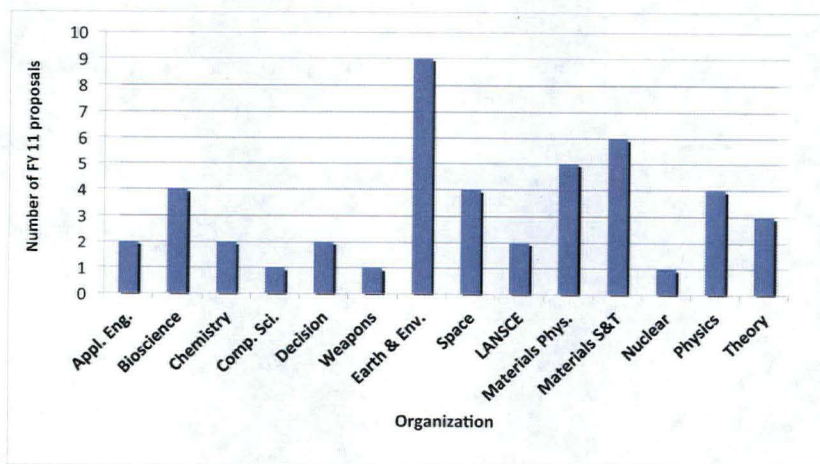


## Imprint of division strategy: FY12 DR pre-proposals



Green = passed to final round

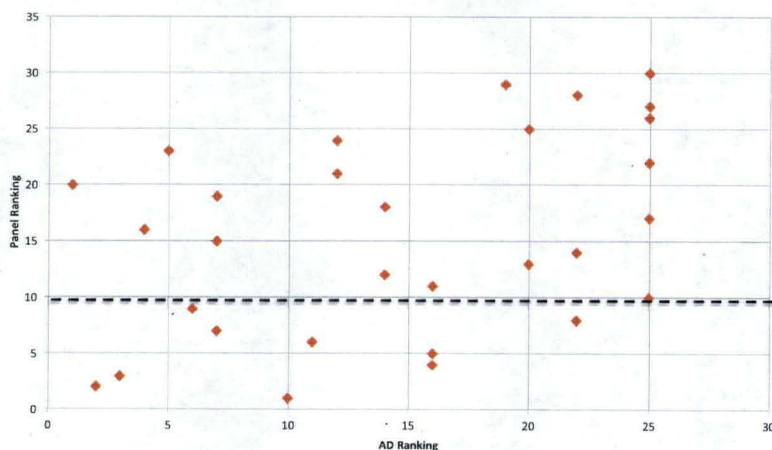
## Organizational distribution of FY11 Early Career proposals





## Working to Improve Impact of AD Strategy on Early Career Decisions

Correlation with Endorsements



## Early Career Stars



Nate McDowell

- Fulbright Scholar Award (2010)
- DOE Early Career Award (2010)
  - Started as a postdoctoral fellow in 2003
  - Converted to staff scientist in 2004
  - Serves on advisory committees for the NSF, DOE, and the Laboratory
  - Associate editor for two international journals
  - Testified before congress regarding DOE's climate-change research

- DOE Early Career Award (2010)
  - Started as a Director's Postdoctoral Fellow in 2005
  - Converted to staff scientist in 2007
  - American Physical Society Outstanding Doctoral Thesis in Beam Physics Award
  - Los Alamos Distinguished Performance Award



Evgenya Smirnova