LA-UR- 11-03037

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Title: Los Alamos LDRD and our Stockpile Stewardship Mission (U)

Author(s): Mark B. Chadwick, XCP-DO, DL

Intended for: NNSA 2011 LDRD Symposium, Washington, D.C.

Los Alamos NATIONAL LABORATORY EST. 1943

Abstract:

These viewgraphs describe LANL's LDRD program as it relates to our stewardship mission.

Los Alamos LDRD and our Stockpile Stewardship Mission

Mark Chadwick

X – Computational Physics Division Leader, Los Alamos National Laboratory

Thanks to: Malcolm Andrews, Nels Hoffman, XCP

Unclassified: DC:MBC

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Overview

LDRD Grand Challenges at Los Alamos

Past: Examples of major impacts of previous LDRD investments

Present: Introduction to the LANL posters this afternoon

Future: Thrusts in LDRD

People

8 LDRD Directed Research Grand Challenges: Many of These Support our Stewardship Mission

- Nuclear Performance
- Materials: Discovery Science to Strategic Applications
- Information Science & Technology
- Energy and Earth Systems
- Sensing and Measurement Science for Global Security
- Intelligent Adaptive Engineered Systems
- Complex Biological Systems
- Beyond The Standard Model

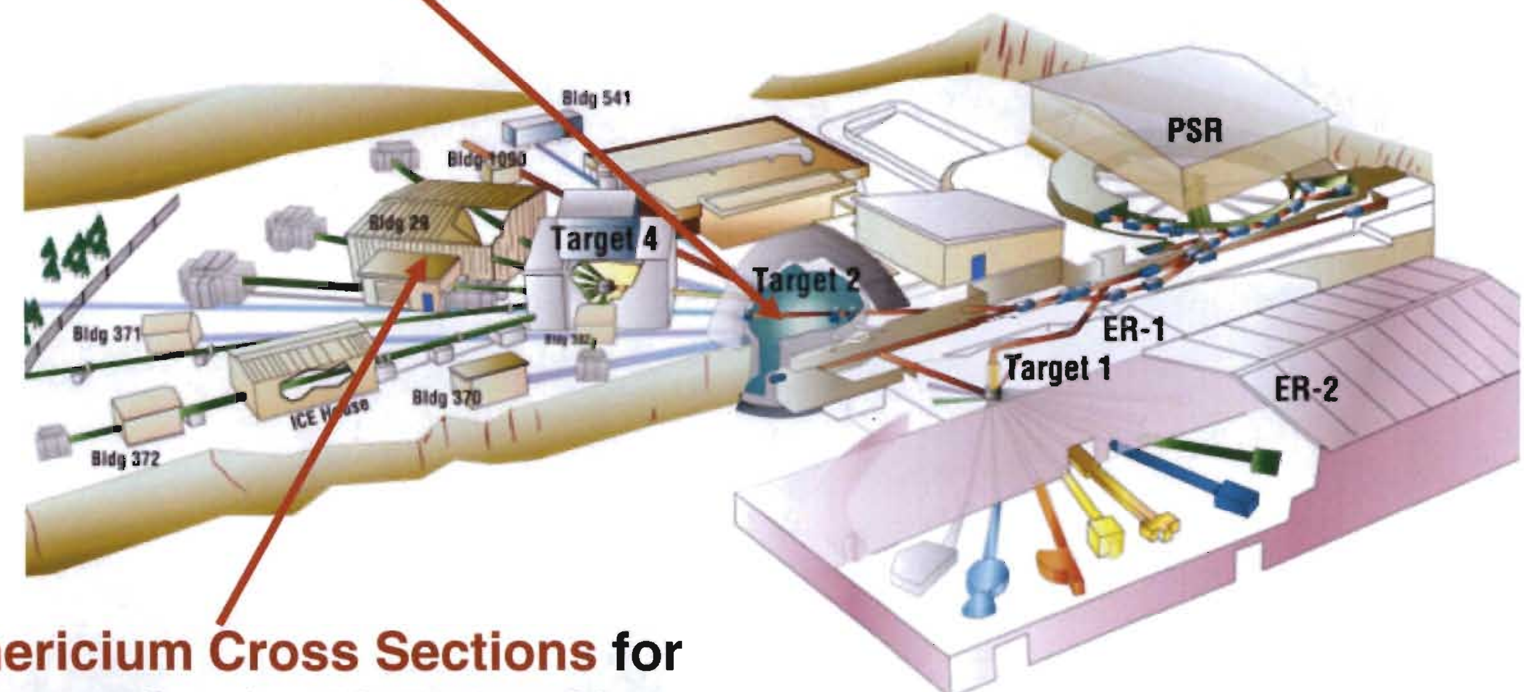
+ New Co-design thrust

- **Nuclear weapons program looks to LDRD to:**
  - Develop innovative capabilities for improved, more efficient, more predictive approaches to science/engineering problems
  - Build multi-disciplinary teams that
    - Cut across program elements
    - Transition to new programs
    - Provide scientific vibrancy for future

2 Examples of Past LDRD Investments Impacting our Increased Confidence in Certifying the Stockpile

Proton radiography: 1 GeV protons for imaging dynamic systems, *Chris Morris*

LANSCE



Americium Cross Sections for Diagnostics (at Weapons Neutron Research Facility) *Mark Chadwick*

Proton Radiography – Grew from LDRD in the 1990s, Chris Morris

Add info on early LRD/DR origins

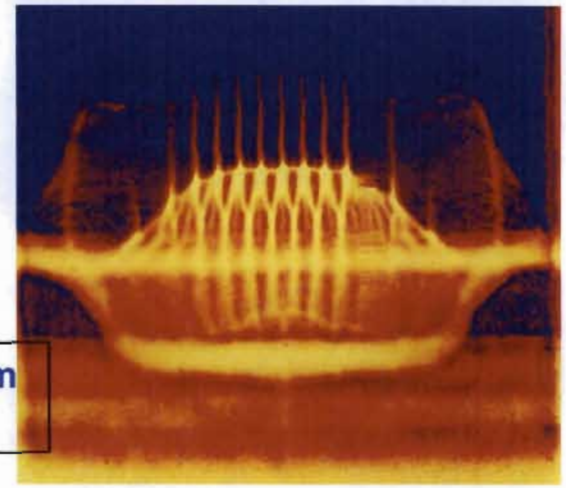
Enables multiple (17?) images of dynamical systems

Certain advantages regarding resolution

Now, Proton Radiography is Impacting a Wide Variety of Topics in Dynamical Material Response

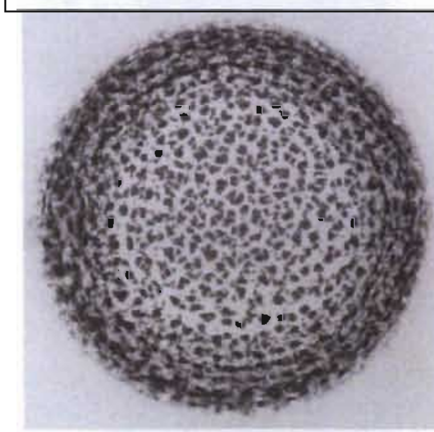
Materials damage evolution, including Pu

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



Strength at high strain rates, from suppression of instability growth

Fragment distribution from shear band formation



High-explosive burn

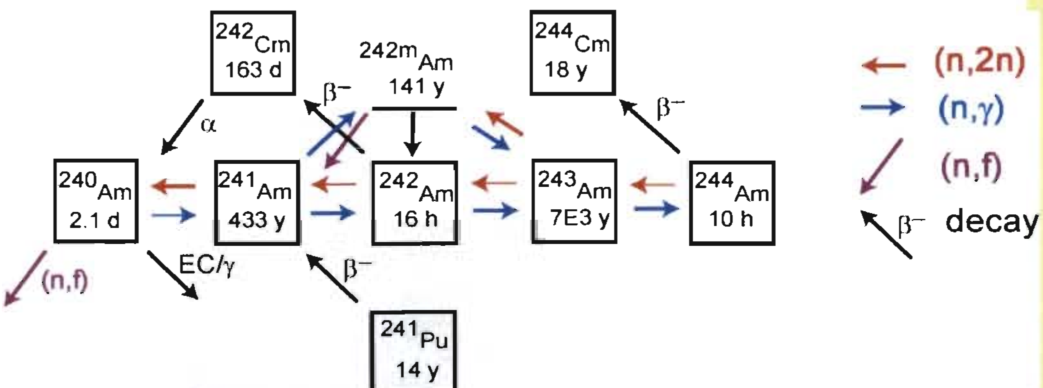
Americium Cross Sections for Diagnostics: LDRD Developed the Vision into a Reality

DANCE (n,γ)

- ^{241}Am grows in from ^{241}Pu, $t_{1/2}$=14 yr.

Transmutations tell us about neutron fluence and spectrum:

- (n,2n) tells us about higher energy neutrons (6-14 MeV).
- (n,γ) tells us about low energy neutrons especially < 500 keV



Historical post-explosion debris data are available, but previously underutilized because of cross section uncertainties

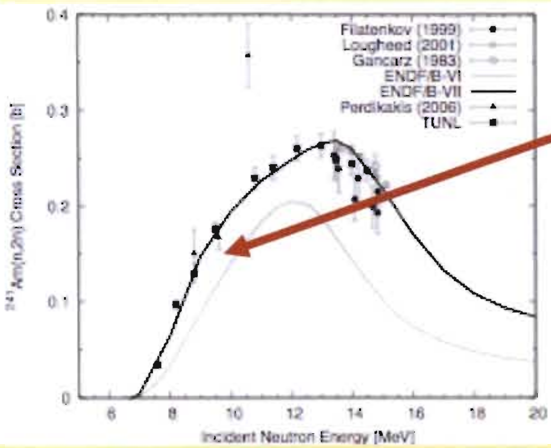
LDRD measurements and theory reduced unc. from >20% to <5%

- now routinely used to improve and validate our boost models

(With LLNL)

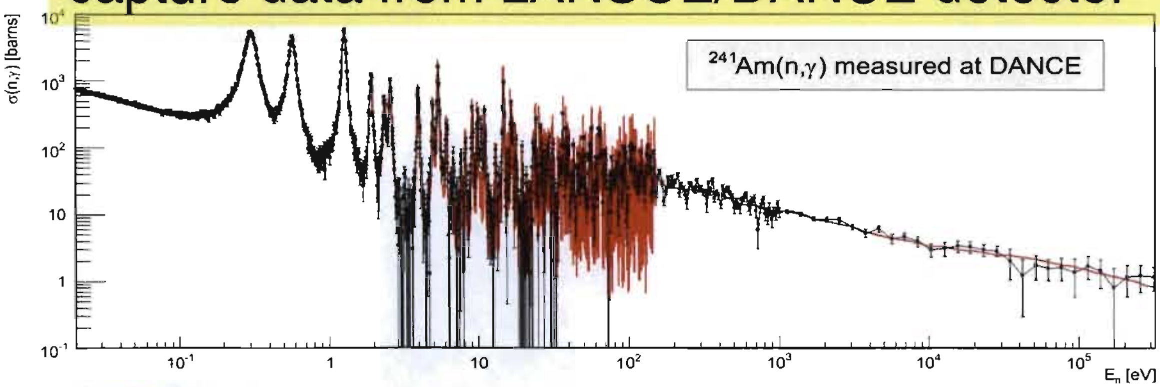
Results Incorporated into ENDF, Published, Also Impacting Fast Reactor Programs in US, Europe, Japan

(n,2n) now known very well – even better than ^{239}Pu(n,2n)



Our theory predictions agreed very well with the new measurements

capture data from LANSCE/DANCE detector



Other fast reactor impacts:
(a) Curium waste production; and (b) Criticality of plutonium decreases with time because:

^{241}Pu: high fission, low capture

^{241}Am: low fission, high capture

LANL Poster: "Material Response to Shockwaves"
PI: Darcie Dennis-Koller

Achieving a future of materials by design requires an understanding of materials response in extreme environments like shock loading.

<u>Goal</u>: controlled experiments to probe parameters of shock loading that affect damage initiation, growth, and ultimately failure of a material. These results advance our damage models.

Example: a sapphire flyer plate incident on copper, leading to material porosity and damage

Simulation

Experiment

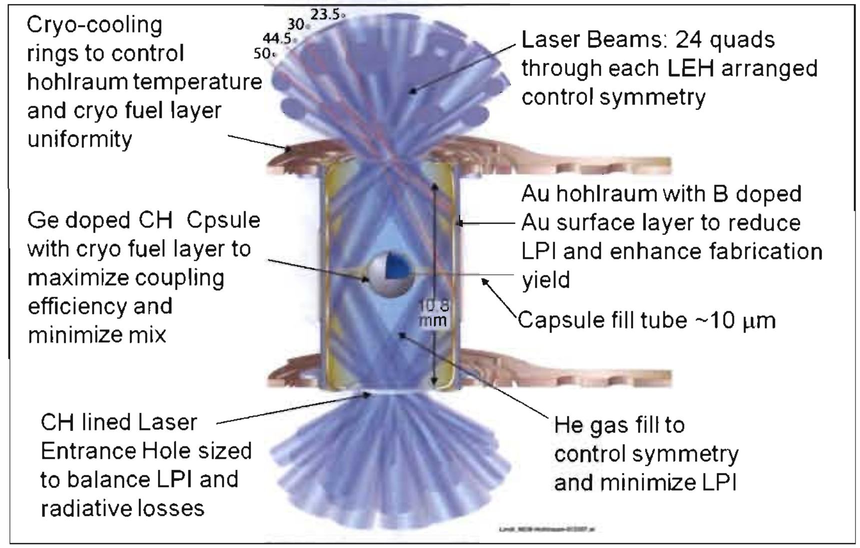
Why is this important for our nation?

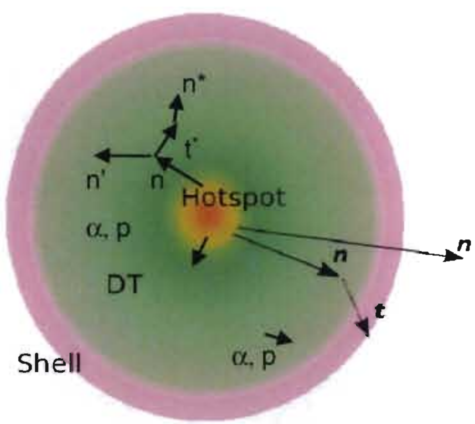
Functionally designed materials needed:

- Ensure US nuclear deterrent
- Reduce global threats
- Solve emerging energy challenges

LANL Poster: Leveraging NIF To Better Understand Turbulence, PI: Michael Steinkamp

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.



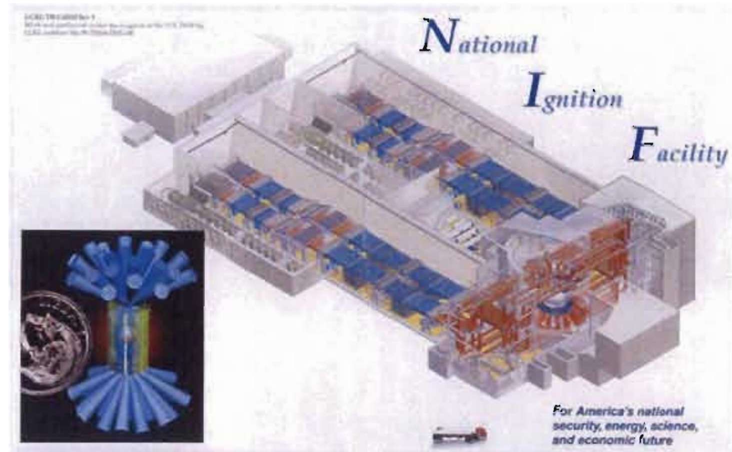


This research would provide a new class of experimental data to increase our understanding of turbulence in these flows, including the first thermonuclear data to test LANL's state-of-the-art turbulence models at *small scales*. To date, LANL's turbulence transport models in ASC codes have only been validated with data insensitive to these small scales.

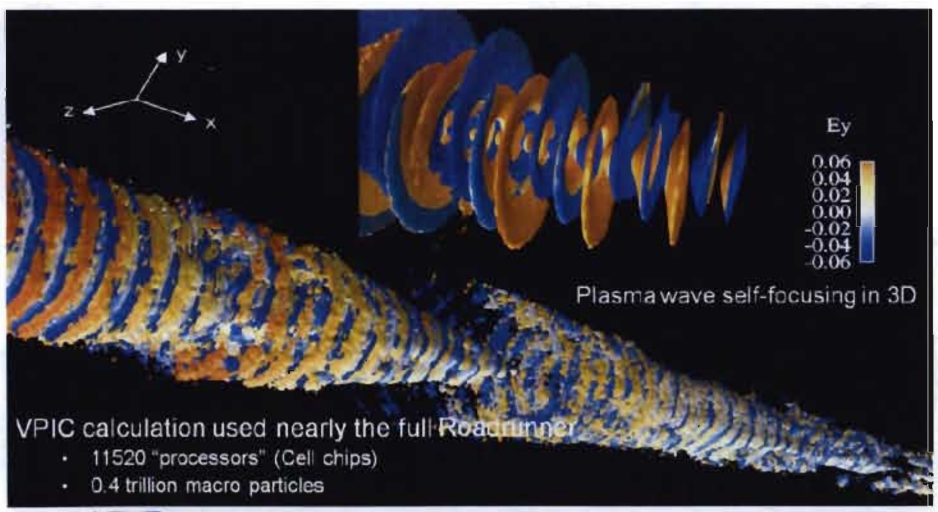
LANL Poster: Laser Plasma Interaction - Science Underpinning Fusion Energy and National Security Science, PI: Yin Lin

VPIC code describes the plasma from first-principles, and can run efficiently on HPCs

We perform 3D simulations over 100 times larger than before, enabling us to capture the very complex, nonlinear behavior



(image compliments of LLNL)

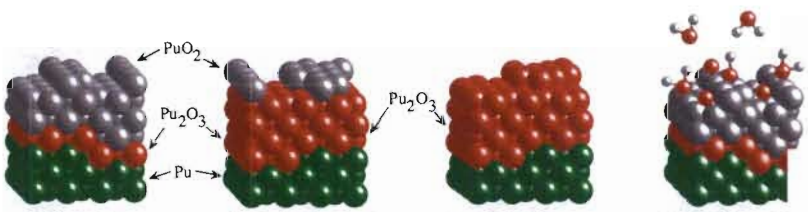


This LDRD work underpins the use of leading experimental facilities to advance frontier HEDP science.

LANL Poster: Predictive Capabilities for Transuranic Materials, PI: Richard L. Martin

The *f*-electron challenge:

There is currently no first principles predictive tool capable of even a qualitatively correct description of the motion of electrons in actinide metals.



(a)Room T (b) 25 C/Vacuum (c) 150 C/Vacuum (d) Ambient, H

Significance – Accelerated materials by design involving strongly correlated systems:

Small, portable, hand-held gamma ray detectors for homeland security

Advanced nuclear energy systems

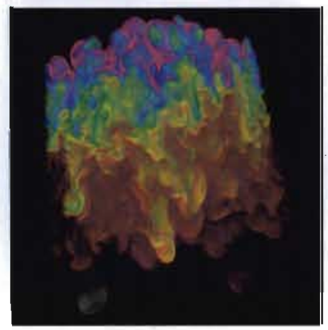
Organic photovoltaics

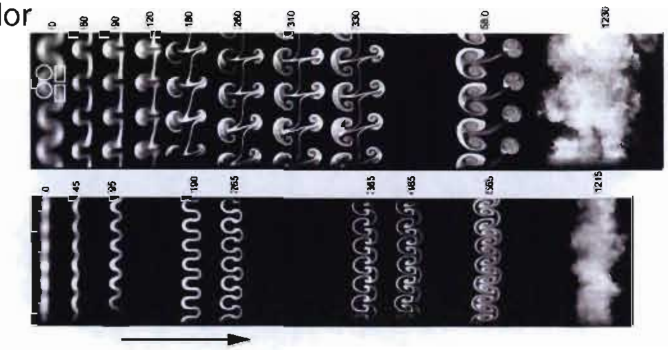
Next generation batteries

LANL Poster: Turbulence By Design,
PI: Malcolm J. Andrews

Initial conditions can influence the development of hydrodynamic turbulence and material mixing flows – a strategic problem in energy production, the environment, and in the stewardship mission

3-D DNS of Rayleigh-Taylor on Roadrunner





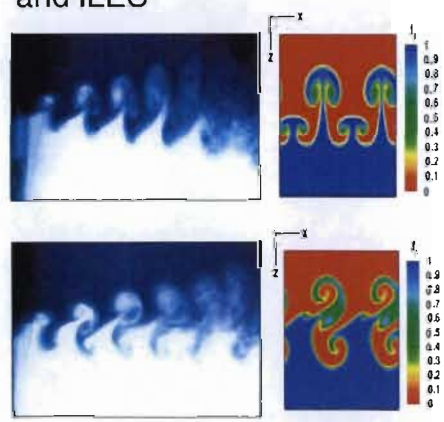
Richtmyer-Meshkov Experiments

ICF

Climate

Sprays

Rayleigh-Taylor Experiments and ILES



Goal: A new understanding of transitions to turbulence, and how they can be controlled and employed

2011 Nuclear Performance Grand Challenge Recognizes Five Strategic Thrust Directions

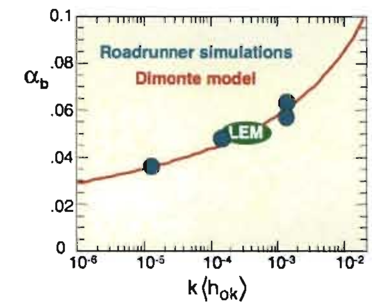
- Surrogacy and scaling
- Boost
- Materials-aware predictive capability; from observation to control; impact of grain microstructure
- (Avoiding) technological surprise, evaluate foreign threats
- Exascale computing, co-design, advanced physics applications

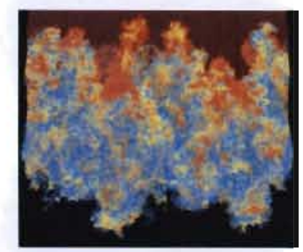
  - Building on Roadrunner peta-scale hybrid computer experience *(see next viewgraph)*

Roadrunner Science@Scale Petascale Simulations Have Led to Numerous Scientific Breakthroughs, and Set Directions for Exascale Computing

Nature – VPIC first-ever 3D plasma simulations give a new understanding of the development of turbulent magnetic reconnection in astrophysics, earth science, & fusion, *Daughton et al. (XCP, CCS)*

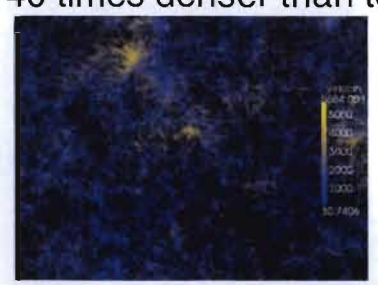
Turbulence – NECDC plenary talk - PPM code used to study effect of broadband initial conditions on RT instability with record resolution for mix-model validation, *Woodward, Rockefeller, Fryer, Dimonte et al (UM, CCS, XCP)*





Phys Rev Lett, & Phys. Plasmas – VPIC laser-plasma simulations of Raman backscatter at NIF, *Yin, Albright et al. (XCP, CCS)*

Astrophysical J & Comp Sc. and Eng. *Large-scale structure of the universe:* dark matter clumps termed "halos", colored with respect to their velocity magnitude when the universe was 40 times denser than today, *Habib et al.*



LDRD supported the initial open-science RR work

People – LDRD is Essential for Recruitment & Career Development: Examples of Staff Advancing Mission Goals and Fundamental Discoveries

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, a 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: As the PI of an LDRD DR the opportunity to explore new realms of turbulence and fundamental problems, that transition into new opportunities with programmatic impact has facilitated my career and the **opportunity to work with post-docs across multiple disciplines.**

Tim Germann: The LDRD program - exploratory research (ER), directed research (DR), and postdoctoral fellowships - have greatly benefitted my career path at LANL, **providing the intellectual freedom and flexibility to explore new (and often risky) ideas.** As a postdoctoral fellow; then as a newly minted staff member contributing to DRs I progressed to leadership roles, as the PI of an ER, a team leader within a larger DR effort, or mentoring a postdoctoral fellow; and most recently leading a DR project which has pushed the spatio-temporal frontiers of peta-scale atomistic simulations further into the experimental regime.