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Title: Briefing Book for 2009 Weapons Science Capability Review

Author(s): Mary Y. Hockaday

Intended for: 2009 Weapons Science Capability Review



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Weapons Science Capability Review

March 25 – 27, 2009

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Weapons Meeting Room
TA-03, Bldg. 1400, Room 6413B

Wednesday, March 25, 2009 (7:00 am – 7:30 pm)

- 7:00 Meet Committee Members in Lobby of Holiday Inn Express Evan Sanchez
Protocol Planner, Protocol Office
- 7:10 Bus leaves Holiday Inn..... LANL Taxi Service
- 7:15 Arrive at Otowi Building for badging Evan Sanchez

Institutional Requirements and Weapons Science Capability

- 7:30 **Executive Session – (closed session)** **Roy Schwitters**
Chair, Weapons Science Capability Review
- 7:50 Introductions, Agenda, Meeting Logistics Charles McMillan
Associate Director, Weapons Physics
- 8:00 Security Briefing Michael Irving
Security Program Leader, Weapons Physics
- 8:10 Director's Welcome & Committee Charge Terry Wallace, Jr.
Principal Associate Director, Science, Technology, and Engineering
- 8:45 Overview and Strategic Directions Charles McMillan
Associate Director, Weapons Physics

Institutional Host(s): Charles McMillan, ADWP 505-667-8711
Technical Host(s): Mary Hockaday, ADWP, 505-667-8711
Protocol POC: Evan Sanchez, CGA-GAO/505-667-5223/Cell 699-1121

Classification Level: Unclassified/SRD Sigma 1-10 Page 1
Dress: Business/Business Casual
RED: Classified Presentation



10:30 Break

Modeling and Simulation Capabilities

10:45 Modeling and Simulation Capability Futures and Discussion..... John Hopson
Program Director, ADWP

11:55 Depart for Working Lunch – University House

12:00 Working lunch with Early Career Staff (by invitation only) – University House

1:00 Return to Weapons Meeting Room

1:05 Code Strategy..... Bill Archer
Acting R&D Manager/Program Manager, X-3

1:50 Roadrunner
Hardware..... Andy White
Deputy Associate Director, Theory, Simulation, and Computation
Codes..... Paul Henning
R&D Scientist, CCS-2

3:00 Break

3:15 Spatial Temporal Frontiers of Atomistic Simulations Timothy Germann
R&D Scientist, T-1

Publication, Peer Review, and Recognition

4:00 Overview of Publication Record, Peer Review, and Recognition..... Bryan Fearey
Executive Advisor, ADWP

4:30 Defense Research Review (DRR) Process..... Joyce Guzik
Scientist/Laboratory Fellow, X-2

5:15 Executive Session (closed session)..... Roy Schwitters
Chair, Weapons Science Capability Review

5:45 Depart for No Host Dinner at Central Avenue Grill.....LANL Taxi Service

Agenda

6:00 No Host Dinner at Central Avenue Grill

7:30 Depart for Holiday Inn Express.....LANL Taxi Service

Thursday, March 26, 2009 (7:00 am – 7:30 pm)

7:00 Meet Committee Members in Lobby of Holiday Inn Express Evan Sanchez
Protocol Planner, Protocol Office

7:10 Depart for TA-3-1400, Weapons Meeting Room. LANL Taxi Service

7:15 **Executive Session (closed session)** Roy Schwitters
Chair, Weapons Science Capability Review

Experimental Science Capabilities

8:00 Experimental Science Capabilities..... Mary Hockaday
Deputy Associate Director/Program Director, Science Campaigns

9:10 MaRIE: Matter-Radiation Interactions in Extremes John Sarrao
Program Director, SPO-SC

9:40 **DARHT Update**..... David Funk
R&D Manager, HX Division

10:15 Break

Diversification

10:30 Capability Sustainment through Diversification.... Jay Dallman
R&D Manager, DE Division

11:00 Lunch with Senior & Mid-career Staff (by invitation only) – Weapons Meeting Room

Nuclear Design

12:15 **Advanced Certification**..... Don Haynes
R&D Manager, X-4

1:15 **Sustaining Nuclear Design** Michael Bernardin
R&D Manager, X Division

Agenda

2:15 Break

2:20 Executive Session (closed session)..... Roy Schwitters
Chair, Weapons Science Capability Review

2:55 Depart for Poster Session – Oppenheimer Study Center

3:00 Poster Session – Oppenheimer Study Center – Upper Level

5:15 Depart for Working Dinner - Otowi Cafeteria

5:30 Working Dinner (by invitation only) - Otowi Cafeteria

7:30 Depart for Holiday Inn Express..... LANL Taxi Service

Friday, March 27, 2009 (8:00 am – 3:00 pm)

7:15 Committee Members arrive (via private vehicle) at TA-3-1400 (Weapons Meeting Room)

7:30 Executive Session..... Roy Schwitters
Chair, Weapons Science Capability Review

8:30 Meeting with Capability Leaders

9:45 Break

10:00 Executive Session (closed session) Roy Schwitters
Chair, Weapons Science Capability Review

12:00 Working lunch Committee Members only

1:30 Closeout Meeting (DIR, PADs, AD, DAD)..... Terry Wallace, Jr.
Principal Associate Director, Science, Technology, and Engineering

2:30 Closeout Meeting (Open to All) Roy Schwitters
Chair, Weapons Science Capability Review

3:30 Adjourn

**Weapons Science Capability Review
2009 Committee Members' Contact Information**

Committee Member	Mailing Address	E-mail Address	Phone Numbers
Marvin Adams	Texas A&M University 129 Zachary 3133 TAMU College Station, TX 77843-3133	mladams@tamu.edu	(979) 845-4198 (office) (979) 845-6075 (fax)
Kimberly (Kim) Budil	LLNL Physics 7000 East Avenue Livermore, CA 94550	budil1@llnl.gov	(925) 423-8098 (office) (925) 424-2723 (fax)
John Cornwall	UCLA Depart of Physics and Astronomy Los Angeles, CA 90095-1547	cornwall@physics.ucla.edu	(310) 825-3162 (office)
Paul Drake	University of Michigan 2455 Hayward St. Ann Arbor, MI 48109-2143	rpdrake@umich.edu	(734) 763-4072 (office) (734) 647-3083 (fax)
Ted Hardebeck	SAIC 6825 Pine St. Omaha, NE 68106	theodore.m.hardebeck@saic.com	(402) 554-4742 (office) (402) 554-4759 (fax)
Daniel (Dan) Meiron	Caltech Engineering & Applied Science MC-256-80 Pasadena, CA 91125	dim@caltech.edu	(626) 395-4563 (office) (626) 568-9102 (fax)
Lee Peddicord, (STC POC)	Director, Texas Engin. Exper. Station Texas A&M University 301 Wisenbaker Engin. Research Center 3577 TAMU College Station, TX 77843-3577	k-peddicord@tamu.edu	(979) 845-5802 (office) (979) 845-0423 (fax)
Roy Schwitters, Chair	University of Texas at Austin Physics 1 University Station, C1600 Austin, TX 78712-0264	schwitters@physics.utexas.edu	(512) 471-9962 (office) (512) 471-9637 (fax)

**Weapons Science Capability Review
2009 Committee Members' Contact Information**

Committee Member	Mailing Address	E-mail Address	Phone Numbers
James Siegrist	Lawrence Berkeley National Laboratory 1 Cyclotron Road, 50-4049 Berkeley, CA 94720	jsiegrist@lbl.gov	(510) 486-4397 (office) (510) 486-6003 (fax)
Robbie Vogt	Department of Physics California Institute of Technology 2170 N. Altadena Drive Pasadena, CA 91108 (626) 398-5066	vogt@caltech.edu	(626) 398-5066

Marvin L. Adams

HTRI Professor of Nuclear Engineering

Director, Institute of National Security Education and Research

Texas A&M University

B.S., Nuclear Engineering
Mississippi State University

M.S., Nuclear Engineering
University of Michigan

Ph.D., Nuclear Engineering
University of Michigan

Marvin L. Adams served in the weapons program at LLNL from 1986 until he joined the faculty at Texas A&M University in 1992. He is past Chair of the American Nuclear Society's Mathematics and Computations Division and served for several years on the U.S.-Russian Joint Technical Working Group for disposition of weapons Pu. He has served on the LANL Science and Technology Committee, the LLNL Science and Technology Committee, the ASC Predictive Science Panel, the LANL X-Division Review Committee, and many other advisory and review committees at the NNSA labs. He has also served on National Academy committees including the recent QMU committee and the ongoing committee studying Nuclear Forensics, and he has participated in several indepth studies for NNSA. "I claim to have learned something at every committee meeting," Marv says.

He has authored or coauthored over 100 technical papers and advised a dozen M.S. graduates. He has advised more than a dozen Ph.D. graduates, ten of whom have held staff positions at NNSA laboratories.

Kimberly S. Budil

Associate B Program

**Leader of Science,
Technology, and
Experiments**

**Weapons and Complex
Integration Directorate**

**Lawrence Livermore
National Laboratory**

Ph.D., Applied Science
University of California at Davis

M.S., Applied Science
University of California at Davis

B. S., Physics
University of Illinois at Chicago

Kimberly S. Budil manages the fundamental weapon science research program supporting WCI including the Dynamic Material Properties Campaign, the ASC Physics and Engineering Models Program, and the Dynamic Plutonium Experiments Program. During her career at LLNL she has pursued research in a number of areas including experimental High Energy Density Physics (HEDP) investigating hydrodynamic instabilities, equations-of-state, and radiation transport, as well as computational studies of weapon physics issues.

Kim is currently a member of the American Physical Society (APS) Panel on Public Affairs and participated in their recent study *Nuclear Weapons in 21st Century National Security*. She is also in the first National Security Leadership Program class from LLNL pursuing a certificate in National Security Leadership from the Bush School of Public Policy at Texas A&M University.

Prior to this assignment, Kim was detailed to NNSA headquarters in Washington, D.C. for two years where she was assigned to the Office of Defense Science. She managed the Dynamic Materials Properties Campaign, served as the Chair of the Pit Lifetime Working Group, was the NNSA representative for the development of the National Ignition Campaign Plan, and provided technical advice on a variety of issues.

Kim was a member of the Committee on the Status of Women in Physics of the APS and has served on and chaired a number of CSWP site visit teams assessing the climate for women in physics at national laboratories. She was a member of the U.S. delegation to both the 1st (2002) and 2nd (2005, U.S. co-chair) International Union of Pure and Applied Physics Conference on Women in Physics and has participated in numerous other activities focused on increasing the participation of women in physics.

Kim has received two Defense Programs Awards of Excellence for her HEDP work. In 2002 Kim was selected to be the Scientific Editor for the LLNL publications *Science and Technology Review* and *National Security Review*.

John M. Cornwall

Professor of Physics

**University of California at
Los Angeles**

B.A.
Harvard University

M.S.
Denver University

Ph.D.
University of California at
Berkeley

Professor Cornwall is a faculty member at UCLA where he does research in elementary particle theory. He has written some 40 papers on space plasmas such as the aurora. He has been a visiting professor at many institutions in the US and abroad, and for some years was a Professor of Science and Policy Analysis at the RAND Graduate School in Santa Monica. He served for many years as a consultant to the Space Sciences Laboratory of the Aerospace Corporation, where he wrote papers on the magnetosphere and the aurora.

He has served on the Defense Science Board. He is a consultant to the Institute for Defense Analyses, where he serves on the White Team reviewing ballistic missile defense technology, and to Los Alamos and Livermore national laboratories, serving as Chairman of the Weapons Complex and Integration Directorate Review Committee at Lawrence Livermore National Laboratory as well as Chairman of the Advanced Strategic Computing Predictive Science Panel at Los Alamos and Livermore.

He is a member of the Jason group, advising the government on subjects such as ballistic missile defense, ultrasound technology, and the human genome project, among others, and has coauthored more than 150 Jason reports. He has authored several works on, and testified to Congress concerning, ballistic missile defense, including as coauthor of the report "Countermeasures" of the Union of Concerned Scientists. Among other contributions, he has been an adviser to, and lecturer in, the Public Policy and Nuclear Threats program of the Institute for Global Conflict and Cooperation at the University of California, San Diego; has served on a National Research Council review panel; and has chaired a workshop for the Panel on Public Affairs of the American Physical Society.

He is a Fellow of the American Association for the Advancement of Science and of the American Physical Society.

R. Paul Drake

Henry Smith Carhart
Professor of Space Science
Professor, Applied Physics
University of Michigan

B.A., Philosophy & Physics
Vanderbilt University

M.S., Physics
Johns Hopkins University

Ph.D., Physics
Johns Hopkins University

Professor R. Paul Drake has played a leading role in the development of two related fields of inquiry – High-Energy-Density Physics (HEDP) and High-Energy-Density Laboratory Astrophysics (HEDLA). This has grown from his scientific work, encompassing experiment, theory, and simulation in several topical areas. He now directs the Center for Radiative Shock Hydrodynamics, supported by the Predictive Science Academic Alliance Program of NNSA. His work at Michigan, since 1996, has emphasized hydrodynamics and radiation hydrodynamics with an emphasis on connections to supernovae and other applications to astrophysics. He also directed the 13 M\$/yr Space Physics Research Laboratory from 1998–2002.

Dr. Drake was a Professor at the University of California Davis (Associate from 1989-91 and Full from 1991–93), while also serving as Director of the Plasma Physics Research Institute at the Lawrence Livermore National Laboratory (LLNL). A number of his discoveries in laser-plasma interactions made during the period from 1982 to 1996 are quite well known. From 1982 to 1989 he conducted research in the LLNL laser fusion program, while leading various projects including the activation of target experiments on the Nova laser facility during 1984-85, and serving as Group Leader for Plasma Physics from 1985-89. Prior to that, his doctoral research was in plasma spectroscopy, after which from 1979 to 1982 he studied magnetic confinement and plasma-surface interactions for the magnetic fusion program at LLNL.

He has authored more than 190 scientific papers and has published a book entitled *High Energy Density Physics: Foundations, Inertial Fusion, and Experimental Astrophysics* [Springer, Berlin (2006) ISBN-10 3-540-29314-0].

He is a Fellow of the American Physical Society.

Theodore M. Hardebeck

**Vice President and Director
of Science, Technology, and
Strategy**

**Science Applications
International**

Ph.D., Mathematics
Case Western Reserve University

M.S., Mathematics
Case Western Reserve University

B.S., Mathematics and physics
Ball State University

Theodore M. Hardebeck serves as a consultant to the Departments of Defense (DoD) and Energy (DOE) on nuclear weapon issues. He served as a member of the National Research Council committee examining the quantification of margins and uncertainty methodology used by the NNSA to certify the reliability and safety of the nation's nuclear weapons stockpile. He was a member of the National Academy of Sciences Committee studying the Nuclear Earth Penetrator. He is also a consultant to Johns Hopkins University Applied Physics Laboratory; to Sandia, Lawrence Livermore, and Los Alamos national laboratories; DoD's Threat Reduction Advisory Committee; and to USSTRATCOM's Strategic Advisory Group. In addition, Dr. Hardebeck was a member of the Defense Science Board 2005/2006 Task Force examining U.S. nuclear capability. In 2004, he served on the DSB Task Force which examined the employment of the National Ignition Facility. Dr. Hardebeck is an advisor to the 2008 U.S. Nuclear Command and Control System Comprehensive Review Advisory Committee.

As USSTRATCOM's Associate Director, Plans and Policy and the Commander's Science and Technology Advisor, Dr. Hardebeck chaired or served as a member of numerous groups overseeing stockpile management and evolution. In 2003, he chaired the Future Arsenal Panel of the Stockpile Stewardship Conference, which developed a transformational vision of the future nuclear stockpile, leading a change to align the stockpile to the national security environment. He created and guided annual assessments of the nuclear stockpile, the results lauded by Presidential and Congressional reviews. He also guided analytical baselines for Nuclear Posture Reviews and Arms Control proposals. Results were used to formulate treaty details. As Director for Force Assessments at the Strategic Air Command, Dr. Hardebeck led a comprehensive examination of guidance, target base, weapon requirements, reserves, support requirements, and stability issues, the results providing the foundation of the 1991 Presidential Nuclear Initiative.

Dan Meiron

**Professor of Applied and
Computational
Mathematics and Computer
Science**

**California Institute of
Technology**

Sc.D., Applied Mathematics
Massachusetts Institute of
Technology

Dan Meiron is a professor of applied and computational mathematics and computer science at Caltech. His research interests include computational fluid dynamics and materials science. Specifically, those interests include nonlinear water-wave theory, Rayleigh-Taylor and Richtmyer-Meshkov Instability, dynamics of inviscid flows, and pattern formation in nonequilibrium systems. Other research interests have covered theory of turbulence, computer extension of perturbation series and methods of series analysis, numerical simulation of free surface flow, spectral methods, and parallel scientific computation.

Dan is a member of several review committees including the LANS BOG Mission Committee and the ASC Predictive Science Panel.

Kenneth L. Pedicord

**Associate Vice
Chancellor for Federal
Relations, and
Professor of Nuclear
Engineering**

Texas A&M University

B.S, M.S., Mechanical
Engineering,
University of Notre Dame

M.S., Ph.D., Nuclear
Engineering,
University of Illinois

Kenneth Peddicord is the associate vice chancellor for federal relations and a professor of nuclear engineering at Texas A&M University. He is also a registered professional engineer in the State of Texas. Before joining Texas A&M in 1983, he was an associate professor of nuclear engineering at Oregon State University.

Dr. Peddicord has acted as a consultant to the Department of Energy, the national laboratories, the Nuclear Regulatory Commission, and to universities and industry. His fields of specialization are the behavior of nuclear fuels, disposition of weapons plutonium, space nuclear power systems and missions, international engineering education, and curriculum policy.

In addition, he has served on numerous committees, commissions, and boards, including the International Coordinating Committee, Youth and the Plutonium Challenge; Educational Programs, Eagle Alliance; the Amarillo National Resource Center for Plutonium Governing Board; and the Universities Space Research Association Council for Science and Engineering Education. He is a frequent keynote speaker at meetings and conferences on such subjects as nuclear materials, radiation protection, weapons disposition, and disarmament.

Dr. Peddicord is a member of the American Nuclear Society, the American Society for Engineering Education, the American Society of Mechanical Engineers, and the Society of Mexican American Engineers and Scientists.

Roy F. Schwitters

**S.W. Richardson
Foundation Regental
Professor of Physics and
Former Chair of the
Department of Physics
University of Texas, Austin**

Ph.D., Physics
Massachusetts Institute of
Technology

B.S., Physics
Massachusetts Institute of
Technology

Roy F. Schwitters is the S.W. Richardson Foundation Regental Professor of Physics and former Chair of the Department of Physics at the University of Texas at Austin, where he teaches and conducts research in experimental high energy physics. Dr. Schwitters has been involved with research in experimental high energy physics and related developments in particle detectors and accelerators for more than thirty years.

Dr. Schwitters joined the Harvard faculty in 1979. Previously, he was assistant and then associate professor at the Stanford Linear Accelerator Center in Stanford, California. During the period 1980–1988, he was co-spokesman and head of construction for the Collider Detector at Fermilab in Batavia, IL, a \$100M-level construction project and related international scientific collaboration. From its founding in 1989 until canceled by Congress in 1993, he was director of the Superconducting Super Collider (SSC) laboratory in Dallas, Texas.

Since 1996, Dr. Schwitters has been a member of JASON, a group of academic scientists and engineers who advise agencies of the U.S. government on technical matters related to issues of national security. Currently, he is chair of the JASON steering committee.

Dr. Schwitters is a fellow of the American Academy of Arts and Sciences, the American Physical Society, and the American Association for the Advancement of Science. He received the 1980 Alan T. Waterman Award of the National Science Foundation, the 1996 Panofsky Prize of the American Physical Society, and was awarded a Research Prize by the Alexander von Humboldt Foundation of Germany in 1998.

James L. Siegrist

**Assoc. Director of
General Sciences,**

**Director of Physics
Division,**

**Lawrence Berkeley
National Laboratory**

**Professor,
Department of Physics,
UC Berkeley**

B.S., Physics,
University of Texas at Austin

B.A., Mathematics,
University of Texas at Austin

Ph.D., Physics,
Stanford University

James Siegrist has worked since the late 1980s on the physics of electroweak symmetry breaking. His current work centers on the ATLAS experiment at CERN. Recent physics interests include applications of instrumentation to problems in nuclear energy, especially non-proliferation.

In academics, James has taught physics for more than 10 years and is currently a professor at the Department of Physics at the University of California at Berkeley.

Since 1999, James also has served as Associate Lab Director of General Sciences at Lawrence Berkeley National Laboratory. He has been Physics Division Director at the Laboratory since 1997.

His group's current experimental program includes: study of the production of candidate dark matter particles at ATLAS; study of the production and decay of the top quark, including improved techniques for top quark mass measurement; searches for unexpected new phenomena, such as supersymmetric particles or extra dimensions.

Other hardware activities center on further development of state-of-the-art Silicon Detectors for charged particle track reconstruction. This work involves VLSI electronics, modeling of the details of the silicon response, and understanding the behavior of silicon systems in the intense radiation environment expected at future proton colliders.

Nuclear energy studies center on the use of instrumentation and techniques originally developed for High Energy Physics in monitoring of fissile material as part of the nuclear fission fuel cycle. This work involves simulation and modeling of nuclear fuel systems and proof-of-principle hardware projects to demonstrate detection techniques.

In his professional activities, James is a fellow of the American Physical Society and a member of the American Association for Advancement of Science. He has more than 360 publications in high-energy physics research, instrumentation development, particle phenomenology, and accelerator physics.

Rochus E. Vogt

R. Stanton Avery Distinguished Service Professor, and Professor of Physics, Emeritus, California Institute of Technology

Cand. Physics, Technische
Hochschule Karlsruhe,
Universitaet Heidelberg,
Germany

M.S., University of Chicago

Ph.D., University of Chicago

Robbie Vogt has been involved in teaching, research, and consulting with government and industry for more than 40 years.

He became emeritus at Caltech in 2002, where he had been teaching for more than 40 years and had become the R. Stanton Avery Distinguished Service Professor in 1982.

He served as Chief Scientist of JPL (Caltech/NASA), 1977–1978. He was the Chairman of the Division of Physics, Mathematics, and Astronomy at Caltech from 1978 to 1983. He was Vice President and Provost at Caltech (1983–1987) and later the Director of the Caltech/MIT Laser Interferometer Gravitational Wave Observatory (LIGO) Project at Caltech (1987–1994).

He has served on numerous advisory panels for the University of California. Currently, he is a member of the UC President's Council on the National Laboratories, a member of its National Security Panel, a member of its Project Management Panel, and chairman of its Science & Technology Panel.

His research has focused on astrophysical aspects of cosmic rays, gamma-ray astronomy, and gravitational wave astronomy.

He is a Fellow of the American Physical Society and a Fellow of the American Association for the Advancement of Science.

He is participating in this review as a member of the UC Science and Technology Panel.

Weapons Science Capability Review Presenters
March 25 - 27, 2009

Presenter/Title	Organization	Presentation Title	Thrust Area	Capability Title	E-Mail Address
Bill Archer, Acting R&D Manager/Program Manager	X-3	Code Strategy	Computation, Codes, and Platforms	High-Performance Computing	barcher@lanl.gov
Michael Bernardin, R&D Manager	X-DO	Sustaining Nuclear Design	Nuclear Weapons Design	Weapon Design	mpb@lanl.gov
John Dallman, R&D Manager	DE-DO	Capability Sustainment through Diversification			dallman@lanl.gov
Bryan Fearey, Executive Advisor	ADWP	Overview of Publication Records and Recognition	People	All	bfearey@lanl.gov
David Funk, R&D Manager	HX-DO	DARHT Update	Penetrating Imaging	Integral Experiments and Validation/Weapon Design	djf@lanl.gov
Tim Germann, R&D Scientist	T-1	Spatial Temporal Frontiers of Atomistic Simulations	Computation, Codes, and Platforms	Computational Math and Physics	tcg@lanl.gov
Joyce Guzik, R&D Scientist/Laboratory Fellow	X-2	Defense Research Review (DRR) Process	People		joy@lanl.gov
Donald Haynes, Group Leader	X-4	Advanced Certification	Nuclear Weapons Design	Weapon Design	dhaynes@lanl.gov

Presenter/Title	Organization	Presentation Title	Thrust Area	Capability Title	E-Mail Address
Paul Henning, R&D Scientist	CCS-2	Roadrunner Updates - Codes	Computation, Codes, and Platforms	High-Performance Computing	phenning@lanl.gov
Mary Hockaday, Deputy Associate Director/Program Director	ADWP	Experimental Science Capabilities	Weapons Science	All Experimental Capabilities	mhockaday@lanl.gov
John Hopson, Program Director	ADWP	Modeling and Simulation Capability Futures and Discussion	Computation, Codes, and Platforms	High-Performance Computing	jhopson@lanl.gov
Michael Irving, Security Specialist	PS-4/ADWP	Security Briefing			irving@lanl.gov
Charles McMillan, Associate Director	ADWP	Overview and Strategic Directions			mcmillan1@lanl.gov
John Sarrao, Program Director	SPO-SC	MaRIE: Matter-Radiation Interactions in Extremes	Facilities		sarrao@lanl.gov
Terry C.Wallace Jr., Principal Associate Director	PADSTE	Committee Charge			terryw@lanl.gov
Andrew White, Deputy Associate Director	ADTSC	Roadrunner Update – Hardware	Computation, Codes, and Platforms	High-Performance Computing	abw@lanl.gov

**Weapons Science Capability Review
Poster Session Presenters
March 26, 2009**

Presenter(s)	Organization	Poster Title	Thrust Area	Capability	E-Mail Address
Tariq Aslam	DE-9	Capturing Material Variability and Environmental Conditions in Detonation Shock Dynamics (DSD)	Weapons Science	Dynamic & Reactive Material Properties & Characterization	aslam@lanl.gov
Markus Berndt	T-5	Feasible Set Untangling of Multi-material Meshes	Computation, Codes, and Platforms	Computational Math & Physics	berndt@lanl.gov
Donald W. Brown	MST-8	Neutron Diffraction Study of the Strain Rate Dependent Development of Microstructure in Beryllium	Weapons Science	Weapons Material Properties & Characterization	dbrown@lanl.gov
Geoff Brown	DE-1	Understanding and Predicting Detonator Powder Aging	Weapons Science	Dynamic & Reactive Material Properties	geoffb@lanl.gov
Ellen Cerreta	MST-8	Shear Localization of U-6Nb: Experiments to Support Process Aware Damage Modeling	Weapons Science	Weapons Material Properties & Characterization	ecerreta@lanl.gov
Jimmy Fung	X-3	Ejecta Modeling in FLAG	Weapons Science	Theory & Modeling	fung@lanl.gov
Tim Goorley	X-3	Nuclear Weapon Effects for Urban Consequences	Weapons Design	High-Performance Computing	jgoorley@lanl.gov





Presenter(s)	Organization	Poster Title	Thrust Area	Capability	E-Mail Address
Margo Greenfield	DE-9	Towards Coherent Control of Initiation & Detection of Explosives	Weapons Science	Dynamic & Reactive Material Properties & Characterization	margog@lanl.gov
Bob Hackenberg	MST-6	Aging Mechanisms & Lifetime Prediction in Uranium-Niobium Alloys	Weapons Science	Weapons Material Properties & Characterization	roberth@lanl.gov
Tony Hill	LANSCE-NS	A Time Projection Chamber for High Precision Fission Cross Section Measurements at LANSCE	Weapons Science	Radiochemistry and Nuclear Science	tony.hill@lanl.gov
David Holtkamp	P-23	Phase Change Experiments on Multiphase Materials	Weapons Science	Dynamic Model Validation	holtkamp@lanl.gov
Dan Horner	T-1	Quantum Molecular Dynamics Simulations of Warm Dense Matter	Weapons Science	Theory & Modeling	dahorner@lanl.gov
Marian Jandel	C-NR	New Neutron-Induced Reactions Measurements for Nuclear Forensics and Stockpile Stewardship using DANCE	Weapons Science	Radiochemistry and Nuclear Science	mjandel@lanl.gov
Andrea Labouriau	MST-7	Probing Polymer Aging Mechanisms for Weapons Applications	Weapons Science	Weapons Material Properties & Characterization	andrea@lanl.gov
Frank Merrill	P-25	The 2008 pRad Scientific Program	Penetrating Imaging	Dynamic Model Validation	fmerrill@lanl.gov

Presenter(s)	Organization	Poster Title	Thrust Area	Capability	E-Mail Address
David Montgomery	P-24	High Energy Density Science & Initiatives of the Trident User Program	Weapons Science	Dynamic Model Validation	montgomery@lanl.gov
Paulo Rigg	DE-9	Obtaining Multiphase Equation of State Information Using 1D Compressional Loading	Weapons Science	Dynamic & Reactive Material Properties & Characterization	prigg@lanl.gov
Krista Stalsberg-Zarling	X-4	Evolving the Molecular Mix in the BHR Turbulence Transport Model in RAGE	Weapons Science	Dynamic Model Validation	ksz@lanl.gov
Chris Tomkins	P-21	Quantification of Density Errors in DARHT Radiography Using the French Test Object (FTO)	Penetrating Imaging	Integral Experiments & Validation	ctomkins@lanl.gov
Wendy Vogan-McNeil/ Matt Briggs	HX-4	Fundamental Photon Doppler Velocimetry Capabilities	Weapons Science	Integral Experiments & Validation	vogan@lanl.gov


	Audits & Ethics Director Terry Brendlinger
	Community Programs Office Kurt Steinhaus
	Chief Prime Contracts Mike Rafferty
	Office of Equal Opportunity & Diversity Charles (CJ) Bacino
	Ombuds Office John Armijo (Acting)
	Comm. & Gov. Affairs Lisa Rosendorf




Terry Wallace
Principal Associate Director
Science, Technology & Engineering

			
Chemistry, Life, & Earth Sciences Assoc. Director Mary Neu	Engineering & Engineering Sciences Assoc. Director Scott Gibbs	Experimental Physical Sciences Assoc. Director Susan Seestrom	Theory, Simulation, & Computation Assoc. Director Alan Bishop
ADCLES Chemistry	ADE Applied Engineering & Technology	ADEPS Physics	ADTSC Theoretical
Biology	Accelerator Operations & Technology	Materials Science & Technology	High Performance Computing
Earth & Environmental Sciences	Departmental Computing Services	Materials Physics & Applications	Computer & Computational Sciences
	Engineering Services	Los Alamos Neutron Science Center	
	Software and Applications Engineering		
	Network Infrastructure and Engineering		
	Prototype Fabrication		
Laboratory-Directed Research & Development Program Office	Science Program Office		
Science & Technology Base	Technology Transfer		
	LANL Institutes		


Institutional Leaders




Michael R. Anastasio
Laboratory Director




Isaac E. Richardson
Deputy Laboratory Director







Executive Director
Rich Marquez



Executive Office Manager
Peggy Gonzales









Glenn Mara
Principal Associate Director
Weapons Programs

			
Stockpile Manufacturing & Support Assoc. Director Carl Beard	Weapons Engineering Assoc. Director Bret Knapp	Weapons Physics Assoc. Director Charles McMillan	Threat Reduction Assoc. Director Mike Burns (Acting)
ADSMS Program Management & Production Planning	ADWE Weapons Technology	ADWP Applied Physics	ADTR Decision Applications
Plutonium Manufacturing & Technology	Weapons Systems	Dynamic and Energetic Materials	International & Applied Technology
Weapons Component Manufacturing	Hydrodynamic Experiments		International, Space, & Response
Manufacturing Quality			Nuclear Nonproliferation
RAD Liquid Waste			



Mike Mallory
Principal Associate Director
Operations & Business

					
Nuclear & High Hazard Operations Assoc. Director Robert McQuinn	Project Management & Site Services Assoc. Director Thomas McKinney	Environment, Safety, Health, & Quality Assoc. Director Chris Cantwell	Safeguards & Security Assoc. Director Michael Lansing	Business Services Assoc. Director Doris Heim	Environmental Programs Assoc. Director Michael Graham
ADNHQ Safety Basis	ADPMSS FIRP Projects	ADESHQ Radiation Protection	ADSS Security	ADBS Human Resources	ADEP Waste Services
Operations Support	Program Projects	PAAA Office	Safeguards	Central Training	TRU Waste Disposition
CMR Facility Operations	Construction Management	Occupational Medicine	Emergency Operations	Information Resource Management	TA-21 Closure
TA-55 Facility Operations	Cost & Schedule	Environmental Protection		Acquisition Services	LANL Water Stewardship Project
LANSCE Facility Operations	CMRR	ISMS/Worker Safety Office			Environment & Remediation Support Services
Weapons Facility Operations	Infrastructure Planning	Quality Assurance			Corrective Actions
Environmental & Waste Management Facility Operations	Maintenance & Site Services	Industrial Hygiene and Safety			
Institutional Facilities & Central Services Operations					
Science & Technology Facility Operations					
Utilities & Infrastructure Facility Operations					
Fire Protection Division					

	Contractor Assurance Officer Roland Knapp
	Cyber Security Office Director Vacant
	Chief Information Officer Tom Harper
	Chief Counsel David Sosinski
	Chief Financial Officer Glenn Kizer
	National Security Officer Patrice Stevens (Acting)

Weapons Science Capability Review

March 25 – 27, 2009

SECURITY NOTICE: Electronics, including cell phones, two-way pagers, PDAs (Blackberry, PalmPilot, etc.), laptop computers, thumb-drives, cameras, etc. are NOT allowed in cleared Laboratory areas. It is suggested that visitors going behind the security fence leave all personal belongings in vehicles or hotel rooms or they will be subject to a complete search to include coats, purses, briefcases, etc.

Weapons Meeting Room
TA-03, Bldg. 1400, Room 6413B

Wednesday, March 25, 2009 (7:00 am – 7:30 pm)

- 7:00 Meet Committee Members in Lobby of Holiday Inn Express Evan Sanchez
Protocol Planner, Protocol Office
- 7:10 Bus leaves Holiday Inn..... LANL Taxi Service
- 7:15 Arrive at Otowi Building for badging..... Evan Sanchez

Institutional Requirements and Weapons Science Capability

- 7:30 **Executive Session – (closed session)** Roy Schwitters
Chair, Weapons Science Capability Review
- 7:50 Introductions, Agenda, Meeting Logistics Charles McMillan
Associate Director, Weapons Physics
- 8:00 Security Briefing..... Michael Irving
Security Program Leader, Weapons Physics
- 8:10 Director's Welcome & Committee Charge Terry Wallace, Jr.
Principal Associate Director, Science, Technology, and Engineering
- 8:45 Overview and Strategic Directions Charles McMillan
Associate Director, Weapons Physics

Institutional Host(s): Charles McMillan, ADWP 505-667-8711
Technical Host(s): Mary Hockaday, ADWP, 505-667-8711
Protocol POC: Evan Sanchez, CGA-GAO/505-667-5223/Cell 699-1121

Classification Level: Unclassified/SRD Sigma 1-10 Page 1
Dress: Business/Business Casual
RED: Classified Presentation

10:30 Break

Modeling and Simulation Capabilities

10:45 Modeling and Simulation Capability Futures and Discussion..... John Hopson
Program Director, ADWP

11:55 Depart for Working Lunch – University House

12:00 Working lunch with Early Career Staff (by invitation only) – University House

1:00 Return to Weapons Meeting Room

1:05 Code Strategy..... Bill Archer
Acting R&D Manager/Program Manager, X-3

1:50 Roadrunner
Hardware..... Andy White
Deputy Associate Director, Theory, Simulation, and Computation
Codes..... Paul Henning
R&D Scientist, CCS-2

3:00 Break

3:15 Spatial Temporal Frontiers of Atomistic Simulations Timothy Germann
R&D Scientist, T-1

Publication, Peer Review, and Recognition

4:00 Overview of Publication Record, Peer Review, and Recognition..... Bryan Fearey
Executive Advisor, ADWP

4:30 Defense Research Review (DRR) Process..... Joyce Guzik
Scientist/Laboratory Fellow, X-2

5:15 Executive Session (closed session)..... Roy Schwitters
Chair, Weapons Science Capability Review

5:45 Depart for No Host Dinner at Central Avenue Grill..... LANL Taxi Service

Agenda

6:00 *No Host Dinner at Central Avenue Grill*

7:30 Depart for Holiday Inn Express.....LANL Taxi Service

Code Strategy (U)

Bill Archer, ASC Integrated Codes Program Manager

Our strategic vision for simulations is to establish a capability base both in staff and codes that can respond to a wide variety of national requirements. This talk gives an overview of the capability drivers and the resulting responses for staff and code capabilities. (U)

Applications Development for Roadrunner: Saving Scientific Computing

Paul Henning, CCS-2

The next wave of computer processor designs requires users to radically rethink the way they develop algorithms and applications, adding new complexity to the software development process. These changes have particular impact on the scientific computing community, which is already struggling with complicated software on advanced computers. Fortunately, the *Roadrunner* petascale computer at Los Alamos National Laboratory already embodies the architectural changes underway, providing an early opportunity to tackle the challenges and prepare scientific computing for the future. This talk will illustrate some of the hardware changes that we are seeing in the market, discuss application development on *Roadrunner*, and demonstrate how this experience can help scientific computing as a whole.

WEAPONS SCIENCE CAPABILITY REVIEW

Applications Development for *Roadrunner*: Saving Scientific Computing

Paul Henning

CCS-2/Roadrunner Project
Los Alamos National Laboratory
phenning@lanl.gov

March 25, 2009



Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

UNCLASSIFIED

ADC: Paul Henning



Slide 1

Why talk about hardware in an applications talk?

- The days of “cookie-cutter” systems are over (again)
- Hardware diversity provides unprecedented computational power to software designed to take advantage of it
- At this point, high-performance software is tied to specific hardware
- Computational science will fail if we don’t change our software development practices
- LANL has a leadership opportunity with *Roadrunner*

Recent announcements illustrate the diversity in computer systems

■ New machine specifications

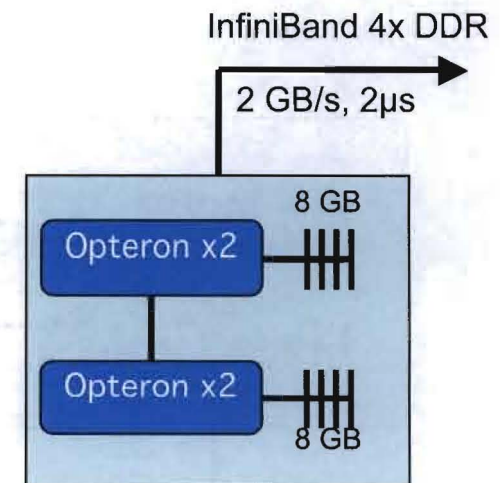
- *Blue Ice*: AMD quad-core + CELL
- *AMD Fusion Render Cloud*: >1000 GPUs, >1 PF/s
- *NSF Blue Waters*: > 200K Power7 cores, ≥ 2 GB/core
- *LLNL Sequoia*: 1.6 M BG/Q cores, 1 GB/core, SMP + MPI, >98K nodes

■ Interesting “tidbits”

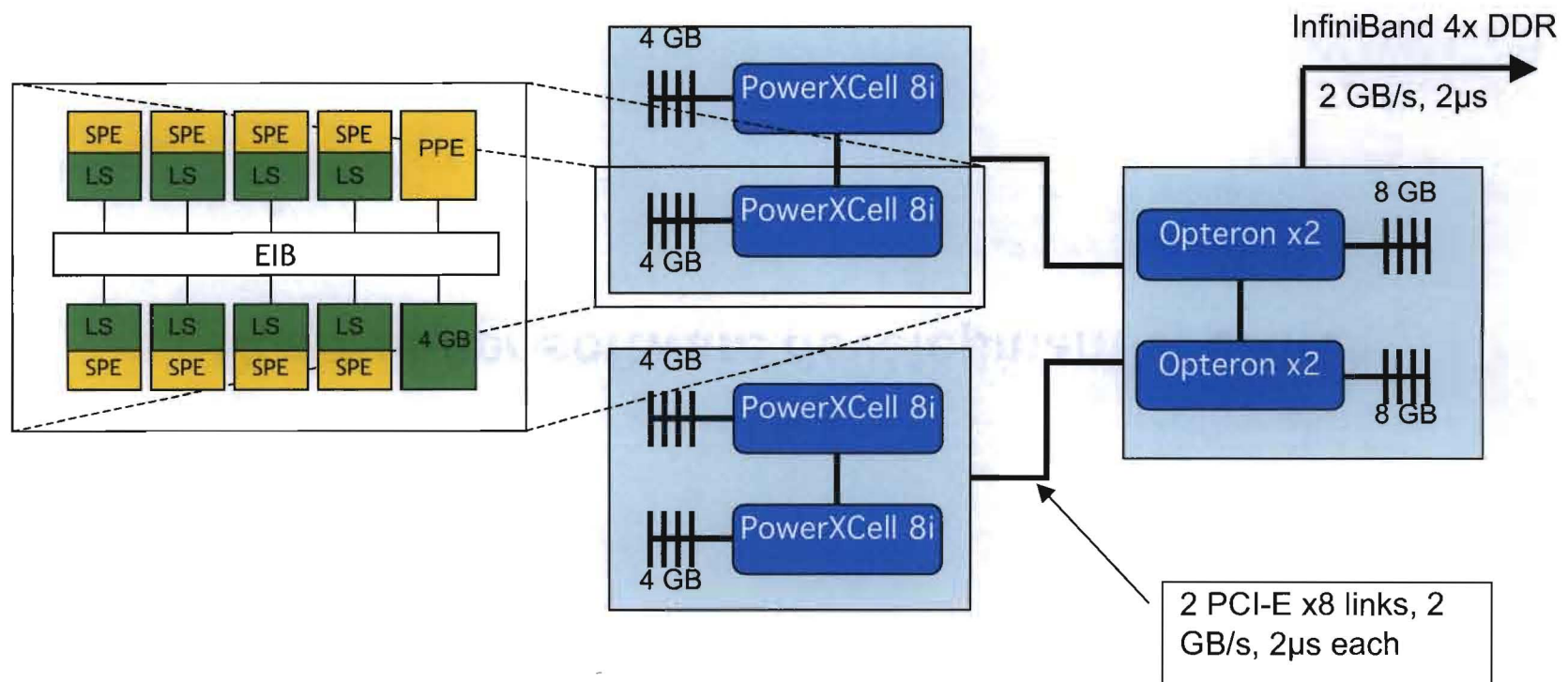
- IBM hybrid strategy: mix-and-match BlueGene, Cell, x86
- Quad-quad AMD configurations swamp memory system (Renci TR-09-01)
- Many calls for conferences and papers in “emerging architectures”
- A multitude of new processor designs are on the way

Roadrunner embodies new features of emerging architectures, while remaining familiar

- A node starts as two dual-core Opteron
- Nodes are assembled as a traditional cluster
- Existing codes can run unchanged on this portion of the machine (~50 Tflop/s)



The *PowerXCell 8i* is a heterogeneous network on a chip, and the floating point workhorse of a Triblade



Open science projects will advance both science and programming knowledge

<i>Principal Investigator</i>	<i>Project Name</i>	<i>Code Base</i>
Albright	Kinetic Thermonuclear Burn Studies with VPIC on Roadrunner	VPIC
Germann	Multibillion-Atom Molecular Dynamics Simulations of Ejecta Production and Transport using Roadrunner	SPaSM
Bhattacharya	New Frontiers in Viral Phylogenetics	ML
Daughton	Three-Dimensional Dynamics of Magnetic Reconnection in Space and Laboratory Plasmas	VPIC
Habib	The Roadrunner Universe	MC ³
Hungerford	Implicit Monte Carlo (IMC) Calculations of Supernova Light-Curves	IMC + Rage
Livescu	Instabilities-Driven Reacting Compressible Turbulence	CFDNS
Sanbonmatsu	Cellulosomes in Action: Peta-Scale Atomistic Bioenergy Simulations	GROMACS
Voter	Parallel-replica dynamics study of tip-surface and tip-tip interactions in atomic force microscopy and the formation and mechanical properties of metallic nanowires	SPaSM + PAR-REP
Yin	Saturation of Backward Stimulated Scattering of Laser In The Collisional Regime	VPIC

Roadrunner knowledge is being transferred to a broader community

- **Technical seminar series**
 - Application porting experiences
- **Tutorials**
 - Lecture-style presentations on *Roadrunner* features
- **Hands-on programming classes**
 - Intensive classroom programming courses
 - In high demand
- **Knowledge preservation**
 - <http://www.lanl.gov/roadrunner>
 - Internal wiki and mailing lists
- **Proposal writers are planning for changes due to emerging architectures**

Nostalgia is prevalent in scientific computing

- We try to make all computers look like a single processor
- We want to pretend that there is a single, flat, global memory
- We assume hardware executes our instructions perfectly
- We treat our *code* as the apex of computational science

***This is understandable,
but not sustainable!***

**While change is disruptive to productivity,
we *need* to embrace system diversity**

**“Conventional programming languages are
growing ever more enormous, but not stronger. ”**

John Backus, developer of FORTRAN.

**Backus, J. “Can Programming Be Liberated from the von
Neumann Style? A Functional Style and Its Algebra of
Programs,” CACM 21(8), August 1978.**

High-performance computing has even more challenges

- Applications must fully exploit specialized network topologies
- Applications must survive node failures in the network (resilience)
 - Checkpoint-restart activities would dominate available system time
- We must account for incorrect results (error detection/recovery)
- Power efficiency is a major driver in system *and software* design
- Large data = large problems²: I/O, analysis, visualization
- Applications must be able to run on the “next big machine”

LANL is organized for internal and external collaboration

- **LANL Center for Advanced Architectures and Usable Supercomputing (CAAUS)**
- **LANL Information Science and Technology Center (IS&T)**
- **Several institutes leverage university research:**
 - Scalable Scientific Data Management (UC-Santa Cruz)
 - Reliable High Performance Information Technology (CMU)
- **Many inter-agency collaborations in I/O, storage, and performance modeling**
- **Partnerships with all major chip vendors**
- **Actively pursuing new collaborations**

LANL is seizing the leadership opportunity

- There is an institutional commitment to tackling the challenges of emerging architectures
- CCS Division is putting into place an organizational structure that will draw together the core expertise that made *Roadrunner* a success and point them at science applications for the future for various programs
- The opportunities presented by *Roadrunner* encourage computational scientists to reconsider the design of their applications
- *Roadrunner* is not the end-goal: it is a catalyst for broad change

Spatio-Temporal Frontiers of Atomistic Simulations in the Petaflop Computational World

Timothy C. Germann, T-1

Atomistic-scale simulations are playing an increasing role in fundamental and applied materials science. Los Alamos has two distinct internationally recognized capabilities in this area: large-scale (parallel) molecular dynamics simulations, specifically the SPaSM code supported primarily by the weapons program (ASC), and accelerated molecular dynamics algorithm development and implementation under the auspices of LDRD and BES. The goal of this project is to develop and demonstrate the coupling of these two capabilities to address heretofore inaccessible problems in materials science, building a transformational capability with potential future applications in the basic energy sciences (BES), nuclear energy, and weapons programs. Two different routes are being pursued to couple large-scale and accelerated Molecular Dynamics (MD), one involving the spatial isolation of small regions where activated events are expected to occur, and the other applying acceleration techniques (“hyperdynamics”) locally, with a global synchronization. These methods are being applied to two specific problems: (1) the nucleation, growth, and coalescence of voids leading to ductile failure of metals (“spall”) following shock release; and (2) the interaction of a dislocation pileup forced against a grain boundary, a fundamental issue underlying material strength.

WEAPONS SCIENCE CAPABILITY REVIEW

**Spatio-Temporal Frontiers of
Atomistic Simulations in the
Petaflop Computational World***

Timothy C. Germann

T-1: Physics and Chemistry of Materials

tcg@lanl.gov

***LDRD-20090035DR**



Operated by Los Alamos National Security, LLC for the U.S. Department of Energy's NNSA

ADC Reviewed by Joel D. Kress (T-1 DGL)



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Charge to Capability Review Committee

1. Performance: Is the project making good progress against its first year milestones? Has the PI assembled the appropriate team, collaborators, and facilities? Is the project plan re-assessed on a regular basis, in the light of new opportunities and unanticipated difficulties, to maximize the project's impact at the end of 3 years?
2. Quality: Are the initial S&T results of high quality compared to national and international peers? *If the project is past its first year, then are project participants publishing in the archival literature and prestigious conferences?*
3. Relevance: How do the project goals relate to the strategic directions of the Laboratory? Have the PI and program development mentor (PDM) developed a transition plan, mapping out the project's future S&T direction after the LDRD funding concludes? Have the first steps of the transition plan been taken?

Spatio-Temporal Frontiers of Atomistic Simulation in the Petaflop Computational World

Goal: Develop a transformational atomistic simulation capability to enable studies of previously inaccessible materials science issues, by bringing together world-class LANL leaders in both large-scale and accelerated molecular dynamics algorithms.

Initial target applications on which we will demonstrate this capability include:

- Spall failure: develop an improved understanding of void nucleation, growth, and coalescence dynamics at length and time scales that cannot be directly probed experimentally, enabling development of a science-based model
- Dislocation pileup against a grain boundary: determine the nature of the critical event controlling material strength, a fundamental long-standing problem

• Performance Period: October 1, 2008 - September 30, 2011

• Project Budget: \$1.3 M / year



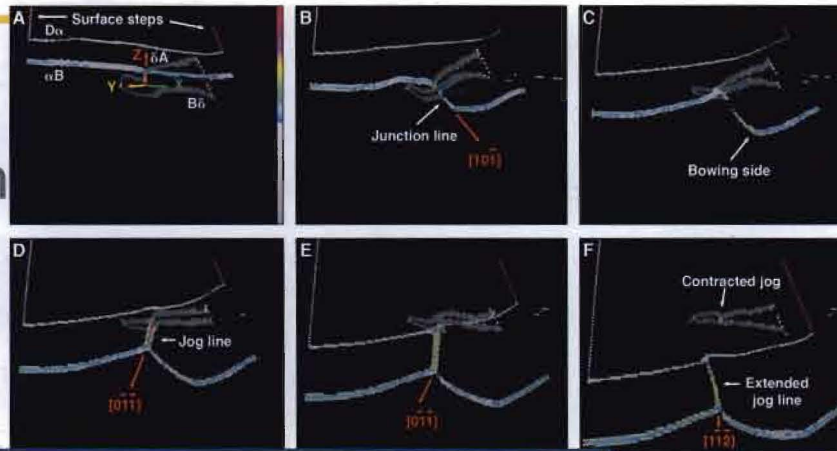
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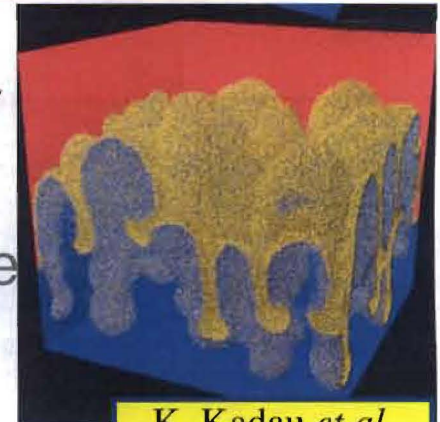
SPaSM simulations have helped to gain insight into fundamental materials and physics processes

Strength
of
metals



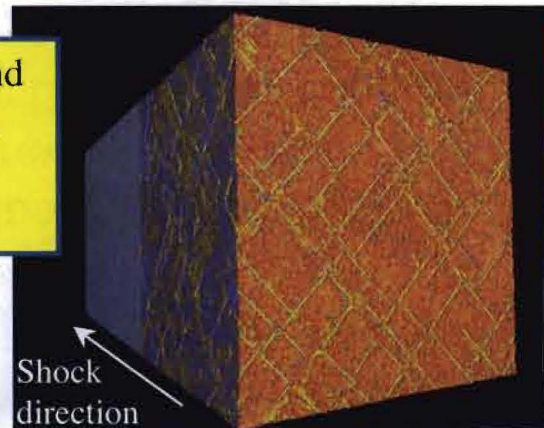
S. J. Zhou, D. L. Preston, P. S. Lomdahl, and D. M. Beazley, *Science* **279**, 1525 (1998).

Fluid
instability
and the
onset of
turbulence



K. Kadau *et al*,
PNAS **101**, 5851
(2004).

B. L. Holian and
P. S. Lomdahl,
Science **280**,
2085 (1998).



Shock-
induced
plasticity
and phase
transitions



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There are three key challenges in atomistic simulations that must be confronted in the next few years

This LDRD-DR

- Extending simulation *time* scales

Petascale simulations with $\sim 10^9$ atoms can access ns timescales; can we cleverly accelerate simulations to reach μ s-ms by focusing on key dynamical processes, and not just watch atoms vibrate endlessly? Or must we wait for exascale platforms to study processes on μ s timescales?

ASC PEM Program

- Improving interatomic *force* descriptions

Exascale computing will enable *ab initio* calculation of forces each timestep for the types of simulations we are doing now; ideally we would only resort to such calculations for local configurations beyond the regime of validity of a simpler (e.g. EAM, MEAM) empirical force field!

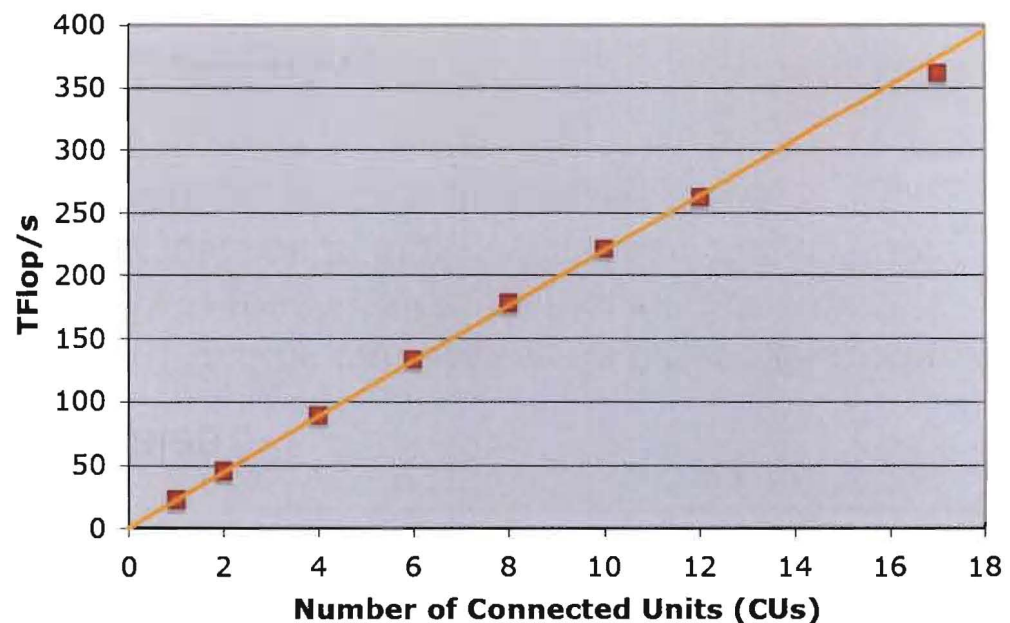
- Incorporating insights from the atomistic scale into higher length-scale models, e.g. polycrystal plasticity and strength/damage models

The parallel molecular dynamics code SPaSM achieves excellent performance on Roadrunner

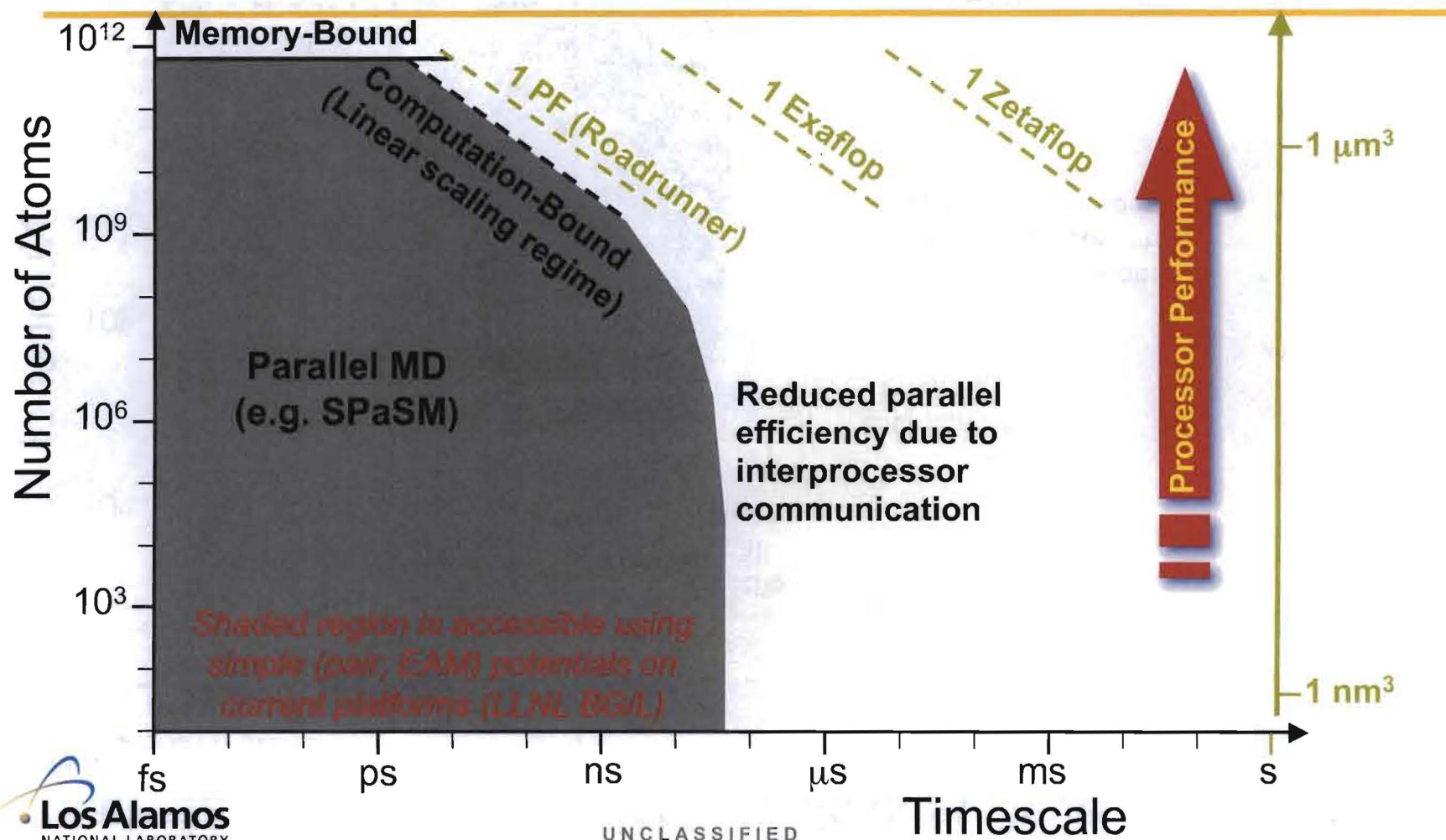
- The initial “evolutionary” port for the FY07 assessment, off-loading the CPU-intensive force subroutine to the Cell processors, was projected to reach 100 TF/s (double precision) on the full Roadrunner, a ~2.5x speedup.

- The “revolutionary” rewrite of SPaSM in FY08 takes much better advantage of the Cell accelerators, reaching ~50% of their theoretical peak performance, and 28% (**369 TF/s**) overall in initial tests done at IBM Poughkeepsie (June `08), a **10x speedup**.

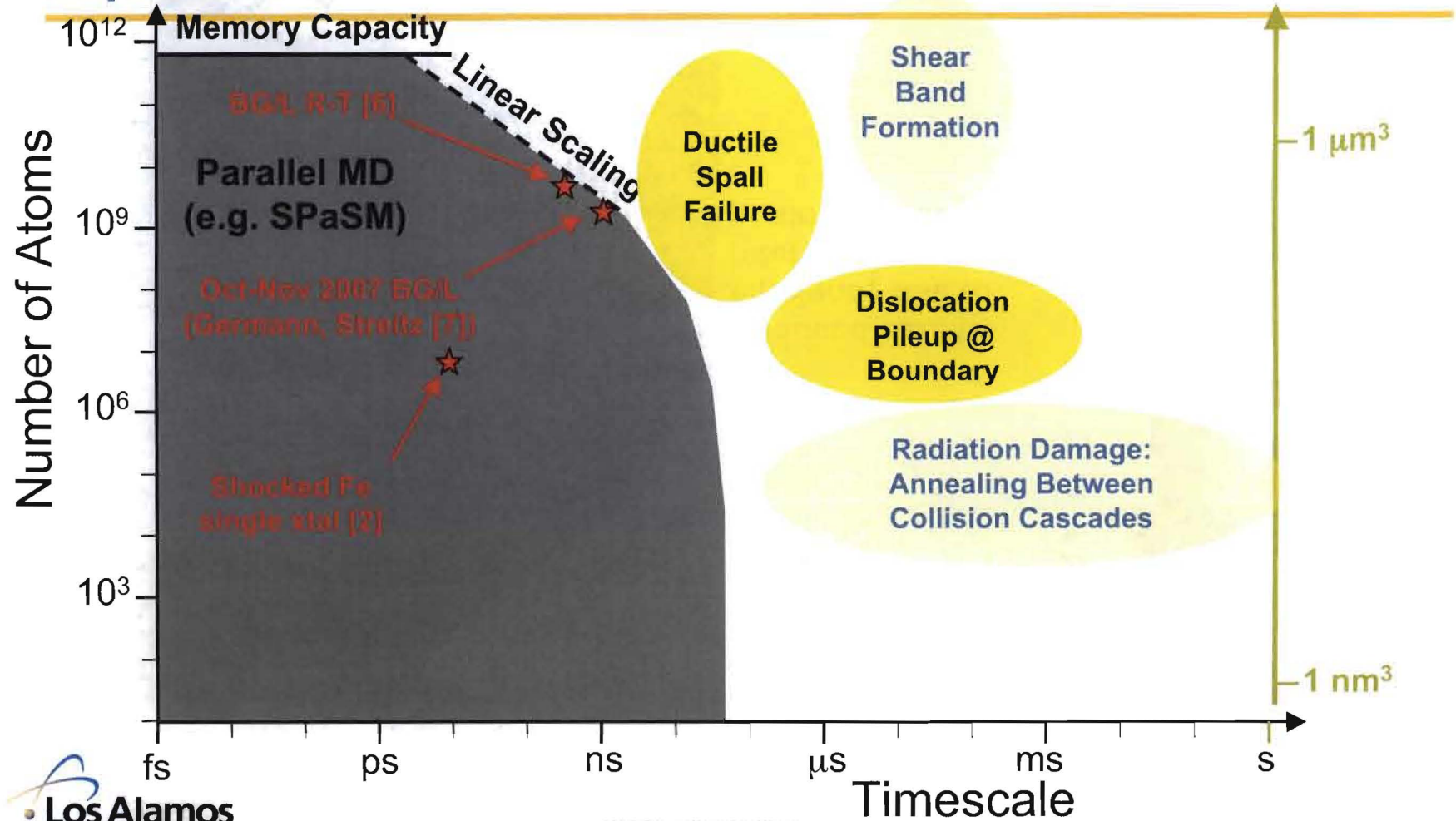
SPaSM weak scaling on Roadrunner



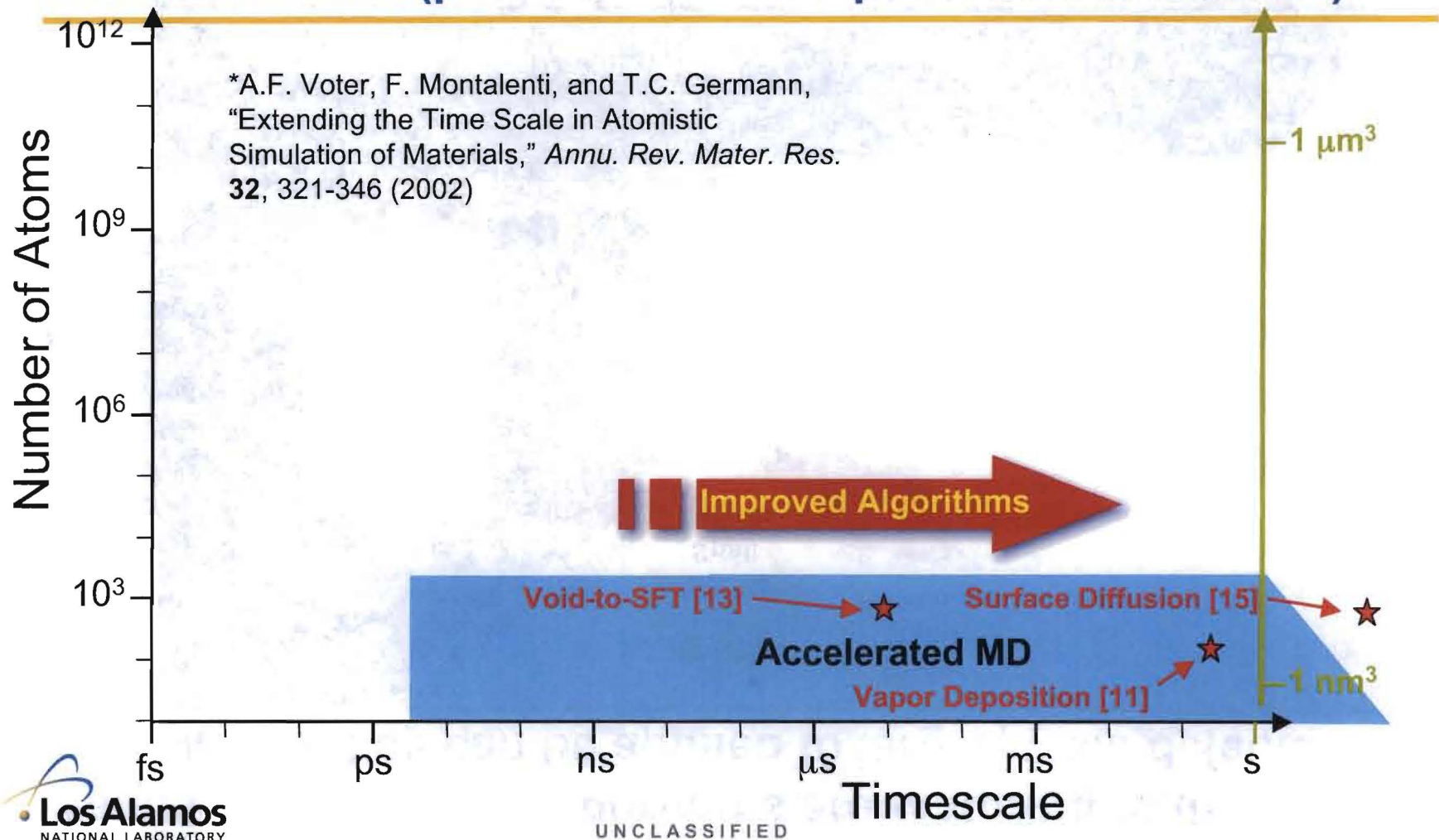
Atomistic Materials Simulations are Limited by Different Machine Characteristics in Different Regimes



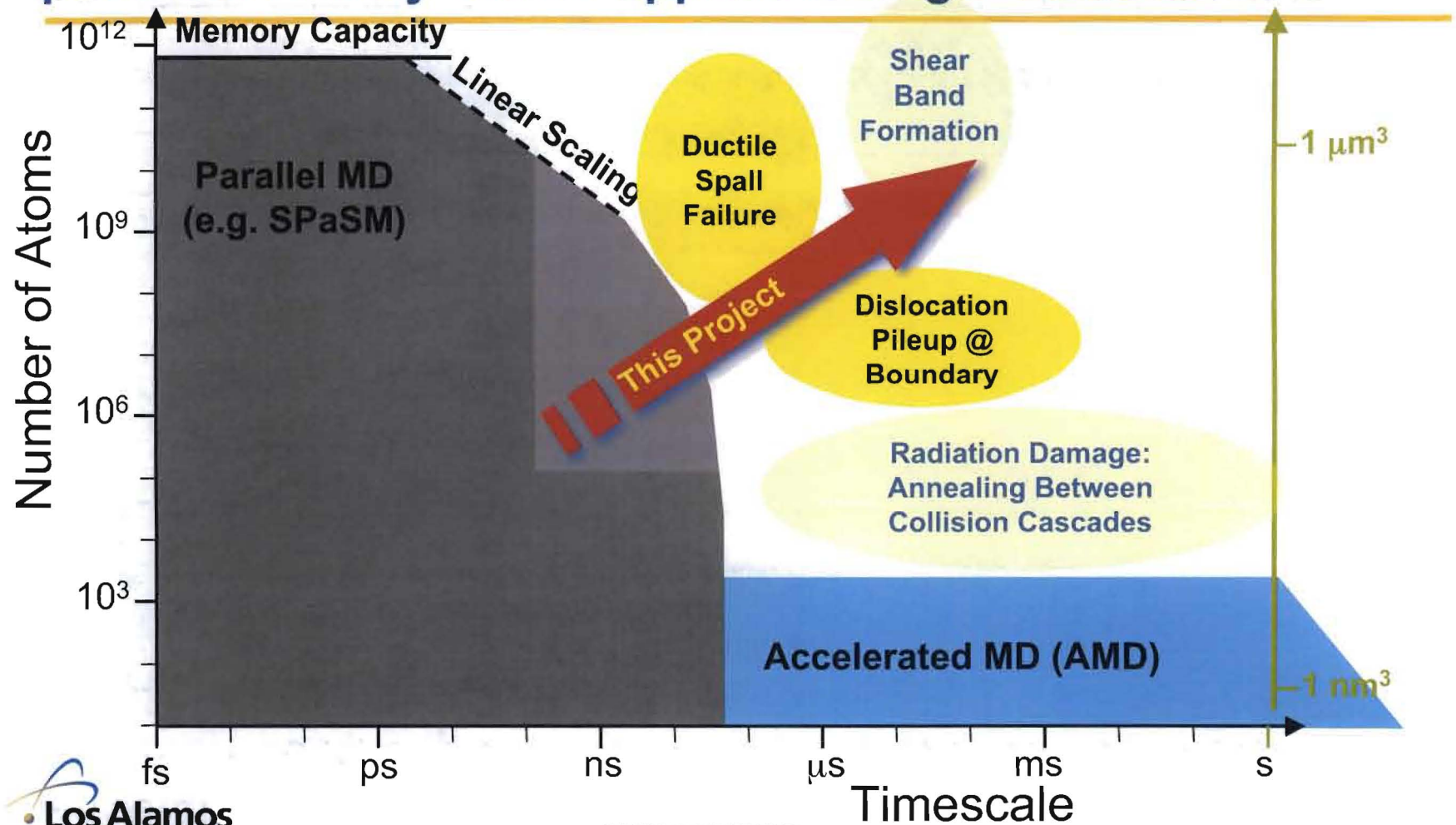
Many Materials Science Issues Lie Just Beyond Current Capabilities



Accelerated MD techniques* have been demonstrated on small scales (point defects and point defect clusters)



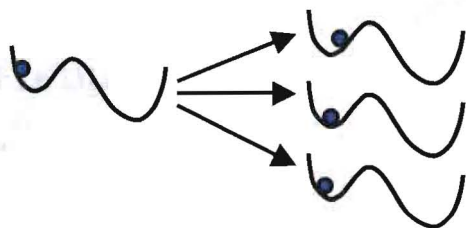
We believe that AMD algorithms are maturing to the point where they can be applied to larger-scale defects



LANL* has pioneered methods to reach long timescales for systems involving a sequence of activated processes

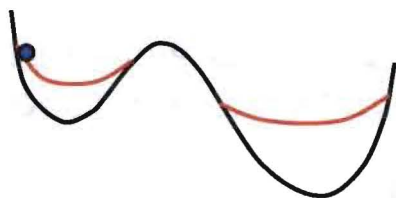
- The key concept is to let the trajectory find appropriate escape pathways
- Accelerated Molecular Dynamics (AMD) methods developed include:

Parallel Replica Dynamics



- Parallelizes time.
- Very general -- any exponential process.
- Gives exact dynamics.
- Boost requires multiple processors

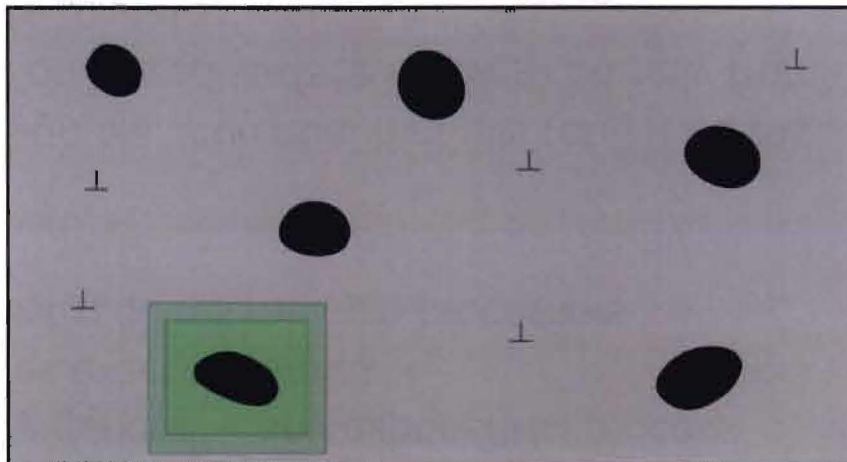
Hyperdynamics



- Design bias potential that fills (only!) basins.
- MD on biased surface evolves correctly from state to state.
- Accelerated time is statistical quantity.

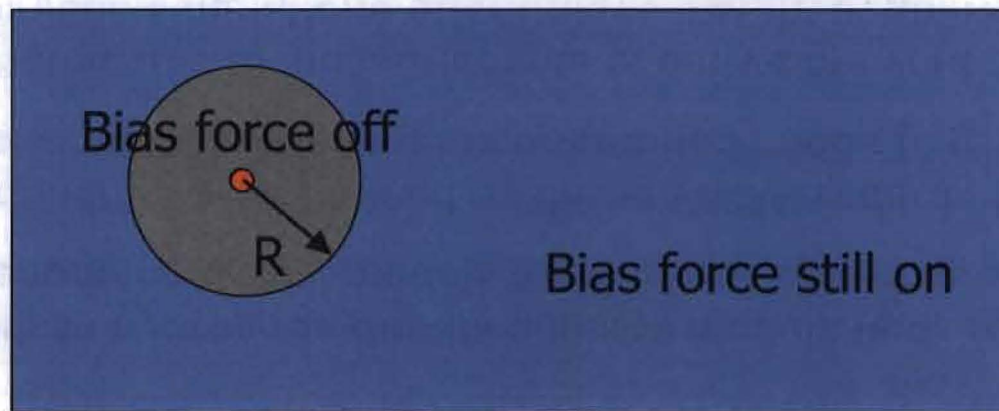
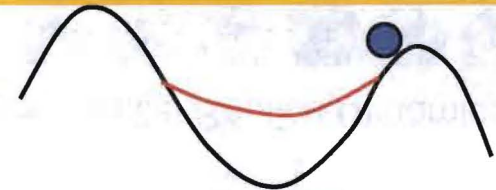
A concurrent SPaSM-AMD approach can accelerate “active” regions within a large-scale atomistic simulation

- Carve out small active regions from the full, large-scale system.
- Carry out parallel replica on the active regions using thousands of processors.
- Insure that proper boundary conditions are applied to each replica.
- The treatment of the replica boundaries is important: the boundary should respond and fluctuate as if the replicas were part of the large-scale system.
 - Enforce an average strain state as dictated by the large-scale system
 - Provide appropriate thermal fluctuations to each replica from the knowledge of the full phonon dispersion relation
 - Allow for a dynamically adequate strain relaxation in response to events occurring in the small-scale system through the use of time-dependent Green's functions
 - Provide a re-embedding scheme to allow for seamless and timely recoupling of the small and large-scale systems



Under previous LDRD funding, we proposed a *local* extension of hyperdynamics

- In hyperdynamics, if the (global) system comes close to making a transition (i.e., comes close to the dividing surface), the bias potential must go to zero.
- As the system size increases, there is an increasing probability that this is happening *somewhere* in the system at any given time. Thus, any proper bias potential *must* give vanishing boost as system size increases towards infinity.
- Under prior LDRD-ER funding, we proposed a *local-bias hyperdynamics*, in which the bias force is only turned off for atoms near the possible event.

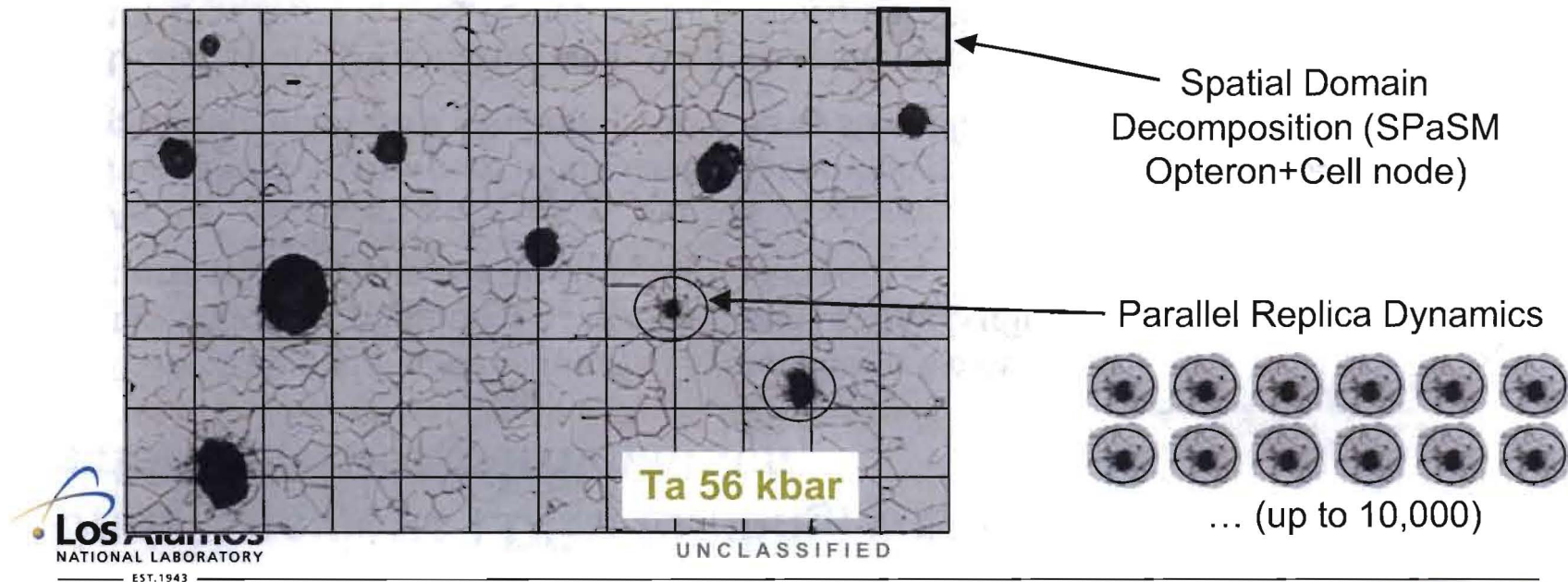


● = atom close to making a jump

R = locality range

Our first application is to study void nucleation, growth, and coalescence leading to ductile spall failure

- Modern hydrocode ductile damage models (e.g. Tonks) are based on phenomenological models for void nucleation, growth, and coalescence
- Parameters are obtained by fitting VISAR records from integrated experiments, adjusting unconstrained knobs (e.g. void volume fraction)
- Dynamic *in situ* measurements of early-time void dynamics are impossible; atomistic simulations offer unique insight at $\mu\text{m}/\text{ns}$ - μs scales



Our studies are expected to significantly enhance the realism of atomic-scale materials damage simulations

- **AMD will greatly extend simulation times for small systems, which will:**
 - Reduce strain rates from excessively high 10^9 s^{-1} to $\sim 10^5$ to 10^6 s^{-1}
 - Provide insight into the nucleation and growth of very small voids
 - Allow us to observe high barrier processes
- **Roadrunner-scale simulations will greatly extend simulation length scales, which will:**
 - Allow us to treat systems of $\sim 1 \text{ }\mu\text{m}$ size (instead of 10 nm size)
 - Compare with experimental damage structures from recovered specimens (EBSD, SEM) from a previous LDRD-DR (A. Koskelo, PI)
 - Include realistic stress concentrators (grain boundaries, inclusions)
 - Treat realistic inertial effects
 - Compare results with gas gun / laser driven experiments, as well as FEM simulations

Our second application involves a dislocation pileup forced against an obstacle (grain boundary)

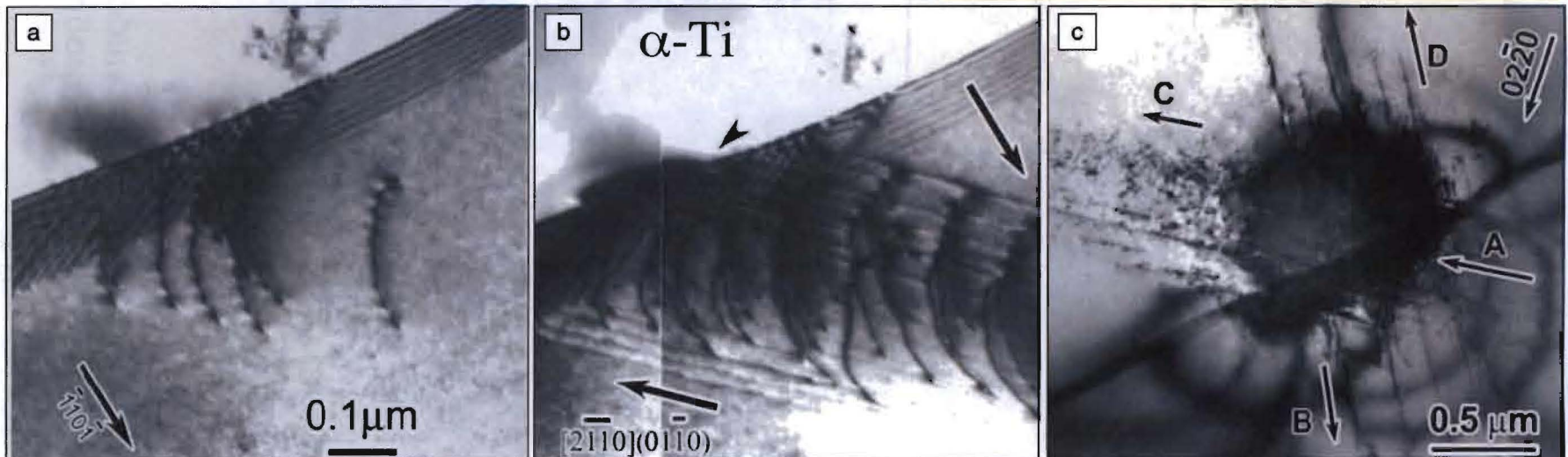
- **Dislocation pileups play a key role in the macroscopic deformation behavior of polycrystalline materials under an applied stress.**
- **When the stress near the leading dislocation in a pileup approaches a critical threshold,**
 - The dislocation may break through the barrier,
 - Initiate plastic yielding on the other side of the barrier,
 - Or lead to some other type of failure (e.g. intergranular fracture).
- **The time and length scales of this event have been too short for direct experimental observations, and (until now) too large for atomic-scale models.**

Key, rate-limiting processes controlling dislocation pileup dynamics should be discoverable

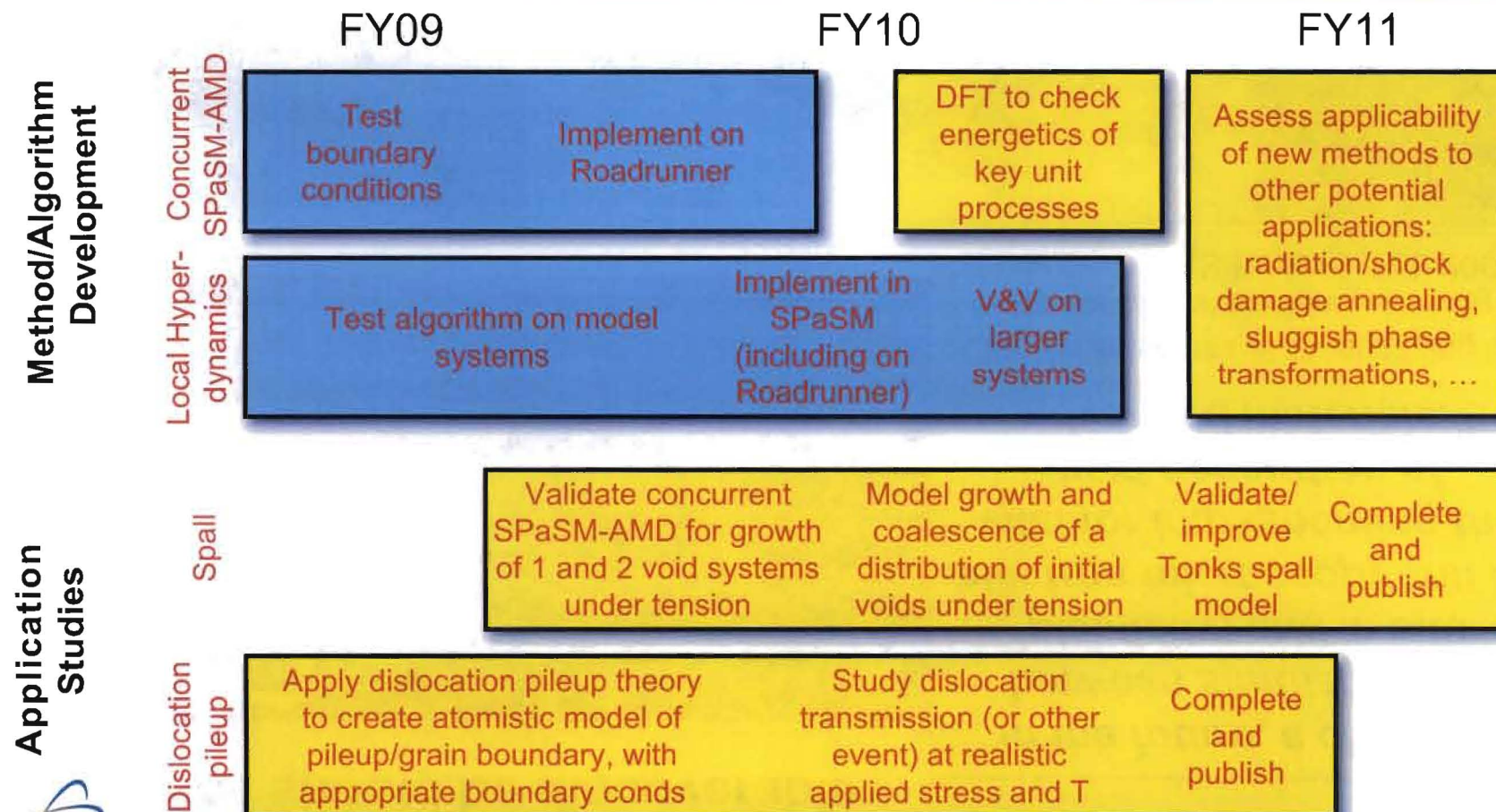


“In the future, a close link between simulation (of plasticity) and in situ electron microscopy will be vital for implementing the next generation of advanced materials.”

I.M. Robertson *et al*, “Visualizing the Behavior of Dislocations - Seeing is Believing”, MRS Bulletin (Feb 2008)



Research Schedule and Deliverables



We have assembled a strong team with complementary expertise

PI: Tim Germann

Co-PIs: Jim Hammerberg, Art Voter

Algorithm Development

Lead: **Art Voter (T-1)**

Coupling large-scale and accelerated MD:

Tim Germann (T-1)

Danny Perez (T-1 PD)

PD, TBD (T-1)

Cell/Roadrunner:

Balu Nadiga (CCS-2)

Sriram Swaminarayan (CCS-2)

Testing/scoping studies:

Kai Kadau (T-1)

Blas Uberuaga (MST-8)

Weapons Science Studies

Lead: **Jim Hammerberg (X-1)**

Simulation design/analysis:

Brad Holian (X-1)

Kai Kadau (T-1)

Shengnian Luo (P-24)

Davis Tonks (X-1)

PD, TBD (X-1)

Spall model & integration with experiments:

Shengnian Luo (P-24)

Davis Tonks (X-1)

External collaborators:

Jim Belak (LLNL)

Marc Meyers (UCSD)

Fundamental Materials Science Applications

Lead: **Dick Hoagland (MST-8)**

Simulation design:

Blas Uberuaga (MST-8)

Steve Valone (MST-8)

Zhiqiang Wang (T-3 PD)

Visualization/analysis:

Kai Kadau (T-1)

Stephen Sintay (CCS-2 GRA)

External collaborators:

John Hirth (WSU, emeritus)

Ian Robertson (UIUC)

Program Development Mentor:

John Sarrao (SPO-SC)



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VASP calculations:

Joel Kress (T-1)

Ramon Ravelo (X-1)

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(M)EAM potentials:

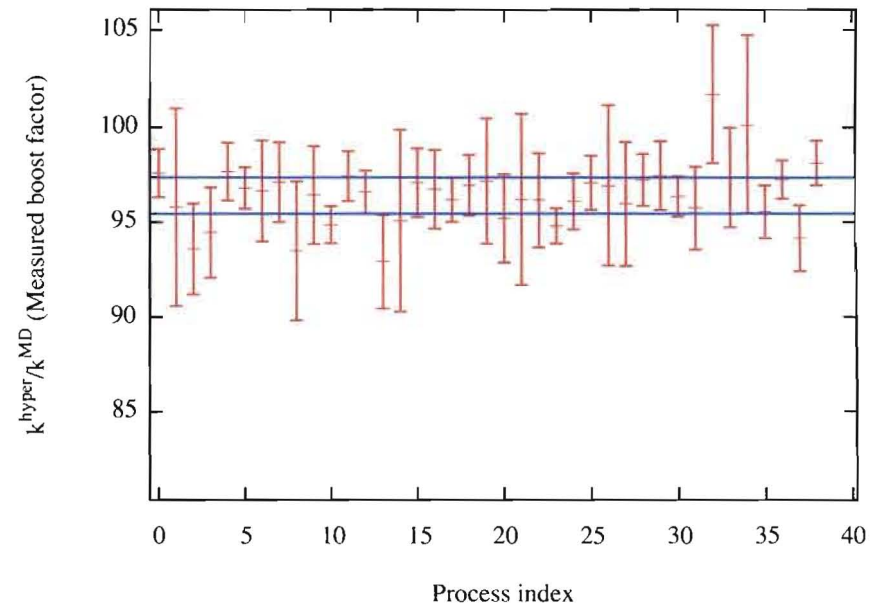
Ramon Ravelo (X-1)

Steve Valone (MST-8)



Initial tests of the local hyperdynamics algorithm are quite promising

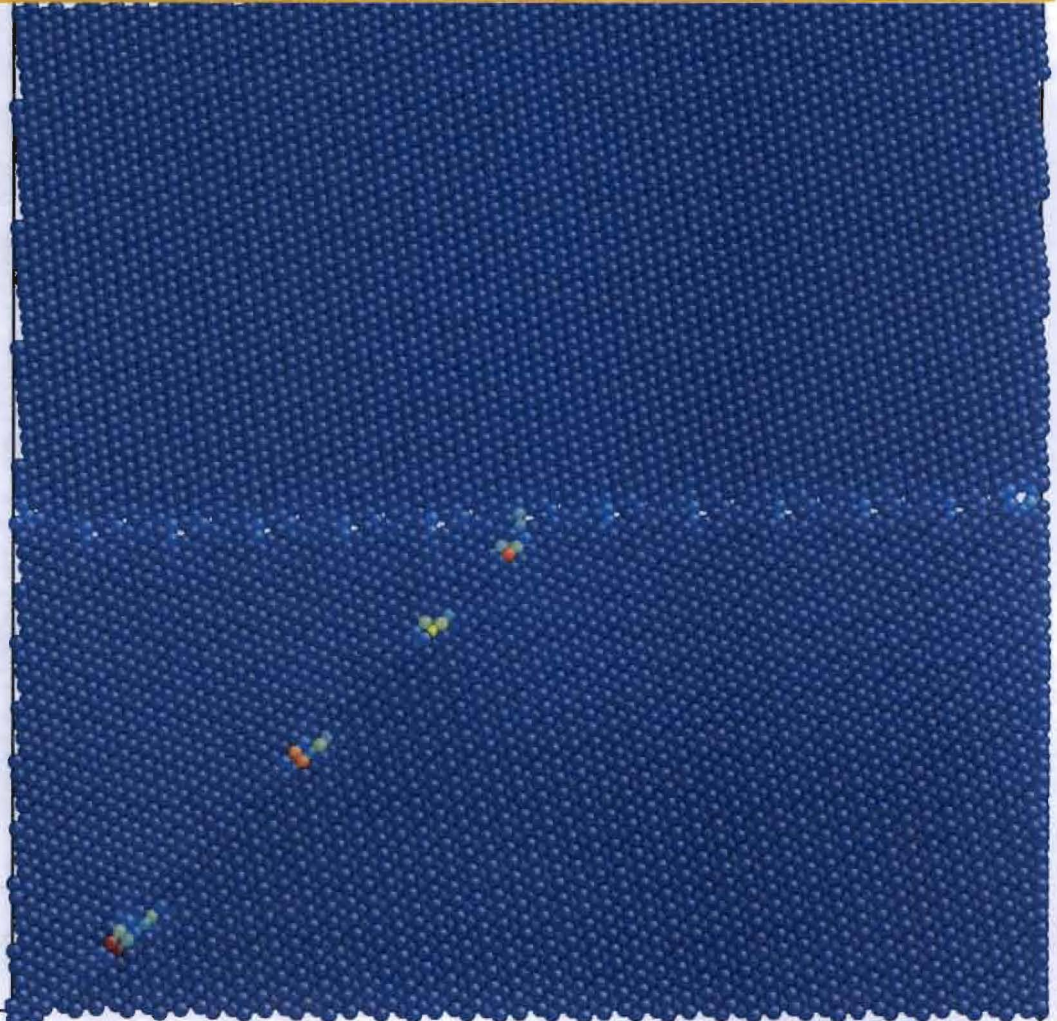
- Results on a finite, disordered 1D Frenkel-Kontorova model show excellent accuracy (uniform increase of various crossing rates, differing by a factor of ~ 50).
- The locality significantly improves the scaling of the method.
- Work is underway to speed up the parameterization of the bias potential and implement the algorithm in SPaSM (including on Roadrunner/Cerrillos).



- 3D tests are currently underway on our model EAM Al grain boundary, prior to introducing the dislocation pileup.

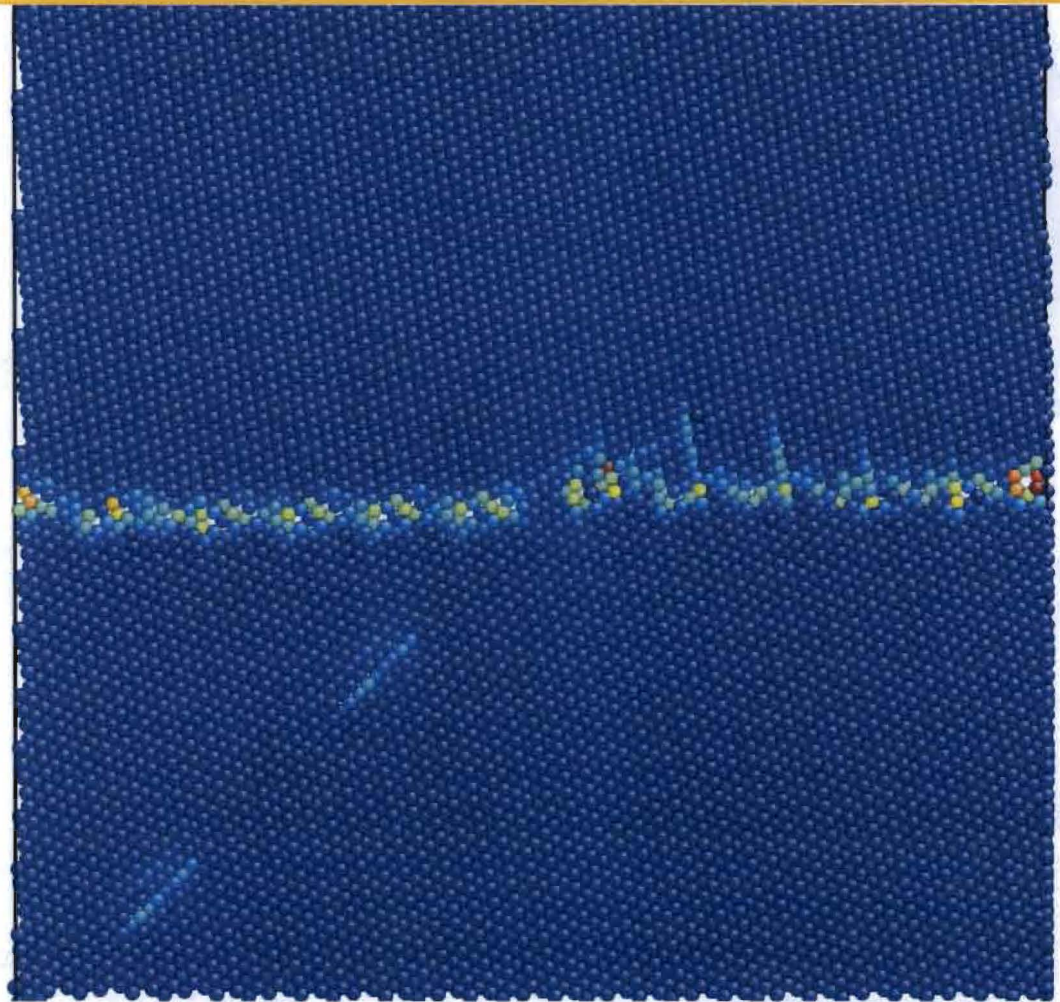
We have chosen an asymmetric $\Sigma 11$ grain boundary in aluminum for our initial pileup study

- The pileup contains 19 dislocations distributed over a distance of 2 microns.
- Only the head of the pileup is shown here.
- The shear stress acting on the pileup is very large: 4 GPa.
- Atoms are colored by excess energy.
- This shows the ideal (linear elasticity) configuration before relaxation.



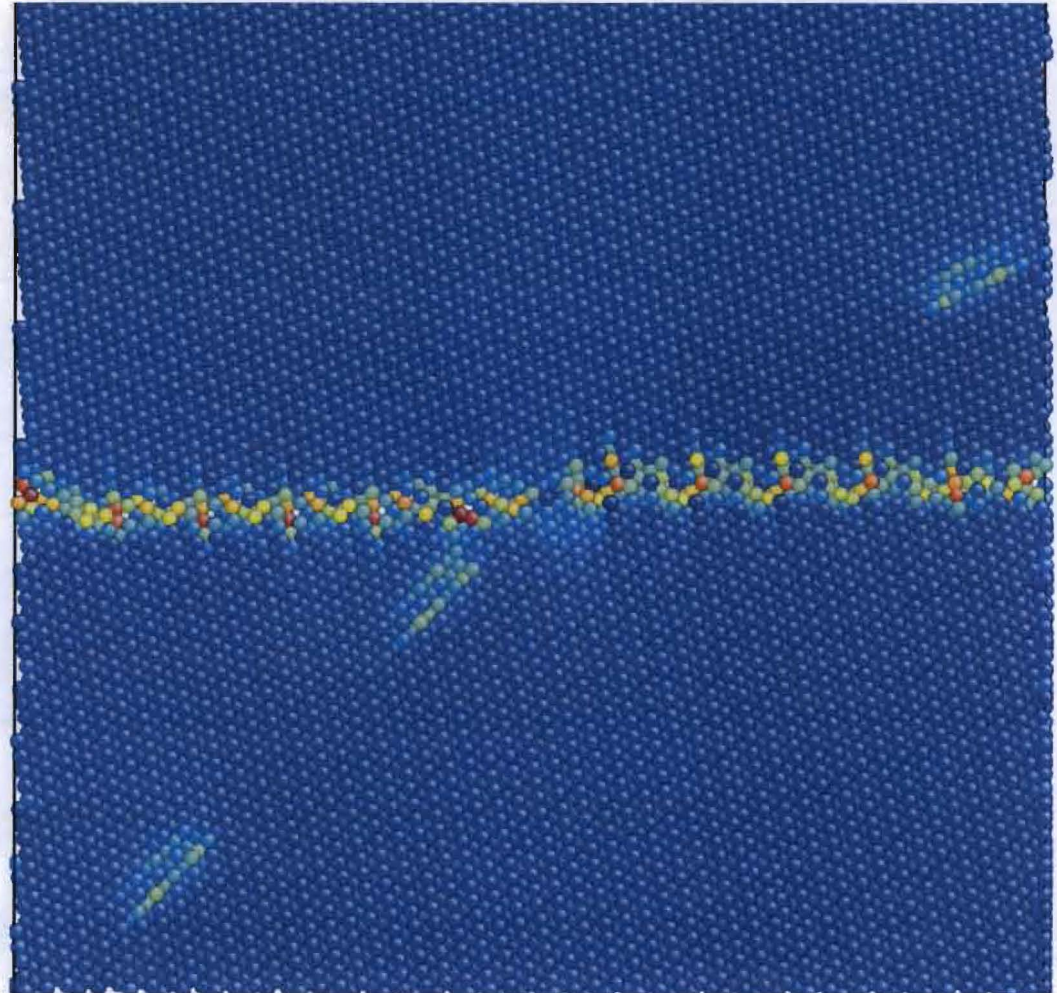
Upon relaxation, the leading two dislocations are absorbed into the grain boundary

- The pileup has been relaxed at a temperature of $\sim 0\text{K}$.
- The first two dislocations have entered the grain boundary and have become part of the grain boundary structure which has changed significantly.
- Slip transmission through the grain boundary has not occurred.

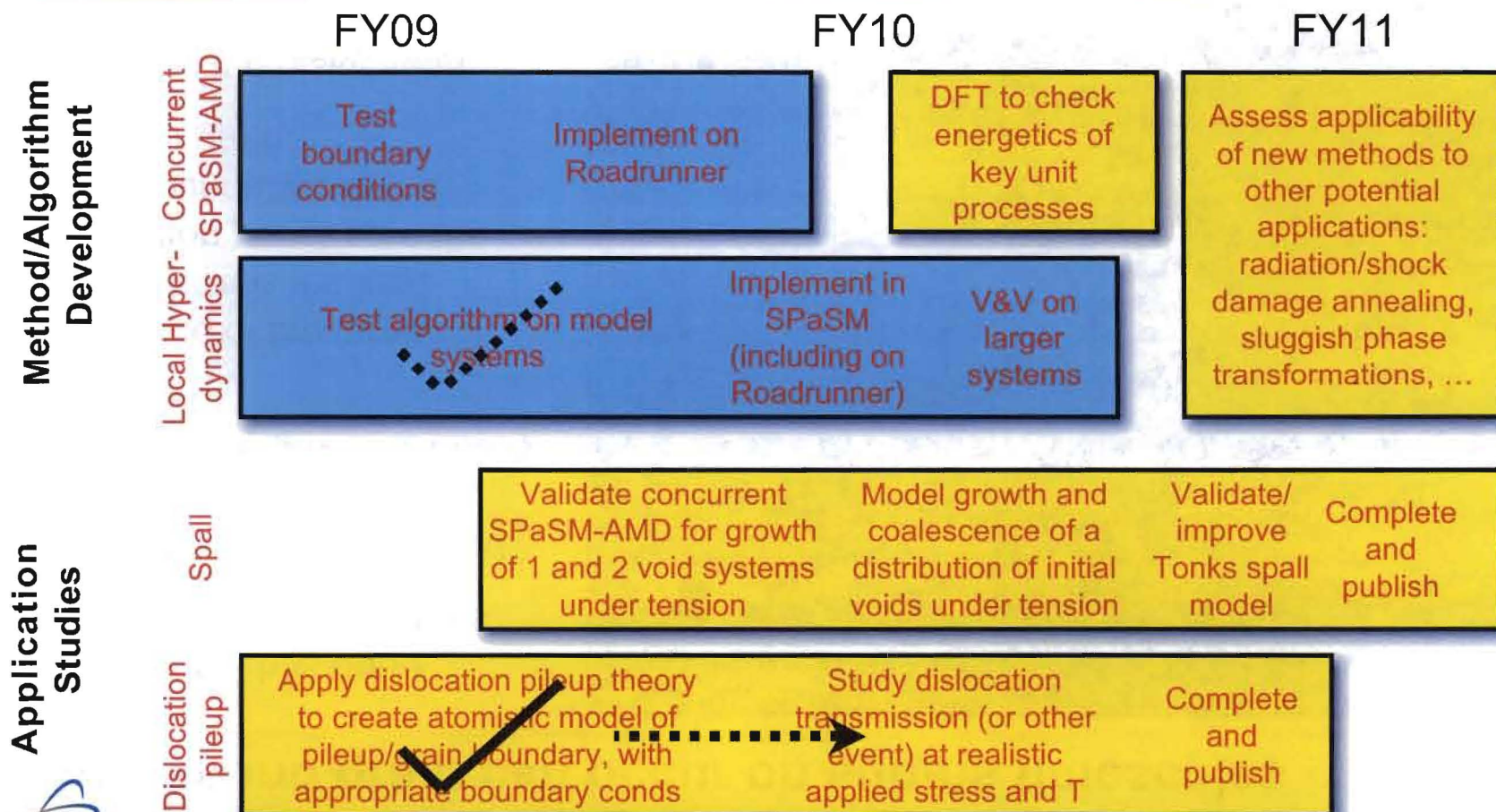


Under a high applied stress, dislocation emission into the second grain can occur on sub-ns timescales

- The model has been relaxed at 300 K for 20 ps.
- The pileup has interacted with the grain boundary changing the grain boundary structure.
- Because of the large applied stress the lead dislocation penetrated the grain boundary into the adjacent grain.
- The second dislocation entered the grain boundary and became trapped within it.



We are making good progress against our first-year milestones



We have developed a transition plan with multiple potential customers identified

Our original proposal included a transition plan with the following:

- BES, e.g. *Basic Research Needs for Advanced Nuclear Energy Systems* which called out the critical role of modeling in the development and assessment of candidate structural materials for next-generation nuclear reactors
- Nuclear Energy, e.g. GNEP or NEAMS (Nuclear Energy Advanced Modeling and Simulation)
- Weapons Programs, e.g. ASC or DOD-DOE Joint Munitions Program

We are actively involved with each of these:

- Germann, Hoagland, Uberuaga, Voter in the proposed BES EFRC *Extreme Environment-Tolerant Materials via Atomic Scale Design of Interfaces* (M. Nastasi, PI)
- Germann as co-PI (starting 1 Apr 09) of the BES project *Deformation Physics of Ultrafine Scale Materials: A Framework for Development of Engineering Materials with Near Theoretical Strength* (with A. Misra, PI)
- AFCI seed money for *Large Scale Atomistic Simulations of Thermal Conductivity in Oxide Nuclear Fuel* (with C. Stanek)
- Germann invited talk at SC08 NEAMS workshop
- Collaboration with mesoscale and macroscale modelers (e.g. Beyerlein, Bronkhorst) interested in dislocation-GB interactions, including shared postdoc and summer student from Purdue ASC PSAAP Center this fall

We have considered potential challenges and developed appropriate risk mitigation strategies

- **Coupling large scale and accelerated MD may not be as straightforward as expected**
 - Two completely different techniques, concurrent SPaSM-AMD and massively parallel local-bias hyperdynamics, are being pursued.
- **Rigid boundaries around defect regions in concurrent SPaSM-AMD algorithm may artificially constrain some transition states**
 - We will develop a flexible boundary treatment, a dynamic version of the flexible boundary conditions developed by Hoagland, Hirth, and colleagues for atomic-scale modeling of dislocations.
- **Acceleration factors will shrink as defect (void) regions grow**
 - Initial nucleation and growth steps are still accessible by AMD, and late-time coalescence is thought to be a rapid process directly amenable to large-scale (unaccelerated) MD.
- **Unexpected obstacles may be encountered in either of the two planned applications**
 - As soon as feasible, we will assess the applicability of the developed techniques to other problems of interest to potential customers.

Weapons Science Capability Review

March 25 – 27, 2009

SECURITY NOTICE: Electronics, including cell phones, two-way pagers, PDAs (Blackberry, PalmPilot, etc.), laptop computers, thumb-drives, cameras, etc. are NOT allowed in cleared Laboratory areas. It is suggested that visitors going behind the security fence leave all personal belongings in vehicles or hotel rooms or they will be subject to a complete search to include coats, purses, briefcases, etc.

Weapons Meeting Room
TA-03, Bldg. 1400, Room 6413B

Thursday, March 26, 2009 (7:00 am – 7:30 pm)

- 7:00 Meet Committee Members in Lobby of Holiday Inn Express Evan Sanchez
Protocol Planner, Protocol Office
- 7:10 Depart for TA-3-1400, Weapons Meeting Room. LANL Taxi Service
- 7:15 **Executive Session (closed session)** **Roy Schwitters**
Chair, Weapons Science Capability Review

Experimental Science Capabilities

- 8:00 Experimental Science Capabilities..... Mary Hockaday
Deputy Associate Director/Program Director, Science Campaigns
- 9:10 MaRIE: Matter-Radiation Interactions in Extremes John Sarrao
Program Director, SPO-SC
- 9:40 **DARHT Update**..... **David Funk**
R&D Manager, HX Division

10:15 Break

Diversification

- 10:30 Capability Sustainment through Diversification.... Jay Dallman
R&D Manager, DE Division

11:00 Lunch with Senior & Mid-career Staff (by invitation only) – Weapons Meeting Room

Nuclear Design

12:15 Advanced Certification.....Don Haynes
R&D Manager, X-4

1:15 Sustaining Nuclear DesignMichael Bernardin
R&D Manager, X Division

2:15 Break

2:20 Executive Session (closed session)..... Roy Schwitters
Chair, Weapons Science Capability Review

2:55 Depart for Poster Session – Oppenheimer Study Center

3:00 Poster Session – Oppenheimer Study Center – Upper Level

5:15 Depart for Working Dinner - Otowi Cafeteria

5:30 Working Dinner (by invitation only) - Otowi Cafeteria

7:30 Depart for Holiday Inn Express..... LANL Taxi Service

1:30 Closeout Meeting (DIR, PADs, AD, DAD) Terry Wallace, Jr.
Principal Associate Director, Science, Technology, and Engineering

2:30 Closeout Meeting (Open to All) Roy Schwitters
Chair, Weapons Science Capability Review

3:30 Adjourn

MaRIE

John Sarrao, Office of Science Program Office

MaRIE, for Matter-Radiation Interactions in Extremes, is LANL's signature facility concept for providing transformational materials solutions for today's and tomorrow's national security needs. In this presentation, we'll discuss the why, what, and how of MaRIE, including progress on facility definition since last year's Weapons Science Capability Review, and provide an update on MaRIE's current planning activities. These planning activities include a roadmap of needed capabilities for achieving process aware materials performance.

Dual-Axis Radiographic Hydrodynamic Test (DARHT) Facility Update

David J. Funk, Hydrodynamics Experiments (HX) Division Leader

This talk will discuss the current status of the DARHT facility, emphasizing progress made on the project, the impact of the damage to the beam stop by the accelerator, and the path forward. An overview of the Resumption plan and progress to date on the restart plan will be presented.

The Defense Research Review Publishing Process

Joyce Ann Guzik, X-2-N2

The Defense Research Review is a tri-laboratory refereed classified journal devoted to nuclear weapons science. The DRR began in 1987, and has published 49 printed issues, with 310 articles. Historically 3-4 issues per year, containing 3-5 articles per issue have been published. The DRR currently has over 300 subscribers, with 200 at LANL, 130 at LLNL, about 10 at SNL, and 3 at DOE. At LANL the DRR is managed under ADWP. Technical editing and layout are completed at LANL, and the issues are printed at LLNL. The DRR will be the venue for a special boost issue that is the focus of a Level II milestone to document and archive our understanding of boost as recommended by the JASONS in their 2008 summer study. The DRR has several near-term goals and challenges, including moving to monthly electronic-only publication; improving readership, distribution, and access; engaging AWE as a partner; and improving the processes for tracking and expediting articles from submission through publication.

WEAPONS SCIENCE CAPABILITY REVIEW

The Defense Research Review Publishing Process

Joyce Ann Guzik

X-2-N2

Los Alamos National Laboratory

March 25-26, 2009

The Defense Research Review is a Tri-Lab Classified Refereed Journal Dedicated to Nuclear Weapons Science

- **Current Scientific Editors**

- Joyce Ann Guzik, LANL (since 2004, overlap with Jack Brownell 2002-2004)
- Dennis McNabb, Oleg Schilling LLNL
- Carol Adkins, Peggy Jo Christensen, SNL

- **Editing and layout are done by Louise Mendius and Garth Tietjen (IRM-CAS, LANL) who are supported by ADWP and have offices in X Division**

- **Adobe InDesign software (IRM standard) is used for layout**

- **After proofreading by authors and scientific editors, final pdf file is sent to LLNL for printing**

- **Distribution is currently 343 printed copies (200 LANL, 130 LLNL, 10 SNL, 3 DOE))**

- **Articles are archived on X-division on-line vault and LLNL secure web, and E-mailed to LANL subscribers**

DRR articles are peer reviewed

- Articles are submitted to local scientific editor and checked for content and suitability
- Articles are sent to other two laboratories for anonymous peer review
- Editor at recipient lab chooses a referee, sometimes with advice from colleagues or the local members of the editorial board
- Referee submits review to local laboratory scientific editor. Editor reviews report and returns report to both laboratories
- Editor at article's originating laboratory reviews report, and sends to the authors for article revision and iteration, if necessary
- Article rejection rate is about 30%
- A resolution process for contentious articles needs to be defined

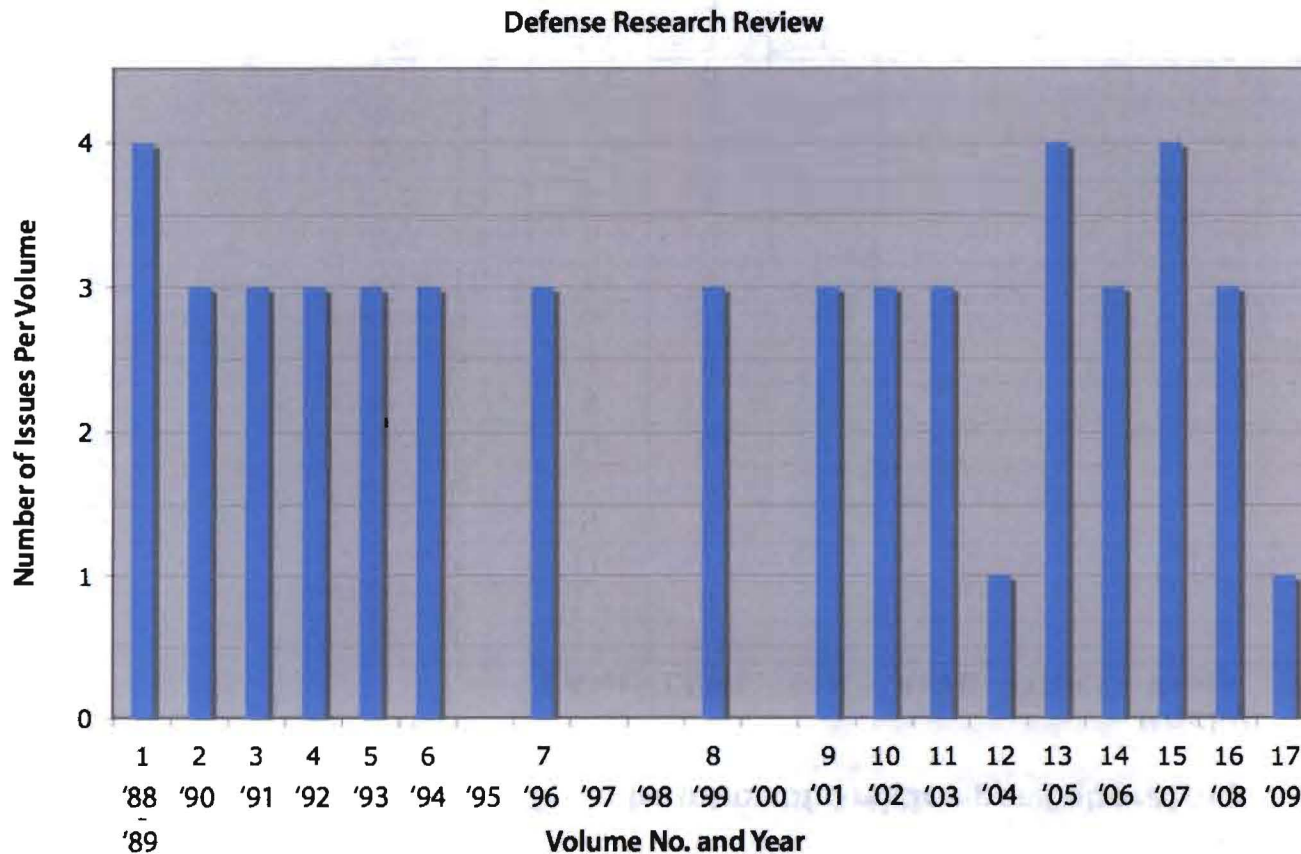
The DRR has an Advisory and an Editorial board

- **Members from three laboratories and academic institutions outside the laboratories, including high-level managers and senior scientists**
- **Boards meet infrequently, and are consulted for policy advice and recommendations for article referees**
- **Board memberships should be updated, and board members could be called upon more often to set policy**

- **Advisory Board Members**
Anastasio, Goodwin, Hagengruber, Hecker, Hunter, Jeanloz, Jones, Juzaitis, McMillan, Miller, Seestrom, Vogt

- **35 Editorial Board members**
 - Members listed in first pages of each issue

The Defense Research Review publication has been sporadic since the journal began in 1987



- **17 volumes (years)**
- **49 issues**
 - Latest issue is 17.1 (in preparation) for 2009
- **310 articles**
- **Several special topical issues**
 - Pu (2 issues)
 - Proceedings: Physics of Radiatively Driven ICF Targets
 - QMU
 - V&V
 - Diagnostics
- **Planned special issues**
 - Boost
 - Commemorative joint issue with AWE
- **2004 issues limited by stand-down**

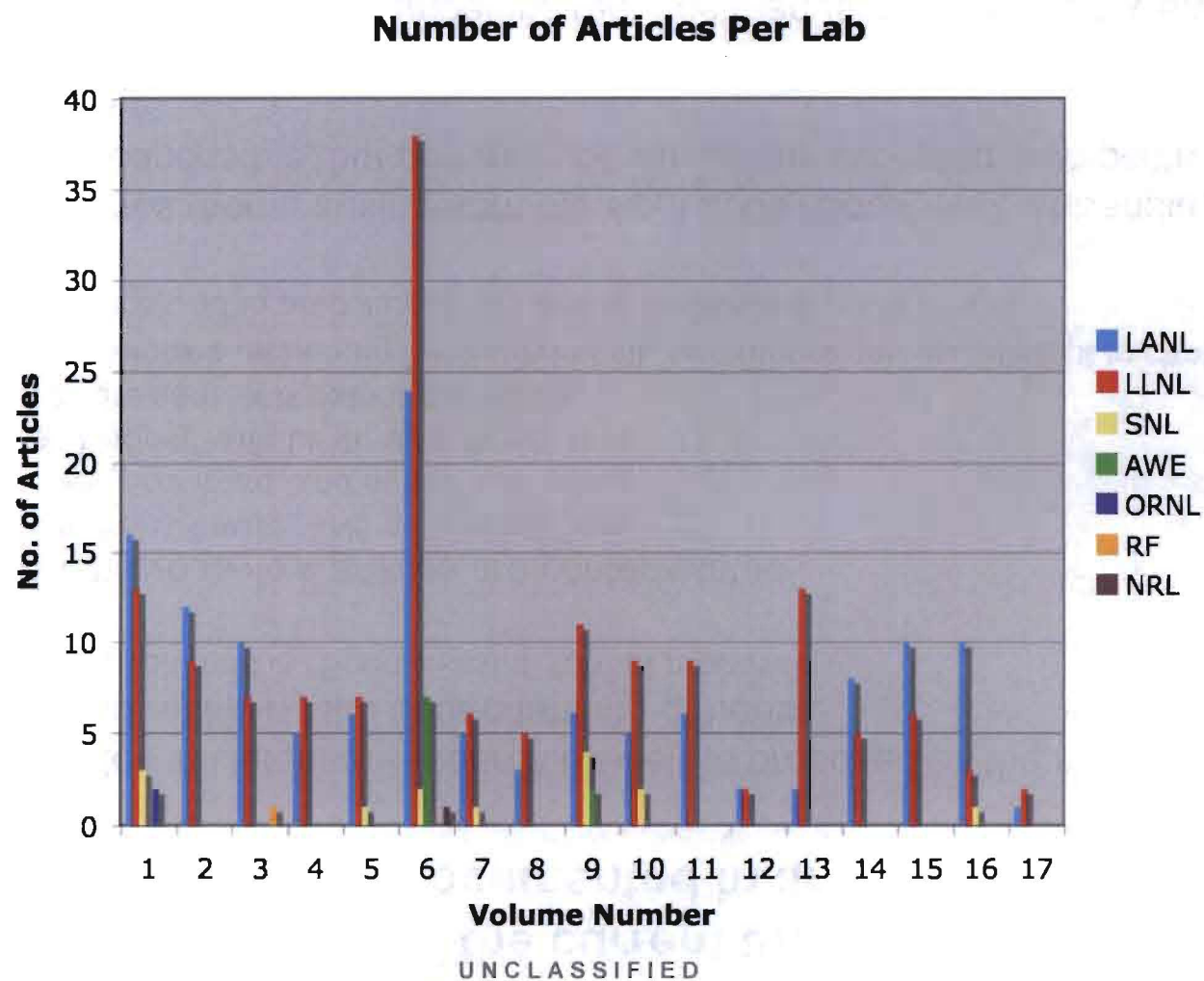
The DRR publishes three to four issues per year with four to five articles per issue, most from LANL and LLNL

Total Number of Articles per Laboratory

	LANL	LLNL	SNL	AWE	ORNL	Rocky Flats	NRL
Vol. 1	16	13	3		2		
Vol. 2	12	9					
Vol. 3	10	7				1	
Vol. 4	5	7					
Vol. 5	6	7	1				
Vol. 6*	24	38	2	7			1
Vol. 7	5	6	1				
Vol. 8	3	5					
Vol. 9	6	11	4	2			
Vol. 10	5	9	2				
Vol. 11	6	9					
Vol. 12	2	2					
Vol. 13	2	13					
Vol. 14	8	5					
Vol. 15	10	6					
Vol. 16	10	3	1				
Vol. 17	1	2					
Total	131	152	14	9	2	1	1

*Special ICF conference proceedings issue

Most articles have been authored by LANL and LLNL



The 2008 Jason Summer Study on Boost recommended that a comprehensive description of the current understanding of the boost process be undertaken and documented in an archival form

- A series of articles in Defense Research Review is proposed as the mechanism for documenting and archiving the understanding of boost.
 - One or more volumes in “Special Issue” format proposed
- Two comprehensive review articles are contemplated
 - “History of Boost” with LANL as editorial lead
 - Maurice Sheppard lead author and editor
 - “Physics of Boost” with LLNL as editorial lead
 - Frank Graziani lead author and editor
 - Both review articles have both LANL and LLNL co-authors and will attempt to capture common understandings and to articulate areas where understanding is lacking .
- Contributed articles (some arising from the April 2009 “Boost-fest” at Sandia) offer opportunity for responsible, but perhaps not universally accepted, perspectives to be captured as well.
- Level II milestone in Science Campaigns requires manuscripts for the review articles to be completed Sept 2009.

The Defense Research Review has a number of goals and challenges

- **Increase publication frequency to 1 issue/month**
- **Resolution process for controversial or rejected articles**
 - Take debate to DRR letters format
 - Acquiring more than one referee per article
 - Appeals process involving advisory or editorial boards
- **Engaging AWE as a partner laboratory in DRR**
 - Additional peer review desired
 - JAIEG transmissibility rules and delays in document transfers

Several tasks must be completed to achieve goal of one issue/month

- **Move to electronic publishing**
 - Need to establish an effective distribution process
 - Some current or desired subscribers do not have classified electronic web access or classified E-mail
 - Classified web need-to-know
 - Restricted/limited X-division on-line vault access
- **Improve turn-around time between submission and publication**
 - Desire a 2-3 month turnaround
 - 4-6 week referee process
 - Management encouragement for refereeing
- **Database system to track status of articles in submission, refereeing, and production process that is linked to three laboratories**

A project plan is being developed to achieve an October 2009 goal of one electronic issue published monthly

- | | |
|---|--------------|
| ■ Tri-Lab Management Buy-in | April |
| ■ Agreement of understanding | April |
| ■ Call for articles | End of April |
| ■ Receipt of articles for review | Mid-May-June |
| ■ Review process | Mid-May-July |
| ■ Resources in place | September |
| ■ First monthly issue ready for classification review | September 15 |
| ■ First monthly issue electronic print | October 15 |

Advanced Certification

Don Haynes, X-4 (Design 2)

The Advanced Certification Campaign was introduced at the 2008 Weapons Science Capability Review. Now that we are one year into the Campaign, I will show technical results in three areas:

- 1) definition and application of the first generation of generally applicable failure metrics and thresholds,
- 2) definition and application of a “nearness” metric on design space, and
- 3) exploration of the relative importance of parametric and model form uncertainties.

Weapons Science Capability Review

March 25 – 27, 2009

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Weapons Meeting Room
TA-03, Bldg. 1400, Room 6413B

Friday, March 27, 2009 (8:00 am – 3:00 pm)

7:15 Committee Members arrive (via private vehicle) at TA-3-1400 (Weapons Meeting Room)

7:30 **Executive Session.** **Roy Schwitters**
Chair, Weapons Science Capability Review

8:30 Meeting with Capability Leaders

9:45 **Break**

10:00 **Executive Session (closed session)** **Roy Schwitters**
Chair, Weapons Science Capability Review

12:00 **Working lunch Committee Members only**

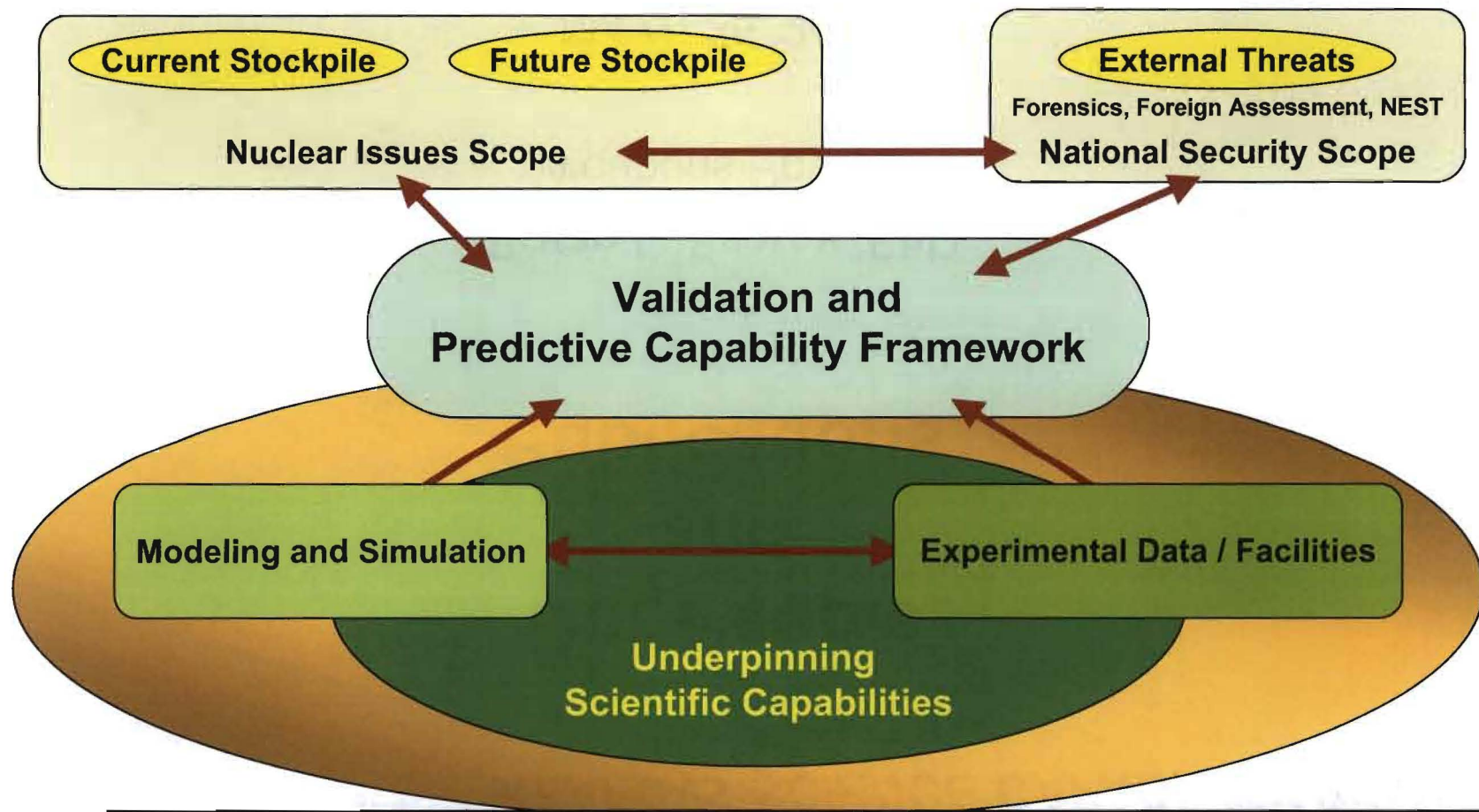
WEAPONS SCIENCE CAPABILITY REVIEW

**Our People
and
Publications**

Bryan L. Fearey, PhD
Weapons Physics

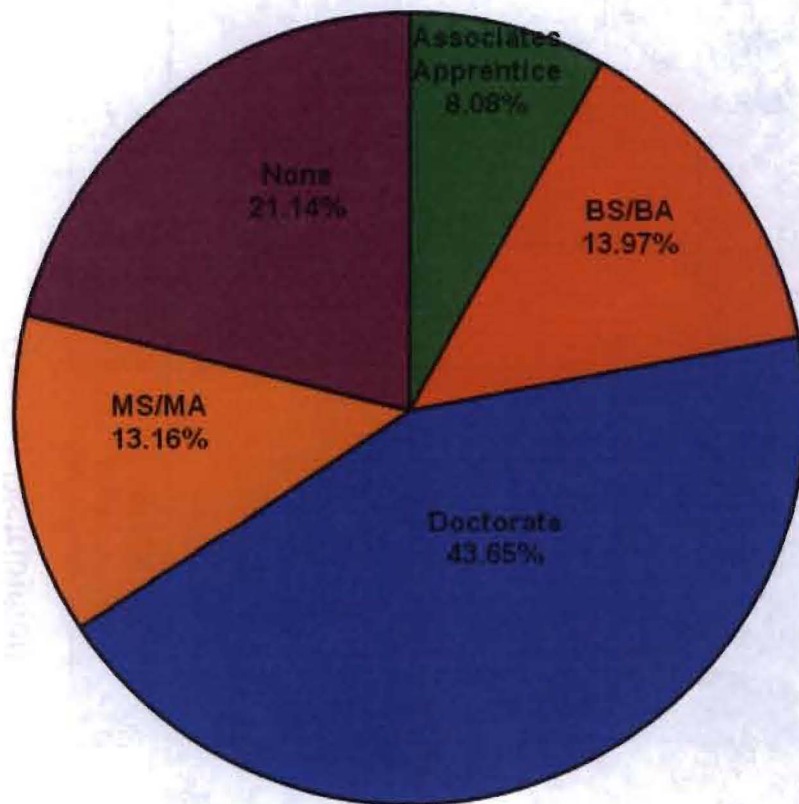
March 25, 2009

We meet our national security responsibilities through validated predictive capability

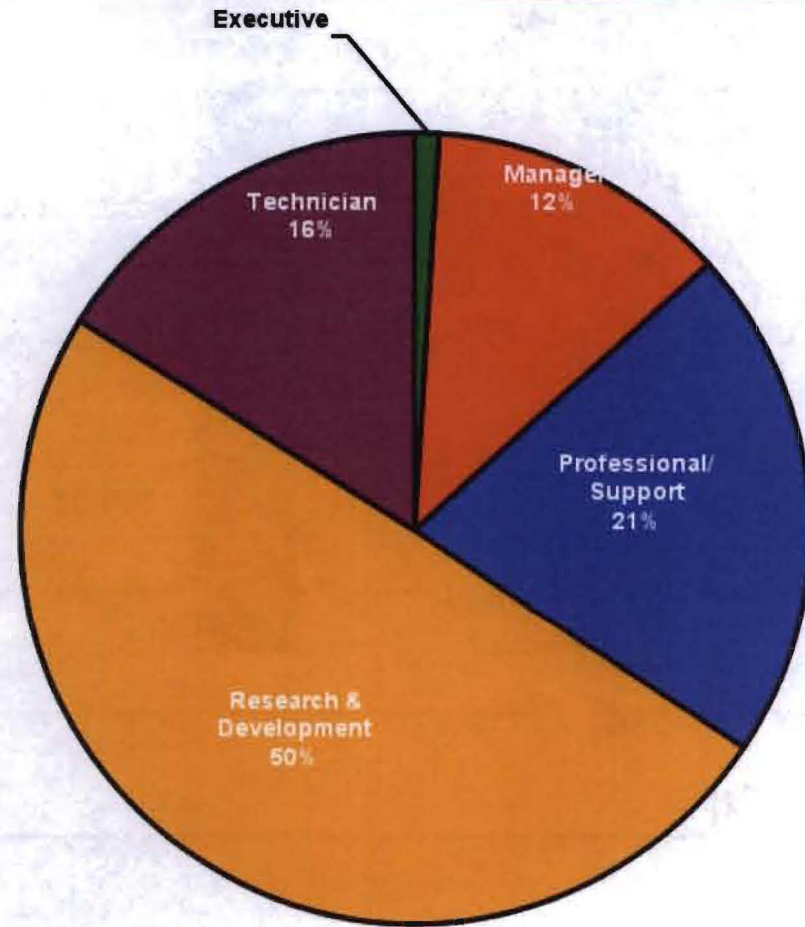


We leverage our Laboratories' science and technology advantage to anticipate, to counter, and to defeat threats and **meet national security needs**

The Weapon Science capability is supported by a well-qualified and dedicated team of employees

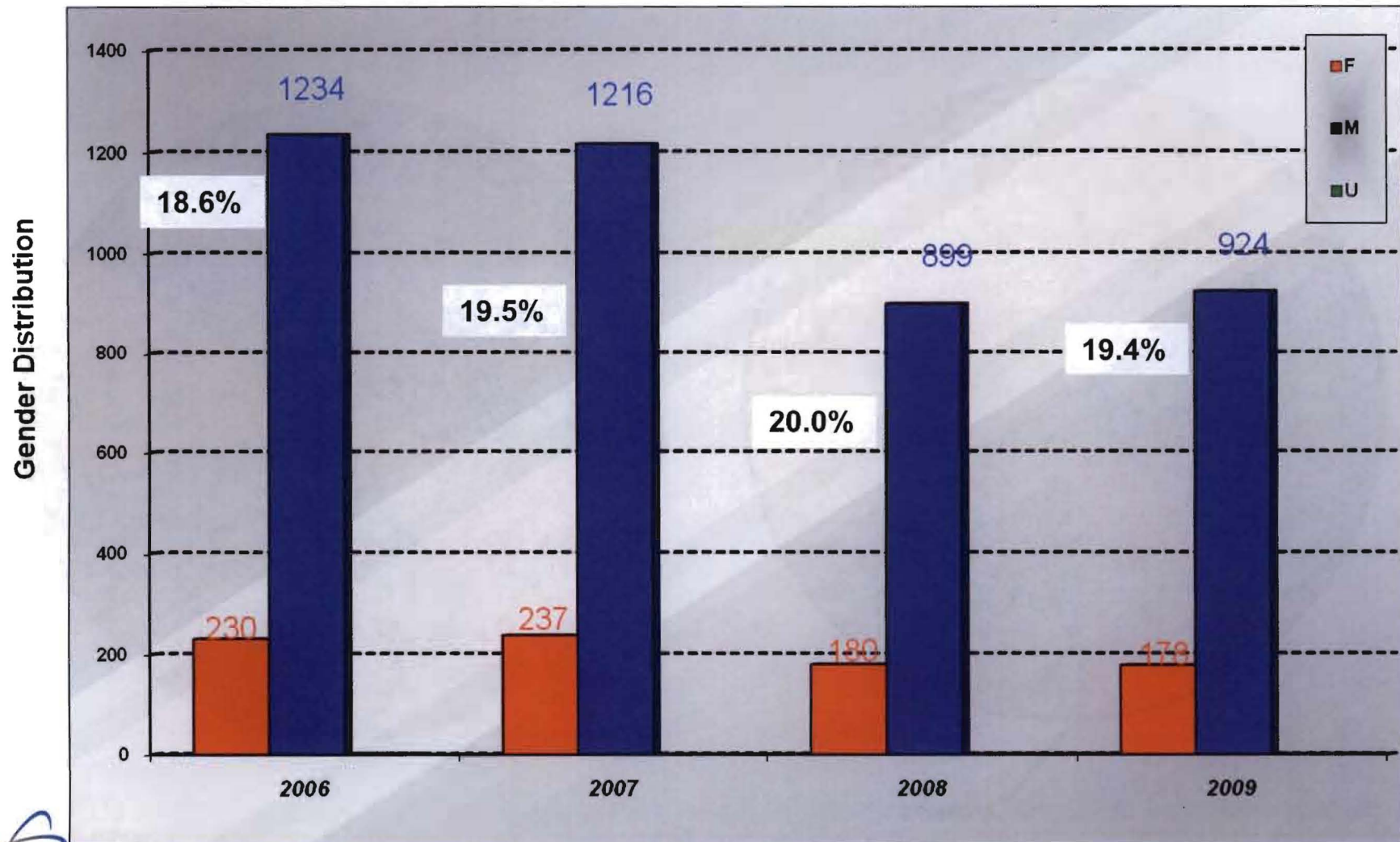


Percentage per Degree

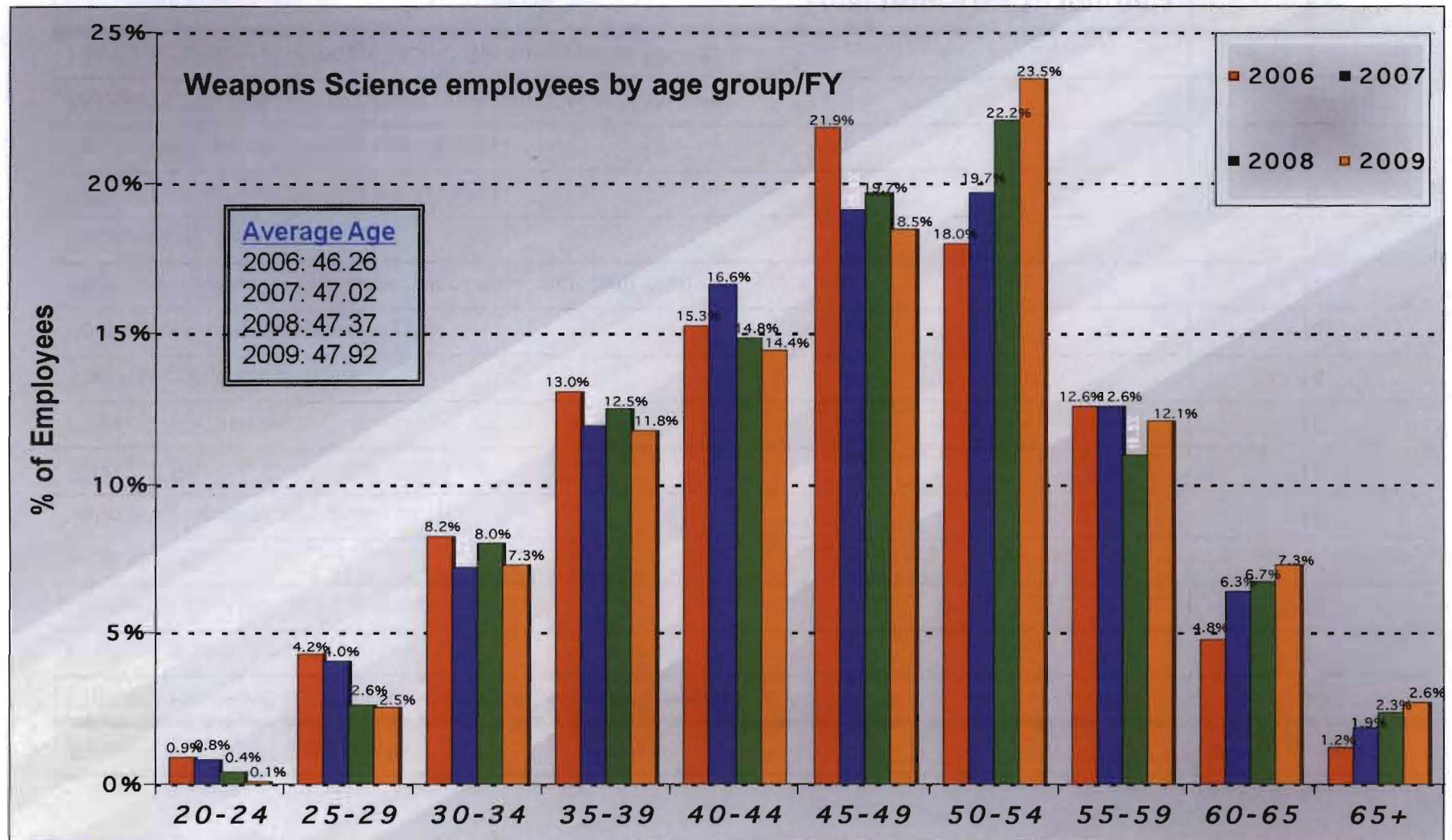


Percentage by Job Classification

Our goal remains to increase the number of female staff in the technical and management arenas



Weapons Science needs to recruit and retain early-career staff



Weapons Science personnel publish in leading peer-reviewed journals

Peer-Reviewed Journals	# Publications
Physical Review B (Condensed Matter & Materials Physics)	36
Physical review Letters	30
Review of Scientific Instruments	24
Acta Materialia	17
Journal of Applied Physics	16
Physical Review C (Nuclear Physics)	15
Physics of Plasmas	15
The Astrophysical Journal	14
Journal of Computational Physics	13
Physical Review E (Statistical, Nonlinear, and Soft Matter Physics)	12
Applied Physics Letters	10
IEEE Transactions on Plasma Science	9
Journal of Physics: Condensed Matter	8
Materials Science and Engineering A: Structural Materials	7
Physical Review A (Atomic, Molecular and Optical Physics)	7
Total from Top 15 journals	233

Weapons Science publications in peer-reviewed journals spans the majority of technical divisions

Organizations (Divisions)	# Publications
Applied Engineering and Technology (AET)	3
Accelerator Operations and Technology (AOT)	8
Chemistry (C)	25
Computer, Computational, and Statistical Sciences (CCS) & High Performance Computing	85
Dynamic and Energetic Materials (DE)	33
Hydrodynamic Experiments (HX)	5
International and Applied Technology (IAT)	2
International, Space and Response (ISR)	1
Materials Science and Technology (MST) & Material Physics and Applications (MPA)	33
Physics (P) & Los Alamos Neutron Science Center (LANSCE)	107
Theoretical (T)	165
Weapons Systems Engineering (W) & Weapons Engineering Technology (WT)	9
Applied Physics (X)	90
Other Organizations	14
GRAND TOTAL	580



Note: this is approximately 31% of the number of peer-reviewed publications at LANL per year-for comparison: LANL ranks 164 on Institute of Science Information list (ORNL 240, LLNL 304)

UNCLASSIFIED



Weapons Science organizations ensure that classified work is published and documented

Organizations (Divisions)	# Classified Publications
Applied Engineering and Technology (AET)	22
Chemistry (C)	98
Computer, Computational, and Statistical Sciences (CCS) & High Performance Computing	173
Decision Applications (D)	48
Dynamic and Energetic Materials (DE)	41
Earth & Environmental Sciences (EES)	7
Hydrodynamic Experiments (HX)	22
International and Applied Technology (IAT)	19
International, Space and Response (ISR)	163
Nuclear Nonproliferation Program (NN)	17
Materials Science and Technology (MST) & Material Physics and Applications (MPA)	261
Physics (P) & Los Alamos Neutron Science Center (LANSCE)	78
Theoretical (T)	78
Weapons Systems Engineering (W) & Weapons Engineering Technology (WT)	224
Applied Physics (X)	891
Other Organizations	130
GRAND (UNIQUE) TOTAL	2272 (852)

The number and range of significant awards (2007-2009) recognizes our outstanding work

- R&D Awards (2007/2008) (4)
- APS/ASA/ASME/HPS Fellow Award (7)
- Laboratory Fellows (2)
- Youden Prize (2)
- E.O. Lawrence Award (2)
- Pollution Prevention Award (2)
- System Safety Award (6)
- Award of Excellence in Tech-Transfer (2)
- Young Professional Development Award
- Young Scientist Award
- Coryell Award in Nuclear Chemistry
- Distinguished Scientist Award
- MacArthur Fellow Award
- Earth Science Award NRC
- National Academy of Engineering
- Defense Science Award of Excellence (45 teams-2007, 17 teams-2008)

Our people continue to demonstrate outstanding scientific performance—concerns for the future are increasing

- Outstanding technical foundation to execute a strong capabilities-based program
- Strong peer-reviewed publication record (unclassified and classified) demonstrate outstanding performance
- The work of our capabilities are represented in top-tier publications
- Our average age of the workforce is increasing, therefore we must attract and retain early-career staff

Our Approach to Diversification in the Weapons Science Capability (WSC)

**Jay Dallman, Division Leader
Dynamic and Energetic Materials (DE) Division**



WEAPONS SCIENCE CAPABILITY REVIEW

Our forward look exercise will generate a number of management recommendations

We have:

- Commissioned a cross-disciplinary team to address diversification of projects in the WSC
- Analyzed the fiscal realities facing the WSC
- Explored the value and need for targeted diversification
- Disassembled the WSC into sub-capabilities (SC) and started a SWOT analysis
- Compiled a set of draft recommendations for management

Our point-of-view is from the Weapons Science Capability within a multi-capability Laboratory

For the WSC we have started a planning process with a forward look of 5-15 years

- **Evolution of the Stockpile—Michael Bernardin**
- **Experimentally-Validated Science Base—Mary Hockaday**
- **Computational Framework—John Hopson**
- **Large Integrating Experiments—Maurice Sheppard**
- **Approach to Diversification—Jay Dallman**

The diversification team has representation from across the Laboratory

- Stephen Becker (X)
- Carol Burns (C)
- Larry Cox (CCS)
- Jay Dallman (DE/ADWP)
- Ed Heighway (ADWP)
- Rich Holmes (X)
- Matt Kirkland (X)
- Ralph Nelson (ADWP)
- Mike Stevens (DE, Foreign Progs)
- John Szymanski (NN-PD)

We have established a number of guiding principles for this process

- **Assumptions:**

- Nuclear design assessment is the core of the central mission
- We will have a skilled, motivated workforce, expected to expand its competency in the underlying science & engineering
- The mission includes significant discovery science
- Diversification beyond core mission must strengthen our competency

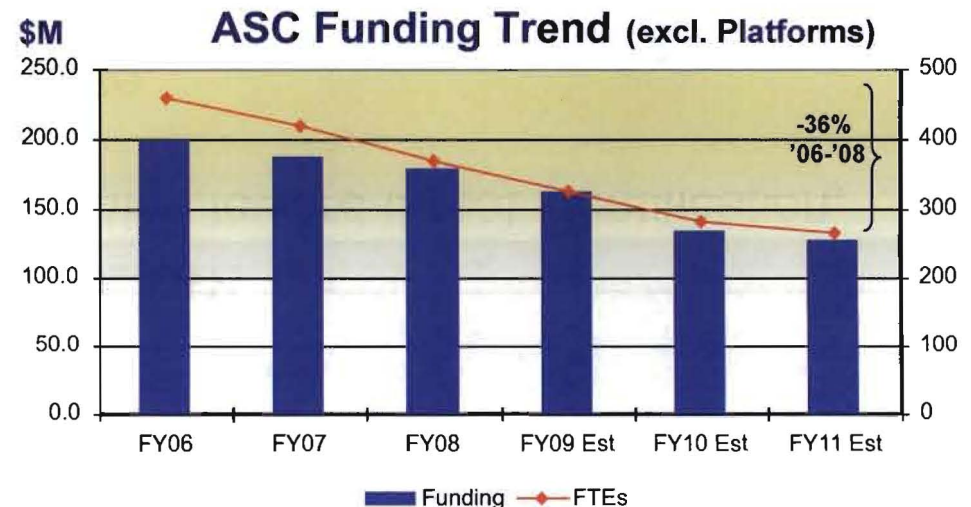
- **Our Approach to Diversification:**

- Prepare for deterrence evolution toward threat identification, denial and attribution
- Prevent technological surprise
- Align new projects with WSC
- Balance diversification with core mission

Fiscal realities drive our diversification efforts

ASC:

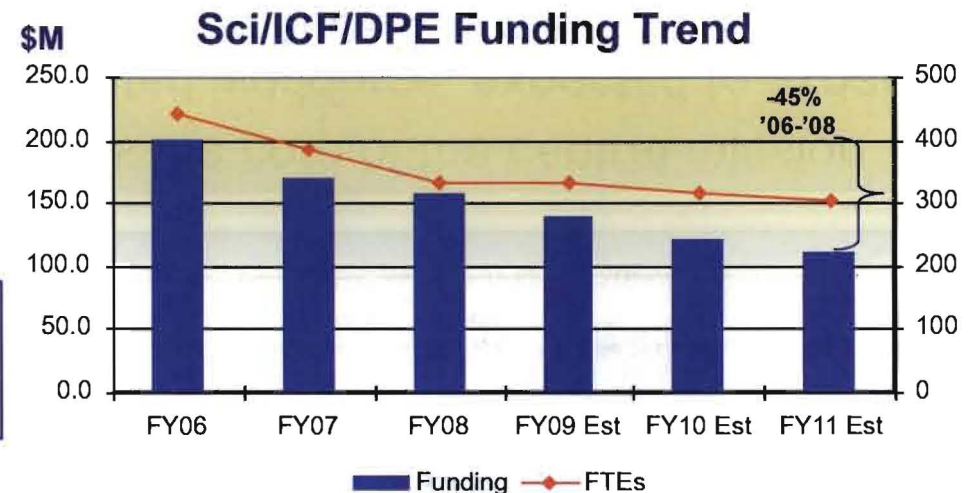
- FY09 LANL omnibus site split \$156M (incl. \$12M for Roadrunner). \$5M less than the currently planned budget
- FY09 omnibus identified \$15M for Zia; Zia infrastructure upgrade on track
- Lab's predictive capability is beginning to see a serious impact in FY09; seeing a rapidly reducing ability to retain expertise



Sci/ICF/DPE:

- FY09 omnibus site split \$123M; does not allow for capital investments
- Experimental Capabilities are at risk

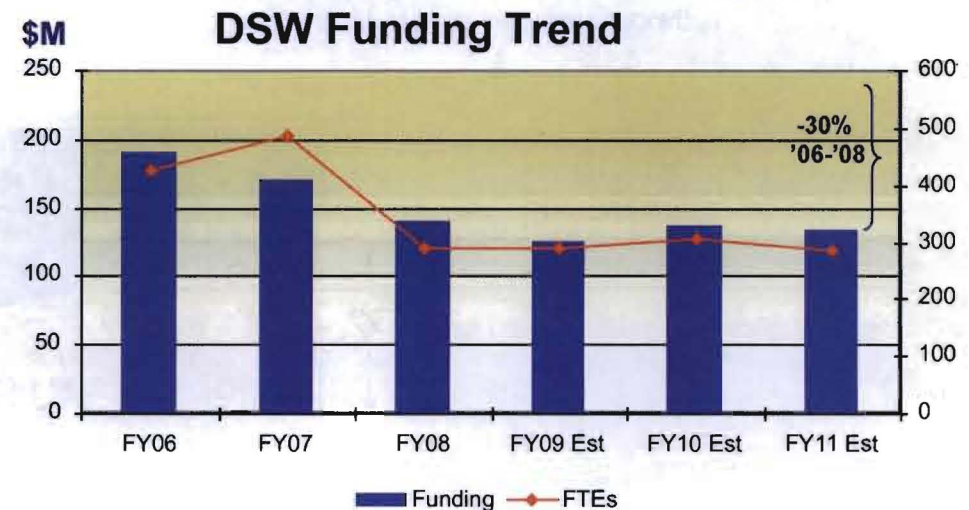
Note: Science has a higher labor/non-labor ratio than ASC, hence greater FTE impact



Fiscal realities drive our diversification efforts

DSW R&D:

- 30% reduction already digested
- No projected growth in DSW budgets

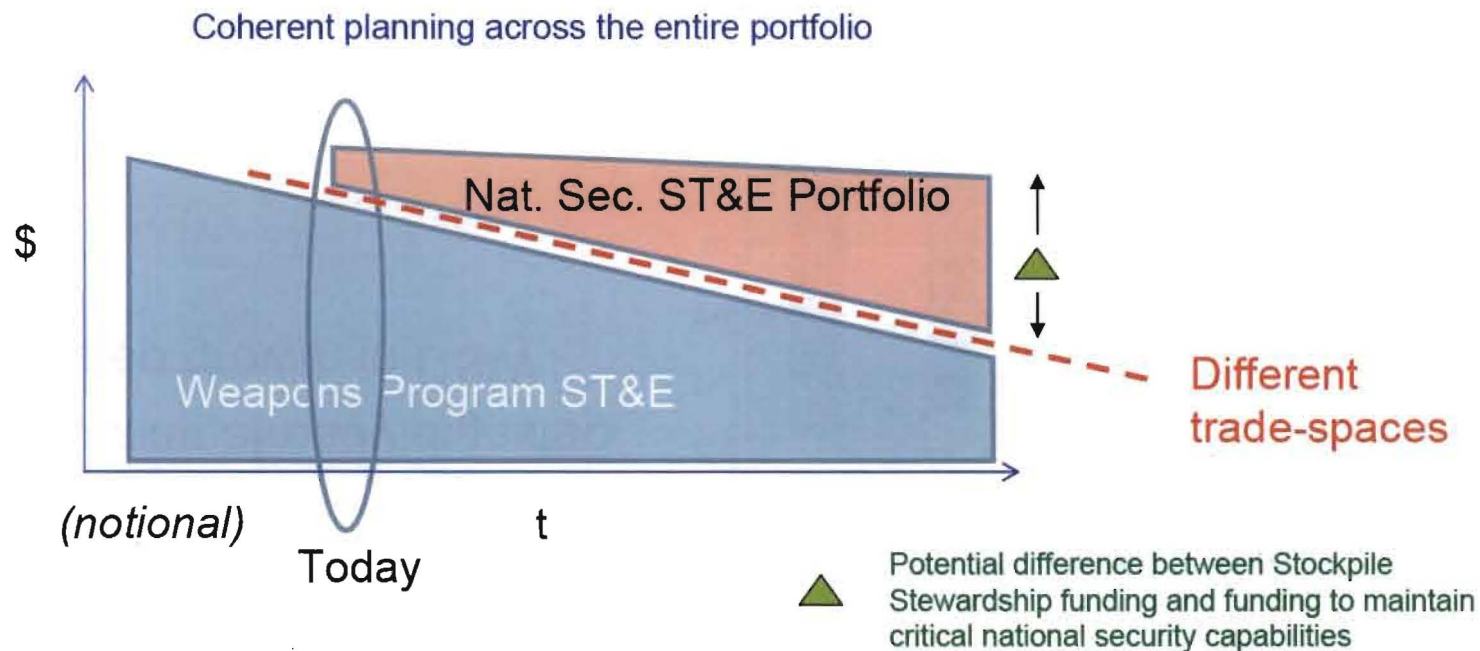


National Security Programs Long-term Funding analysis

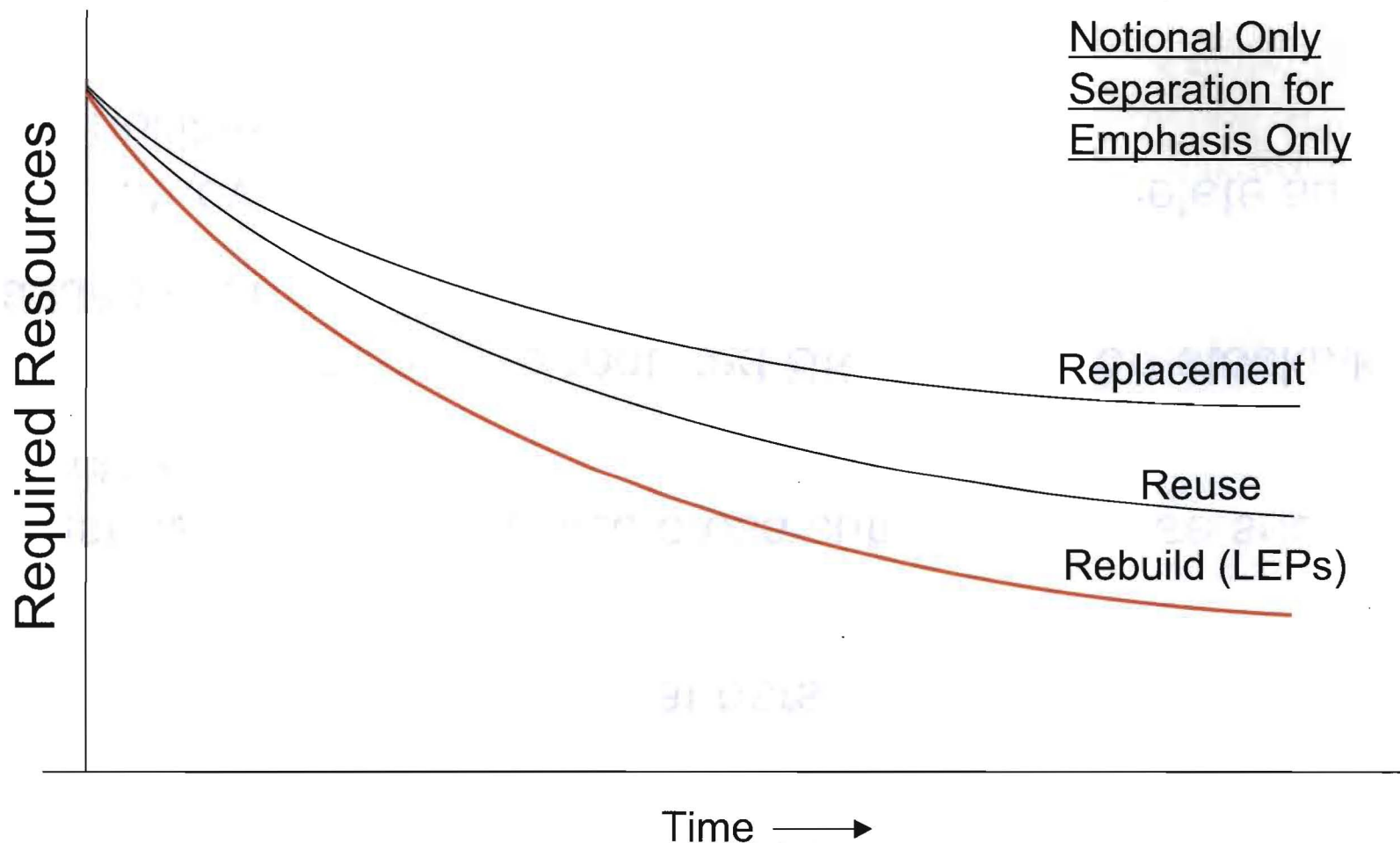
Adapted from Dr. Dimitri Kuznezov, Director
Office of Research & Development for
National Security Science and Technology
NNSA
August 2008 Presentation

Goal: Create a portfolio of National Security ST&E programs that are synergistic with core nuclear weapons responsibilities

Ensure that the essential capabilities of the Laboratories (facilities and people) remain available for the national security enterprise.



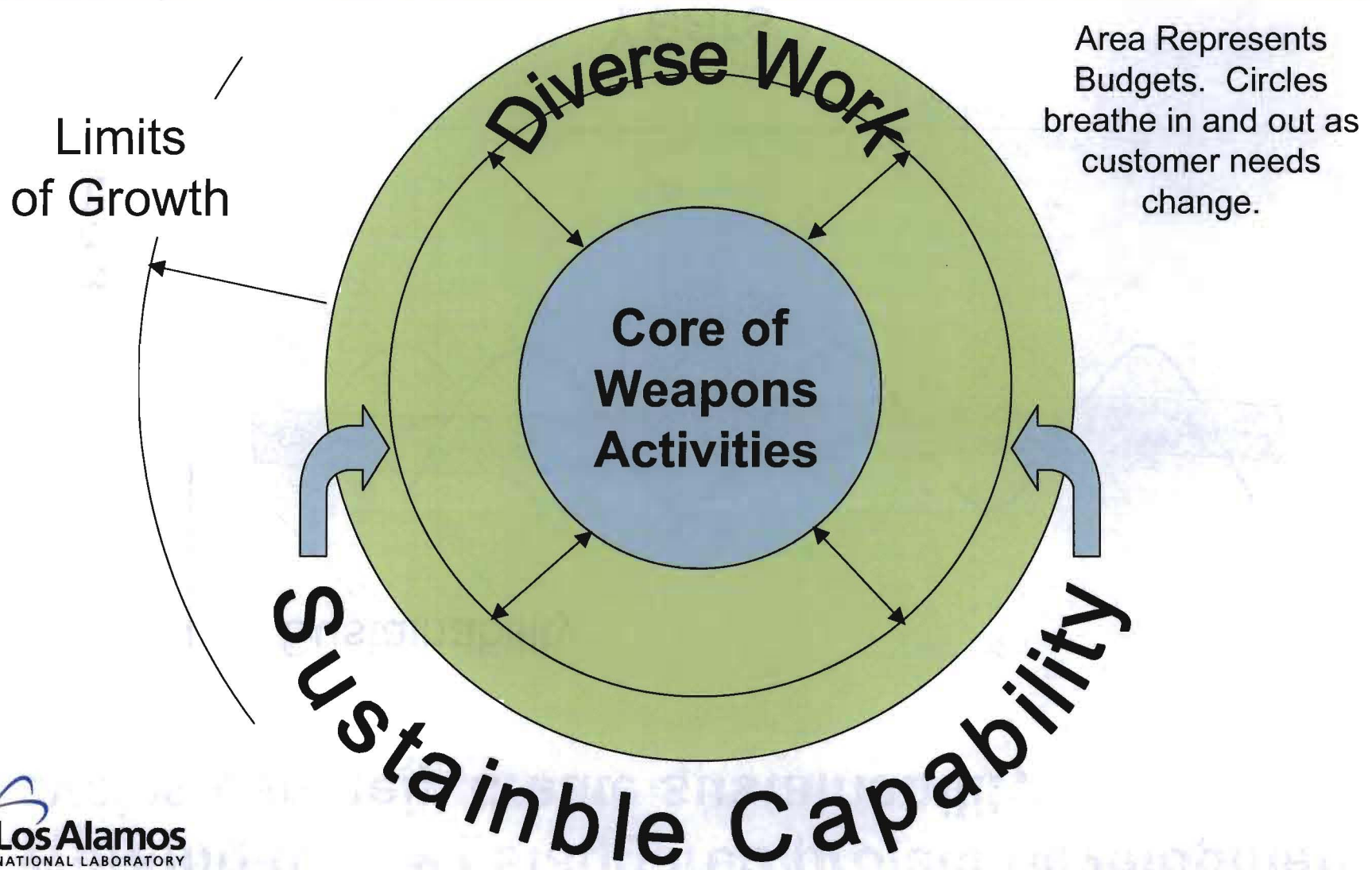
Our purpose is to ensure that essential capabilities as defined by national policy remain sustainable



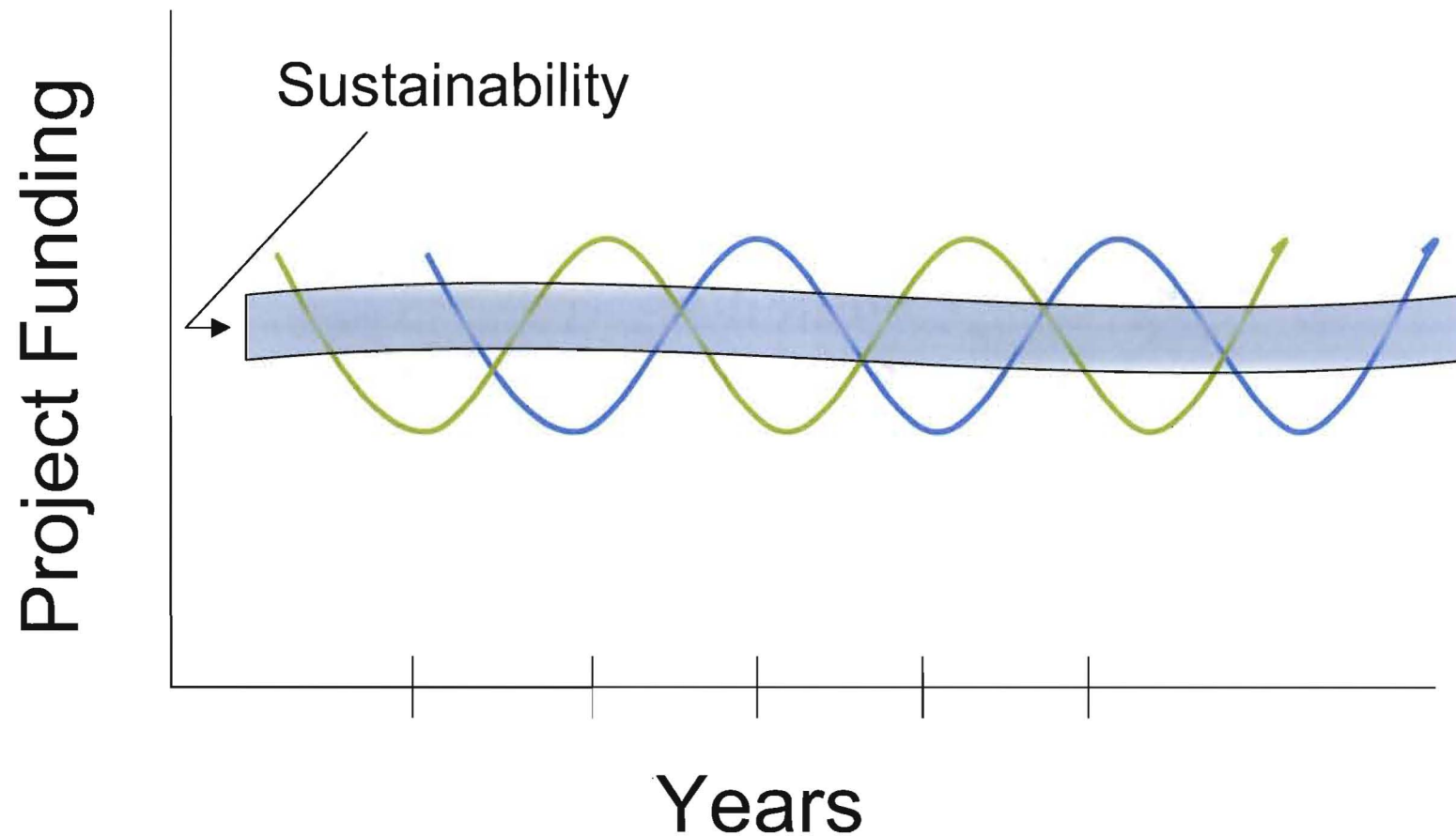
We have divided the WSC into sub-capabilities

- Broad enough definition that personnel (facilities) are fungible within reason
- Must be able to recognize cross cutting expertise such as Nuclear Design
- The totality covers the required SKA to support stockpile assessment and stewardship
- This study has no mandate to discontinue or delete sub-capabilities

Requirements of weapons science vary but resources for a sustainable capability are nearly fixed



Working to have staggered project development cycles can help create sustainability



Team created an initial SWOT analysis of WSC

Capability	Current Hedge	Strth	Op	Threat	Outlook
NW Design	NCT, Foreign Coop., TR applications	S	O	US Intelligence Agencies, SNL	Modest diversification possible
Initiation & Surety Systems*	Special customers, TR	M	O	SNL, Commercial Sector	Must retain Initiation and interface of Init. and Surety, but broader Surety can be diversified
Energetic Materials	DoD, DHS, Special Apps, TR, Surety	S	O	LLNL, SNL, INEL, DoD	Strong opportunity but very competitive
Pu S&T	LLNL	S	O	DAF, INEL, SRS	Strongly diversified
Shock & Detonation Physics	DoD, special customers, TR	M	O	LLNL, SNL, WSU, DC-??	Modest diversification possible
Hydrodynamics, dynamic Testing	DoD, TR, OS (Climate modeling)	S	O	LLNL, SNL, ORNL, Universities	Diversification possible, specialized applications with some other customers
Neutronics, X sections, fission	Nuclear Energy, TR	M	O	ORNL, LLNL	Modest diversification possible
Plasma physi. & complex flows	Astrophysics apps., Fusion Energy, Nuclear Energy	M	N	LLNL, SNL, ORNL, ANL Universities	Some retained investment req'd; modest diversification possible
Radiation transport (photon)	Detection technologies, Nuclear Energy	S	O	ORNL	Must retain strong investment; little diversification possible
Nuclear Test Diagnostics	AGEX, Nuclear Energy (ICF)	W	N	DOE Natl. Labs, Universities	Some retained investment req'd; little diversification possible
Rad Chem Analysis	Non Proliferation, TR	M	O	PNNL, LLNL, SRL	Some retained investment already diversified
Geophysics, containment,	CRADAs (oil), Energy Futures, CTBT Safeguard	W	O	Broad, Anybody can claim to do this, no demand	Small core investment req'd; modest diversification possible
Penetrating Imaging <AGEX Diag's>	TR, NCT, Foreign Coop.	S	O	SNL, LLNL, NSTec	Must retain strong investment;
Prompt diag. for forensics	Nonproliferation, NCT, other TR	M	O	SNL, LLNL, Commercial Aerospace	Very small investment req'd; awareness req'd CTBT support
Computational Science ¹	TR, Nonproliferation, Office Of Science	S	O	ORNL, LLNL, SNL, U centers	Strong national support for CS

Science Campaigns and ASC are doing an “As Is” and minimum needs sizing analysis

- Goal is to maintain complete suite of capabilities to support stockpile stewardship and nuclear weapon assessment and design
- We will use Science Campaigns and ASC “As Is” and “Minimum Needs” sizing analysis as a basis
- Customer base in some areas is well developed others require a development strategy
- Some capabilities will be shared with other NW complex partners but this is beyond the scope of this study

Top ten draft recommendations for management action will support targeted diversification

1. Decide on critical “keeper” SCs
2. Create plan of action for limited diversification and sustainability for each “keeper” including developing management ownership of the SCs
3. Articulate value of targeted diversification in WSC to customers, managers and staff
4. Develop high impact opportunities using C, SMS, and DE Divisions and SNL for pro and con bench marking, TR programs for leverage
5. Identify opportunity targets—NNSA (MOUs) and LANL efforts
6. For MOUs assign well-matched staff to develop relationship
7. For LANL efforts, develop points of responsibility for customer development
8. For LANL led development, measure program success through market assessments, customer satisfaction, and contact management
9. Encourage a spirit of entrepreneurship...where diverse projects provide challenge and growth opportunities
10. Estimate projects potential synergy and resource requirements

We are considering three alternative strategies that may be identity changing

1. Sub-capability (SC) reduction: difficult decision susceptible to champion phenomena
 - Benefit: Management actively decides about critical “keepers”
 - Improved climate/morale for “keepers”
 - Risk: sub-capability lost
2. Reduce certain SCs to a minimum; seeding a future rebuild
 - Benefit: Saves SC and provides path to recovery
 - Risk: A fine-art strategy
3. Thousand points of light
 - Benefit: Customers’ needs set the course
 - Risk: Future determined by sum of customers’ needs

Some closing comments on the benefits and risks to a diversified project base

- **Benefits:**
 - SCs remain sustainable
 - Redirect resources to less diversified SCs
 - Keeps critical capabilities for the future
- **Risks:**
 - Management decisions about SCs “tainted by the marketplace”
 - Redirecting saved \$ punishes the successful teams
 - Redirecting \$, DP might de-invest simultaneously...killing a strong capability
 - Lose or weaken major mission capability
 - Workforce may lose interest in nuclear weapons work

List of Acronyms (LOA)

A

AD	Associate Director
ADTSC	Associate Directorate for Theory, Simulation, and Computation
ADWE	Associate Directorate for Weapons Engineering
ADWP	Associate Directorate for Weapons Physics
AFM	atomic force microscopy
ALE	arbitrary Lagrangian-Eulerian algorithm
AMD	accelerated molecular dynamics
ASC	Advanced Simulation and Computing

B

BES	Basic Energy Research
BBU	beam break-up

C

CAAUS	LANL Center for Advanced Architectures and Usable Supercomputing
CCS	LANL Computer, Computational, and Statistical Sciences Division
CARS	coherent anti-Stokes Raman Spectroscopy

D

DANCE	Detector for Advanced Neutron Capture Experiments
DDC	DARHT Detection Chamber
DE	Dynamic and Energetic Materials Division
DoD	Department of Defense
DOE	Department of Energy
DP	Defense Programs
DR	(LDRD) Directed Research
DRR	<i>Defense Research Review</i>
DSD	detonation shock dynamics

E

EBS	electron back scattered diffraction
EOS	equation of state
EMP	electro magnetic pulse
EMS	Environmental Management System
ER	(LDRD) Exploratory Research

F

FTO	French Test Object
-----	--------------------

G

GC	Grand Challenge
GNEP	Global Nuclear Energy Partnership
GRA	graduate research assistant (LANL)

H

HCP	hexagonal close packed
HE	high explosive
HIPPO	high pressure preferred orientation (diffractometer)
HMX	tetranitro tetrazacyclo-octane
HPC	high-performance computing
HX	Hydrodynamic Experiments Division

I

ISSM Integrated Safeguards and Security Management
IS&T LANL Information Science & Technology Center

J**K****L**

LA-CC Los Alamos Computer Code
LA-CP Los Alamos Controlled Publication
LANS Los Alamos National Security
LANSCE Los Alamos Neutron Science Center
LA-UR Los Alamos Unlimited Release
LDRD Laboratory Directed Research and Development
LEP Life Extension Program
LTSM Limited Term Staff Member

M

MaRIE Matter-Radiation Interactions in Extremes (Signature Experimental Facility)
MCNP Monte Carlo Neutron & Photon transport code
MD molecular dynamics
MPI message passing interface
MST Material Science & Technology Division
MTE Major Technical Effort

N

NEAMS Nuclear Energy Advanced Modeling & Simulation
NIF National Ignition Facility
NNSA National Nuclear Security Administration
NSA National Security Agency
NSF National Science Foundation
NTS Nevada Test Site
NW Nuclear Weapons Program

O

ODF orientation distribution function
OFMD orbital free molecular dynamics

P

PADSTE Principal Associate Director for Science, Technology, and Engineering
PDM program development mentor
PDV Photon Doppler Velocimetry
PETN pentaerythritol tetranitrate
PFN pulse forming network
PIC particle-in-cell
pRAD proton radiography

Q

QMD quantum molecular dynamics
QMU quantification of margins and uncertainties

R

RDX 1,3,5-trinitro-1,3,5-triazacyclohexane (Cyclotrimethylenetrinitramine)

S

SBP	Science-Based Prediction
SC	DOE Office of Science
SFI	significant finding investigation
STC	Science and Technology Committee (LANS, LLC)
STE	Science, Technology, and Engineering

T

TATB	triaminotrinitrobenzene
TEM	transmission electron microscopy
TPC	time projection chamber
TR	Threat Reduction
TSM	Technical Staff Member

U

UQ	uncertainty quantification
----	----------------------------

V**W**

WE	Weapons Engineering
WDM	warm dense matter
WNR	Weapons Neutron Research
WP	Weapons Physics

X**Y****Z**

NOTE: Can't find a Laboratory acronym? See the Acronym Master List at <http://www.lanl.gov/tools/acronyms/AML.html>. This Web site is available to everyone (i.e., users outside the LANL firewall).

WEAPONS SCIENCE CAPABILITY REVIEW

Experimental Science Capabilities (A Strategic Look in Progress)

March 26, 2009

Mary Hockaday

**Deputy Associate Director for Weapons
Physics**



Slide 1

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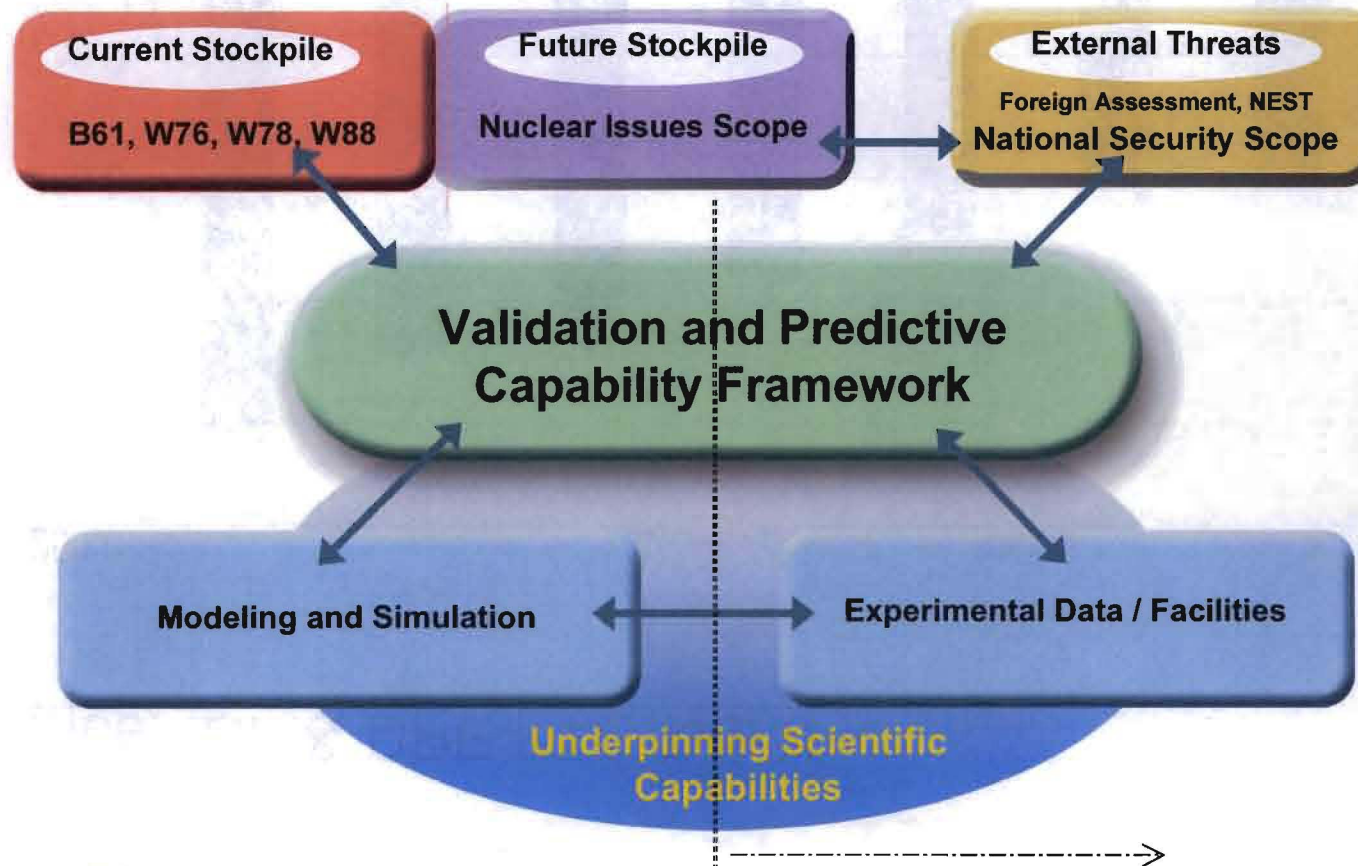
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We are in the middle of a strategic planning process

- Transition brings opportunity
- Facing budget scenarios that require hard decisions on capabilities
- Piggybacking on “Right sizing” or “4 C” exercise across Science Campaigns
- Strength, Weakness, Opportunity, and Threat analysis for capabilities has bubbled up possible “game changers”

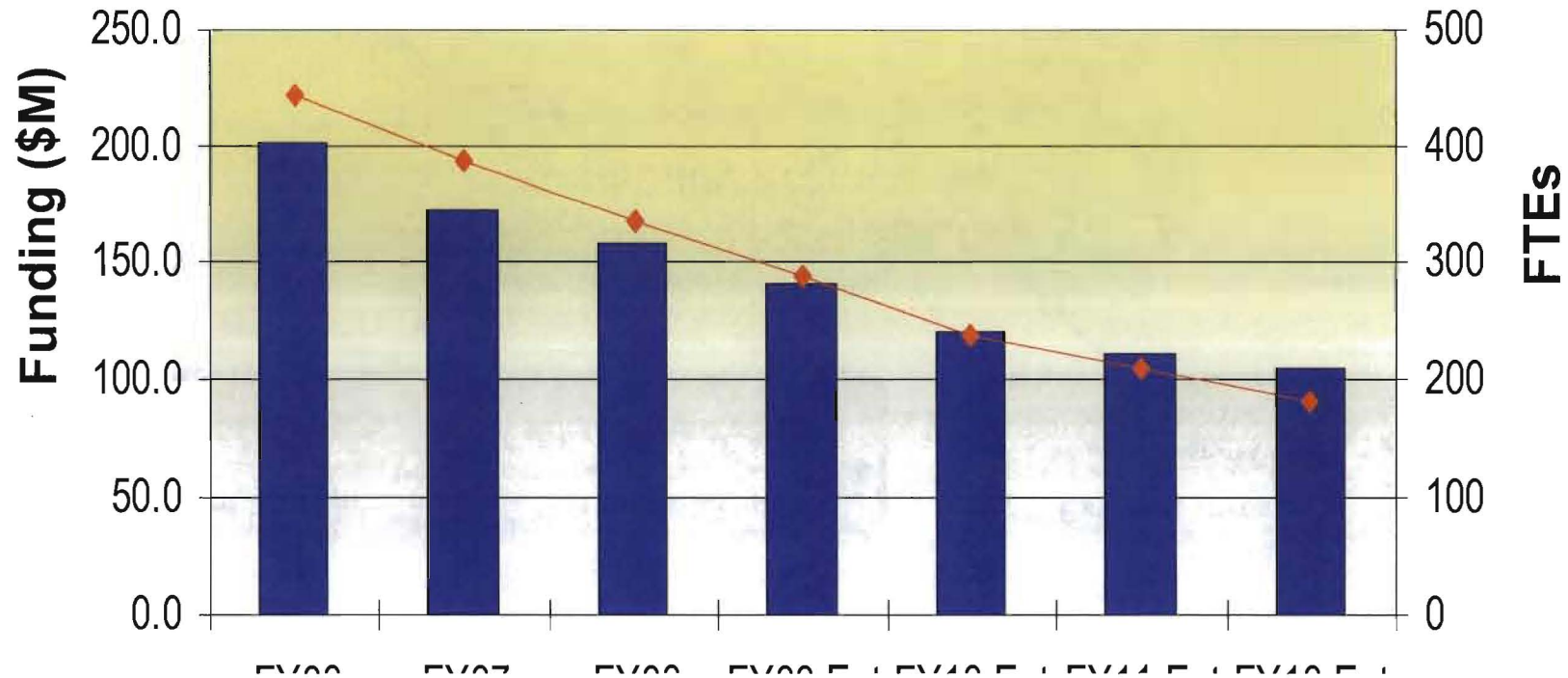
Our planning team consists of the Science Campaign Program Managers and Division Representatives from C, DE, HX, LANSCE, MST, P, T, and X.

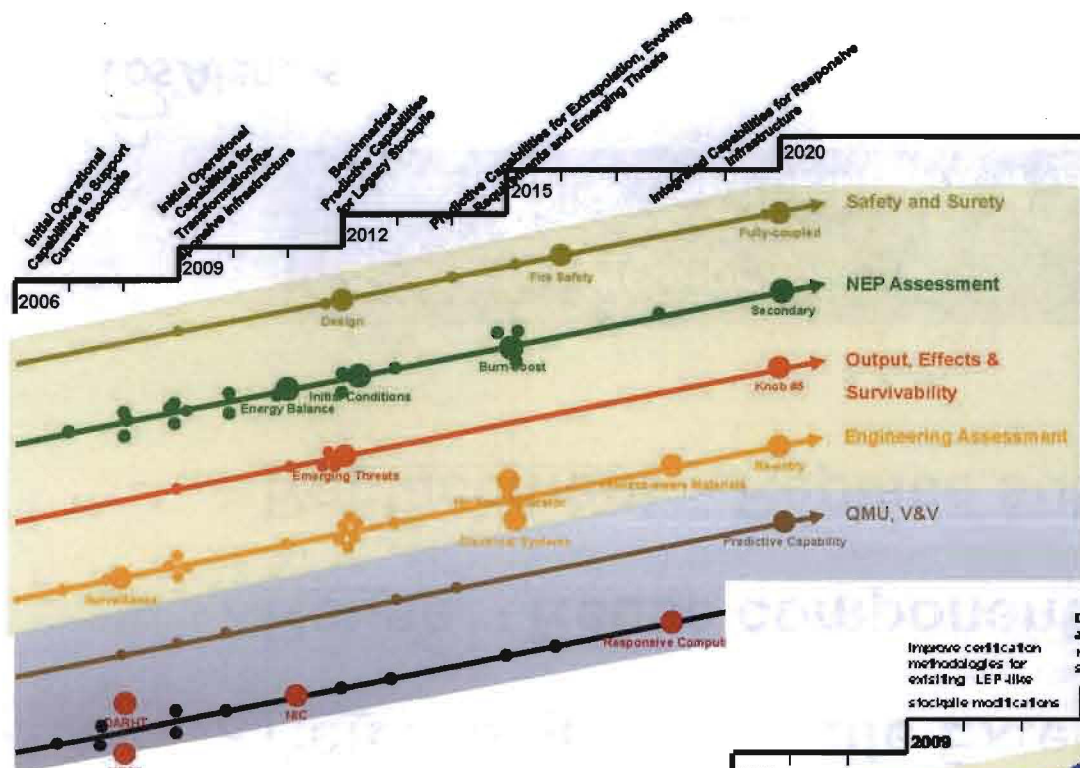
In this talk we will be discussing “the right half” of Weapons Science



Our technical capability base revolves around our people

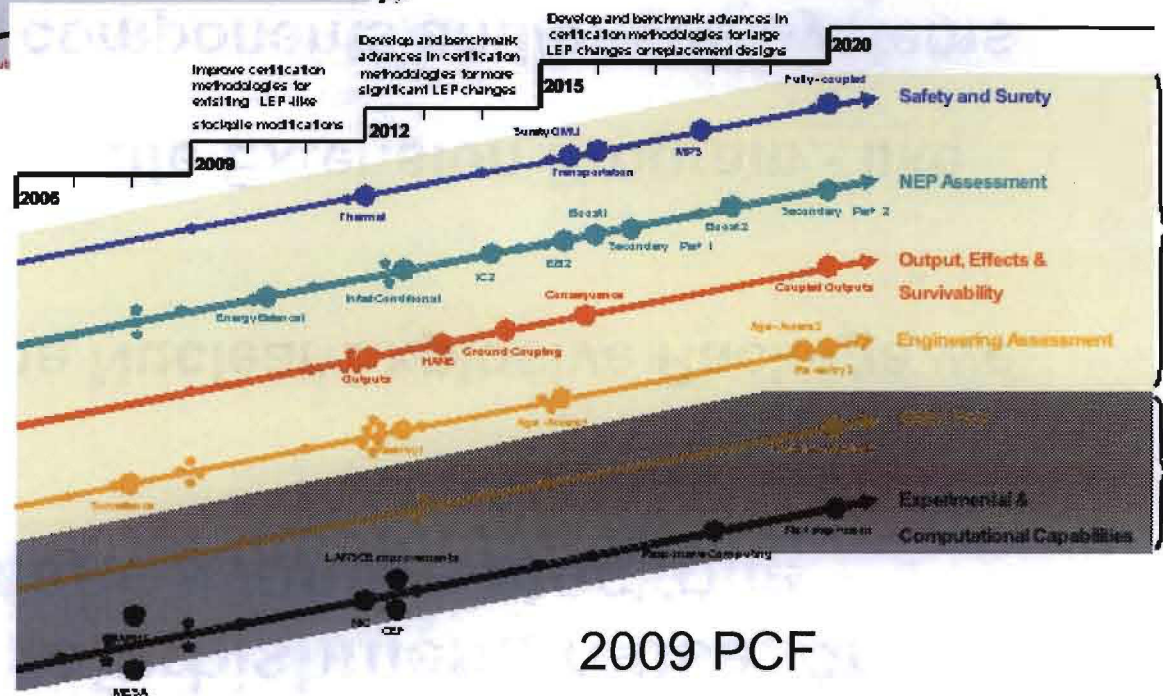
Science, ICF & DPE FTE Trend





PREDICTIVE CAPABILITY ENABLING C

We are already slipping out our PCF pegposts.



As we look out into our strategic horizon we can see possible refurbishment, reuse, or replacement scenarios for the stockpile

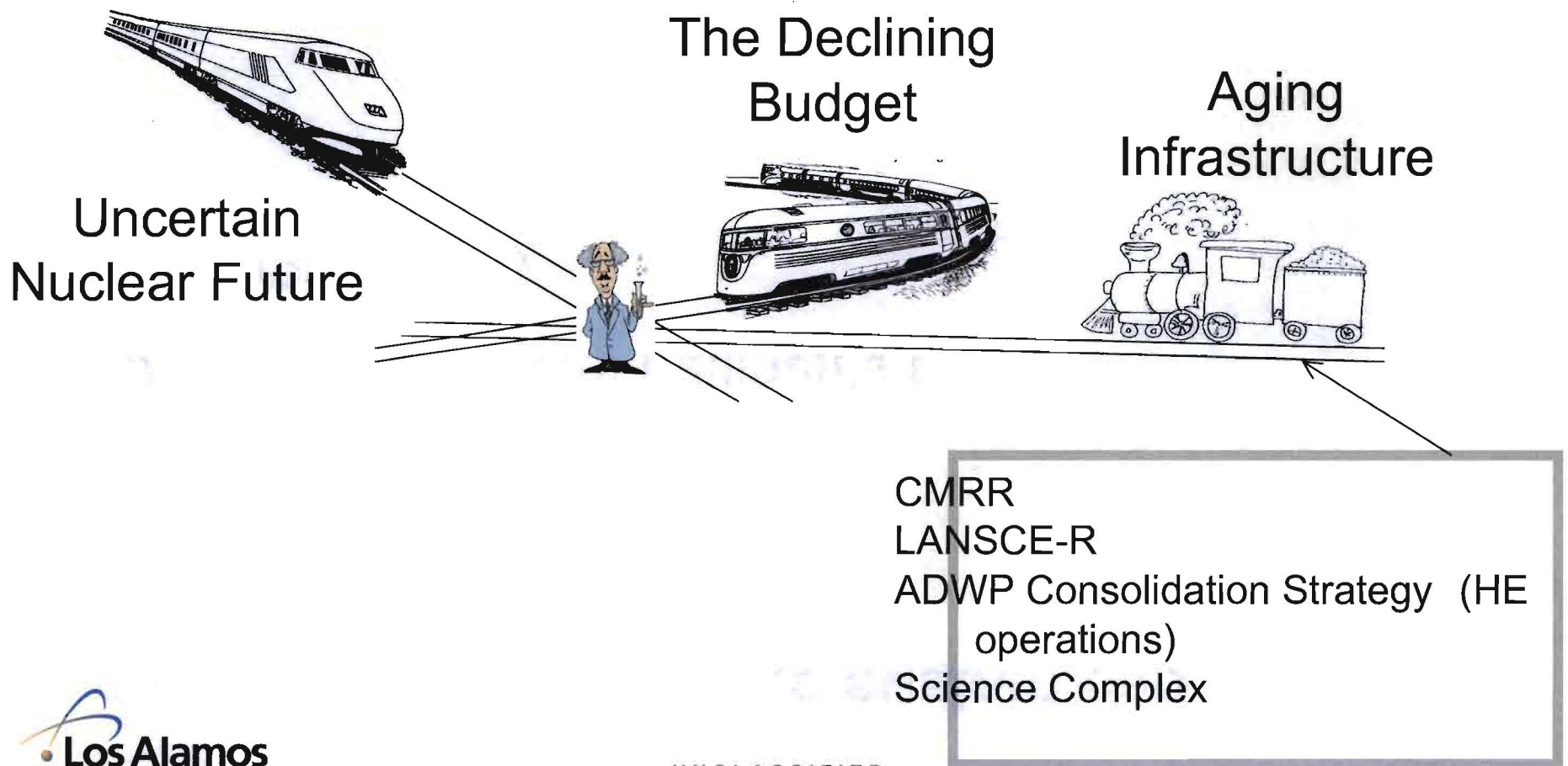
With respect to the Nuclear Explosive Package we see:

- **Refurbishment** - Life Extension Program - like
- **Reuse** - Reuse components and/or sub systems
- **Replacement** - Replace subsystems/systems

Options for the stockpile:

Do Nothing → Refurbishment → Reuse → Replacement

Our challenges are converging



There are several ways to sustain capabilities

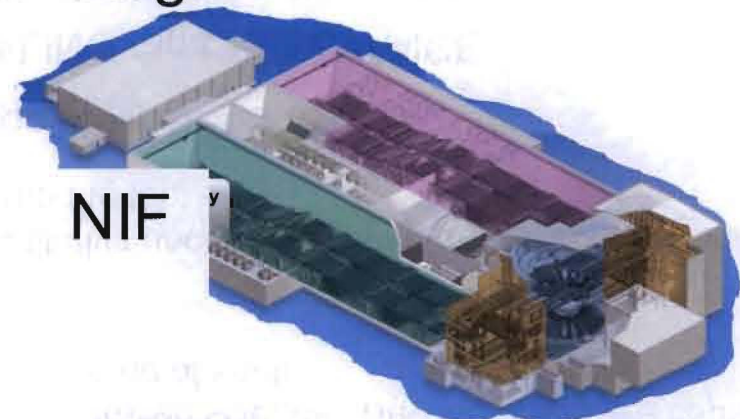
- Find Efficiencies ←
- “Right size” ←
- Diversify --- see Jay Dallman’s talk
- Get more money

Great opportunities are upon us in the experimental realm

Long-term Stewardship investments in DARHT and NIF are just at the “reaping of benefit” stage



LANSCCE-R is here



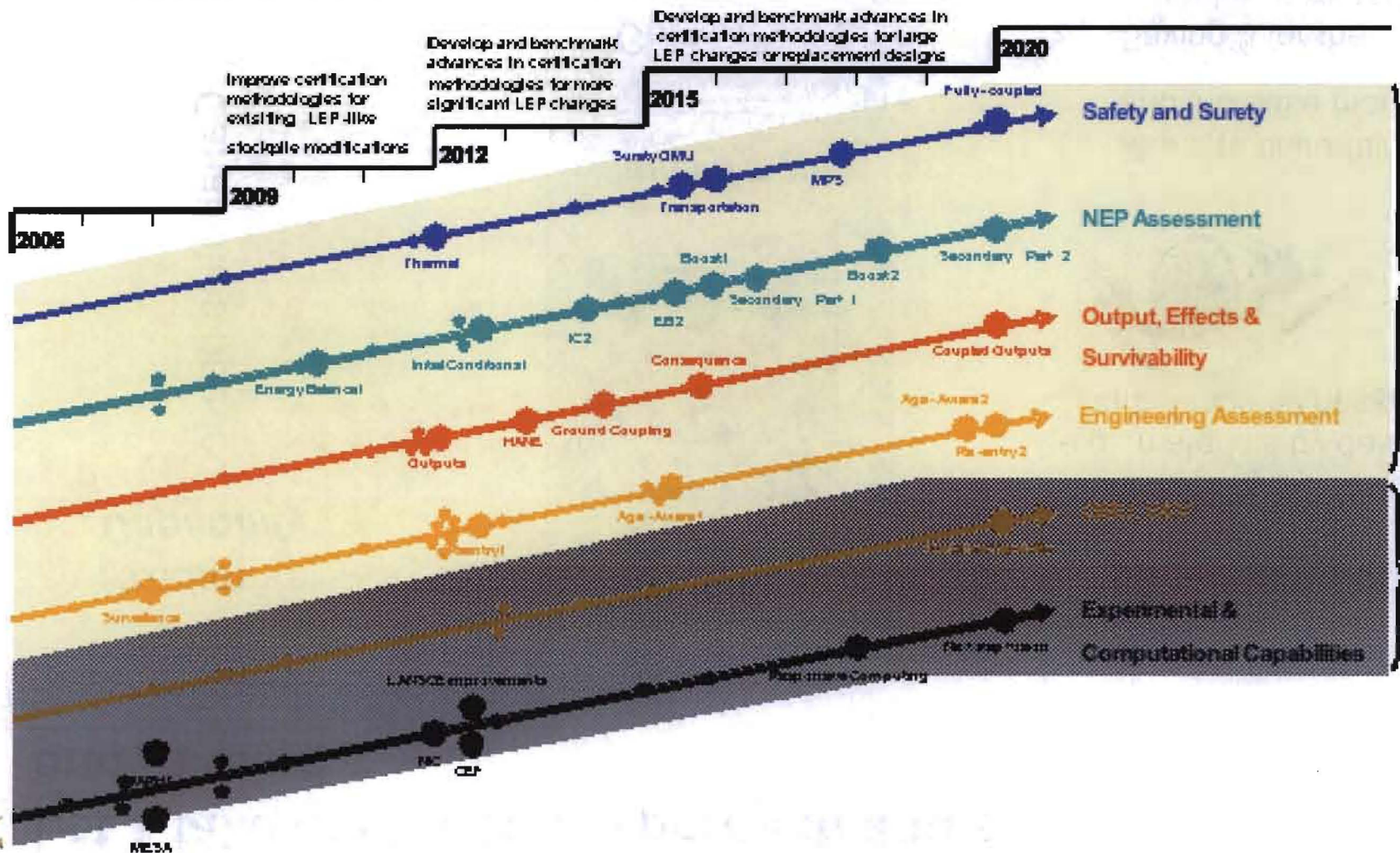
MaRIE is on the horizon



Guiding Principles

- TECHNOLOGICAL ADVANTAGE
 - GOAL: Build and maintain the capabilities needed to the predictive capability to react to technical and/or technological surprises and provide technological advantage for the country.
- OBSERVATION TO CONTROLLED SCIENCE (functionality by design)
 - GOAL: Transition from observation science to controlled science. Beyond predictive capability but balanced with the “sandbox”. More than getting rid of knobs.
- QUANTITATIVE UNCERTAINTIES
 - GOAL: Develop the tool that establishes quantitative uncertainties that are reliable enough for decision makers to decide and provide input into the tool.
- BETTER INTEGRATED MANAGEMENT (goal?)
- WELL UNDERSTOOD SURROGACY, SCALING, and RELEVANCE
 - GOAL: Understanding scaling, surrogacy, and relevance to maximize return on our investment.
- DELIVER ON OUR CURRENT WORK

We have been asking ourselves “What is beyond the Predictive Capability Framework of today?”

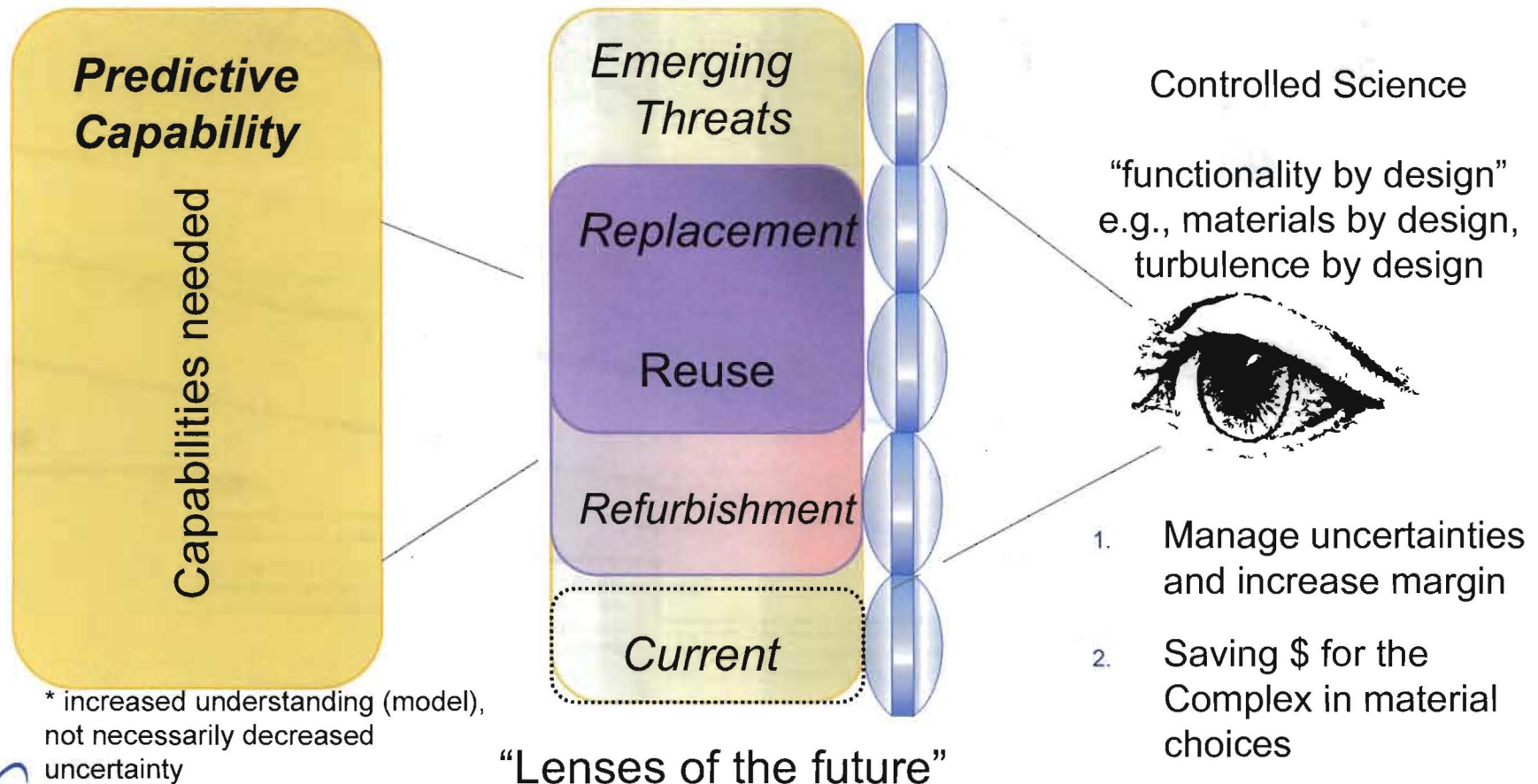


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Let's take the Vic Reis approach and start with the end in mind



The Draft Science Campaign Experimental capabilities are quite broad

Experimental Science:

- Pulsed Power Science
- Laser Science
- Accelerator Science
- HEDP diagnostics
- HEDP experiments
- Radiography
- Integral experiments
- Containment
- LEDP diagnostics
- Dynamic compression techniques (e.g. magnetic, lasers, gas guns...)
- LED materials characterization (e.g. quasi-static techniques)
- High pressure science (e.g. DAC)
- Experimental chemistry
- Image analysis
- UGT data analysis and processing

Nuclear Physics:

- Fission
- Fusion
- Radiochemistry

Hydrodynamics

- Fluid dynamics (includes turbulence)
- Hydrodynamics (integral hydro)

High Energy Density Physics (HEDP):

- Radiation-matter interactions
- Opacity
- MHD
- Plasma physics
- Non-LTE physics
- Inertial confinement fusion
- Target design (includes hohlraums)

Material Science:

- Actinide science
- Energetic materials (includes detonation and burn, chemistry)
- Polymers and foams
- Ceramics
- Low-Z materials (includes hydrogen, other gases)
- Thermodynamics (EOS)
- Constitutive properties of metals (includes strength and damage)
- Material chemistry (includes compatibility and corrosion)
- Materials processing and fabrication

Weapon assessment:

- Design
- QMU methodology
- Outputs and effects
- Validation (models and codes)



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Making a list is the easy part – how to think about it is the hard part--- Material Science

Material Classes

- Actinide science
- Energetic materials (includes detonation and burn, chemistry)
- Polymers and foams
- Ceramics
- Low-Z materials (includes hydrogen, other gases)

Materials Fundamental Disciplines/Activities

- Thermodynamics (including EOS)
 - Condensed matter electron bonding and phonon interaction
 - Alloy theory
 - Phase stability
 - T & P
- Constitutive properties of metals (includes strength and damage)
 - Microstructure influence (e.g. grain size or second phase strengthening)
 - Crystallography (texture)
 - Deformation mechanisms (dislocations, shear localization, twinning etc.)
- Material chemistry (includes compatibility and corrosion)
 - Thermodynamic reactivity
 - Electrochemical reactions
 - Transport theory and boundary kinetics (crevice, wear, microstructural discontinuity, residual stress)
 - Localization and probability
- Materials processing and fabrication
 - Synthesis – research alloys and new materials
 - Fabrication – ingot metallurgy, powder processing, deposition, etc.
 - Precision machining
 - Assembly technologies, tolerancing, welding, bonding etc.
 - Metrology and Inspection

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We have come up with different questions to help guide us as we look out into the future

What is the evolution path for validation e.g. re: Admiral's tests? Will we need one? We relied on UGTs, now we rely on hydros, is there another credible evolution? Will we have it when we need it?

What is beyond PCF? What is needed to support complex transformation?

We have come up with different questions to help guide us as we look out into the future

Critical work needs to be done to improve the tie of investments to payoff in performance – re: surrogacy, scaling, relevance?

Is our emphasis on surety and safety sufficient if the goal is intrinsic safety and surety?

What are the pacing technologies that would most reduce yield uncertainty?
Advanced diagnostics are critical.

Plutonium experimental capability at NTS is underfire– how do we change the paradigm to get the data we need?

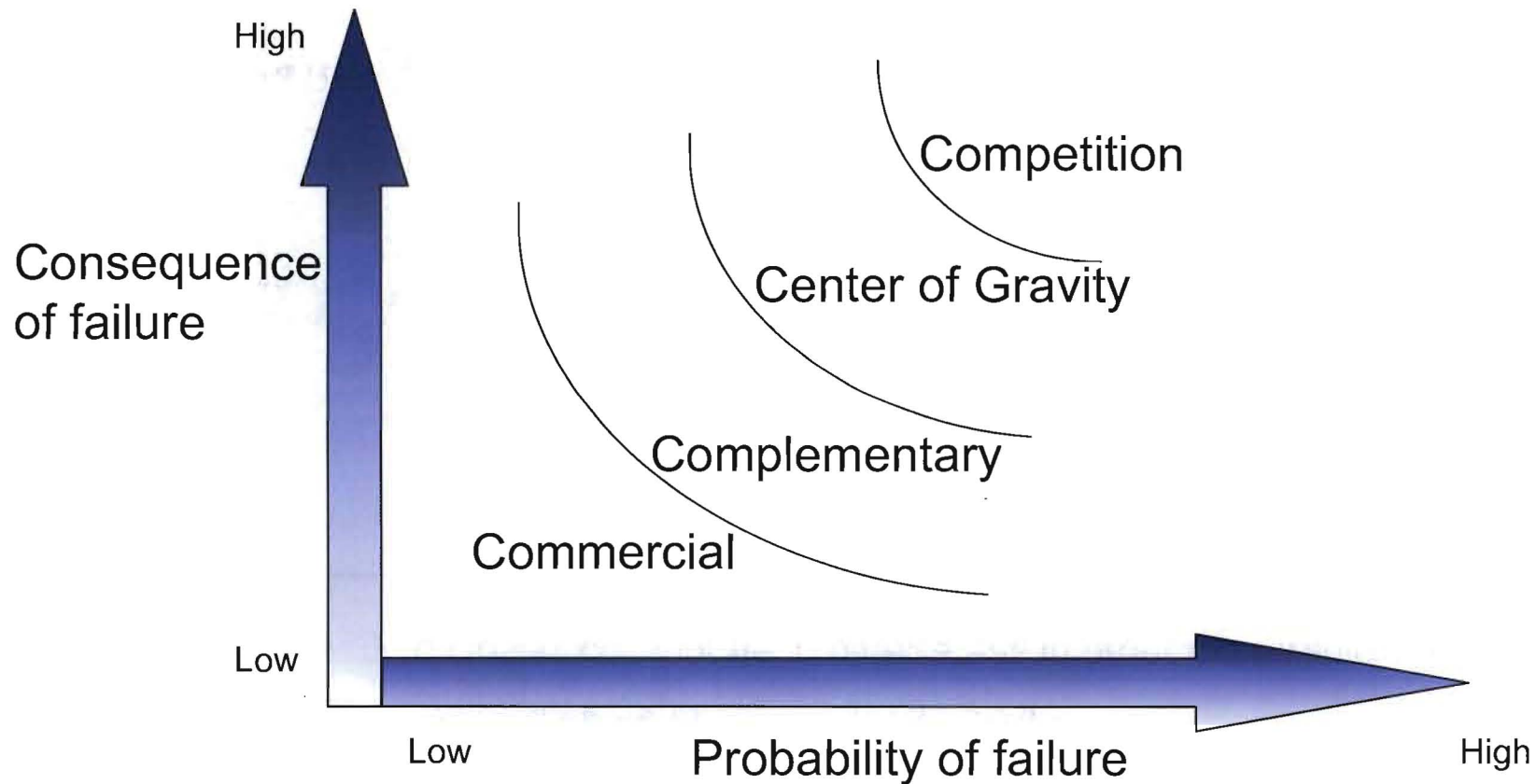
- Is there a central argument for MaRIE's role in complex transformation decisions as we move from refurbishment through reuse to replacement?
- We have identified on a smaller scale that there may be consolidations, changes in focus that would increase efficiency, and effectiveness? Are there further optimizations on the “way we do experiments” that would strengthen our capabilities and increase efficiency?

About the time we got down to discussing capabilities, HQ requested an ASC-like “right size” or “4C’s” exercise for Science Campaigns

- The 4C’s model recognizes that it is
 - Essential to maintain independence in key areas
 - Necessary to closely collaborate in other areas in order to fit within a limited budget

Category	Description	ASC Examples	FTES
Competition	Multiple significant efforts; independent depth and review capabilities	Nuclear Performance Codes, Pu EOS, Advanced Architecture Platforms	
Center of Gravity	One lab has a leading role, with key experts at other labs	Engineering Codes, Material Damage, HE EOS, Archival Storage	
Complementary	Moderate efforts at one or more labs integrating to achieve a common goal	Linear solver libraries, Capacity Computing Platforms & Environment	
Commercial	Off the shelf tools available	Configuration Management tools, Compilers	

Categories are used to manage risk in the disciplines



Multiple efforts are necessary in areas where risk is high

Competition

80%

S

W

Experiments, Modeling, and Simulation
Gas guns to integral
End-to-end design, construction, fielding, analyze
Weapon designers
Plutonium "center of excellence"
High explosives synthesis, formulation and manufacturing
Materials Laboratory

ASC codes
Implementing models in codes
Aging infrastructure
Potential to develop false confidence in ability to "calculate".....

O

T

MOXIE: Movies Of X-rays Imaging Explosives (DARHT continuous imager)
MaRIE (e-radiography, phase contrast imaging at and coherent diffractive imaging at 50 keV)
X-rays at pRad
Process Aware
Strategy to move from Observation Science to Control Science
Threat Reduction Apps

LLNL
ORNL
Economic Downturn
Cost of experimentation

Center of Gravity

80%

S

W

- LANSCE
- C-div radioactive prep
- IPF and sample prep
- Integration with T Division evaluation and modeling
- Strong outside collaboration
- Outside sponsors

- LANSCE costs, especially WFO
- Run-time
- Low-intensity 40/100 Hz w/o LANSCE-R

O

T

- Digital Signal Processing opens up new experiments
- Pulse-stacking
- Forensics and TR growth
- FRIB

- LANSCE closure
- LANSCE-R will reduce run-time
- ORNL is now the neutron lab

Cross sections for nuclear and thermonuclear reactions

Center of Gravity

80% S

W

"best in class" combo of
theory/experiment/modeling
University contacts

Fragmented LANL community - Lack of unifying vision
Separation of engineering and physics communities
No other sponsors support
Cost of doing business at the Lab

O

T

Could cheaply build water tunnels,
vertical shock tube
Could (should) make "Center"
▪ investment in other drivers
Leverage for other fields
Recruiting tool

No National vision (No DFD
leadership)
Rest of world cares about other
kinds

Turbulence and Mix

Center of Gravity

80%

S

W

DARHT

pRad

Outdoor firing and X-ray access

Containment Science (Vessels)

Distributed Image Analysis (no LANL "center of excellence")

Connecting data to performance

of Hydros per year

No JOPINs

ASC Codes

PRAD

DARHT integrating
vision

O

T

MOXIE: Movies Of X-rays Imaging

Explosives (DARHT continuous imager)

MaRIE (e-radiography, phase contrast imaging at and coherent diffractive imaging at 50 keV)

X-rays at pRad

Scaling

HEDP on DARHT



Penetrating Radiography

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Competition

80%

S

W

- Experiments, Modeling and Simulation
- Gas guns to integral
- End-to-end design, construction, fielding, analyze
- Weapon designers
- Plutonium “center of excellence”
- High explosives synthesis, formulation and manufacturing
- Materials Laboratory

ASC codes

Implementing models in codes
aging infrastructure

Potential to develop false confidence in ability to
“calculate”

O

T

- MOXIE: Movies of X-rays Imaging Explosives (DARHT continuous imager)
- MaRie (e-radiography, phase contrast imaging at and coherent diffractive imaging at 50 keV)
- X-rays at pRad
- Process Aware
- Strategy to move from observation science to control science

- LLNL
- ORNL
- Economic Downturn
- Cost of experimentation

Threat Reduction Apps
Los Alamos

NATIONAL LABORATORY

EST. 1943

MULTI-SCALE PHYSICS

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Complementary

80%

S

W

Diagnosability: B transparent to X-rays and light
Geometry of cylindrical liners (axial, radial access)
2-D convergence (eg 2D strains in condensed liners)
Dialable and reproducible
Large Targets (compared to Lasers) eg continuum > grain size
Fundamentally isentropic (off Hugoniot states) planar, cylinder
Higher material velocities (compared to HE) because "c"
Easier containment (transmission & energy without mass)
Experience
Pulsed power technology (HEPP) NHMFL

Not HE – not a Laser
MTF is not a weapons mission
Very small team
Limited (No) sponsors
(Weak coupling between physics & expt)

O

T

PHLIX on LANSCE/DARHT
Avenue to assess Tech'lgry Surprise (eg. Russia)
Joint program in HEDLP
TYPE III Experiments

Sandia ownership (short pulse), precludes consideration of PPH (long pulse)
(No clear path forward)



Magnetic Compression

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Competition

80%

S

W

Excellent performance model (DSD) - highly tuned to experimental data, which we can provide

Full suite of experimental capabilities, (SCO, FCO, Fragment Impact, Bullet Impact,)

Equation of State

Ignition, propagation, and chemical kinetics

Unique diagnostics to study underlying physics

Reactive flow hydrodynamics

Ability to work with non-traditional energetics

Specialized technicians to field diagnostics and specialized diagnostics (not assoc. w/ facilities)

Lack a true reactive burn capability

HE fabrication/machining is costly

Lack integrated thermal-chemical-mechanical capability **Game Changer**

Funding decreasing

Lack direction on experimental needs that will most impact predictive burn development

O

T

Experimental characterization to other explosives for DoD, DHS, TR,

Congressional call for EM research status in US and abroad shows a national desire to excel in this area

Have the people, and capability to generate the next generation reactive burn models

Several DoD initiatives are interested in detonation and burn (MSI, fuse, JIMTP)

Other programs are interested in detection and risk mitigation

Modernize exp. facilities as outdoor sites close

Continued decrease in funding

Lack of strategic coordination of capability maintenance and basic long-term payoff science is a critical threat as funding balances change (this is a capability, but it is not managed as one at LANL, and there is no national interagency coordination)

Many core capabilities at near-threshold levels (pressing, machining, formulation, scale-up, etc.)

Planned loss of outdoor firing without credible alternatives will reduce throughput and eliminate some capabilities (i.e. testing thermobarics)



Detonation and Burn

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We have started addressing scale, training time, and risk

Materials Science	Size	Training Time
Materials Classes		
Actinide science	large	> 10
Energetic materials (includes detonation and burn chemistry)		
Polymers and foams	medium	5
Ceramics	small	5
Low-Z materials (includes hydrogen, other gases)	small	5
Materials Fundamental Disciplines/Activities		
Thermodynamics (including EOS)	medium	
• Condensed matter electron bonding and phonon interaction	small	1
• Alloy theory	small	5
• Phase stability	small	5
• T & P	small	10
Constitutive properties of metals (includes strength and damage)	large	5
• Microstructure influence (e.g. grain size or second phase strengthening)	medium	5
• Crystallography (texture)	medium	5
• Deformation mechanisms (dislocations, stress localization, twinning etc.)	small	5
Material chemistry (includes compatibility and corrosion)	small	5
• Thermodynamic reactivity	small	1
• Electrochemical reactions		
• Transport theory and boundary kinetics (creep, wear, microstructural discontinuity, residual stress)		
• Localization and probability		
Energetic Chemistry		
• Degradation and Detonation		
Materials processing and fabrication	large	5
• Synthesis - research alloy and new materials	large	5
• Fabrication - ingot metallurgy, powder processing, deposition etc.	large	5
• Precision machining	medium	5
• Assembly technologies, tolerancing, welding, bonding etc.	medium	5
• Metrology and inspection	small	5

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We are about 90% through our first cut SWOT analysis

Experimental Science:

- Pulsed Power Science ✓
- Laser Science ✓
- Accelerator Science ✓
- HEDP diagnostics ✓
- HEDP experiments ✓
- Radiography ✓
- Integral experiments ✓
- Containment
- LEDP diagnostics ✓
- Dynamic compression techniques (e.g. magnetic, lasers, gas guns...) ✓
- LED materials characterization (e.g. quasi-static techniques) ✓
- High pressure science (e.g. DAC) ✓
- Experimental chemistry
- Image analysis
- UGT data analysis and processing

Nuclear Physics:

- Fission ✓
- Fusion ✓
- Radiochemistry ✓

Hydrodynamics:

- Fluid dynamics (includes turbulence) ✓
- Hydrodynamics (integral hydro) ✓

High Energy Density Physics (HEDP):

- Radiation-matter interactions
- Opacity ✓
- MHD
- Plasma physics ✓
- Non-LTE physics
- Inertial confinement fusion ✓
- Target design (includes hohlraums) ✓

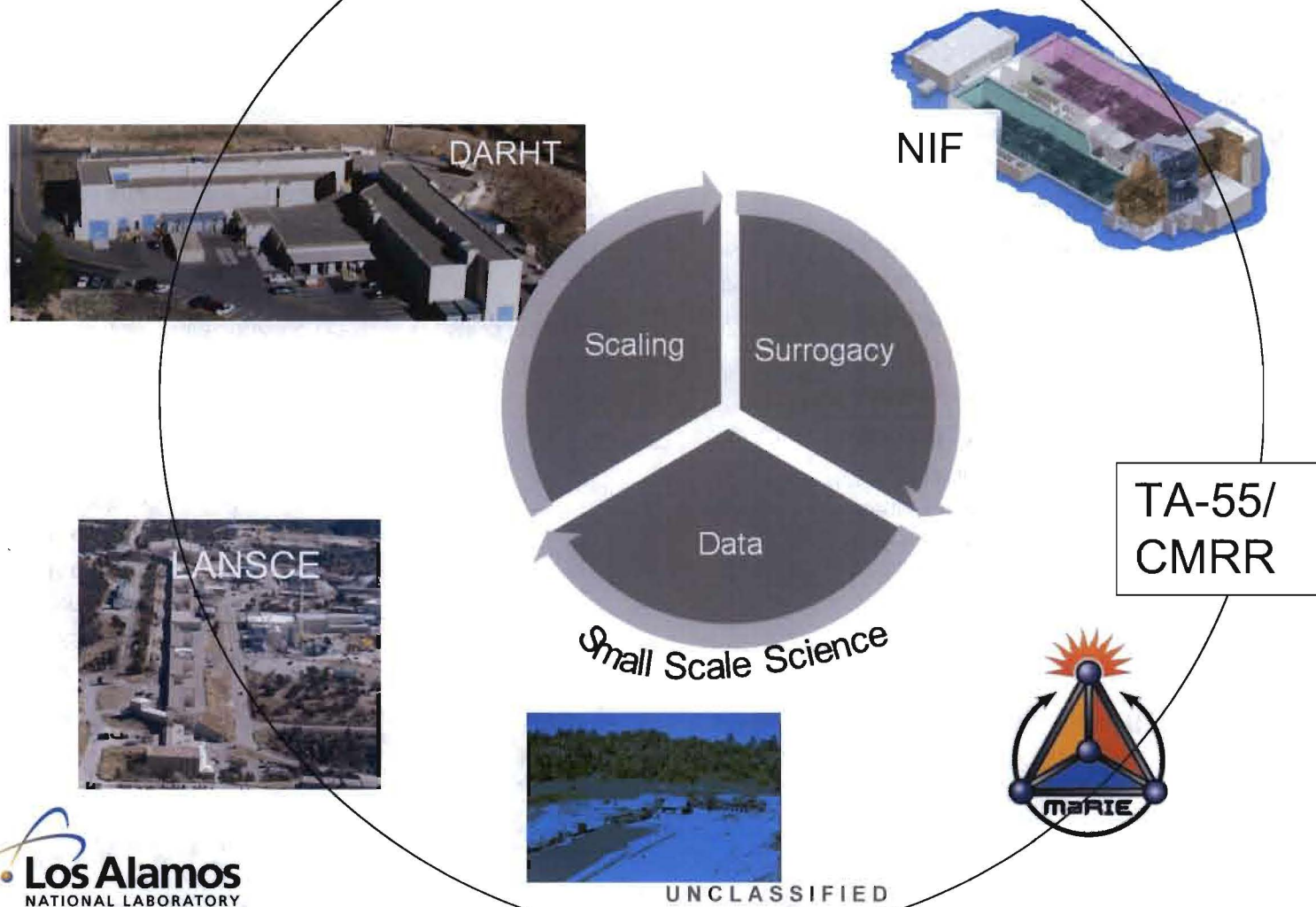
Material Science

- Actinide science ✓
- Energetic materials (includes detonation and burn, chemistry) ✓
- Polymers and foams ✓
- Ceramics ✓
- Low-Z materials (includes hydrogen, other gases) ✓
- Thermodynamics (EOS) ✓
- Constitutive properties of metals (includes strength and damage) ✓
- Material chemistry (includes compatibility and corrosion) ✓
- Materials processing and fabrication ✓

Weapon assessment:

- Design ✓
- QMU methodology ✓
- Outputs and effects ✓
- Validation (models and codes) ✓

Ideas are emerging



This is not a drill because the trains are coming down the tracks

- For the HQ “right size” exercise
 - Cycle through the sub-disciplines to determine if we have right set, and refine categorizations, risks, and scales of effort
 - Get agreement across Laboratories
- For our Strategic Planning
 - Finish up SWOTs and identification of game changers and issues (iterate with other planning groups)
 - Take a higher level look (iterate with other planning groups)
 - Answer the questions we have been generating
 - Prioritize (iterate with other planning groups)
 - Develop implementation plan and execute

WEAPONS SCIENCE CAPABILITY REVIEW

Overview and Strategic Directions

Charles F. McMillan

Associate Director Weapons Physics

March 25, 2009



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We will address your FY08 recommendations throughout our briefings

- **Develop a near-term strategy that can form the credible basis for a future LANL signature capability**
- **Continue to assign high priority to communicating with and mentoring of all laboratory staff to manage the burdens of contractual obligations**
- **Use recent experiences, such as W88 Pit Certification, W76 LEP, and RRW to inform plans for the new Advanced Certification Campaign**
- **Continue to develop the LANL HED physics program**
- **Continue to expand the role of experimental peer review**

Weapons Physics has delivered key milestones for the weapons program

- Physics assessments delivered on all weapons systems for Annual Assessment
- Physics contributions to W76-1 down select
 - Established path forward for alternative material study
- Conducted 40 pRad shots this run cycle
- Using modern ASC codes for Assessment, SFIs, LEPs
 - Transitioning from legacy codes to ASC
 - Enabled closure of 5 recent SFIs
 - Progress in addressing 5 previous test anomalies (including 3D hydrodynamic simulations of long-time primary anomaly)
- Achieved world-record computing on Roadrunner (#1 on Top 500 at >1.1 Petaflops); machine successfully installed in Metropolis Center
- Zia platform CD-0 approved, CD-1 at HQ for approval

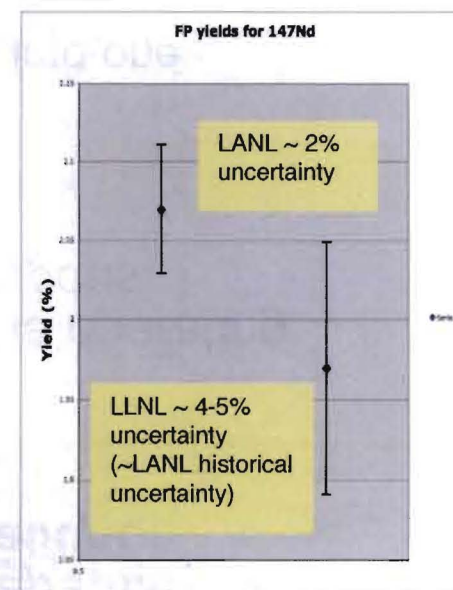
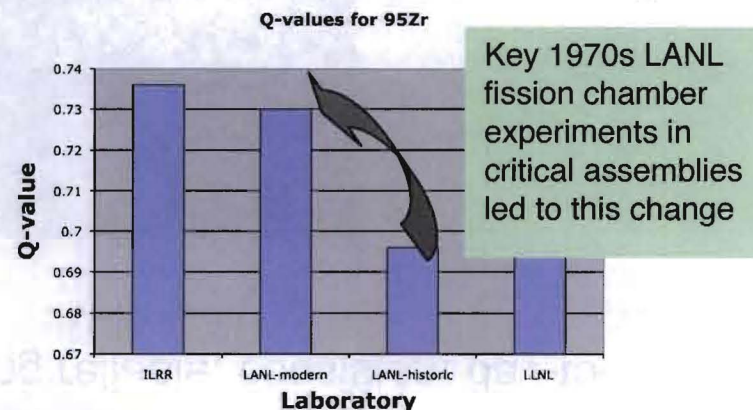


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- **W76-1 Alt Matl slide here**

We are headed to resolving inter-laboratory discrepancies on radiochemistry assessment of yields

- Fission product yields (Q-values) differences for fast ^{239}Pu neutrons have persisted between Los Alamos and Livermore for >10 yrs
- Improved Q-values critical to accurately determine radiochemical nuclear yields from UGTs – essential to reduce QMU uncertainties
- Reassessed evidence based on seminal '70s *dual fission-chamber* experiments significantly improves accuracy and reduces uncertainties
- Laboratories finalizing joint reevaluation of key nuclear data to resolve outstanding differences
- An *Expert Panel* will review the scientific basis used to resolve final fission product yields

$$Q\text{-value} = \text{FP-yield}(^{239}\text{Pu fast}) / (^{235}\text{U thermal})$$



Resolution of RadChem differences will reduce UGT yield uncertainties and enable improved common baselines for all US nuclear tests

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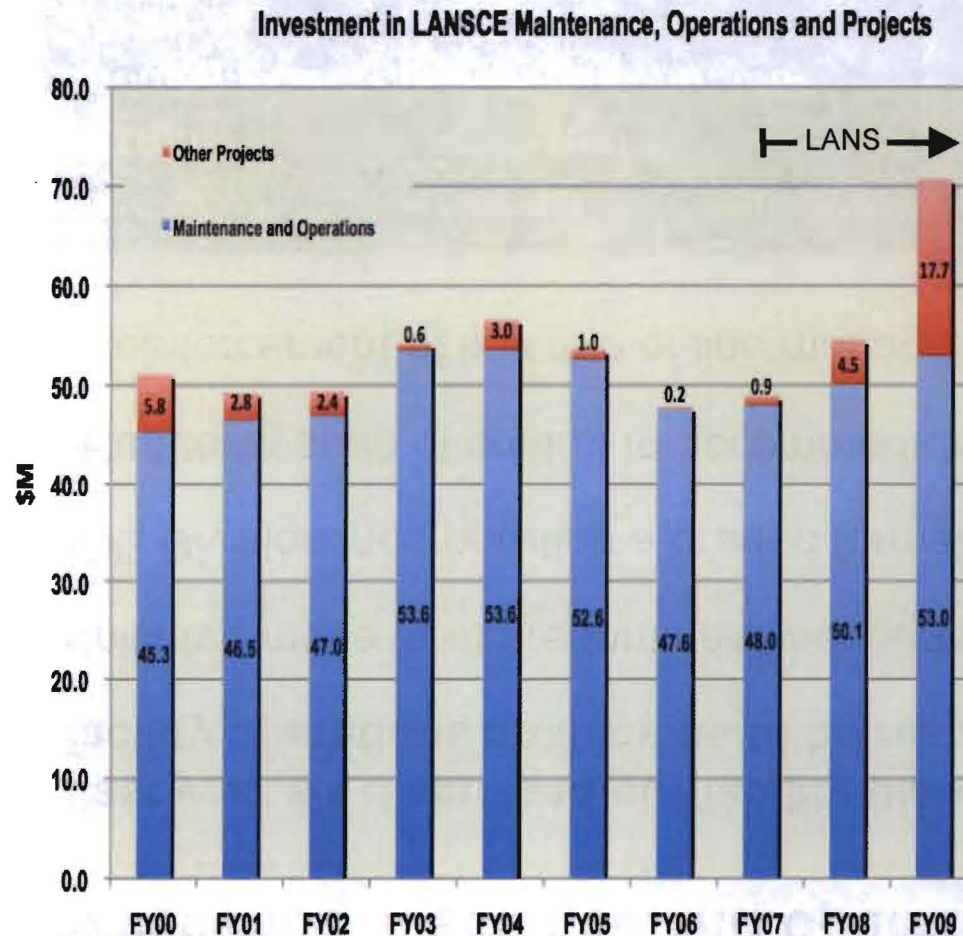


The scientific challenge of developing the DARHT II capability is complete – we now need to turn our attention to formality of operations and conducting experiments

- We have decided to transfer DARHT, HX-Division (the operating line organization), and the Hydrotest program to Weapons Engineering
- The reason is two-fold
 - Integrate experiments and operations with engineering into one organization
 - Engineering is better suited to establishing reliable, consistent day-to-day operations



FY09 RTBF investment in the LANSCE User Facility reflects a continued commitment to a sustainable future



Unique, highly-flexible beam delivery to multiple facilities 6 mo/yr @ 24/7 with ~ 1200 user visits

ADWP is addressing the challenge of simultaneous excellence in science and operations for HE Experimentation

Last year we discussed our facility plans and challenges – excellence in facility operations enables us to be responsive to weapons science issues

- Initiated move from predominantly expert-based to systems approach
- DE Division incorporating a graded formality approach into operations
- Reducing span of control to accommodate increased discipline of operations
- Reinforcement of key role of line manager in risk-based decisions

Careful balance is being struck between customers with a preference for anonymity and quick action with little documentation, and DE requirement to follow formality of operations



Chamber 8 10kg enclosed firing vessel



Chamber 8 control room

Using formal processes to fire shots

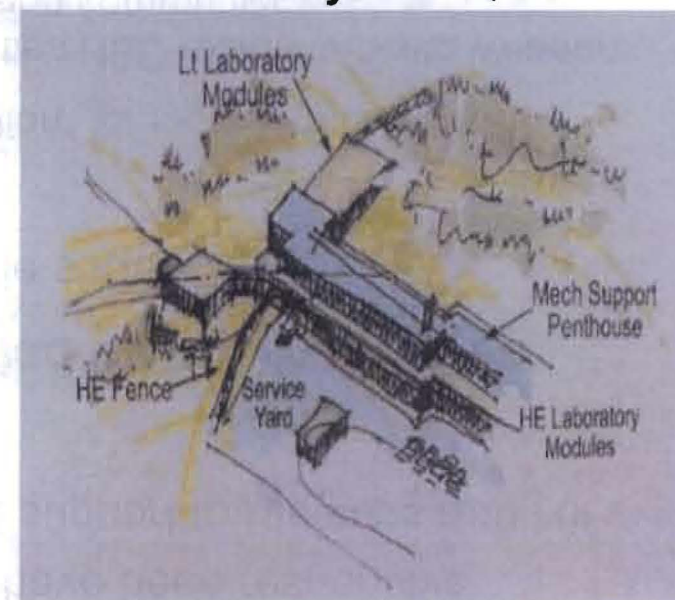
we are on track with our Facility Strategy I told you about last year

Facilities

- Plan is now consistent with SPEIS HE R&D Preferred Alternative
- Line items getting tougher in the future, especially non-nuclear facilities
- ***TechSource report to NNSA on Energetic Materials Characterization Facility validated the business case analysis***

“Without an EMCF to replace extant capabilities, LANL will not have an independent capability for explosive synthesis and characterization of legacy and new explosives”

Preliminary TPC ~\$25 M



Conduct HE synthesis, formulation, and characterization to enable continuation of R&D in advanced energetic materials

Modern, quality HE and Firing Site facilities help attract students, postdocs, new staff

Senior Management has been engaged and has been working our HED portfolio

- **Ignition IS important for the country**
- **LANL is serious about delivering**
 - Made changes in our investments and have been responsive
 - Redirected LANL Z Rad Flow effort and support to Pleiades and NIF
 - Resolved diagnostic log jam
- **We are addressing weaknesses identified by internal review**
 - To consolidate, prioritize, and establish code strategy:
 - Increasing participation in Searchlight
 - Added C1 and C4 effort to C10 “uses of ignition” for long term use of NIF
 - Working on code strategy that more directly ties HED experiments to weapons needs – elevates HED in the eyes of the design community

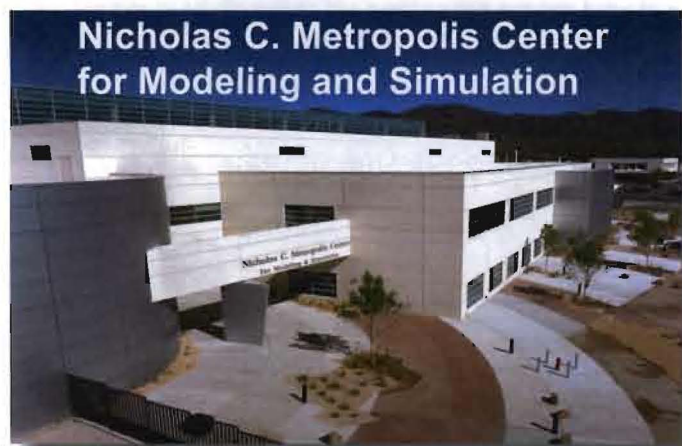
Out year transition budgets are showing upward trend

Boost initiative proposal process: an example of how we are broadening experimental peer review

- **A Sept 2008 invitation for “boost specific” proposals, for work beginning in FY-10 resulted in ~30 pre-proposals**
 - 65% of proposals for mission deliverable projects, 35% for exploratory topics
 - “Renewal/continuation” proposals invited to participate, on equal footing
- **LLNL and SNL participating as reviewers with 12 proposals in final review**
 - Reviewers now ranking and assigning proposals to one of four tiers using criteria:
 - Programmatic relevance to boost-related mission and needs
 - Quality of science proposed, including publish-ability (classified and unclassified)
 - Practicality (scope, budget, schedule)
 - Overall Risk, including adequate ground work
- **Status: presentations done; reviewer input by Apr 1; complete by Apr 17**

We have also implemented proposal processes in LANSCE based experiments, HED, DPE, and JMP/C2 to different extents

We're investing in the infrastructure for Metropolis – one of two premier NNSA high performance computing facilities for Complex



**With Zia, SCC will house ~2.5PF
secure computing**

- Roadrunner – 1.4PF
- Zia ~1PF
- Capacity Systems ~150TF

- ACES Alliance with Sandia will enable a higher return on computing investments
- Roadrunner technology will be explored for developing the path to exaflops
- Forward look at power needs (current capacity: 28MW (20MW for computing and 8MW for cooling))



Los Alamos – Sandia partnering in preparation for Zia installation in 2010

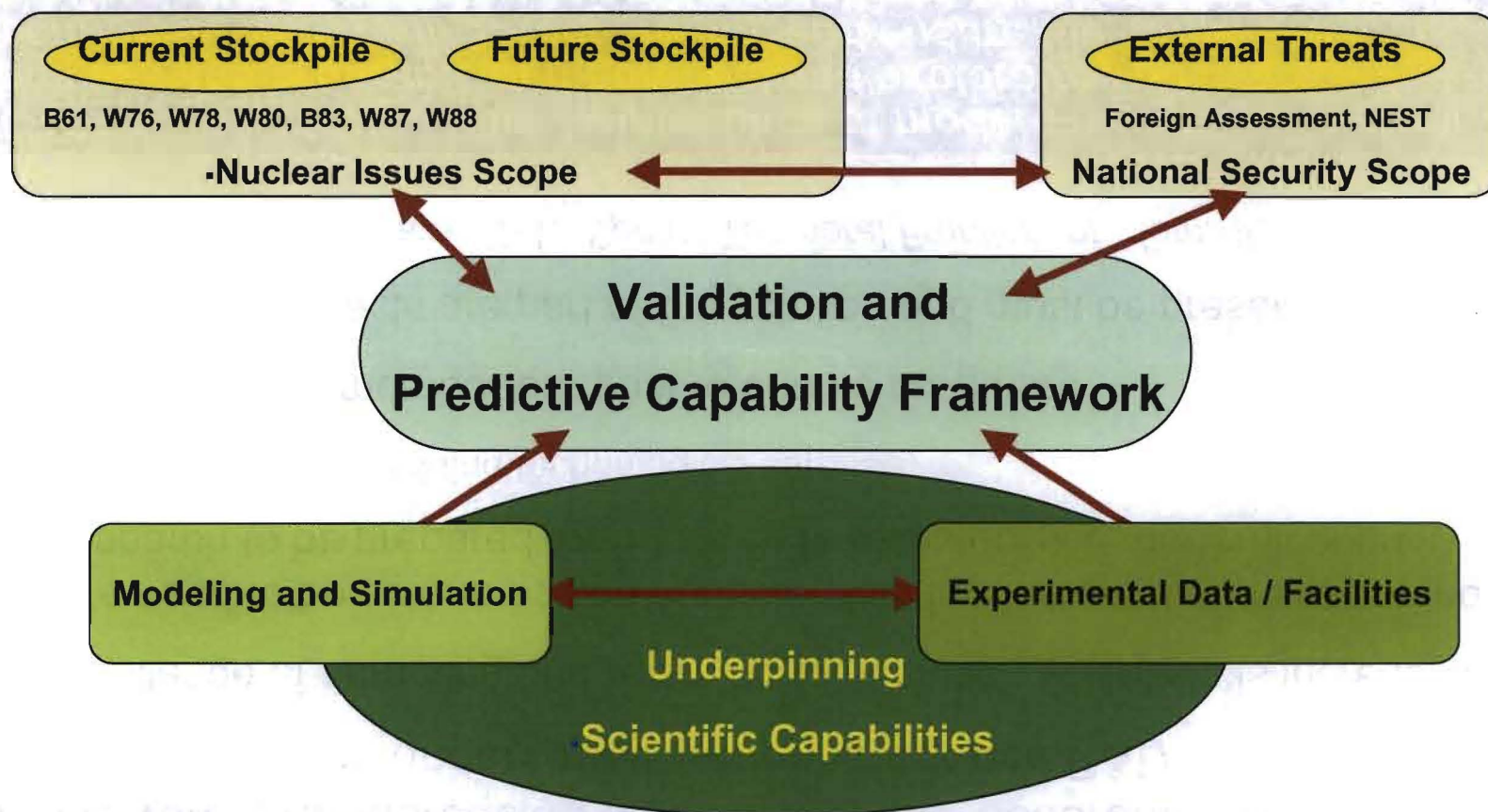


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We meet our national security responsibilities through validated predictive capability — moving from *concept* to *engineering* to *product*



We leverage our laboratories' science and technology advantage to anticipate, to counter, and to defeat threats and meet national security

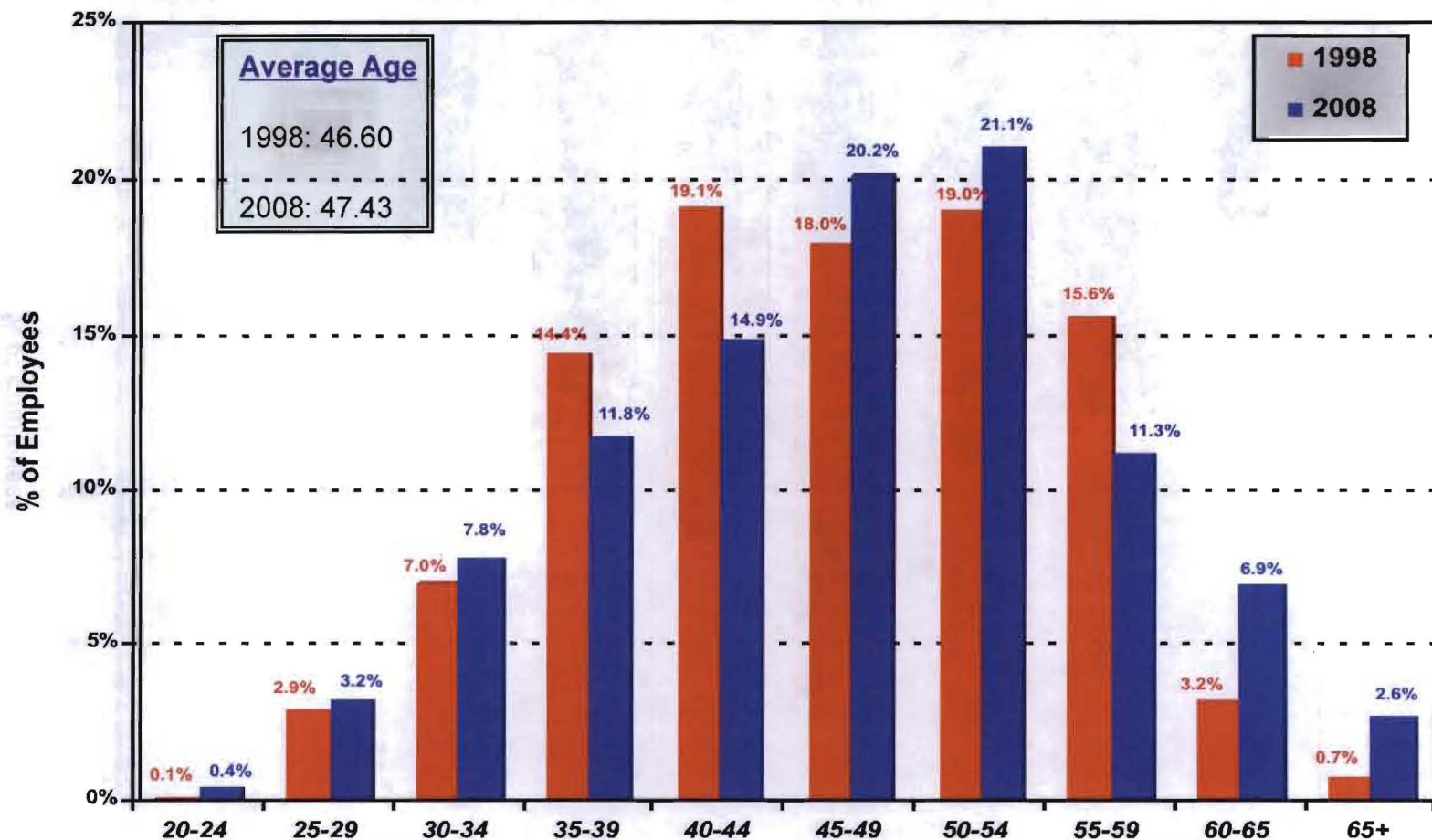
We are concerned about preserving our ability to sustain the existing stockpile and support future stockpile requirements

Driven toward ever-increasing efficiencies, the “headroom” and people available to conduct fundamental weapons science R&D are disappearing

- Challenge of attracting and retaining top-echelon scientists is increasing
- We need to be able to assign our scientists fundamental and supporting research to be prepared for future SFIs and stockpile modernization
 - Essential for avoiding technological surprise
- We need to remember our past to enable our future
- LDRD DR projects are part of the solution and must be preserved
 - **Timothy Germann, T-1:** *Spatial Temporal Frontiers of Atomistic Simulations*

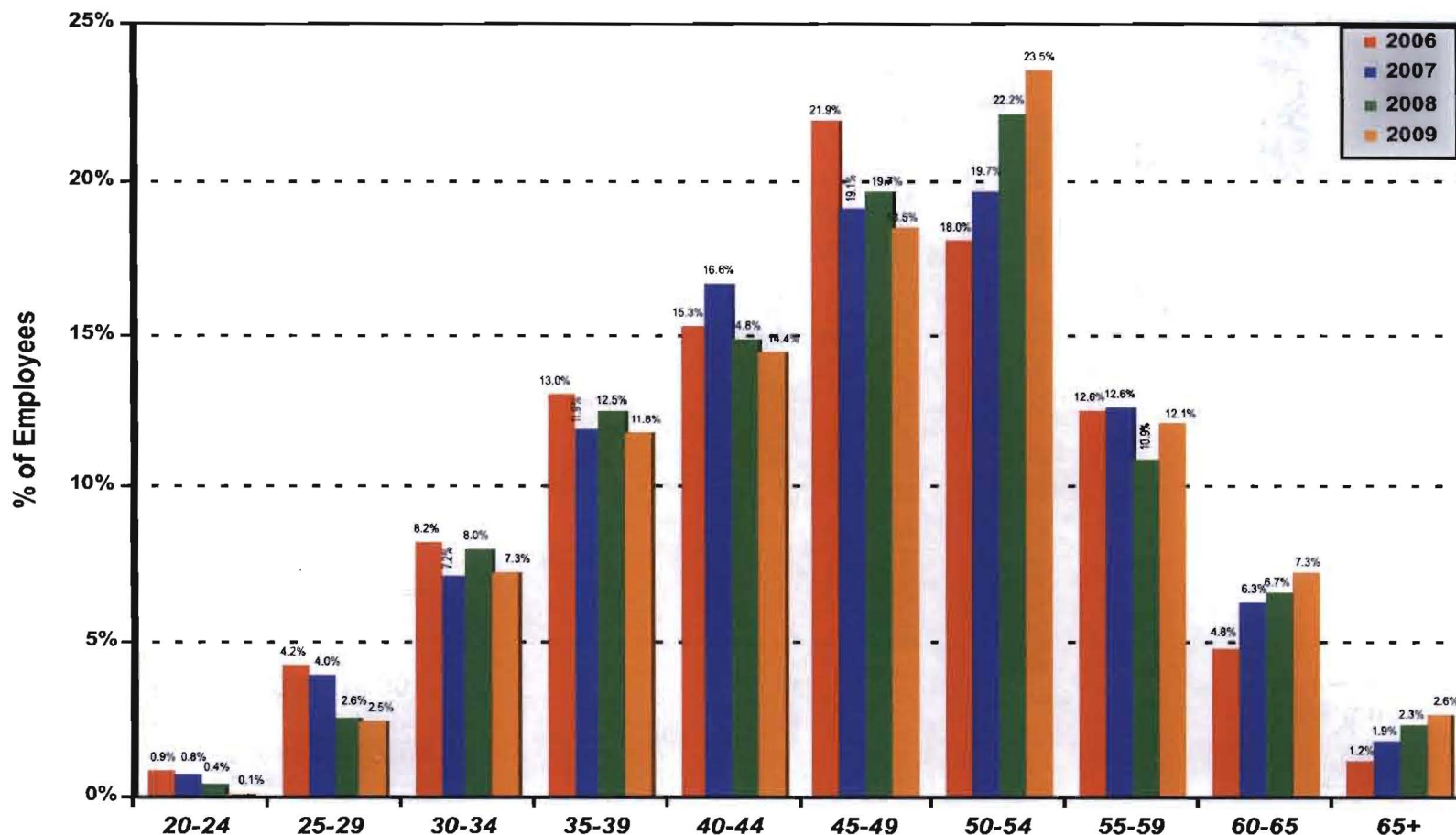
CTBT Safeguard B “The maintenance of modern nuclear laboratory facilities and programs in theoretical and exploratory nuclear technology which will attract, retain, and ensure the continued application of our human scientific resources to those programs on which continued progress in nuclear technology depends”

Our workforce demographics are further cause for concern – aging progressed from Chiles 1999 to Chiles 2008*



Weapons Science Employees by Age Group 1998 vs 2008

A closer look at recent years (FY06 – FY09) indicates we need to recruit more early career employees



Weapons Science % of Employees by Age Group/FY

....and we need to improve the morale of our workforce

Morale as measured by employees has deteriorated at LLNL & LANL since 1999*

DOD (OSD, JS, Agencies)	Army	Navy	DOD Air Force	DOE Labs	DOE Plants	DOE Headquarters
74%	89%	81%	71%	72%	79%	68%

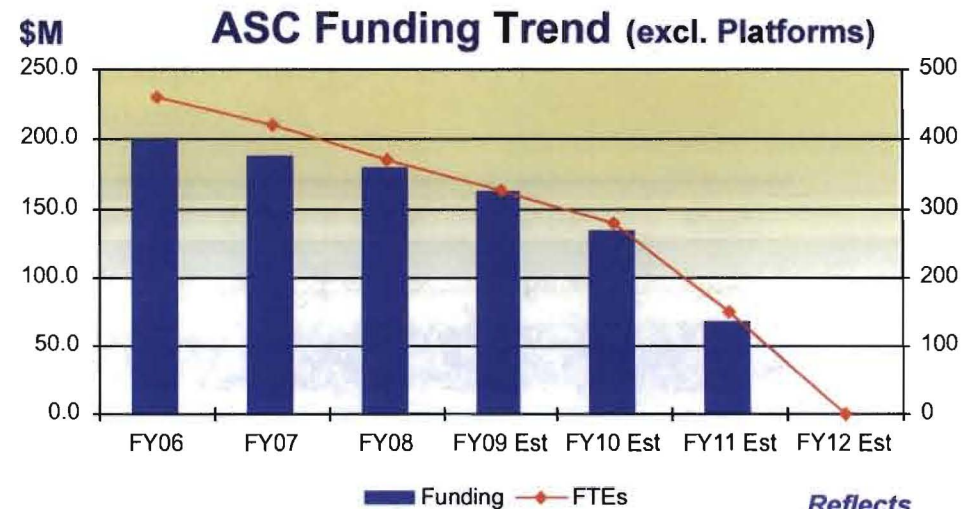
	LANL	Sandia	LLNL	KCP	PANTEX	Y-12	SRS	DOE HQ	NT's
2008	55%	81%	70%	81%	77%	80%	67%	68%	68%
1999	85%	78%	84%	57%	70%	51%	67%	51%	68%

*Table A-4. Would you recommend your organization? (Percent responding "yes")**

The recently-received FYNSP budget is devastating for LANL Weapons Science – killing ASC here is unconscionable

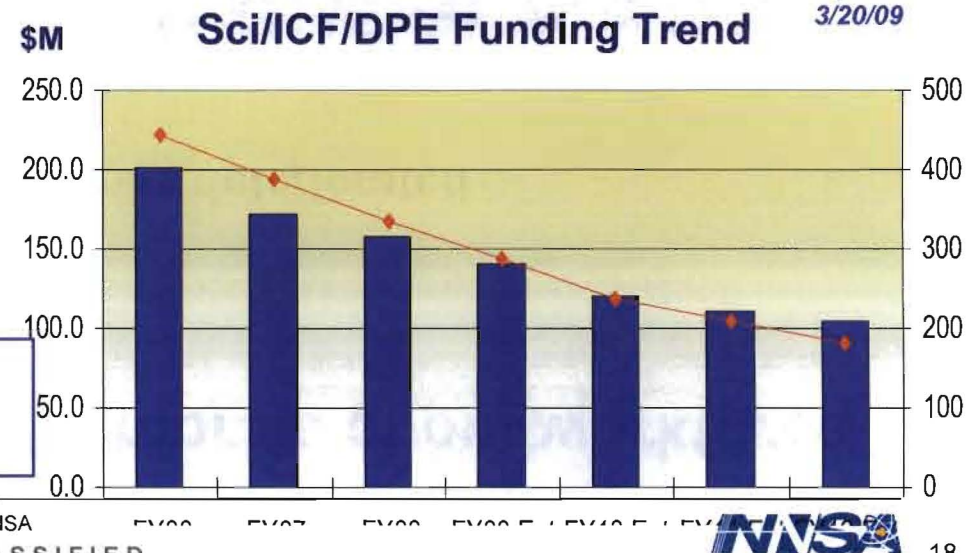
ASC:

- FY09 LANL omnibus site split is estimated to be \$156M (incl. \$12M for Roadrunner). FY09 omnibus identified \$15M for Zia.
- Lab's predictive capability is beginning to see a serious impact in FY09; seeing a rapidly reducing ability to retain expertise.
- Elimination of ASC at LANL makes stewardship of the stockpile impossible



Sci/ICF/DPE:

- FY09 omnibus estimated site split at \$118.7M: \$5M less than the currently planned budget. Assumes DPE is released from HQ at expected \$ level.
- Experimental Capabilities are at risk.

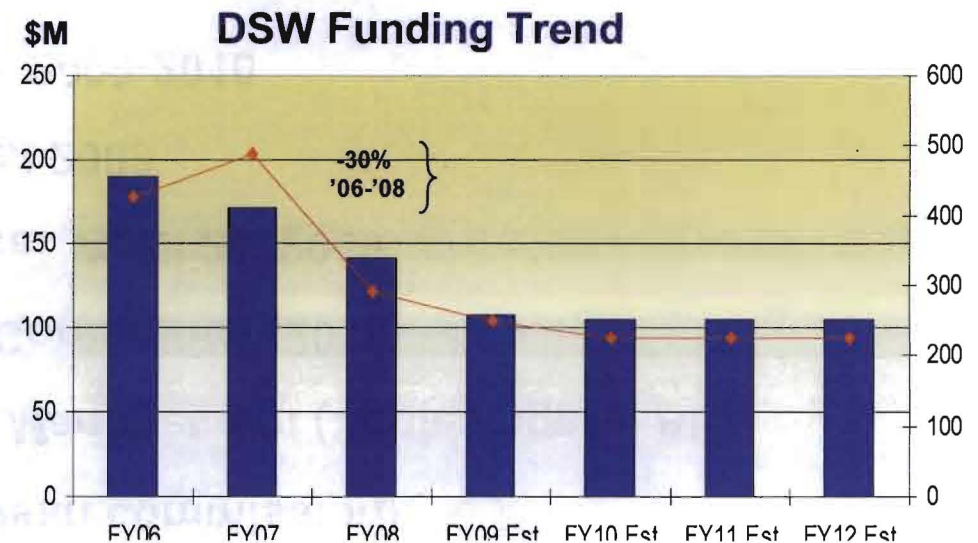


Note: Science has a higher labor/non-labor ratio than ASC, hence greater FTE impact

Our physics assessments come from DSW; also a concern looking to out years

DSW R&D:

- FY09 omnibus site split reduced expected DSW funding from \$125M to \$111M. \$2M included for B61 LEP study.
- FY10-12 assume budgets remain flat from FY09.
- Current FYNSP does not include needed system LEPs. Decisions required at national level.



The national discourse on nuclear weapons issues provides an opportunity to increase attention on the stockpile and its stewardship

- ***Leveraging Science for Security: A Strategy for the Nuclear Weapons Laboratories in the 21st Century*** (Stimson Center)
- ***Defense Science Board Task Force on Nuclear Deterrence Skills*** (Chiles commission)
- ***Congressional Commission on the Strategic Posture of the United States*** (Perry/Schlesinger bi-partisan commission)
- ***Task Force on Nuclear Weapons Management*** (Schlesinger – AF)
- **Non Proliferation Treaty Review Conference** (2010)
- ***Strategic Stewardship Conference***: April 28, 2009
- ***Nuclear Posture Review***: ~August 2009
- ***Comprehensive Test Ban Treaty***: 2009-2010

We are working all issues in close collaboration with LLNL and SNL



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Updating CTBT safeguards is key to sustaining a credible nuclear stockpile

PRIMARY RISK from a *ratified* CTBT:

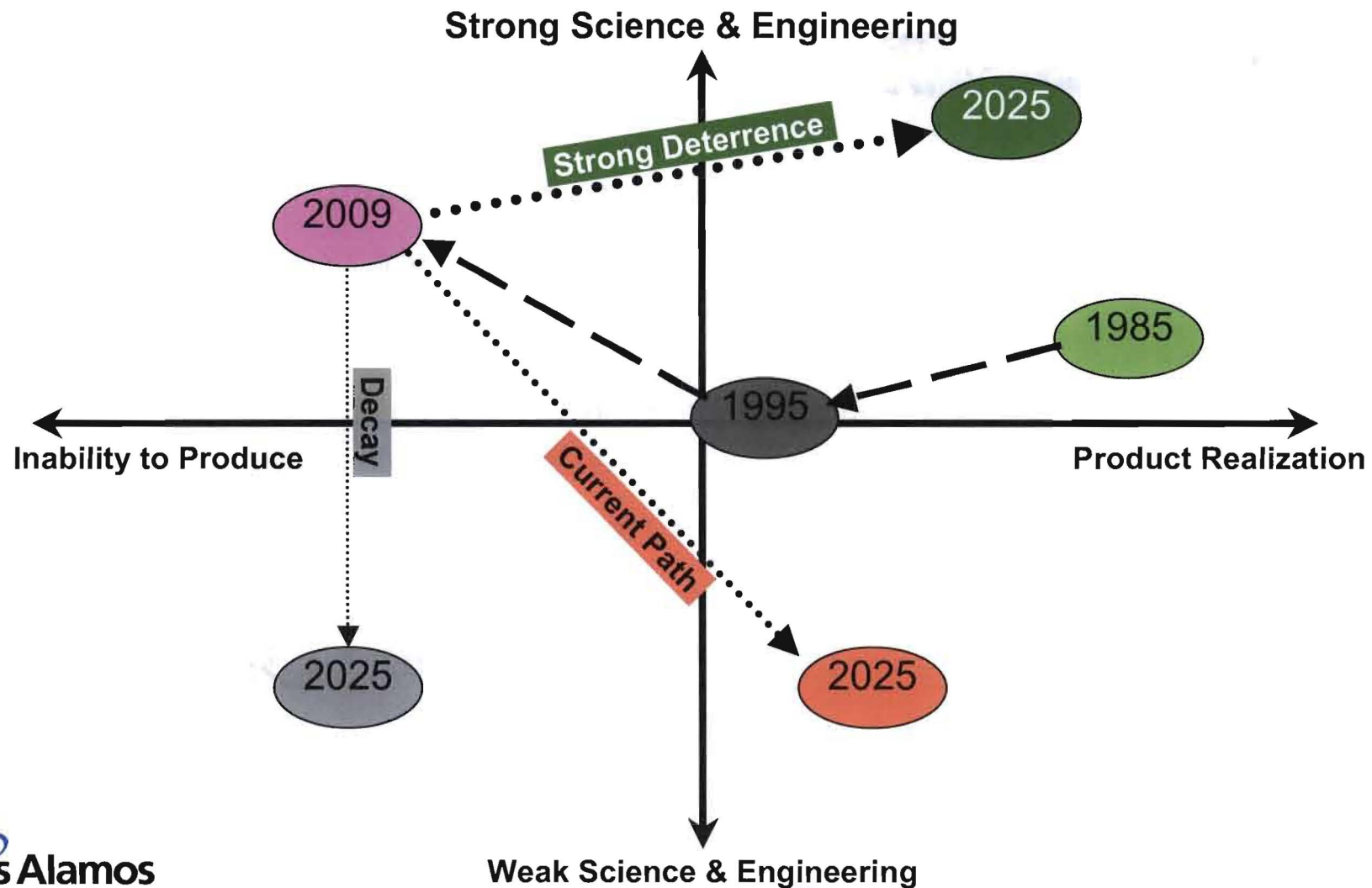
- **Attention** to the nuclear deterrent will likely erode —
 - The effectiveness of the CTBT Safeguards could atrophy quickly
 - *Technically: there is little difference between a ratified CTBT, and the current testing moratorium*

MITIGATION measure:

- Strengthen the language of the safeguards

*We must design mechanisms to counter “intentional inattention”
—Sustaining a credible nuclear deterrent requires enduring safeguards*

The course we undertake today will determine the outcome of tomorrow



Stockpile risk under a CTBT decreases with increased flexibility

- Limited refurbishment with a combination of reuse and replacement provides timely modernization
 - Refurbishment alone cannot meet DoD performances, safety and security standards for much of the stockpile
 - Reuse enables necessary stockpile production timelines
 - Replacement is essential for a viable modernized stockpile with increased flexibility and diversity
- Stockpile modernization can increase confidence and long-term stockpile flexibility and diversity, and provide challenging (attractive) science for our future workforce

Options for the stockpile:

Do Nothing → Refurbishment → Reuse → Replacement

Decreasing Stockpile Risk

CTBT safeguards require continuing national support to ensure the safety, security and reliability of the deterrent

Considerations for inclusion in forward-looking safeguards:

- **Stockpile modernization:** refurbishment, reuse, replacement provide options and maintain needed capabilities for the future
- **Product realization capability:** notably absent in current safeguards
- **Maintaining a hedge capability to test is essential:** complement a strong stewardship program with irreducible set of test-specific activities
- **Surveillance:** more important as stockpile is reduced and ages
- **Annual Assessment:** expand to address projected state of the stockpile and capabilities

We are developing a forward look to guide the evolution of our mission over the next 5-15 years

Five teams focused on the following areas to identify our thinking (asking the right questions) and develop elements of a broader strategy for stewardship

- Chairs have established teams of ~6 leaders to work their areas
- Integration through regular meetings with the chairs and team cross-pollination
- ***Our Computational Framework – John Hopson***
- ***Our Experimentally-Validated Science Base – Mary Hockaday***
- ***Our Approach to Large Integrating Experiments – Maurice Sheppard***
- ***Our Approach to Diversification – Jay Dallman***
- ***Evolution of the Stockpile – Michael Bernardin***

From this exercise we will develop a high-level ADWP strategy that lays out a compelling evolution of weapons physics activities

Some talks will touch on elements of this effort

Modeling and Simulation Capability Futures - Hopson

- Hardware - current requirements, evolution path, power limitations
- Tools for future code development within evolving architectures

Sustaining Capability through Diversification - Dallman

- Hedging and leveraging capabilities across missions

Experimental Science Capabilities - Hockaday

- Looking beyond PCF
- Identification of pacing technologies that increase certification confidence
- Leveraging capabilities between the Labs

Sustaining Nuclear Design - Bernardin

- Transition from current to future weapons systems
- Certification - advanced approaches, common model, QMU
- Evolution of deterrence - external threats, technological surprise

We are asking you to tackle these additional questions for our FY09 review

- 1. In what ever national nuclear security course the nation takes over the next decade have we missed something in our analyses or scenario back drop critical to our capability strategy?**
- 2. Are the technical challenges or problems that need to be resolved (scope of work) providing us the ability to attract the quality of work force necessary?**
- 3. Do we have enough flexibility in our capabilities to handle the inevitable questions that will arise?**

Weapons Science Capability Review Agenda

AGENDA SLIDES



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BACKUP SLIDES

CTBT Safeguards

Safeguard A (Stockpile Stewardship)

The conduct of a Science Based Stockpile Stewardship program to ensure a high level of confidence in the safety and reliability of nuclear weapons in the active stockpile, including the conduct of a broad range of effective and continuing experimental programs.

Safeguard B (Scientists)

The maintenance of modern nuclear laboratory facilities and programs in theoretical and exploratory nuclear technology which will attract, retain, and ensure the continued application of our human scientific resources to those programs on which continued progress in nuclear technology depends.

Safeguard C (Test Readiness)

The maintenance of the basic capability to resume nuclear test activities prohibited by the CTBT should the United States cease to be bound to adhere to this treaty.

Safeguard D (Monitoring)

Continuation of a comprehensive research and development program to improve our treaty monitoring capabilities and operations.

Safeguard E (Intel)

The continuing development of a broad range of intelligence gathering and analytical capabilities and operations to ensure accurate and comprehensive information on worldwide nuclear arsenals, nuclear weapons development programs, and related nuclear programs.

Safeguard F (Annual Assessment)

The understanding that if the President of the United States is informed by the Secretary of Defense and the Secretary of Energy (DOE)—advised by the Nuclear Weapons Council, the Directors of DOE's nuclear weapons laboratories and the Commander of the U.S. Strategic Command—that a high level of confidence in the safety or reliability of a nuclear weapon type which the two Secretaries consider to be critical to our nuclear deterrent could no longer be certified, the President, in consultation with Congress, would be prepared to withdraw from the CTBT under the standard “supreme national interests” withdrawal clause in order to conduct whatever testing might be required.

National discourse surrounding CTBT has provided a focus on the safeguards afforded to the nuclear stockpile

PRIMARY RISK from a *ratified* CTBT:

- **Attention to the nuclear deterrent will likely erode —**
 - **The effectiveness of the CTBT Safeguards could atrophy quickly**
 - ***Technically: there is little difference between a ratified CTBT, and the current testing moratorium***

Additional Risks:

- ***“Modernization”* could be interpreted as precluded under the CTBT**
- ***On-Site Inspections* could interfere with national security missions**

MITIGATION measure:

- **Strengthen the language of the safeguards**

**We must design mechanisms to counter “*intentional inattention*” —
Sustaining a credible nuclear deterrent requires enduring safeguards**

Agenda

Weapons Science Capability Review
March 25 – 27, 2009

SECURITY NOTICE: Electronics, including cell phones, two-way pagers, PDAs (Blackberry, PalmPilot, etc.), laptop computers, thumb-drives, cameras, etc. are NOT allowed in cleared Laboratory areas. It is suggested that visitors going behind the security fence leave all personal belongings in vehicles or hotel rooms or they will be subject to a complete search to include coats, purses, briefcases, etc.

Weapons Meeting Room
TA-03, Bldg. 1400, Room 6413B

Wednesday, March 25, 2009 (7:00 am – 7:30 pm)

- 7:00 Meet Committee Members in Lobby of Holiday Inn Express Evan Sanchez
Protocol Planner, Protocol Office
- 7:10 Bus leaves Holiday Inn LANL Taxi Service
- 7:15 Arrive at Otowi Building for badging Evan Sanchez

Institutional Requirements and Weapons Science Capability

- 7:30 Executive Session – (closed session) Roy Schwitters
Chair, Weapons Science Capability Review
- 7:50 Introductions, Agenda, Meeting Logistics Charles McMillan
Associate Director, Weapons Physics
- 8:00 Security Briefing Michael Irving
Security Program Leader, Weapons Physics
- 8:10 Director's Welcome & Committee Charge Terry Wallace, Jr.
Principal Associate Director, Science, Technology, and Engineering
- 8:45 Overview and Strategic Directions Charles McMillan
Associate Director, Weapons Physics

10:30 Break

Institutional Host(s): Charles McMillan, ADWP 505-667-8711
Technical Host(s): Mary Hockaday, ADWP, 505-667-8711
Protocol POC: Evan Sanchez, CGA-GAO/505-667-5223/Call 699-1121

Classification Level: Unclassified/REF Sigma 1-10 Page 1
Dress: Business/Business Casual
RED - Classified Presentation

Agenda

Modeling and Simulation Capabilities

- 10:45 Modeling and Simulation Capability Futures and Discussion John Hopson
Program Director, ADWP

11:55 Depart for Working Lunch – University House

12:00 Working lunch with Early Career Staff (by invitation only) – University House

1:00 Return to Weapons Meeting Room

- 1:05 Code Strategy Bill Archer
Acting R&D Manager/Program Manager, X-3

- 1:50 Roadrunner
Hardware Andy White
Deputy Associate Director, Theory, Simulation, and Computation
Codes Paul Henning
R&D Scientist, CCS-2

3:00 Break

- 3:15 Spatial Temporal Frontiers of Atomistic Simulations Timothy Germann
R&D Scientist, T-1

Publication, Peer Review, and Recognition

- 4:00 Overview of Publication Record, Peer Review, and Recognition Bryan Fearey
Executive Advisor, ADWP
- 4:30 Defense Research Review (DRR) Process Joyce Guzik
Scientist/Laboratory Fellow, X-2
- 5:15 Executive Session (closed session) Roy Schwitters
Chair, Weapons Science Capability Review
- 5:45 Depart for No Host Dinner at Central Avenue Grill LANL Taxi Service
- 6:00 No Host Dinner at Central Avenue Grill
- 7:30 Depart for Holiday Inn Express LANL Taxi Service

Institutional Host(s): Charles McMillan, ADWP 505-667-8711
Technical Host(s): Mary Hockaday, ADWP, 505-667-8711
Protocol POC: Evan Sanchez, CGA-GAO/505-667-5223/Call 699-1121

Classification Level: Unclassified/REF Sigma 1-10 Page 2
Dress: Business/Business Casual
RED - Classified Presentation

Agenda

Thursday, March 26, 2009 (7:00 am – 7:30 pm)

- 7:00 Meet Committee Members in Lobby of Holiday Inn Express Evan Sanchez
Protocol Planner, Protocol Office
- 7:10 Depart for TA-3-1400, Weapons Meeting Room LANL Taxi Service
- 7:15 **Executive Session (closed session)** Roy Schwitters
Chair, Weapons Science Capability Review

Experimental Science Capabilities

- 8:00 Experimental Science Capabilities: Strategic Look in Progress Mary Hockaday
Deputy Associate Director/Program Director, Science Campaigns
- 9:10 **MaRIE: Matter-Radiation Interactions in Extremes** John Sarrao
Program Director, SPO-SC
- 9:40 **DARHT Update** David Funk
R&D Manager, HX Division

10:15 Break

Diversification

- 10:30 Capability Sustainment through Diversification Jay Dallman
R&D Manager, DE Division
- 11:00 Lunch with Senior & Mid-career Staff (by invitation only) – Weapons Meeting Room

Nuclear Design

- 12:15 **Advanced Certification** Don Haynes
R&D Manager, X-4
- 1:15 **Sustaining Nuclear Design** Michael Bernardin
R&D Manager, X Division

2:15 Break

Agenda

2:20 Executive Session (closed session) Roy Schwitters
Chair, Weapons Science Capability Review

- 2:55 Depart for Poster Session – Oppenheimer Study Center
- 3:00 Poster Session – Oppenheimer Study Center – Upper Level
- 5:15 Depart for Working Dinner - Otowi Cafeteria
- 5:30 Working Dinner (by invitation only) - Otowi Cafeteria**
- 7:30 Depart for Holiday Inn Express LANL Taxi Service

Friday, March 27, 2009 (8:00 am – 3:00 pm)

- 7:15 Committee Members arrive (via private vehicle) at TA-3-1400 (Weapons Meeting Room)
- 7:30 **Executive Session** Roy Schwitters
Chair, Weapons Science Capability Review
- 8:30 Meeting with Capability Leaders
- 9:45 Break
- 10:00 **Executive Session (closed session)** Roy Schwitters
Chair, Weapons Science Capability Review
- 12:00 Working lunch Committee Members only
- 1:30 Closeout Meeting (DIR, PADs, AD, DAD) Terry Wallace, Jr.
Principal Associate Director, Science, Technology, and Engineering
- 2:30 Closeout Meeting (Open to All) Roy Schwitters
Chair, Weapons Science Capability Review
- 3:30 Adjourn

WEAPONS SCIENCE CAPABILITY REVIEW

Roadrunner Update

Andy White

Deputy Associate Director for Theory,
Simulation and Computation

March 25, 2009



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Roadrunner project is on track.

Activity	Schedule
Deliver full Roadrunner system @ LANL	Completed
Repeat LINPACK run @ LANL	Completed
Deliver additional open RR resources	Completed
Accept full RR system	Completed
Begin full system stabilization & integration	In progress
Begin open science applications on full system	In progress
ASC Level 2 Milestone: Weapon Code Initial Capability	4QFY09
Begin classified operations	4QFY09
ASC Level 2 Milestone: Weapon simulation study	4QFY10



Roadrunner team was first to
achieve a petaflop/s

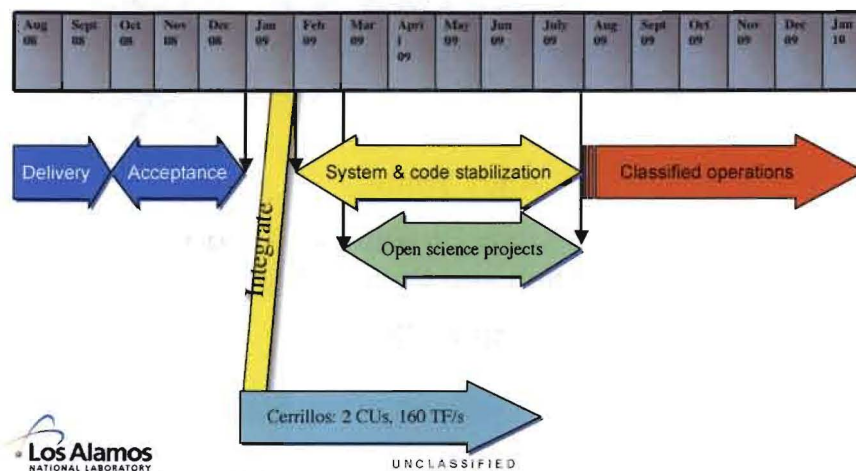


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RR will support open science in FY09 and classified applications in FY10 and beyond.



Open science has a broad, exciting footprint & will develop six new application capabilities for RR.

Project	Code
<i>Kinetic Thermonuclear Burn Studies with VPIC on Roadrunner</i>	VPIC
<i>Multibillion-Atom MD Simulations of Ejecta Production and Transport</i>	SPaSM
<i>New frontiers in viral phylogenetics</i>	ML
<i>Three-D Dynamics of Magnetic Reconnection in Space and Laboratory Plasmas</i>	VPIC
<i>The Roadrunner Universe</i>	MC ³
<i>Implicit Monte Carlo Calculations of Supernova Light-Curves</i>	Cassio
<i>Instabilities Driven Reacting Compressible Turbulence</i>	CFDNS
<i>Cellulosomes in Action: Peta-Scale Atomistic Bioenergy Simulations</i>	GROMACS
<i>Parallel-replica dynamics study of interactions in atomic force microscopy and the formation and mechanical properties of metallic nanowires</i>	SPaSM + PAR-REP
<i>Saturation of Backward Stimulated Scattering of Laser In The Collisional Regime</i>	VPIC

<p>Connected Unit cluster 180 compute nodes w/ Cells 12 I/O nodes</p>	<p>12,240 Cell PowerXCell 8i \Rightarrow 1.33 PF/s, 49 TB 6,120 dual-core Opteron \Rightarrow 0.05 PF/s, 49 TB</p>
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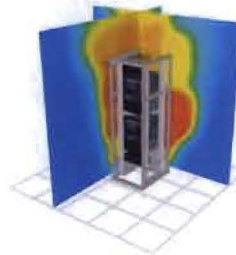


- The future holds both opportunities and threats, some are both.

- [illegible]



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