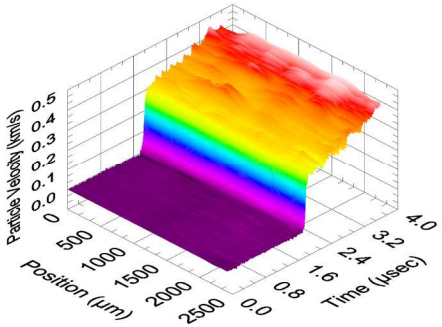
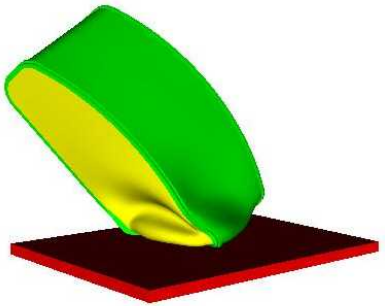
Engineering Sciences Research Foundation (ESRF) Overview

SAND2007-0450C

ESRF External Panel Review
January 15, 2007



LDRD Inside
LABORATORY DIRECTED RESEARCH AND DEVELOPMENT



ENGINEERING SCIENCES RESEARCH FOUNDATION

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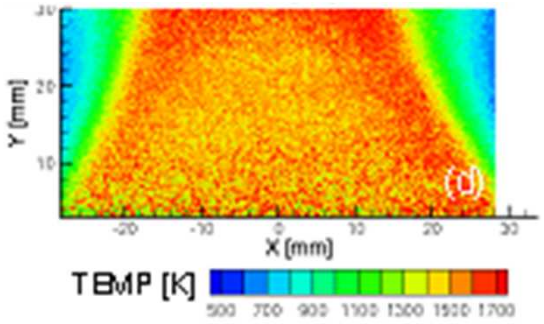
ESRF Objectives

The Engineering Sciences Research Foundation (ESRF) provides capabilities and understanding required to enable predictive simulation in support of the Engineering Sciences needs of Sandia's Strategic Management Units.

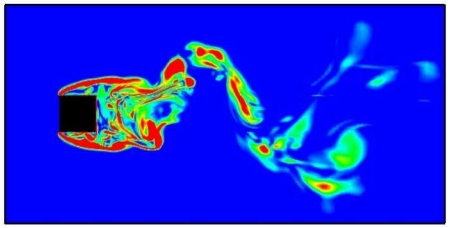
Discipline areas include thermal sciences, fluid sciences, aerosciences, solid mechanics, structural dynamics, material mechanics and electrical sciences.

Research Themes for ESRF

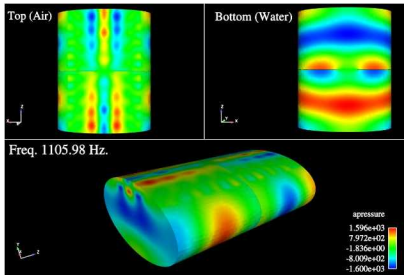
- High fidelity diagnostics and novel experimental approaches:
  - Spatial and temporal resolution
  - Complex/multiple phenomena
  - Range of conditions: continuum to non-continuum
- Constitutive phenomena critical to closure for predictive simulation, e.g.:
  - turbulence, phase change, friction, joints, accommodation coefficients.
- Advanced computational capabilities:
  - Single and multiphysics, e.g. acoustics, noncontinuum, multiphase.



2-D Temperature Imaging w/ FRS

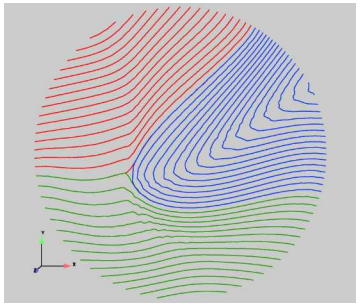


Detached Eddy Simulation



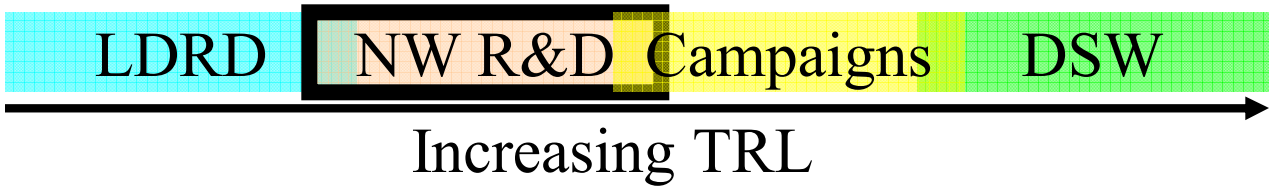
Acoustic simulation capabilities

Multiphase tracking

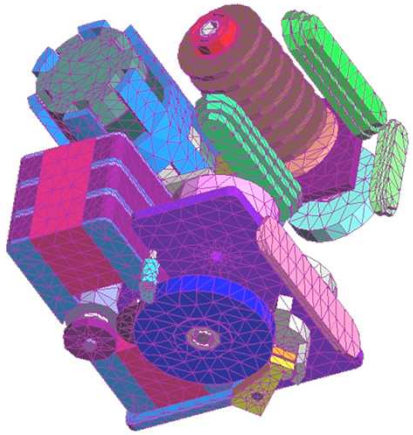


Engineering Sciences Research Foundation (ESRF) has two primary components:

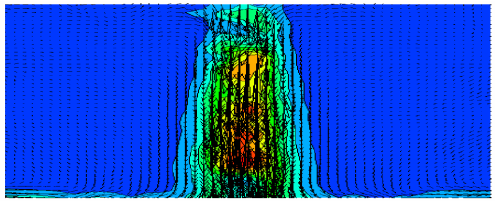
- **Laboratory Directed Research and Development (LDRD)**
  - LDRD is Sandia's **sole source of funding for laboratory-directed technical work** as authorized by Congress and the Department of Energy (DOE) and represents up to 6% of laboratory revenue
  - Focused on **fundamental research and innovative approaches to complex problems of relevance to Sandia's SMUs**
  - **Time horizon is greater than 5 years**
  - Enable Predictive Simulation (EPS) portfolio is approximately $15.4M
- **Tech Base Program (NW)**
  - Research and Development that **builds upon prior fundamental research to build capabilities/understanding to support the needs of the NW program**
  - Combined experimental and computational program
  - **Time horizon is less than 5 years**
  - Engineering science portfolio about $9M (including funding of joint Sandia/NSF program)



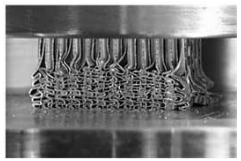
Engineering Sciences Research Foundation (ESRF) provides critical understanding and capabilities for predictive simulation

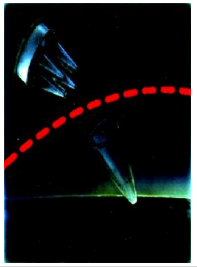


Geometry, Mesh, Algorithms

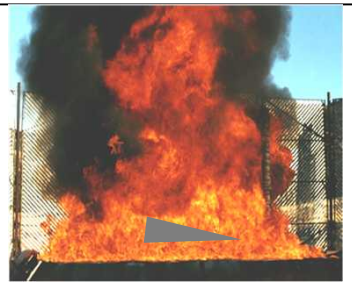


Subgrid Phenomena and Constitutive Models

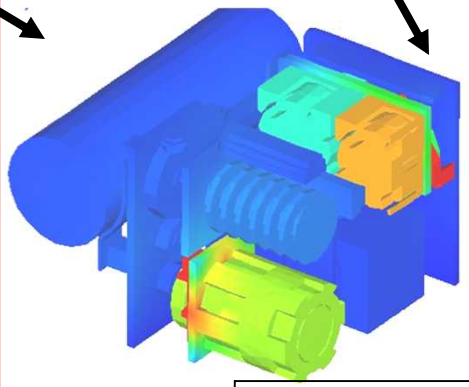


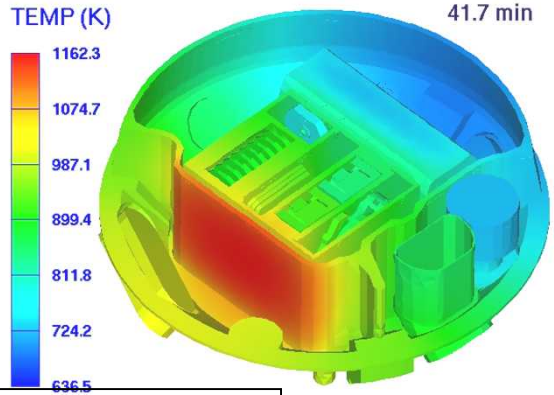


Environments and Initial State



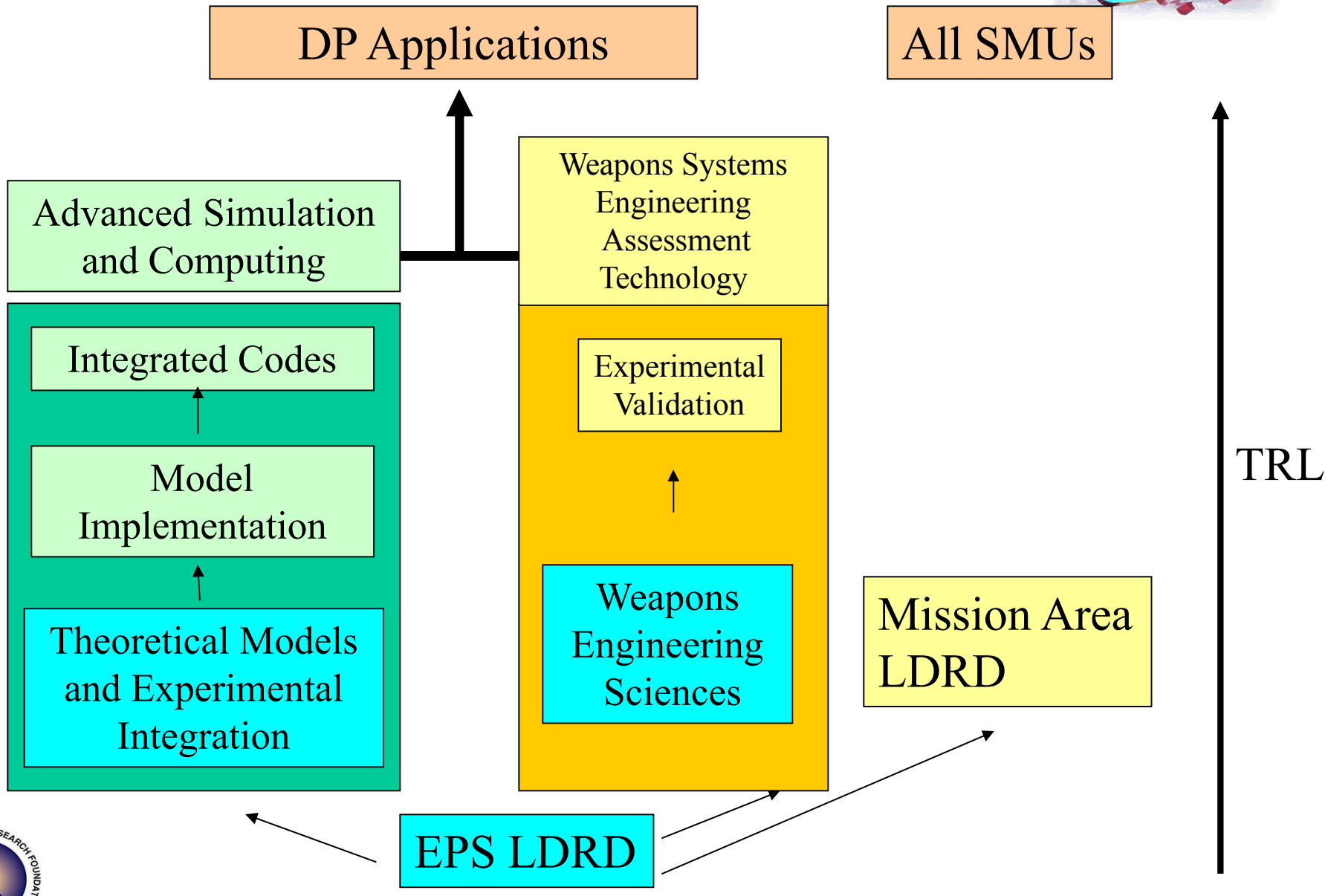
Validation, UQ





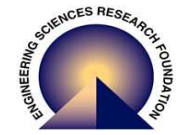
Predictive Simulation based on physics

Programmatic Alignments



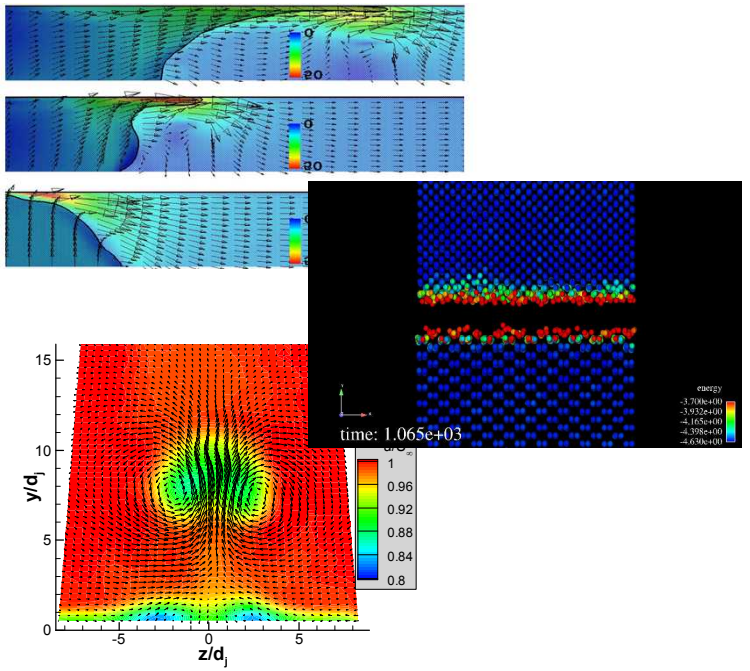
Enable Predictive Simulation (EPS) Investment Area

- Sandia LDRD program restructured by CTO, Rick Stulen
  - Created 8 investment areas including EPS
- Investment area lead by Engineering Sciences Director, with a cross-center Director Team
- $15.4M Portfolio
- EPS Strategic Objective:
  - The Enable Predictive Simulation LDRD Investment area sponsors innovative research and development that builds the knowledge base and capabilities necessary for predictive simulation of complex problems. Scientifically grounded simulation leveraging advanced computational capabilities will revolutionize our ability to understand complex behavior of human and natural systems, and engineer innovative products. This investment area enhances the ability of Sandia's Strategic Management Units to provide solutions to their customers that are grounded in fundamental understanding of underlying principles, and that exceed customer expectations of performance, cost and schedule.



EPS Thrust Areas

- **Physical and Engineering Sciences (P&ES):**
  - Thermal/Fluids/Aero-sciences
  - Solid Mechanics/Material Mechanics/Structural Dynamics
  - Electrical Sciences & Electromagnetics
  - Chemical and Combustion Sciences
  - Material and Geo-sciences
- **Computational & Information Sciences (C&IS):**
  - Algorithm Research & Development
  - Advanced Architectures & Frameworks
  - Future Platforms
  - Optimization/UQ
  - Visualization
  - Informatics



Enable Predictive Simulation (EPS) R&D Goals

- Advanced experimental diagnostics that permit spatial and temporal resolution of key behavior.
- Experimental discovery focused on enhancing our understanding with the intent of building models that codify that understanding.
- Theoretical discovery of new methodologies and models that permit us to describe and predict key behavior.
- Development of computational approaches that codify new methodology.
- Development of computational and statistical approaches for optimization, verification, validation and uncertainty quantification.
- Computer Science that enables all aspects of problem definition, analysis, and prediction. Technologies may include informatics and visualization.
- Discovery and development of computer platforms, architectures and frameworks that enable predictive simulation.

Build knowledge base and capabilities necessary for predictive simulation of complex problems.

EPS IAT Director Team

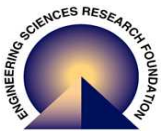
- **Director team consists of 6 Directors across core disciplines:**
  - **Art Ratzel, *Engineering Sciences*, Chair**
  - David Womble, *Computations, Computers, Information and Mathematics*, Co-Chair
  - Bob Carling, *Physical and Engineering Sciences*
  - Duane Dimos, *Materials and Process Sciences*
  - Peter Davies, *Nuclear Energy and Global Security Technologies*
  - Len Napolitano, *Computer Science and Information Technologies*

Physical & Engineering Sciences (P&ES) Thrust Area

- **S&T Activities in Traditional Engineering Disciplines**
  - Thermal/Fluids/Aero-sciences
  - Solid Mechanics/Material Mechanics/Structural Dynamics
  - Electrical Engineering & Electromagnetics
  - Chemical and Combustion Sciences
  - Material and Geo-sciences
- **Focus Areas**
  - Phenomenology Understanding & Quantification (Experiment & Theory)
    - Continuum & Non-continuum processes
    - Multi-scale physics (Bridging micro-to-continuum)
  - Advancing the tools
    - New Diagnostics
    - V&V/QMU methodology

Investment Area Team (IAT) for P&ES

- **Wahid Hermina, ES – Area Lead**
- Mel Baer, ES, reactive processes, chem
- Davina Kwon, ES,
- Jim Redmond, ES, micro, solid, structural
- Tim Trucano, C&IS, validation and UQ sciences
- Sudip Dosanjh, C&IS, thermal-fluids computational
- Justine Johannes, MS&T, materials, processes, chemistry
- Mark Kiefer, Electromagnetics & electrical effects
- Scott Hutchinson, Electrical devices and systems
- John Merson, C&ES, geosciences
- Tim Shepodd, MS&T
- Carl Peterson, Thermal, fluids,aero

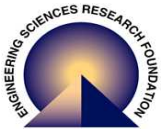


Computational & Information Sciences (C&IS) Thrust Area

- **Focus Areas**
  - Algorithm Research & Development
  - Advanced Architectures & Frameworks
  - Future Platforms
  - Optimization/UQ
  - Visualization
  - Informatics
  - Computational Methods R&D

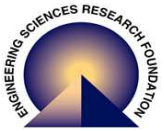
Investment Area Team (IAT) for C&IS

- **Sudip Dosanjh, C&IS – Area Lead**
- Bob Benner, C&IS
- David White, C&IS, informatics
- Scott Collis, C&IS, algorithms
- Heidi Ammerlahn, informatics/algorithms
- Eliot Fang, MS&T, computational mechanics
- Wahid Hermina, ES
- Jim Stewart, computational mechanics and frameworks
- Chris Moen, computational mechanics
- Tom Pfeifle, Geomechanics
- Mitch Sukalaski, architectures
- Mike Hardwick, architectures



EPS LDRD Review Criteria

- Innovation/Creativity
  - **Technical viability**
  - **Boldness – "game-changing"**
- Impact
  - Technical
  - Strategic
    - Has mission thrust insertion potential
    - New business through technology
    - Supports 10 year corporate objective
- Capabilities of Team (factors to be considered)
  - Nurture young staff.
  - Staff track record.
  - Team makeup (someone > 0.5 FTE).
  - University/industry connectivity, if needed.



Process for EPS Full-Proposal Written Reviews/Feedback to PIs

Technical Reviews/Feedback:

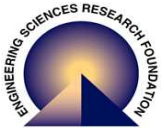
- Identify 1-2 technical reviewers for each proposal- selected principally from DMTS and Senior Scientist community
    - Complete detailed review with submission of review into LDRD Web Page. Submitted to PIs prior to oral review.
    - **Provide list of questions for proposal clarification and issues to PIs to support follow-on review sessions with IAT**

IAT Reviewer Responsibilities:

- Provide written clarification questions to PIs to be addressed during oral review.
- Each IAT reviewer reviews and scores each proposal (H/M/L/NA).

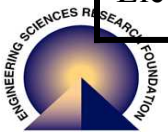
Programmatic Review/Feedback:

- IAT POC for each proposal inputs Thrust Area consensus view on programmatic value



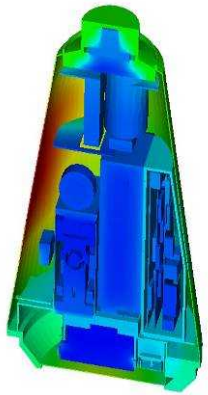
EPS Selection Matrix

Technology Groups (PM areas; PMs TBD)	Discover	Create	Prove
Computational Science	07-1246	07-0010, 07-0873, 07-1286, 07-1328	
Algorithms	07-0872, 07-0013, 07-1249,		
Computer Systems	07-1247, 07-1316, 07-1180	07-0309, 07-1317	
Informatics	07-1314, 07-1315	07-0612, 07-1248, 07-1251	
Materials	07-0206, 07-1257, 07-1329		07-0535
Failure	07-0462, 07-0704	07-0720	
Geophysics and porous media	07-1308	07-1244	
Solids and Structures		07-0166	
Fluid-Structures	07-1259	07-0247	
Thermal-fluids	07-0590, 07-1256	07-1330	
Microsciences & microenergetics	07-1069, 07-0377, 07-0746, 07-1258		
Electrical Sciences		07-0540, 07-1250	

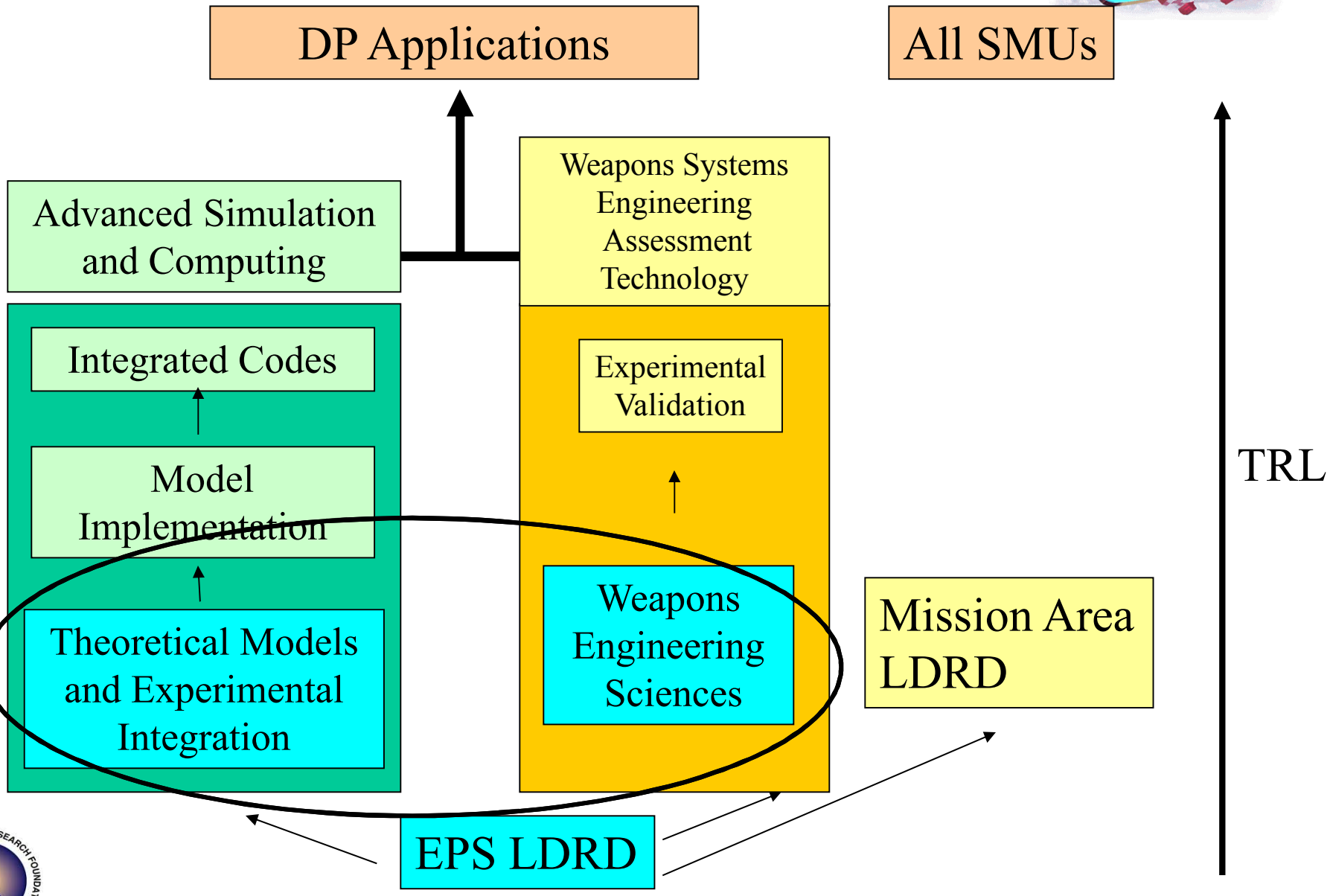


Metrics for Success

- Maturation of research to higher TRL development and application work.
  - Application driven migration of work to NW research foundation and impact to NW campaigns and DSW.
  - Spawn/enable SMU LDRDs and enhance Sandia ability to attract new customers and revenue.
  - Attract CRADA work supporting our core mission areas.
- Publications and citations.
- "Build knowledge base and capabilities necessary for predictive simulation of complex problems."
  - Performance, cost and schedule improvements for Sandia customers traceable to LDRD work.

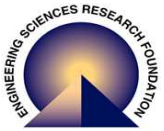


Programmatic Alignments



Engineering Sciences Tech Base Program – NW Funded

- Computational and Experimental Tech Base Program supporting the Engineering Sciences Needs of NW
  - R&D portfolio driven by discipline strategic plans
  - ~ $4M experimental program (C6)
  - ~$4.8M computational program (ASC/PEM)
- Joint funding, with NSF, of university research supporting needs of NW
  - $1M provided by Sandia from ESRF Tech Base Program
  - $1M provided by NSF from Engineering Directorate



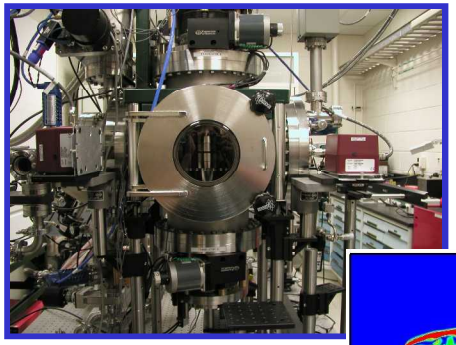
Tech Base Program Management

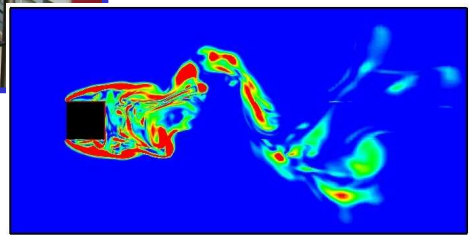
- Research Plans and projects created by Sub-discipline leads (technical managers)
  - **Address needs of NW program**
  - Research plans identify needs/drivers, current state, gaps and subsequent priorities
  - Review existing projects: Objectives, team, budget, applications and accomplishments
  - Propose new projects to address gaps: Objectives, team, budget, applications and deliverables.
- Research plans and projects reviewed by discipline leads (senior managers). Project modifications implemented, as required.
- Research program reviewed and approved by Engineering Sciences Council.
  - ES Council members are Directors or their delegates
  - Representatives from the NW program areas: Accelerated Strategic Computing (ASC), Engineering Campaigns (EC) and Science and Technology (S&T)
  - Representatives from each SMU: NW, DS&A, ER&N, HS&D
  - Representatives from key partner research foundations: computational sciences, microsystems, material sciences, manufacturing sciences.

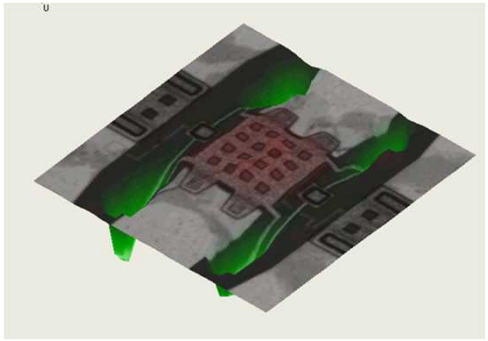
Research Plans are basis for ESRF Tech Base Management

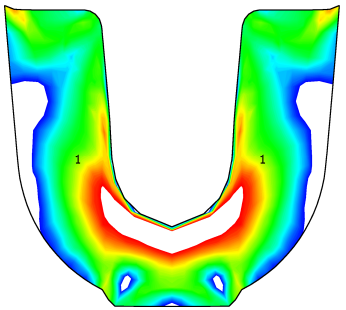
- **Research plans address mission drivers/needs, current state of disciplines, and gaps/priorities.**
  - **Integrated computational and experimental plans**

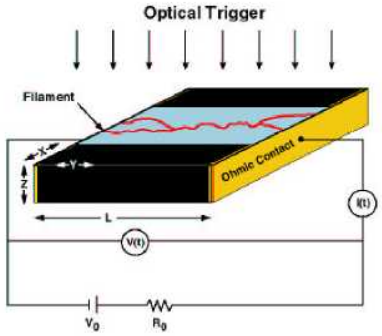
- Thermal, Fluid and Aero Sciences
  - **Microsciences**
  - **Fluid Sciences**
  - **Thermal and Reactive Processes**
  - **Aerosciences**
- Solid, Structural and Material Mechanics
  - **Structural Dynamics**
  - **Solid Mechanics**
  - **Material Mechanics**
- **Electrical Sciences**





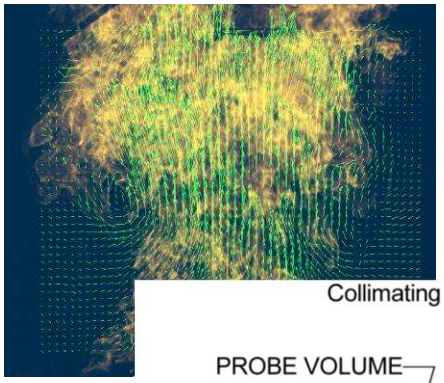


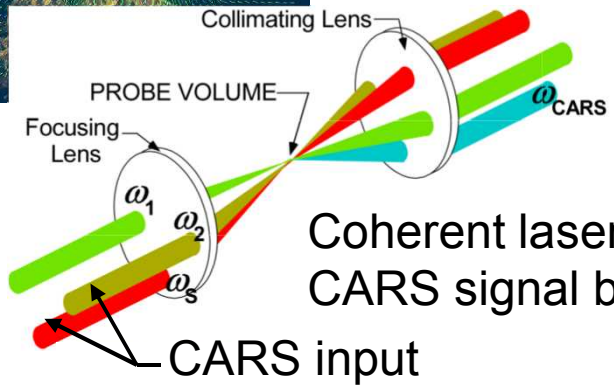


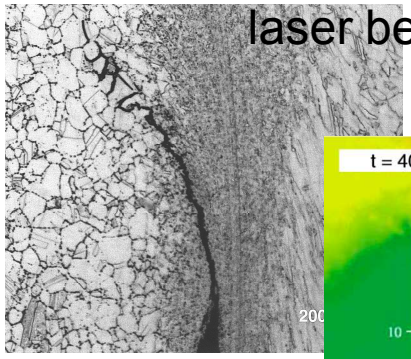


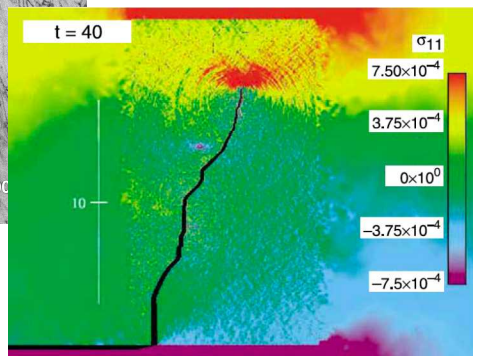
Supporting DP Activity

- Electrical sciences:
  - Electrical breakdown for lightning/safety
- Thermal, Fluids and Aerosciences:
  - Characterizing fire environments for safety. (W76, RRW)
  - Microsystems thermal response and gas-dynamics (Future systems)
  - Bomb/RB flowfields, aerothermal response and surface properties (B61, W76, RRW)
  - Multiphase flows for manufacture. (Neutron Generator, foam potting, NA123 defect free manufacturing)
- Solid, Structures, Material Mechanics
  - Failure models for performance and safety (B61, W76, RRW).
  - Material (foams, metal for gas storage…) response (B61, W76, RRW)
  - Macroscale and microscale structural response (B61 W76, RRW)



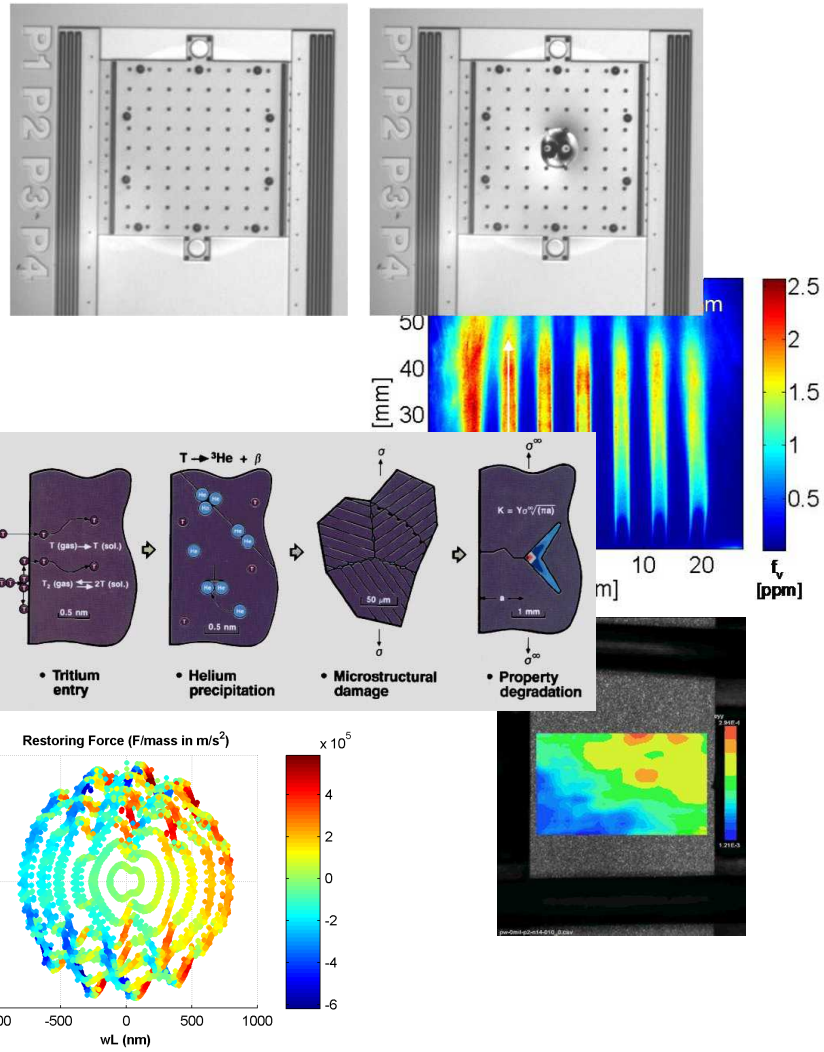






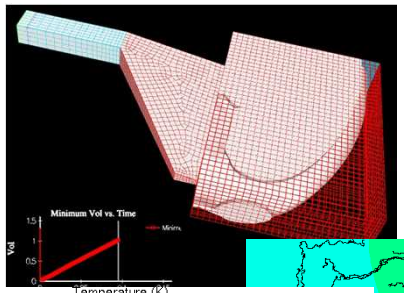
Representative FY06 Experimental Activities

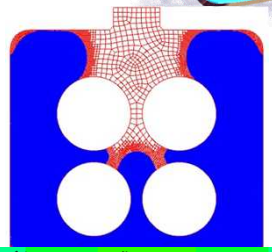
- Optical interations with microsystems
  - Advanced surety applications
- CARS (Coherent Anti-Stokes Raman Spectroscopy) and Raman-Variant Diagnostics for High-Resolution Thermometry
  - Impact on weapon safety
- Hydrogen-Deformation Interactions
  - Support gas transfer
- Optical Measurement Techniques (e.g. Digital Image Correlation)
  - Support safety and performance
- Nonlinear Dynamics of Micro-Scale Structures
  - Advanced surety applications

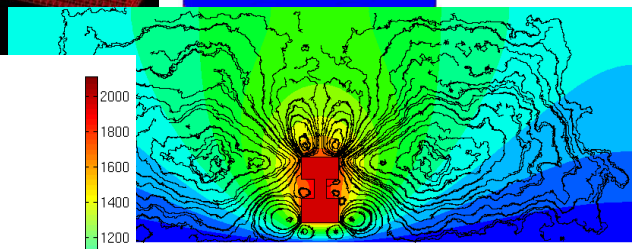


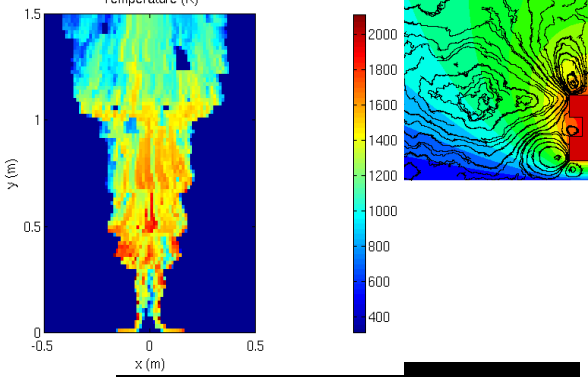
Representative FY06 Computational Activities

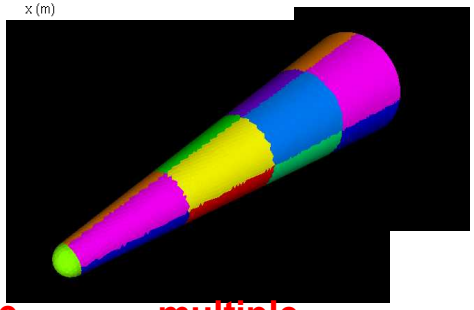
- Stable, efficient formulations of the level set, continuity, and momentum equations for 3-D, low capillary number problems – 100X speedup for 3D mold fill.
- Hosted International DSMC meeting:
- Turbulence model development for fire based on ODT.
- Acoustic analysis of mockup re-entry vehicle with prescribed external pressures due to re-entry. Investigated acoustic pressure buildup inside cavity.
- Developed Viscoplastic Foam Models for PMDI20 Foam and FR3712 foams
- Asperity-level modeling of polysilicon MEMS.
- Computational capabilities for electrical breakdown in solids
- Meshless method development for large deformation failure modeling

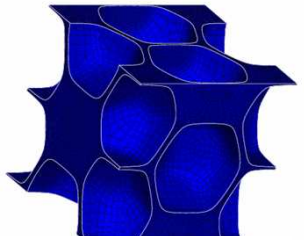


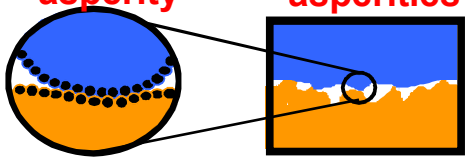


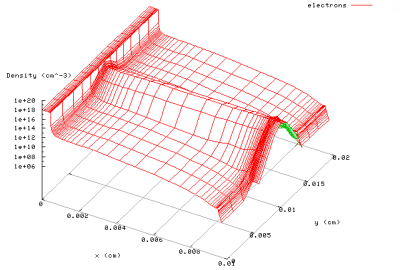






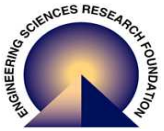






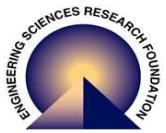
Sandia-NSF Joint Program

- Sandia Engineering Sciences and NSF Engineering Directorate jointly fund $2M/year of university research **responsive to programmatic needs of both organizations**.
  - Sandia portion funded out of Tech Base and PEM (NW) funding
- Program Title: **Engineering Sciences for Modeling and Simulation-Based Life-Cycle Engineering and Manufacturing**
- Projects are chosen through the formal NSF review process.
- We hold yearly workshops to exchange information between participants.
  - Last workshop held in Livermore, CA, on March 1 – 2, 2006 (18 projects)
  - Prior workshop held in Albuquerque, NM, on Feb 10 - 11, 2005. (19 projects)
- 13 new three year projects initiated in FY07



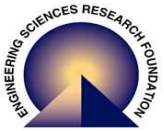
FY2006 NSF-Sandia Workshop Agenda

Solid and Structural Mechanics		**Presenter/Principal Investigator**
8:45 AM	Computational and Modeling Strategies for Damping and Multi-Physics Coupling on Interfaces	Tod Laursen, Duke University (Sandia Funded)
9:15 AM	Development and Analysis of Reduced-Order Models for Mechanical Joints and Interfaces	Edward Berger, University of Virginia, and D. Dane Quinn, University of Akron (SNL Funded)
9:45 AM	Modeling, Simulation and Experimental Study of Thermo-mechanical Degradation in Elastomeric Components	Alan S. Wineman, University of Michigan (SNL Funded)
10:15 AM	Break	
Thermal, Fluid and Aerosciences		**Presenter/Principal Investigator**
10:30 AM	Hot-Wire Measurements of Instability Waves on Sharp and Blunt Cones at Mach-6	Shann J. Rufer, Purdue University (SNL Funded)
11:00 AM	Hypersonic Boundary Layer Stability and Transition Analysis Using STABL	Graham V. Candler, University of Minnesota (SNL Funded)
11:30 AM	Design and Construction of the 3D Digital Particle Image Velocimetry & Thermometry System	Dana Dabiri, University of Washington (NSF Funded)
12:00 PM	Lunch	
1:00 PM	Stochastic Heat Transfer: Algorithms and Applications	George Karniadakis, Brown University (NSF Funded)
1:30 PM	A Posteriori Error Estimators in a Space-Time Framework	Marc Garbey, University of Houston (SNL Funded)
2:00 PM	Experiments on Uncertainty Propagation in Forced Convective Heat Transfer	Tait Pottebaum, University of Southern California (NSF Funded)
Electrical Engineering		**Presenter/Principal Investigator**
2:30 PM	RF MEMS Multiphysics Model, Experimental, Theoretical and Mitigation Studies	Katsuo Kurabayashi, University of Michigan and John L.Volakis, Ohio State University (NSF Funded)
3:00 PM	Break	
3:15 PM	Enabling Methods for Fast Co-Simulation of Electric Circuits Under Uncertainty	Kai Strunz, University of Washington (SNL Funded)
Emerging Technologies - Micro- Nano- Mechanics		**Presenter/Principal Investigator**
3:45 PM	Multiresolution Analysis Mechanics	Wing Kam Liu, Northwestern University (NSF Funded)
4:15 PM	Integrated Atomistic and Continuum Simulation Studies of Stress-Defect Interactions in Semiconducors	Krishna Garikipati, University of Michigan (NSF Funded)



FY2006 NSF-Sandia Workshop Agenda

Emerging Technologies - Micro- Nano- Mechanics		**Presenter/Principal Investigator**
8:00 AM	Electric Field-Driven Transport Phenomena at the Micrometer and Nanometer Scales	Boris Khusid, New Jersey Institute of Technology (SNL Funded)
8:30 AM	Efficient Numerical Solutions of the Boltzmann Equation for Low-Speed Gas Flows	Nicolas G. Hadjiconstantinou, Massachusetts Institute of Technology (SNL Funded)
9:00 AM	Measurements and Modeling of Molecular Motion near Solid Interfaces	Kenneth Breuer, Brown University (SNL Funded)
9:30 AM	Break	
Uncertainty and Engineering Design		**Presenter/Principal Investigator**
9:45 AM	Extrema of Discrepancy Sensitivity Measures	Erik A. Johnson, University of Southern California (NSF Funded)
New Projects		**Presenter/Principal Investigator**
10:15 AM	Finite Temperature Continuum Mechanics Based on Interatomic Potentials	Yonggang Huang, University of Illinois (NSF Funded)

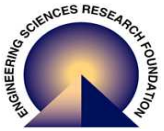


FY07 New Starts in Sandia/NSF Program

Solid Mechanics				
625241	Wierzbicki	MIT	399	Ductile Fracture
625293	Liu	NWU	396	Multi-Res Analysis
625299	Ghoniem	UCLA	400	Multi-scale analysis
626486	Qi	U of Co	293	Shape Memory polymers
Micro/Nano Technologies				
625550	Xu	Purdue	271	Molecular Dynamics of Laser Ablation
Nano/micro processes and manufacturing				
623973	Qiao	Akron	299	Porous Material
626460	Lagoudas	TAMU	347	Thermal-mechanical interfaces
625844	Breuer	Brown	300	Energy and momentum transfer in microfluids
626124	Raman	Purdue	374	Fluid-structure interactions (AFM cantilevers)
Thermal Fluids				
625765	Tryggvason	WPI	320	Computational Boiling
625344	Candler	Uminn	420	Re-entry vehicles
625335	Hu	Upenn	399	microfluids
625865	Yoda	GA Tech	399	microthermometry

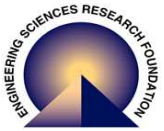
FY2005 NSF-Sandia Workshop Agenda

Solid and Structural Mechanics		**Presenter/Principal Investigator**	**Additional Investigators**
8:45 AM	Computational and Modeling Strategies for Damping and Multi- Physics Coupling on Interfaces	John Dolbow, Duke University (Sandia Funded)	Tod Laursen
9:15 AM	Development and Analysis of Reduced-Order Models for Mechanical Joints and Interfaces	Edward Berger, University of Cincinnati, and D. Dane Quinn, University of Akron (SNL Funded)	Dan Segalman (Sandia)
9:45 AM	Chemorheological response of natural rubber at high temperatures	John A. Shaw, University of Michigan (SNL Funded)	Alan S. Wineman
10:15 AM	Break		
10:30 AM	Material Deterioration in High Temperature Gradients and Transients : Cyclic Loading	Thomas Siegmund, Purdue University (SNL Funded)	Ashwin Hattiangadi
Thermal, Fluid and Aerosciences			
11:00 AM	Mechanisms of Hypersonic Boundary-Layer Transition on Reentry Vehicles: Introduction and Experiments	Shann J. Rufer, Steven Schneider, Purdue University (SNL Funded)	
11:30 AM	Mechanisms of Hypersonic Boundary Layer Transition on Re-Entry Vehicles	Graham V. Candler, University of Minnesota(SNL Funded)	Heath B. Johnson
12:00 PM	Lunch		
1:00 PM	3D Modeling of Flow Behind a Heated Backward-Facing Step Using 3D Digital Particle Image Velocimetry & Thermometry	Dana Dabiri, University of Washington (NSF Funded)	Jim Riley
1:30 PM	Uncertainty Modeling in Convective Heat Transfer	George Karniadakis, Brown University(NSF Funded)	
2:00 PM	The Least Square Extrapolation method for CFD and Heat transfer problems and its application to error estimates	Marc Garbey, University of Houston (SNL Funded)	Christophe Picard, Wei Shyy
2:30 PM	Effects of boundary condition fluctuations on convective heat transfer: measurements and modeling	Tait Pottebaum and Mori Gharib, California Institute of Technology (NSF Funded)	

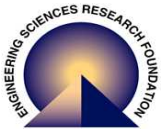


FY2005 NSF-Sandia Workshop Agenda (Cont)

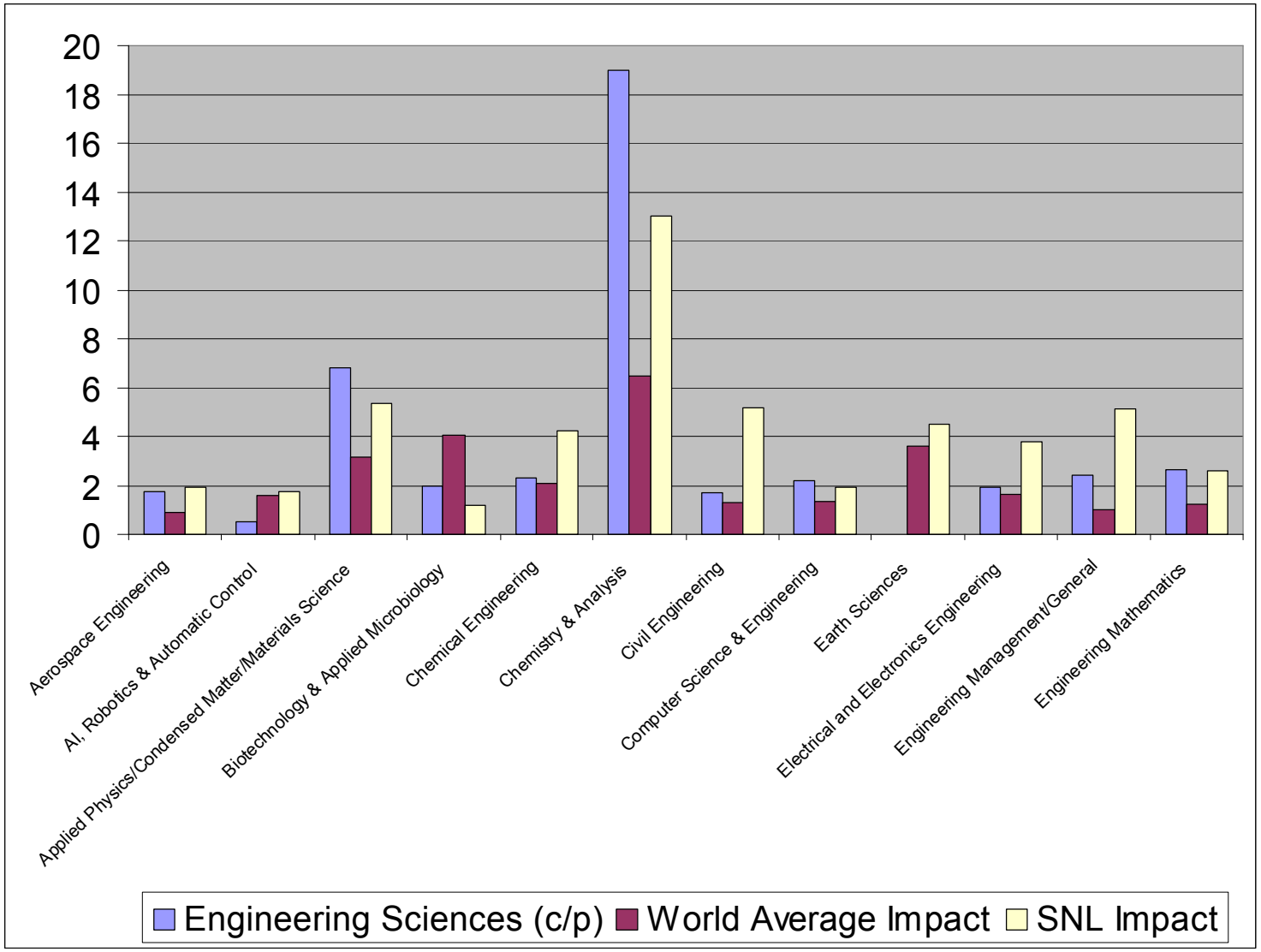
Electrical Engineering		**Presenter/Principal Investigator**	**Additional Investigators**
3:00 PM	Break		
3:15 PM	Design and Integrated Multi-Scale, Multi-Physics Modeling of RF MEMS for Improved Reliability	Katsuo Kurabayashi, University of Michigan and John L.Volakis, Ohio State University (NSF Funded)	Kazuhiro Saitou
3:45 PM	Enabling Methods for Fast Co-Simulation of Diverse Electric Circuits and Networks	Kai Strunz, University of Washington (SNL Funded)	Eric Carlson, Gao Feng
Emerging Technologies - Micro- Nano- Mechanics		**Presenter/Principal Investigator**	**Additional Investigators**
4:15 PM	Multiscale Methods for Materials Design and Bio-Nano Interface	Wing Kam Liu, Northwestern University (NSF Funded)	
8:00 AM	Stress Diffusion Coupling at the Defect Scale	Michael Falk, University of Michigan (NSF Funded)	Krishna Garikipati
8:30 AM	The AC electric field contribution to the fluid energy and stress	Boris Khusid, New Jersey Institute of Technology (SNL Funded)	
9:00 AM	Efficient numerical solutions of the Boltzmann equation for low speed flows	Nicolas G. Hadjiconstantinou, Massachusetts Institute of Technology (SNL Funded)	Lowell L. Baker
9:30 AM	Break		
9:45 AM	Appropriate Fluid-Solid Boundary Conditions at the Nanoscale	Kenneth Breuer, Brown University (SNL Funded)	
Uncertainty and Engineering Design		**Presenter/Principal Investigator**	**Additional Investigators**
10:15 AM	Optimal Material Design in the Presence of Uncertainty	George C. Johnson, University of California, Berkeley (NSF Funded)	Nicolas Rumigny, Panos Papadopoulos, Andrew Packard
10:45 AM	DACE Using Discrepancy Sensitivity	Erik A. Johnson, University of Southern California (NSF Funded)	



External Impact

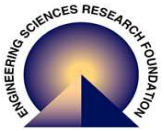


Engineering Sciences Citation Impact



Industrial Activities
(~ $9M in FY06)

- ARCXIS BIOTECHNOLOGIES
- ATOMIC WEAPONS ESTABLISHMENT (AWE) U.K.
- BAE
- CATERPILLAR
- CORNING
- DOW CHEMICAL COMPANY
- EPRI
- GENERAL MOTORS
- GOODYEAR
- INTEL
- LOCKHEED MARTIN
- MINNESOTA MINING AND MANUFACTURING
- NORTHRUP GRMMAN SHIP SYSTEMS
- PROCTER & GAMBLE
- TITAN SYSTEMS
- ULTRAMET



The ESRF provides capabilities and understanding required to enable predictive simulation in support of the Engineering Sciences needs of Sandia's Strategic Management Units.