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Title:	TSC All-Employee Meeting - January 19, 2011
Author(s):	Primary Responsible Author: Alan Bishop
Intended for:	All LANL employees

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Form 836 (7/06)

Abstract:

Annual presentation on TSC accomplishments and state of the Directorate.

This information is general knowledge and intended for all employees within the Theory, Simulation and Computation Directorate.

TSC All-Employee Meeting - January 19, 2011

Celebrating your FY10 success; Looking at road conditions ahead

* Some LANL Updates
  - Terry Wallace: PADSTE/Lab perspectives
  - Frank Alexander: Information Science & Technology Capability Pillar
  - Andy White: DOE Exascale plans
* TSC WSST Message: Alan Gibson
* TSC Update: Alan Bishop

Ladder Safety Share

External Environment

- National Budget Deficit
  - Anticipate "austerity" budgets to replace stimulus of last two years
    - But Simulation and Modeling may be a priority, including decadal Exascale initiative (DOE/OSTP)
  - Impact on Administration agendas
    - But focus on employment, industrial competitiveness will remain
- NW Budget a likely exception (New START…)
  - Administration and Congress alignment
  - Expect growth of NNSA budget over next (few) years

LANL Update

- **Excellent FY10**
  - Growth of programs (NW, ES, Stimulus); partnering strategy
  - Program delivery
  - Infrastructure investments (physical, cyber, IT)
  - VPP on positive path (including WSST)

- **Some Disappointments**
  - Science Complex
  - Impacts of deferred issues from past (infrastructure, pensions, IT,…)
  - Pay Freeze

- **FY11**
  - Deliver on NNSA budget "uplift" and other program growth of last two years
  - Director search
  - May be best budget year for a while: so face long-term issues now (pension/medical costs: compromises with rates, G&A investments)
  - Recruit strategically
  - Diversity and leadership development

LANL FY10 Budget: High Level of Execution

- **Highest level of O&M funding** ($2.1B) in Lab history, steady increases since FY06
- **Program execution just over $2.5B.** Highest level in Laboratory history
- **Early passage of budget** allowed programs to move out early and sustain a higher level of execution

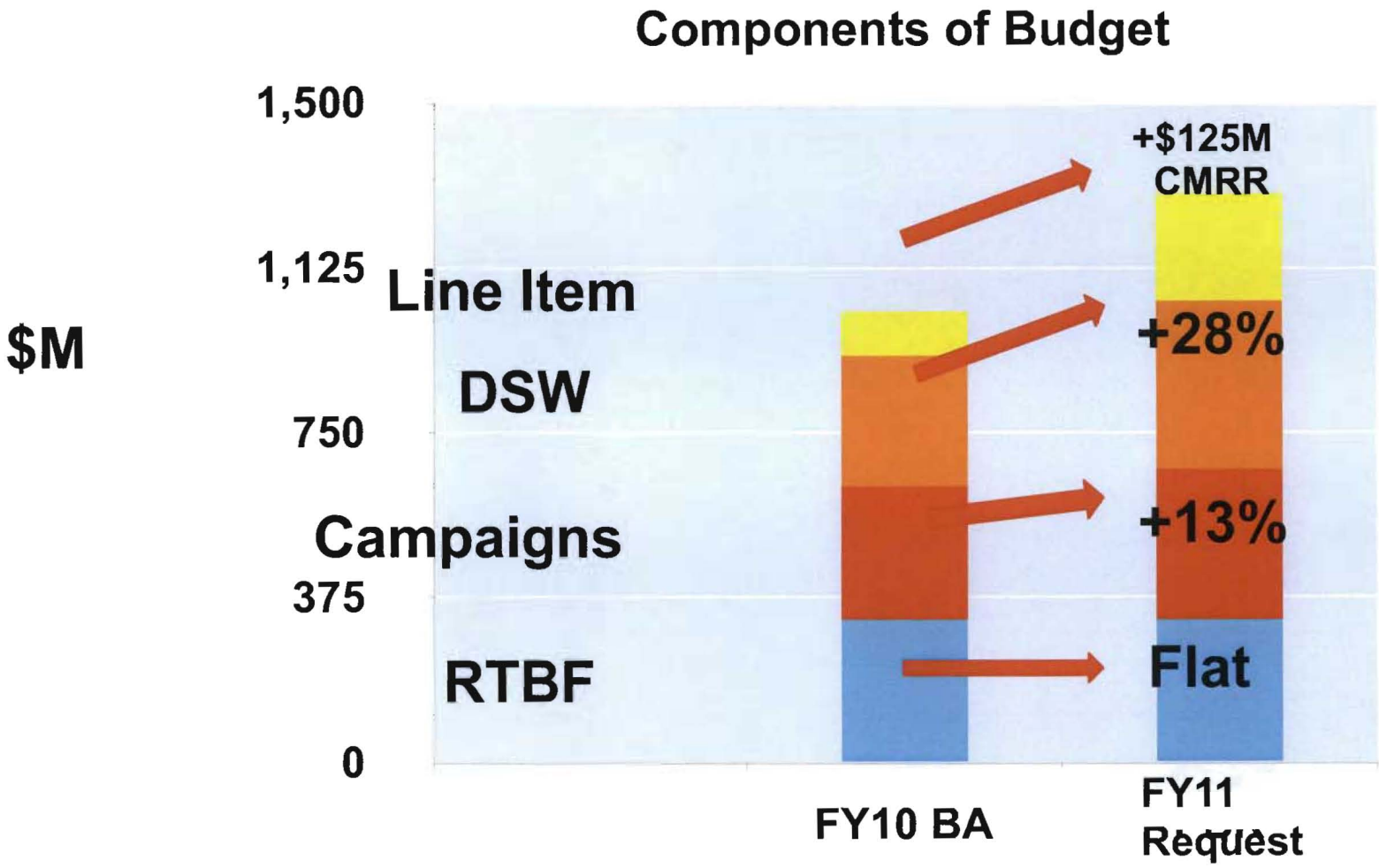
LANL FY10 Budget: Funding increases in all programs

- **Work for Others funding increased $38M (14% increase)** over FY09, reversing downward trend

- **Stimulus added $271M** to LANL budget over past two years. $212M for EM work and $59M for science and Energy projects. $123M in carryover to FY11

- **Pension reprogramming** received Congressional approvals in September – provides additional $40M in FY11 to support increased pension costs.

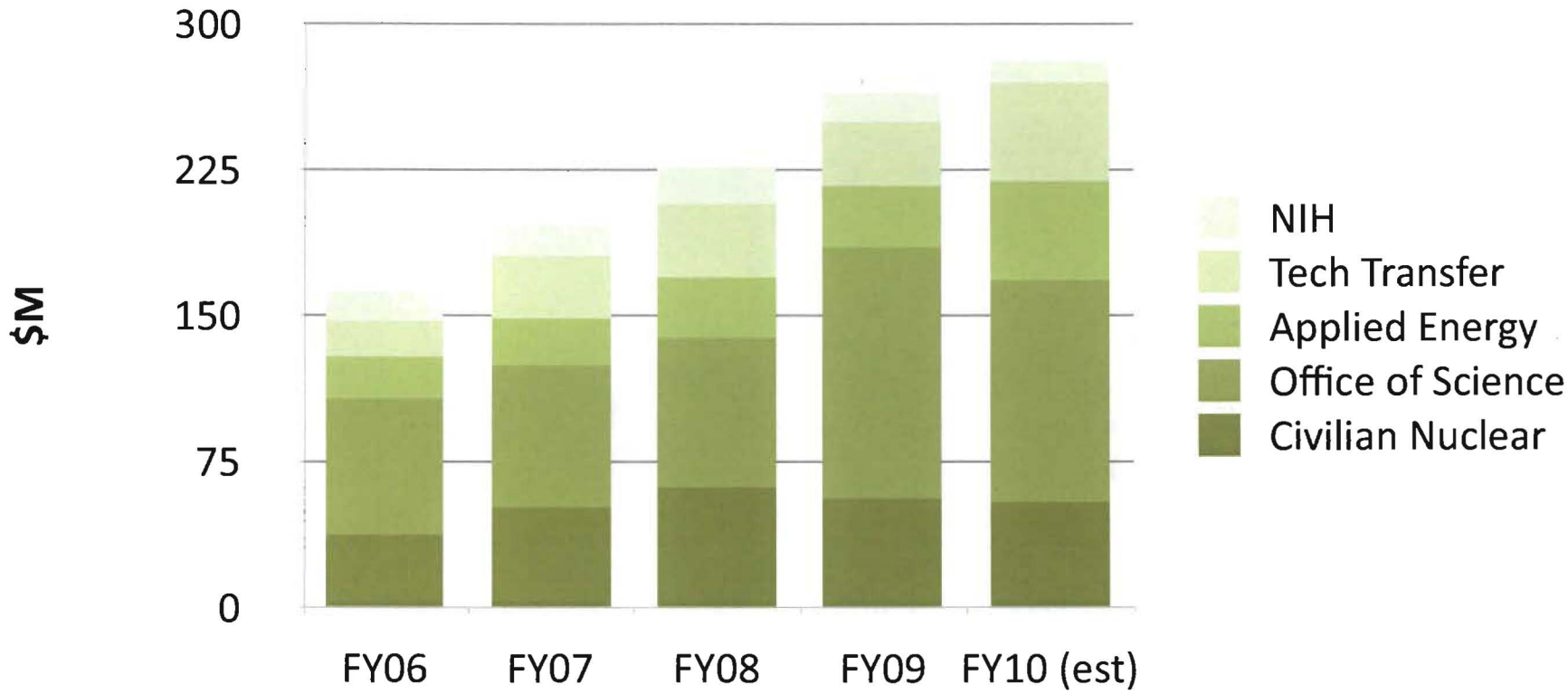
President's NNSA Budget Request at LANL is focused on Line Item, DSW, modest growth in Campaigns, and flat RTBF



Including ASC Program growth

Science and Energy Programs (FY06-FY10)

~ 75% Growth in new funding



Los Alamos successful in competition for funding to address major science issues

Biofuels

- National Alliance for Advanced Biofuels and Bioproducts Consortium
- National Advanced Biofuels Consortium
- LANL leads algal strain development, harvesting, extraction, catalyst development, commercialization

Energy Frontier Research Centers

CMIME
Center for Materials at Irradiation and Mechanical Extremes

- Focus on unique properties of nanomaterials
- CMIME: nanolayered composites provide increased strength and enhanced radiation damage tolerance
- Center for Advanced Solar Photophysics: nanoscale structures boost solar-energy conversion efficiency

Green House Gas Information System

- Global climate models
- Monitoring and verification
- Infrastructure analysis

Nuclear Energy

CASL
Consortium for Advanced Simulation of LWRs

- Hub consortium of 10 principal partners
- Modeling and simulation to improve performance of nuclear power plants
- LANL leads material science and models and numerical methods areas

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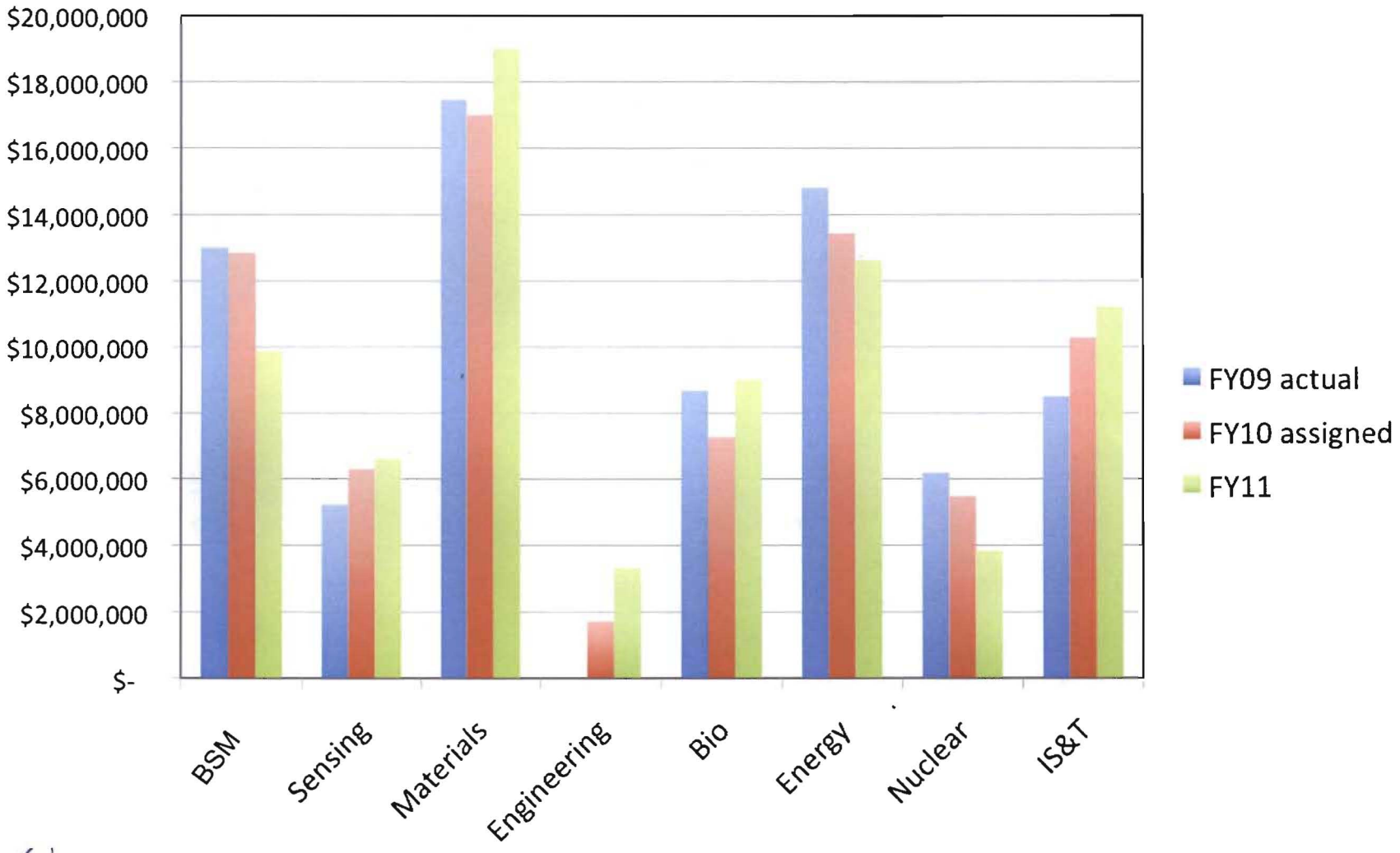
LANL Internal Investments

- G&A/Org Support
  ISS, RTBF (infrastructure)

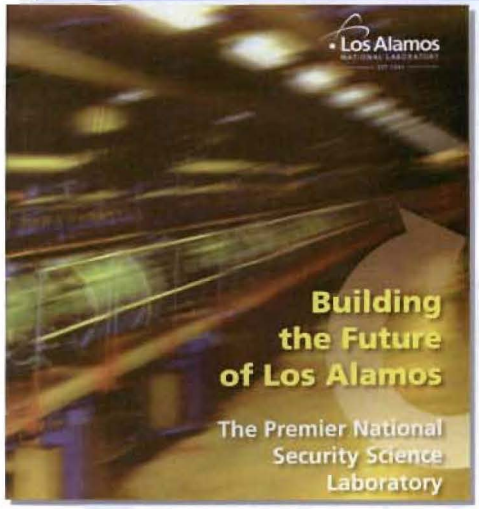
- LDRD (ER & DR [Grand Challenges], Postdocs, Early career)
  Capability Pillars
  Centers/Institutes
  Institutional Computing

- Program Development (NW, GS, ES)

LDRD investment in Grand Challenges supports science pillars and capabilities



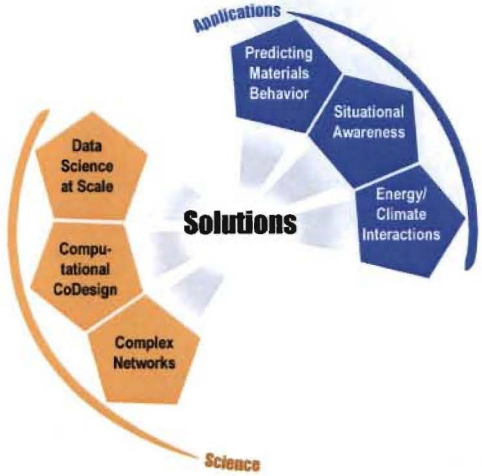
LANL fosters strategy of "Science that Matters" through investments, people, and facilities



- Experimental science focused on materials for the future
- Information science and technology enabling integrative and predictive science
- Science of Signatures for enduring national needs

Materials for the Future

Information Science and Technology for Integrative and Predictive Science



Science of Signatures

Controlled Functionality

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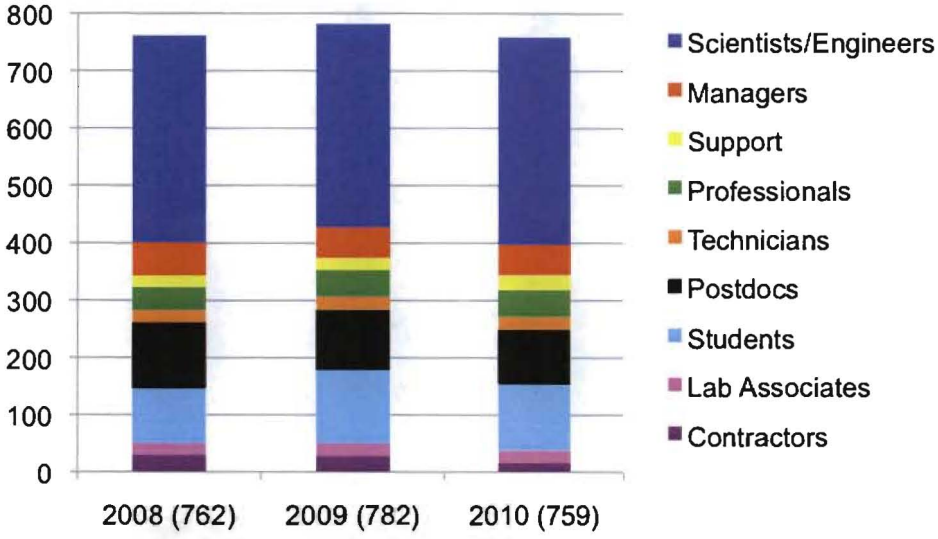
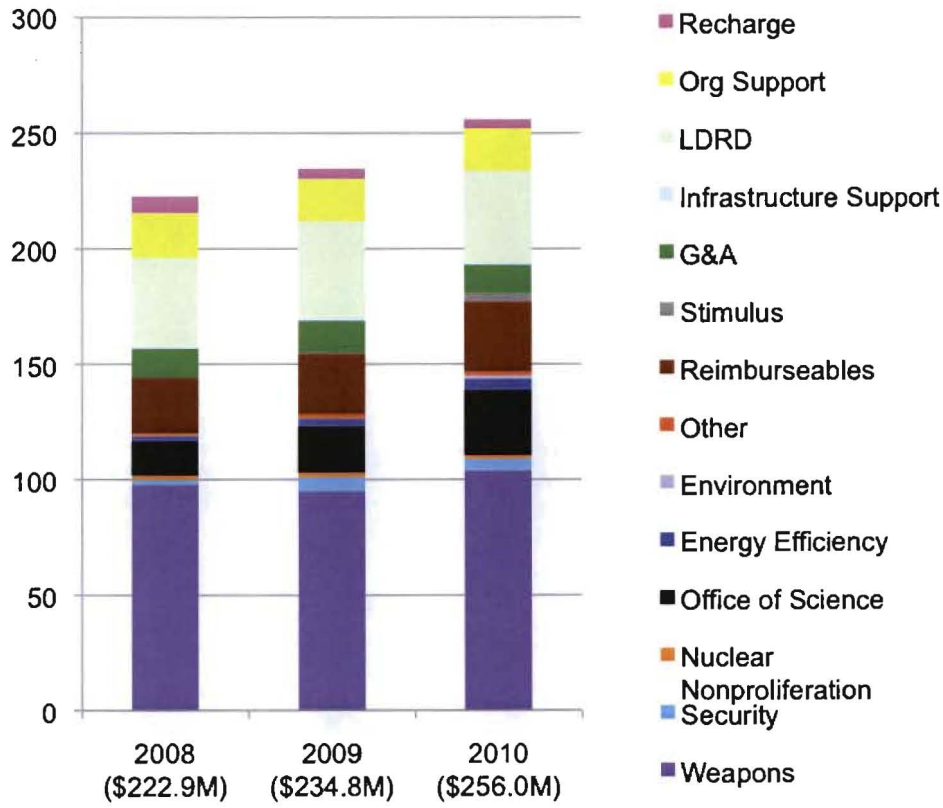
TSC Budget and Staff (FY08-FY10)

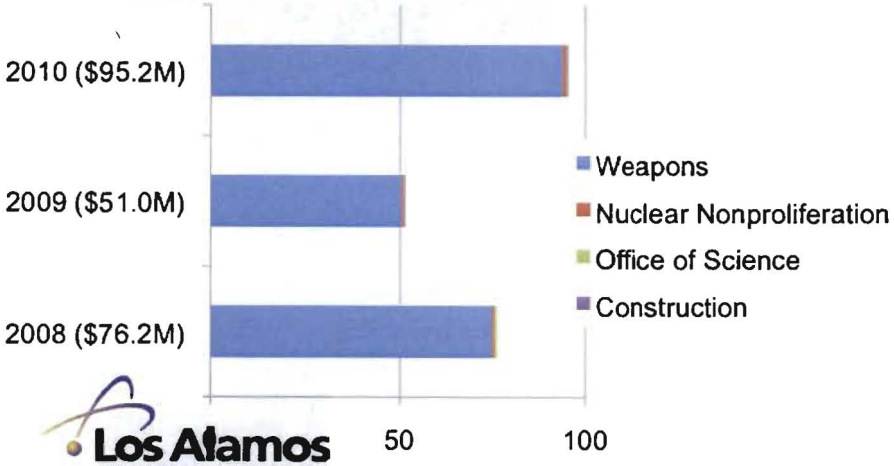
TSC Employee by Series



TSC Total Operating Budget



TSC Total Capital Budget



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A (Small) Subset of TSC Achievements in FY 10

- 2010 Science Highlights (http:www.lanl.gov/orgs/adtsc)
- Meeting significant NW Milestones (ASC, DSW) for Predictive Capability Framework (Models, Databases, Algorithms, Computing environments, Systems UQ…)
- LANL's major roles in DOE Exascale Initiatives planning
- HIV (MOSAIC) vaccine design, moving to human trial (B. Korber et al.)
- Consortium for Advanced Simulation of Light Water Reactors Hub (S. Lee et al.)
- Albert Einstein Visiting Professor at University Ulm (W. Zurek)
- Rapid response to Gulf Oil Spill: dispersal prediction (M. Maltrud et al.)
- LANL selected to lead nationwide Topical Collaboration for DOE in Explosive Astrophysical Events (S. Reddy, PI)
- Cielo System accepted and impressive application performance
- Enterprise Secure Network (ESN) connections to White House and UK: Honorable Mention Award for IT Achievements (M. Boorman)
- Very successful LANL Booth at Supercomputing 2010

etc. etc. etc.

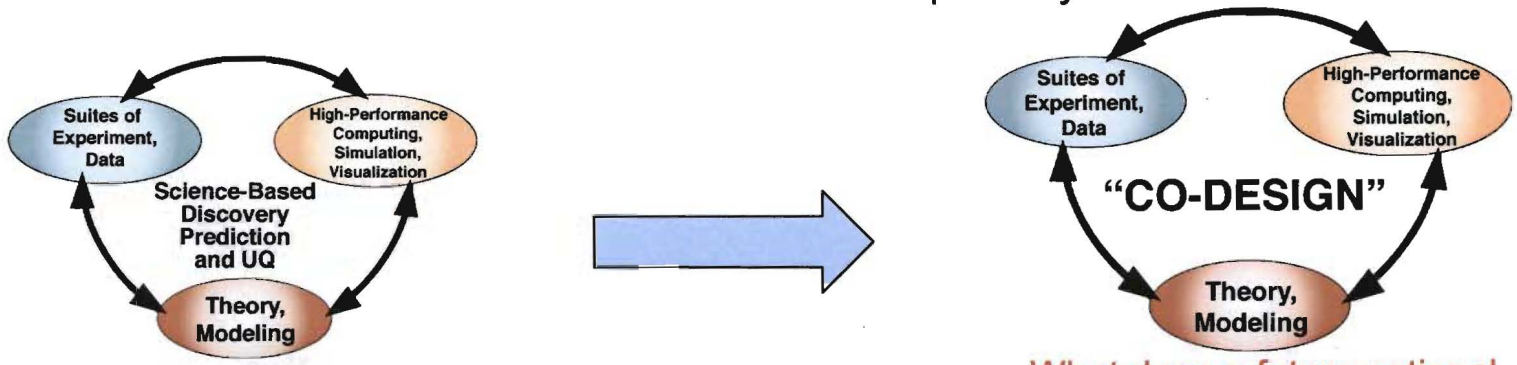
TSC: People, Capabilities, Programs

People

- Focus on quality, mentoring, careers (at LANL or elsewhere)
- Emphasize pipeline (UGS, GRAs, Postdocs) for TSC (and all LANL)
- Hire for excellence, relevance and agility
- Respect and encourage diversity and inclusiveness

Capabilities

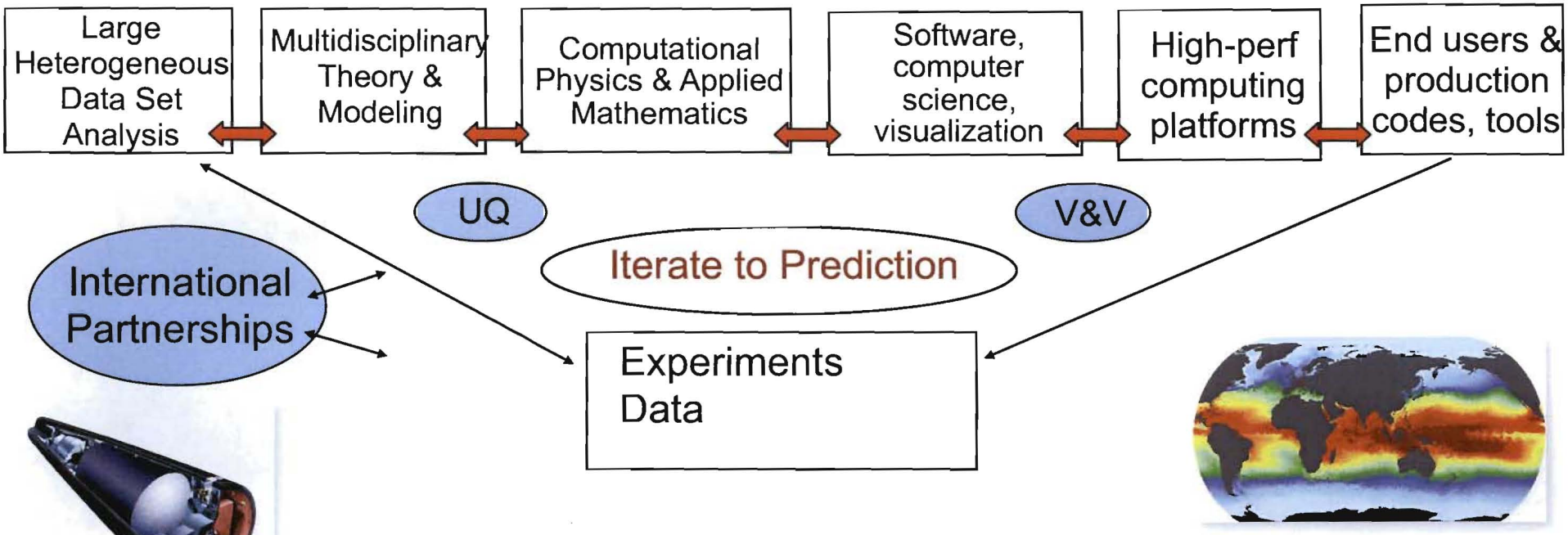
- Balance (impressive) discipline strengths in TSC (Bio to Cosmo!) and LANL's core INTEGRATION strength
- Lead or collaborate strategically — external and internal; support LANL Centers, Institutes, Pillars; multi-Lab MOUs/Consortia
- TSC must lead into the next era of "Advanced Computing and Applications" as a mature tool in the "Scientific Method" for Complex Systems

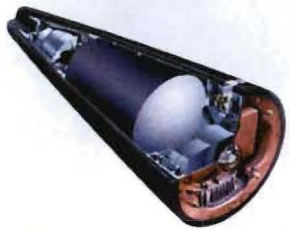


Programs

- Focus on excellent execution of our expanded and diversified program portfolio
- Balance for delivery and capability/career management
- Partner strategically
  - Externally
    e.g. SNL, ORNL, LBNL, ANL,. . .
    Universities, Industry
  - Internally: Seek the next level of INTEGRATING LANL's ASSETS
    e.g. MaRIE
    Energy–Climate
    NE (first DOE "Hub")
    Smart Grid
    EM (ASCEM)
    Cyber S&T
    PRoBE
    •
    •
    •

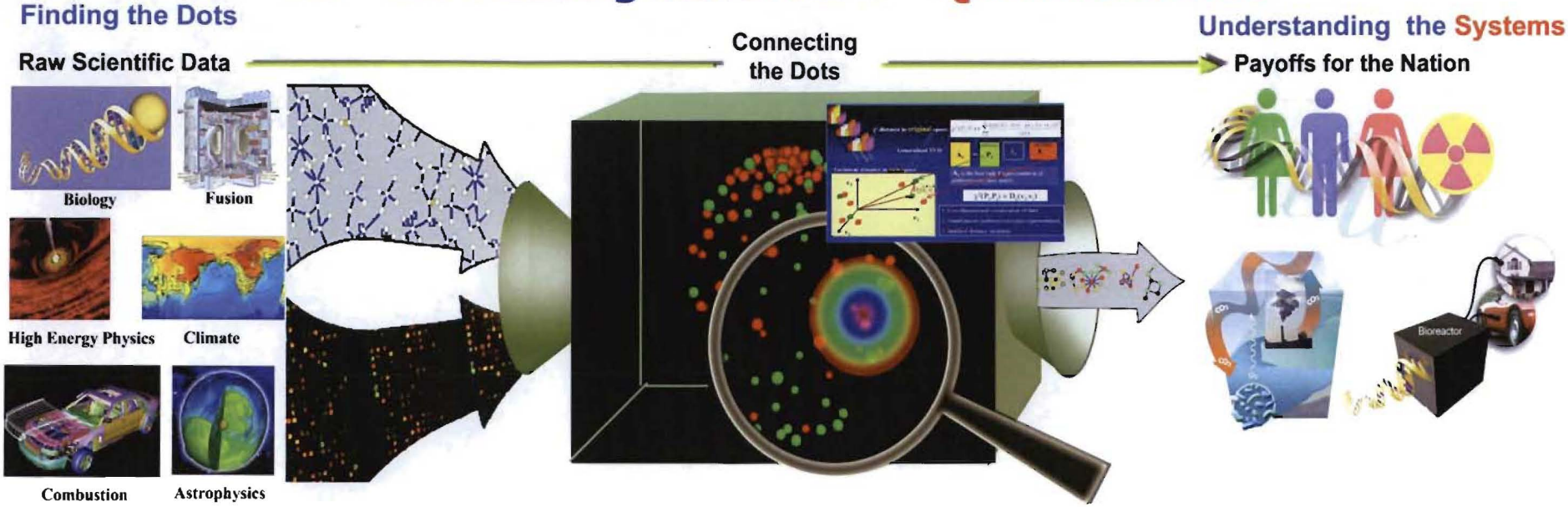
Integration Capability … a nuclear weapons heritage of 65+ years





Elevating this integration to a full "Co-Design" future is central to the huge national need for new generations of ideas, concepts and methodologies to improve the fidelity, reliability, certainty, and usability of tools to guide and interpret experiments, and provide prediction, uncertainty quantification, and control for complex phenomena and systems.

Information Science & Technology must provide the Infrastructure for "Connecting the Dots": "Quantitative X"



Sheer Volume of Data

Climate

Now: 20-40 Terabytes/year

5 years: 5-10 Petabytes/year

Fusion

Now: 100 Megabytes/15 min

5 years: 1000 Megabytes/2 min

Advanced Mathematics and Algorithms

- Requires high-performance computing, advanced theory modeling, data curation

Huge dimensional space

Combinatorial challenge

Complicated by noisy data

Providing Predictive Understanding

- Produce hydrogen-based energy
- Stabilize carbon dioxide
- Clean and dispose toxic waste

Office of Science
U.S. DEPARTMENT OF ENERGY

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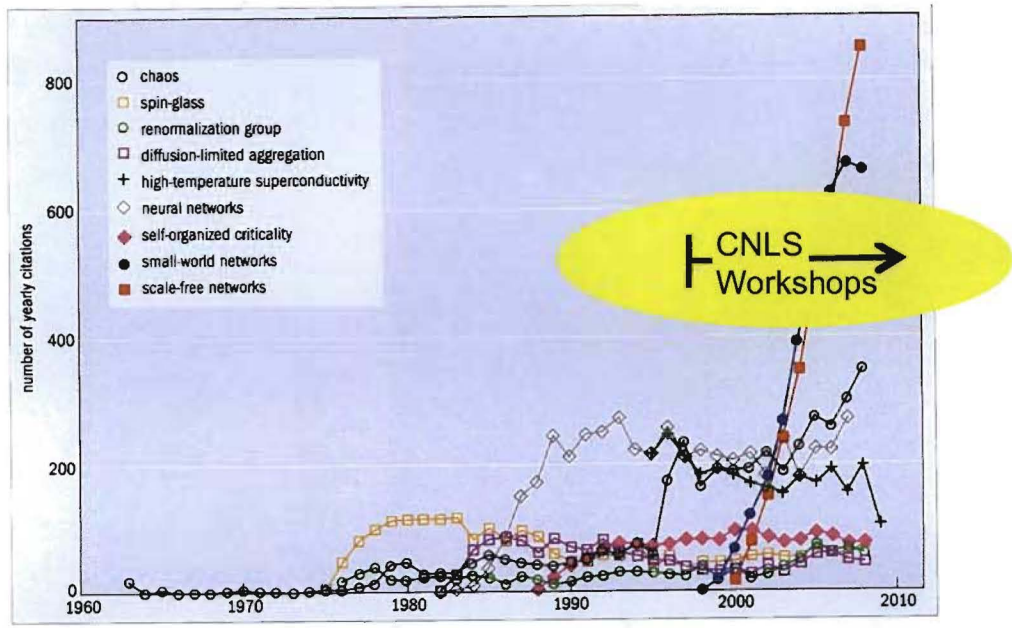
c.f. Raymond L. Orbach, DOE Undersecretary for Science
2006 AAAS Annual Meeting

Complex Networks Science & Programs

- Complex Network Science is an exploding field that is gaining recognition and impact
- Concepts and approaches are being applied to a very broad array of problems: infrastructure, cyber, bio, social networks, etc.
- LANL has notable capability in this area aligned with our multi-disciplinary approach to science
- Natural application areas for Complex Network Science underpin important programmatic directions for the Lab



Networks take off This graph of the number of citation garnered by a handful of groundbreaking physics papers shows that even within this elite group, the popularity of paper on networks has been unprecedented.

Buchanan, Caldarelli, physicsworld February 2010

Recent LANL Successes: Smart Grid, Cyber S&T

Strategic Supercomputing Application & Technologies are Core to LANL's Missions

From LANL's 2011 Performance Evaluation Plan Measures:

- Develop strategies and plans for an exascale technology roadmap in partnership with DOE/NNSA Laboratories, universities, and industry for:
  - Co-design of applications (models, methods, and codes) and exascale computing environment (hardware and software);
  - Next generation file systems;
  - System and application resilience;
  - Uncertainty quantification
  - Science simulation at scale
- Developed multi-year facilities requirements to support exascale applications and systems.
- Successful delivery, acceptance, and utilization of the Cielo supercomputer

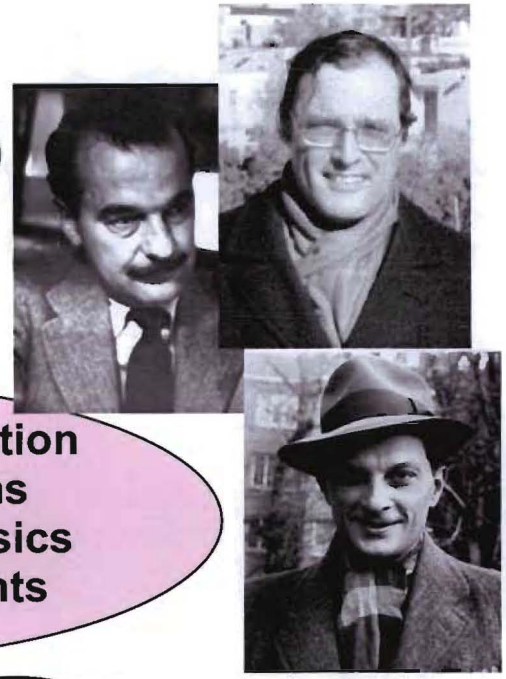
High-Performance/Advanced/Supercomputing and Visualization

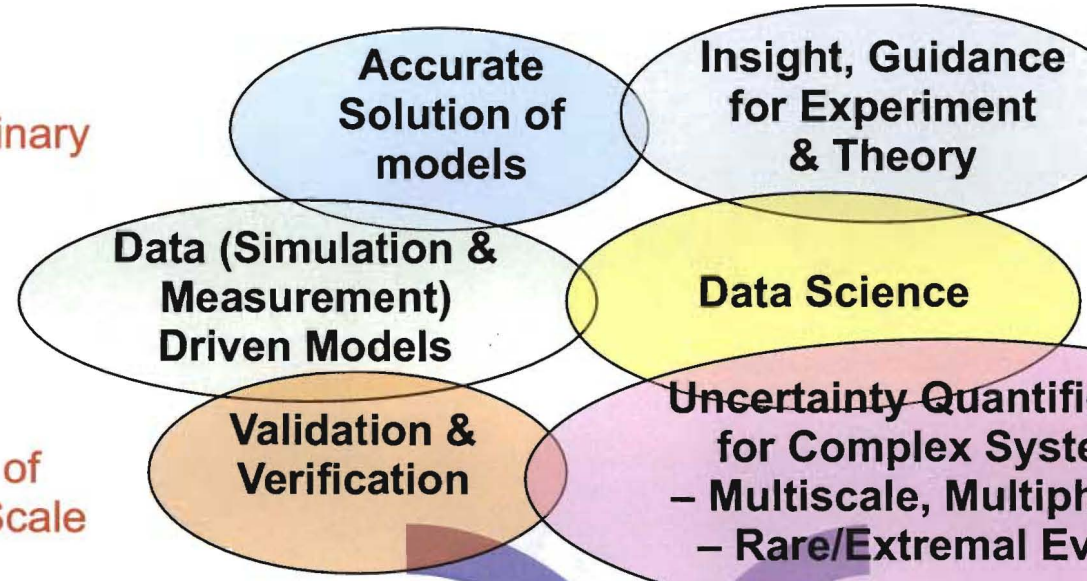
- A "NEWly" mature scientific capability for the scientific method
- Many leaders emerged from traditional disciplines (Physics, Mathematics….); Increasingly an identified discipline at Universities (Computer Science…)

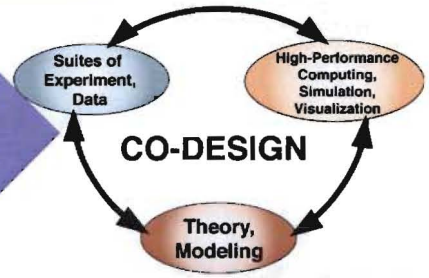
~1950
Interdisciplinary
Teaming
Partnering

Co-Design of
Assets at Scale

2020







Robust Tools for Decision Makers

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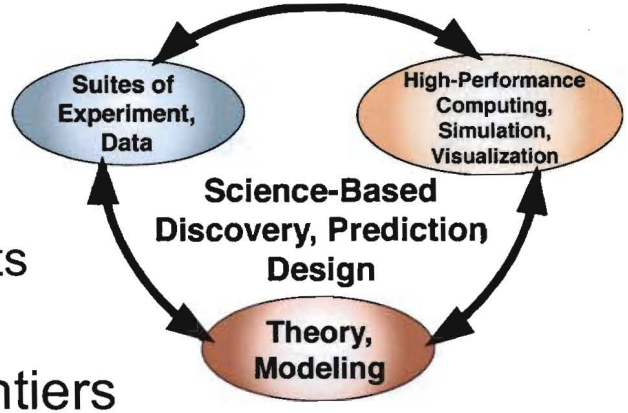
High-Performance Computing at a Fascinating Time — National Challenges and Opportunities

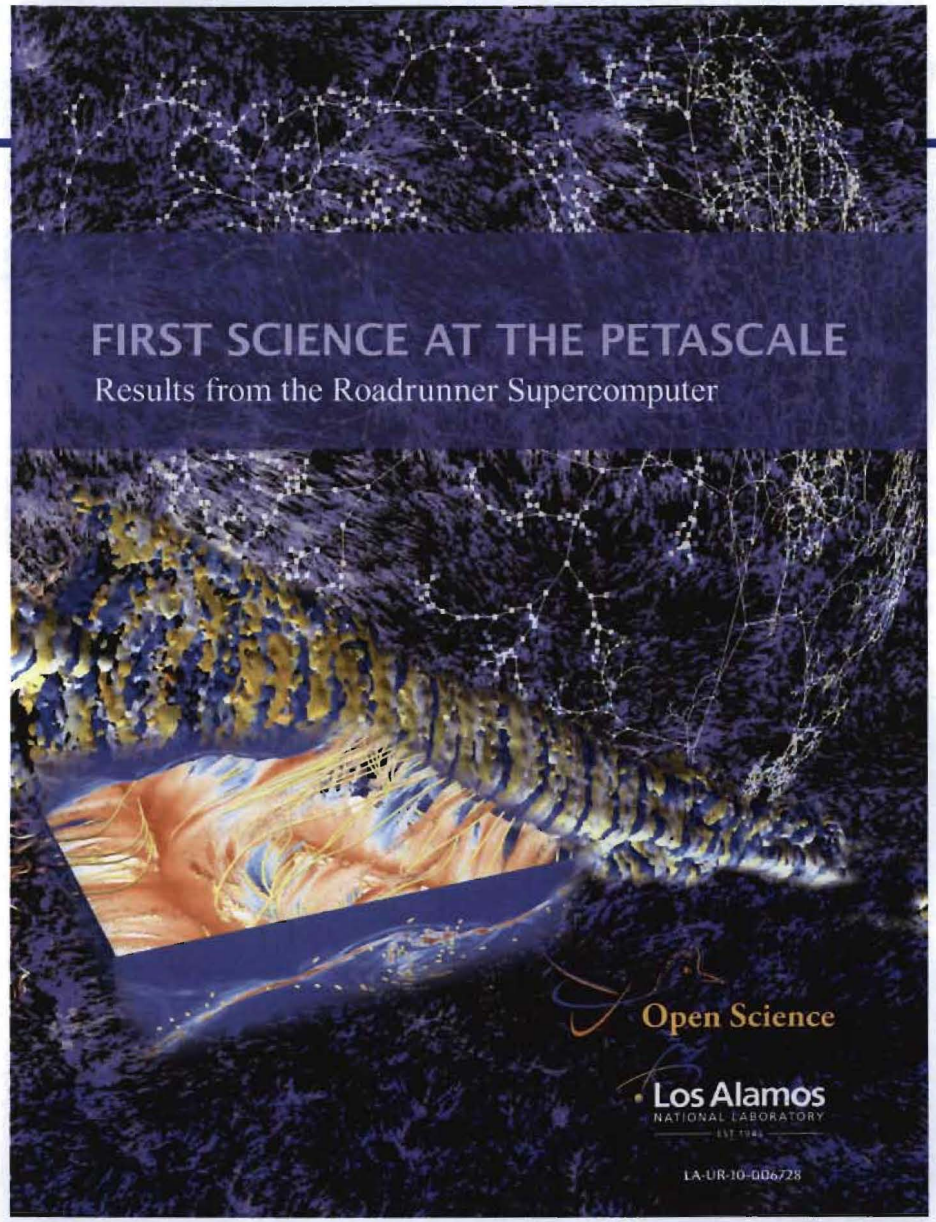
- Heightened expectations (from White House, DOE…) as mature tool in scientific method: Accelerating the "discovery to commercialization" cycle to meet (inter)national imperatives!
- Major technology transitions
  - Hybrid/multi-core…
  - Cooling, Power, Resiliency, File systems, Networking, Agile programming environments for broad S&T portfolio
- Compute-and-store AND data-intensive frontiers
- Training the next generation: "Applied Computer Science"



The DOE road to "Exascale Computing": Multi-Lab Associations, including Industrial Partners : Co-Design Centers with Application Targets

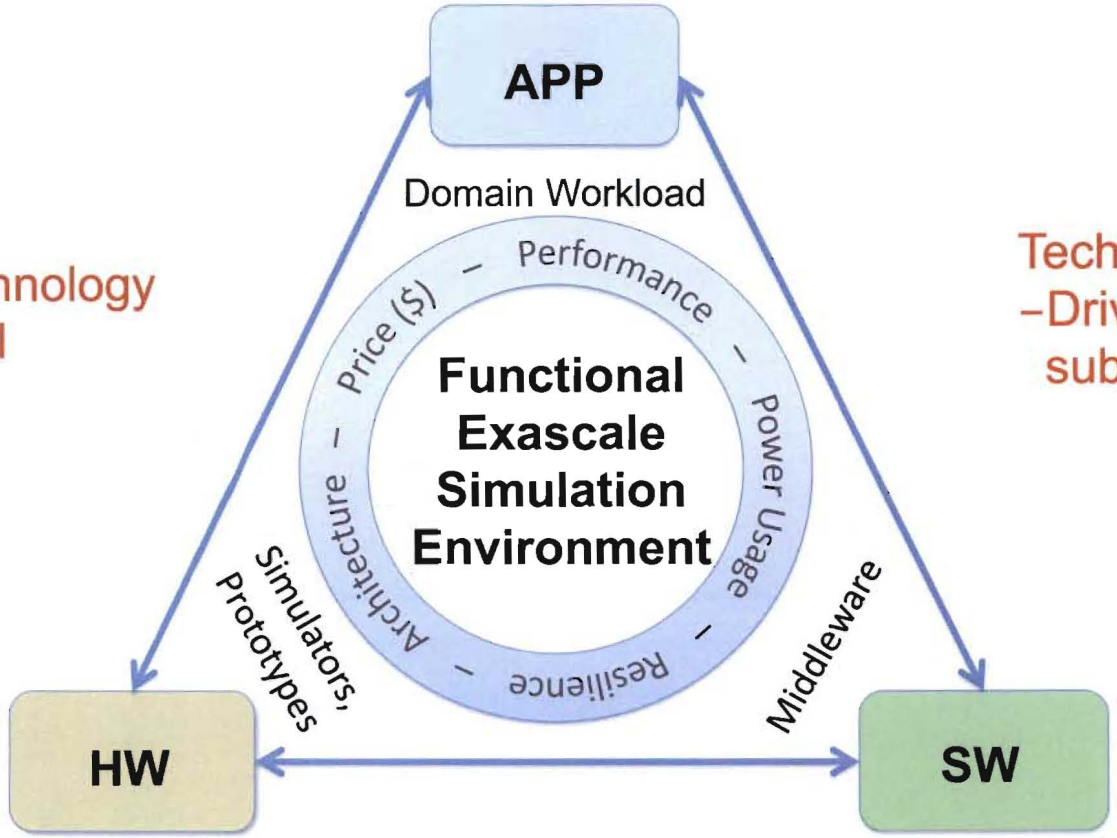
Roadrunner

- Open Science Projects
- Lessons-Learned



Co-Design: Transformational Science & Technology through Integration and Innovation

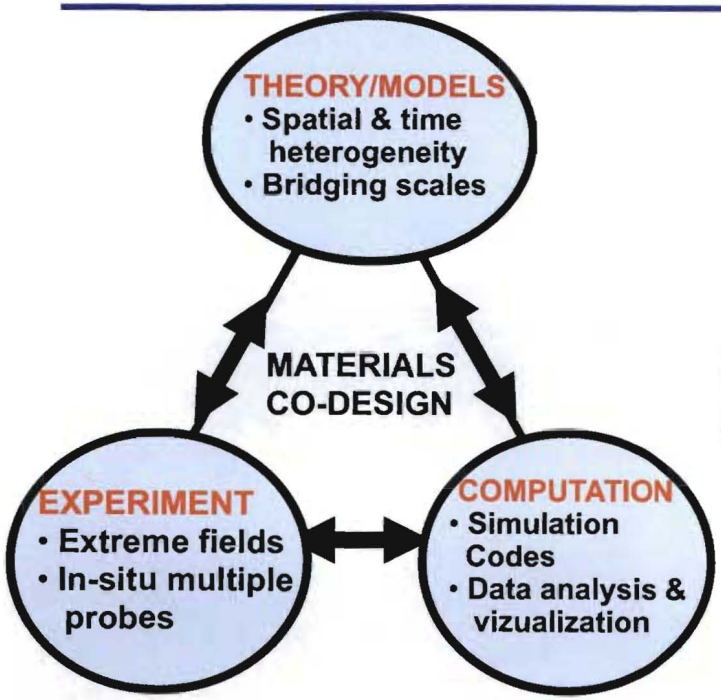
Application
– Driven Technology
sub-optimal

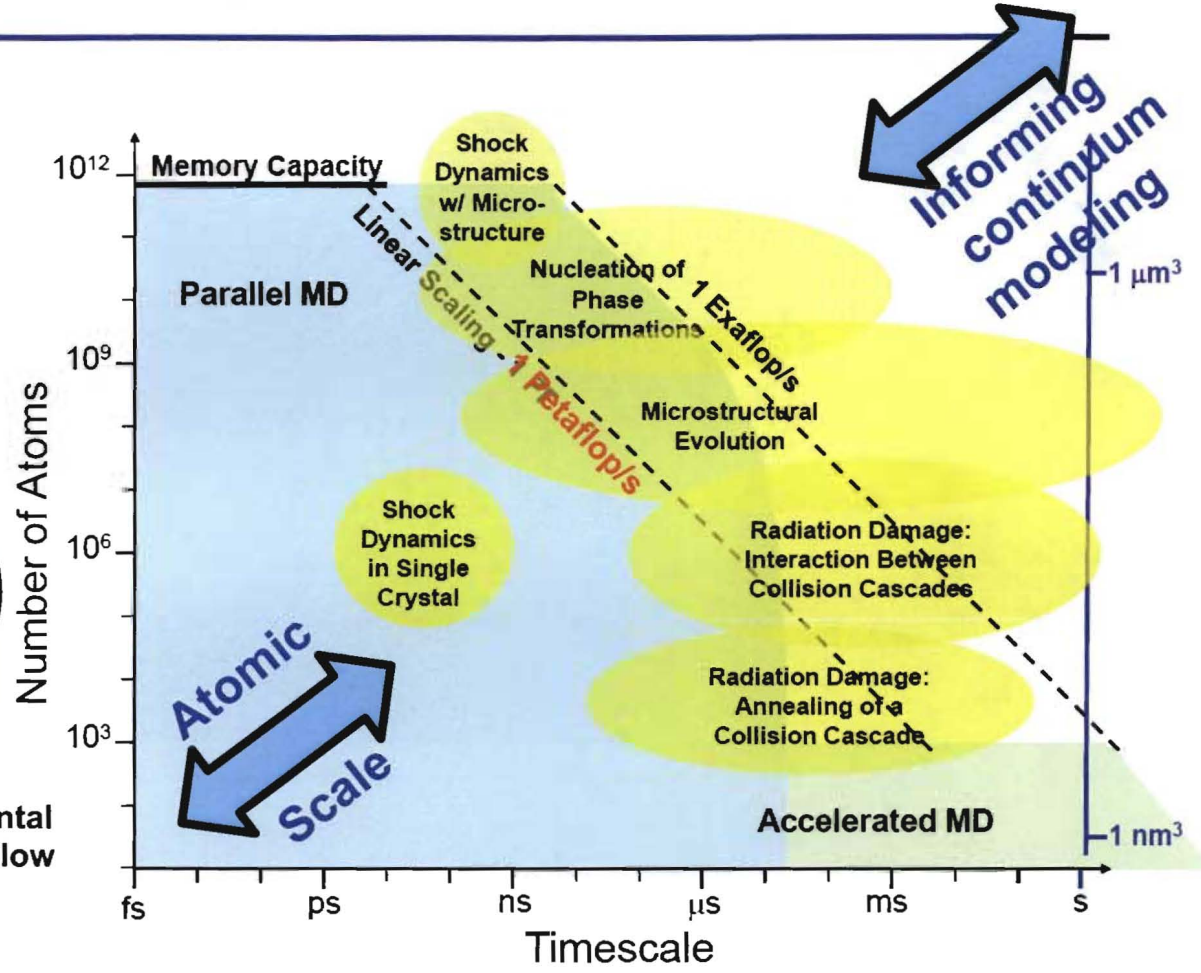


Technology
–Driven Applications
sub-optimal

(Germann, Swaminarayan, et al)

A Decadal Opportunity for Materials Science:
Removing Key Scientific Barriers to Discovery, Prediction and Control





Anticipated advances in modeling, petaflop–exaflop computing, and experimental tools with unprecedented resolution, will allow access to rate-limiting phenomena at the meso (micron) scale

MaRIE: Matter-Radiation Interactions in Extremes
LANL Signature Facility plan (NW, NE, Fission-Fusion…)

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The Consortium for Advanced Simulation of Light Water Reactors (CASL) Team: A unique lab-university-industry partnership

Core partners

Oak Ridge National Laboratory

Electric Power Research Institute

Idaho National Laboratory

Los Alamos National Laboratory

Massachusetts Institute of Technology

North Carolina State University

Sandia National Laboratories

Tennessee Valley Authority

University of Michigan

Westinghouse Electric Company

Building on longstanding, productive relationships and collaborations to forge a close, cohesive, and interdependent team that is fully committed to a well-defined plan of action

Individual contributors

ASCOMP GmbH

CD-adapco, Inc.

City University of New York

Florida State University

Imperial College London

Rensselaer Polytechnic Institute

Southern States Energy Board

Texas A&M University

University of Florida

University of Tennessee

University of Wisconsin

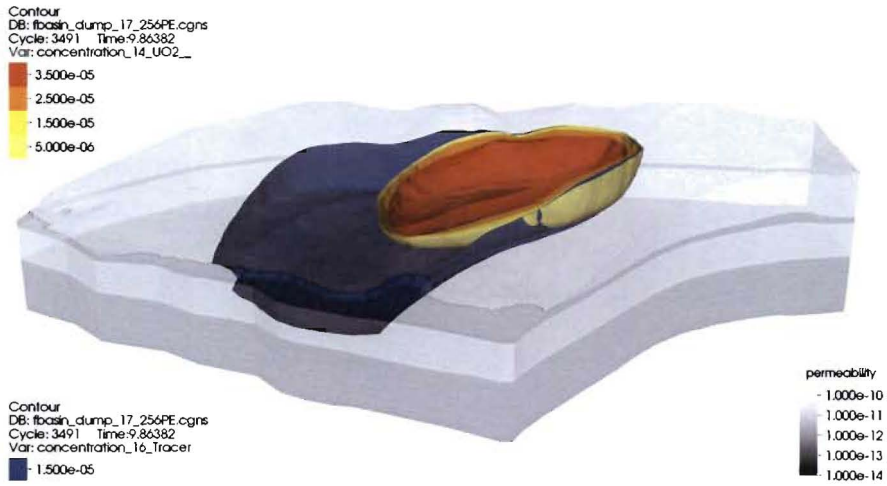
Worcester Polytechnic Institute

(S. Lee et al.)

ASCEM National Laboratory Consortium

The Advanced Simulation Capability for Environmental Management (ASCEM) program is developing a state-of-the-art scientific tool and approach for understanding and predicting contaminant fate and transport in natural and engineered systems. It will facilitate standardized development of performance and risk assessments for EM cleanup/closure activities.

- Multiple Labs: LANL, LBNL, PNNL, ORNL, SRNL (LANL, ANL, INL).
- Bridging Communities: Applied Mathematics, Computational Scientists, Geoscientists.
- Building on advances from ASC, ASCR Applied Math, and SciDAC.
- Members of ADTSC are playing a critical role, and leading the development of Amanzi.



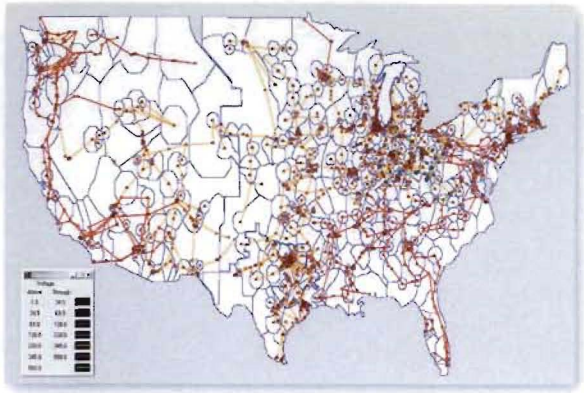
Iso-surfaces of the Uranium plume (yellow and red) and a non-reactive tracer (blue) are shown for a simplified model of the F-Area seepage basins at Savannah River. Results computed with the new parallel open-source ASCEM Multi-Process HPC simulator, Amanzi.

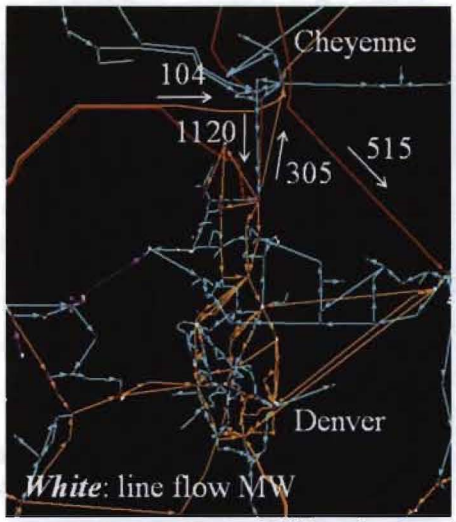
(D. Moulton el al.)

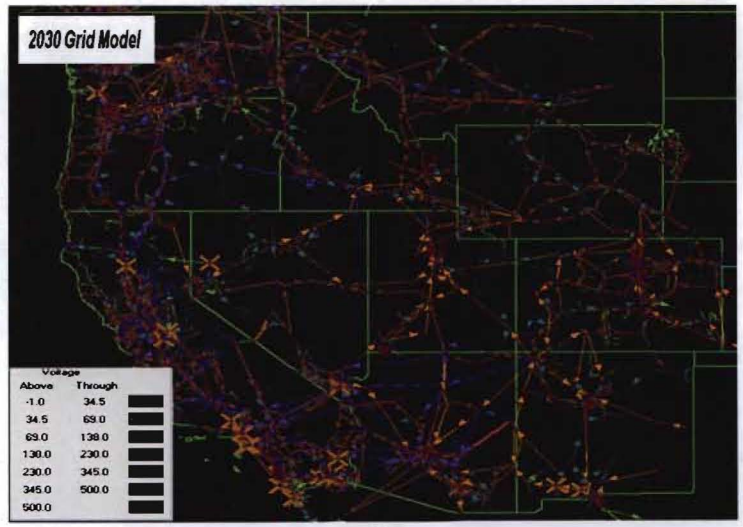
Energy Grid Challenges of the Future: a Complex Network

- Requires predictive simulation and rapid integration of new interdisciplinary technologies for renewable generation, transmission, and storage: "Network S&T"
- Integration is needed to maintain grid stability.
- Cost-effective investment requires predictive simulation.

LANL develops energy infrastructure models to understand impacts and address power options for insertion of renewable and nuclear energy.







(M. Chertkov et al)

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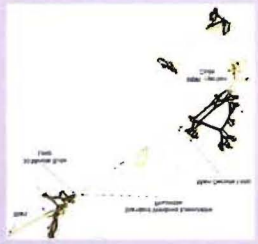
The LANL Cyber Systems Program
An Integrated Set of Technologies and Solutions



Data Intensive Computing

Multi-Domain Analysis, Classification & Detection

Multi-Scale Cyber Experimentation & Validation

Non-Traditional & Multi-Disciplinary Cyber Science

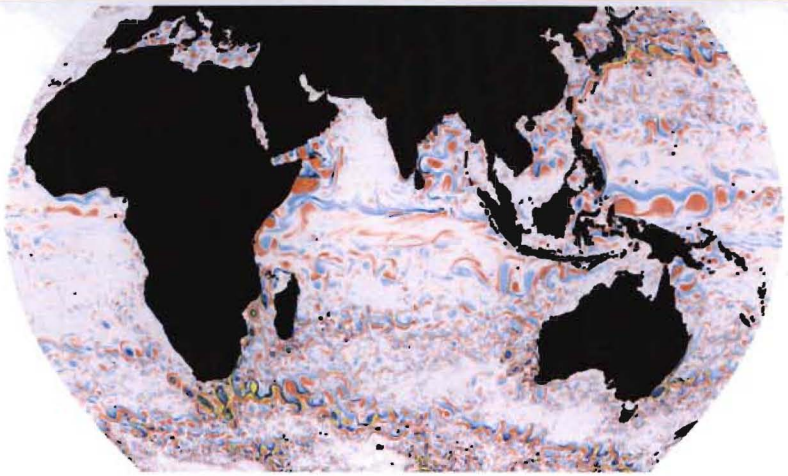
Foundational Cyber Technologies

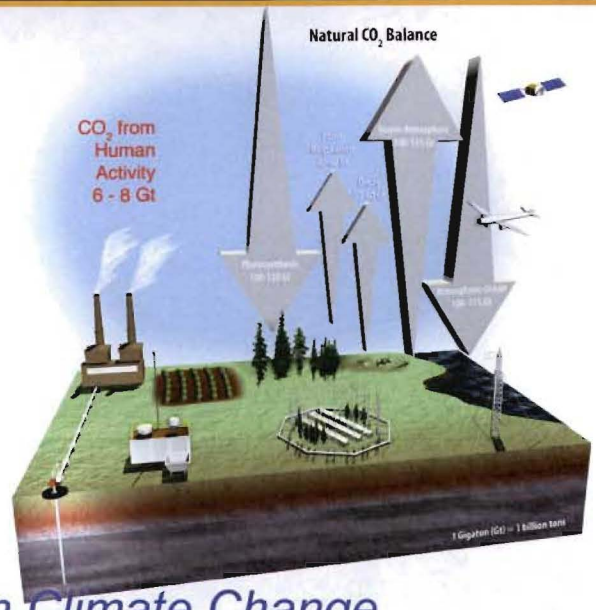
- ***Advanced Threat Analysis, Detection, and Response Tools***
- ***Mobile Cyber Platform Solutions***
- ***Cyber Operation & Decision Support Frameworks***
- ***Experiential Cyber Training***

Differentiating Solutions

(A. Kent et al)

Global Climate Science: Tools for Policymakers





- Los Alamos developed the Coupled Sea-Ice Model: *the global standard used by the Intergovernmental Panel on Climate Change*
- Los Alamos makes key contributions to the DOE/NSF Community Climate System Model: *the first interactive model of molecular to planetary scale*
- National Challenge: *Science-based policies for energy use, regional infrastructure investments, and resource allocation*

Understanding climate change as a global system is required to develop predictive tools for mitigating regional impacts

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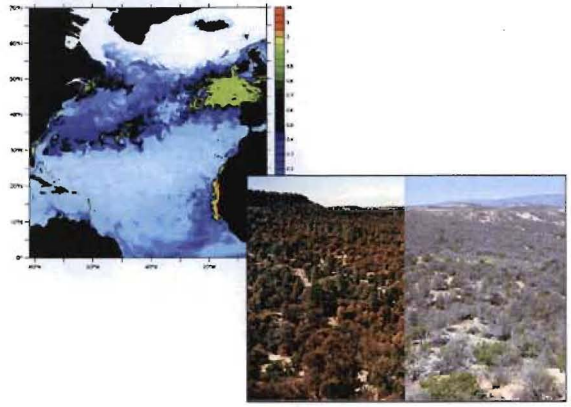
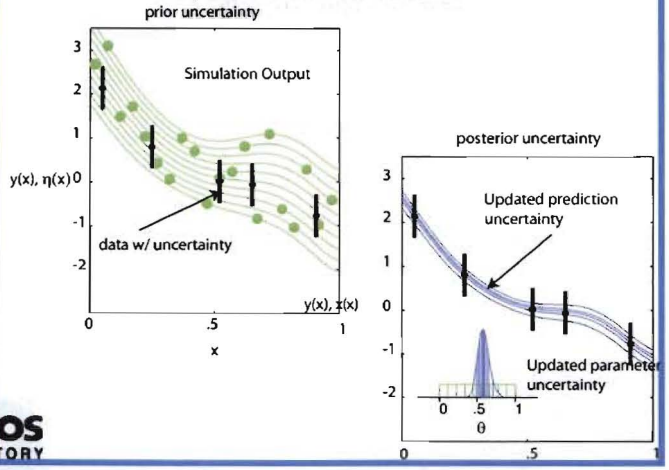
LANL is bringing key assets together:
Co-Design for Energy and Climate Science: Impacts and Mitigations

Measurements & Analysis (Microbes to Satellites!)

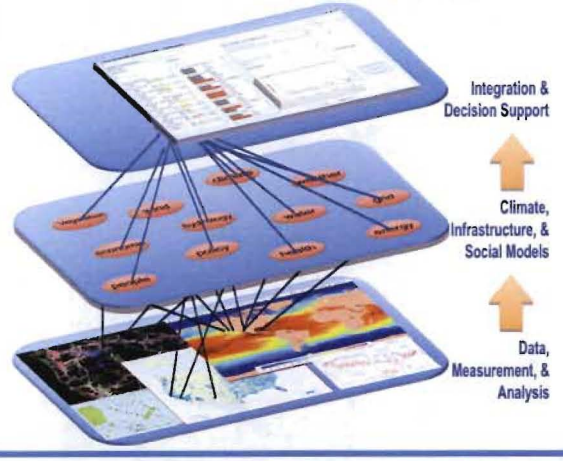
Climate and Modeling



Uncertainty Quantification



Social, Energy, and Infrastructure Modeling



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Uncertainty Quantification: FY11 Activity at LANL

- November 2010 Conference (Higdon, Anderson, Alexander, Ghanem)
  - Report out in early 2011
- Higdon (CCS-6) serving on NAS UQ panel
- Current Applications
  - NW
  - Nuclear Energy
  - Climate
  - ASCEM
  - Carbon Capture
- Future Applications
  - SocioTechnical Simulations
  - CyberSecurity

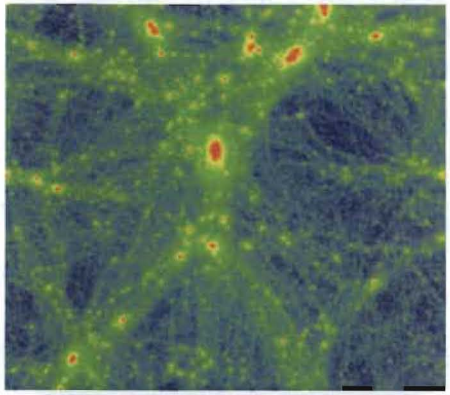
Visualization and Analysis of Massive (including Streaming) Data

- **LANL exploring "Middle Ways" between numerically-intensive and data-intensive supercomputing**
  - Need for interactive scientific visualization of massive data quantities
- **Developing novel ways to use emerging computer hardware to enable real-time visualization and analysis of massive streaming datasets**
  - Use active storage and networks
  - Examples: situational awareness, cyber, space, infrastructure, space . . .
- **Will enable a system that provides real-time:**
  - Processing (correlation) of incoming measurements
  - Analysis of correlated data to identify events of interest, their storage and use

"Data-Intensive Supercomputing" Facility
(G. Grider)

Immersion Visualization (CAVE)

"The Century of Complexity" (S. Hawking)



Cosmology: Filaments, Clusters, and Voids

Science @ Scale

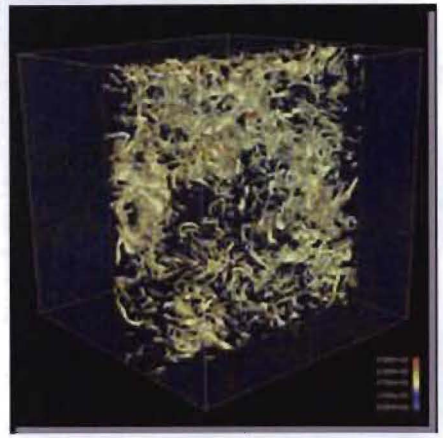
Systems of connected functional scales space, time; Emergent functions; Extreme conditions

Enabled by huge advances in Data, Simulation, Nonlinear Science…

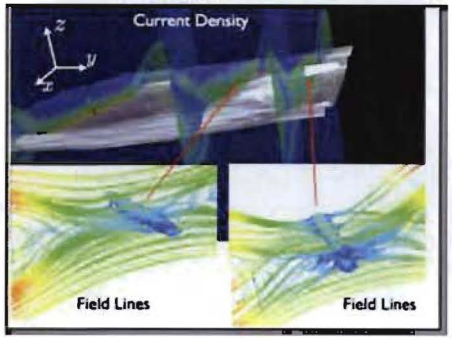
BUT….

? Origins, Measures, Consequences ?

Multiscale Modeling, Simulating, Measuring ≠…at Multiple Scales: Need IS&T

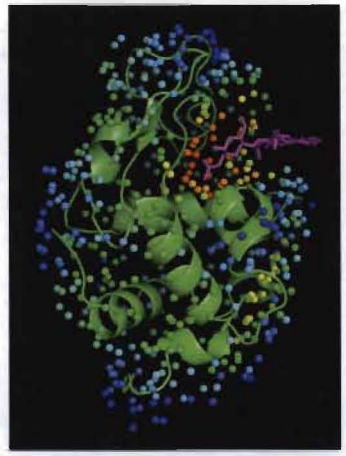


Fluid Turbulence

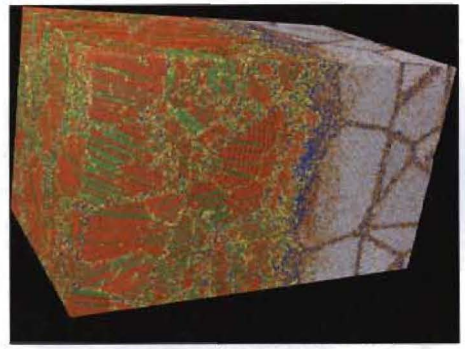


Magnetic Reconnection

Communication Networks



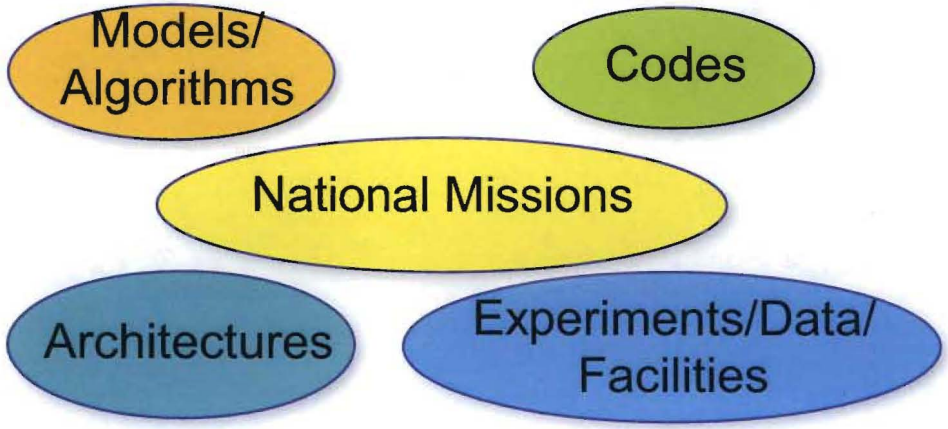
Protein Dynamics

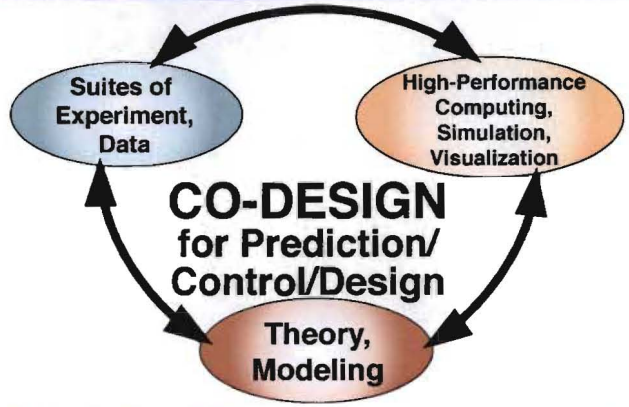


Shocked Metals

Los Alamos NATIONAL LABORATORY

A national S&T management challenge for timely, cost-effective impact on discovery, prediction, design





What should a next-generation user facility look like? Beyond "cottage industries"?

- Resetting integration and collaboration framework for transformational S,T & E at Science & Mission Frontiers (DOE: SciDAC, Hubs, Co-Design Centers…)
- LANL opportunities being developed: NW Predictive Capability Framework, Energy–Climate, Informatics, Environmental Management, Cyber,…MaRIE…

(Interdisciplinary teams, agile codes, IS&T tools, Analysis & Visualization of massive [streaming] data…)

DOE (SC, NNSA, Programs) has a full spectrum of assets for this future: Integrating National Assets for Discovery, Prediction, Control, Design