

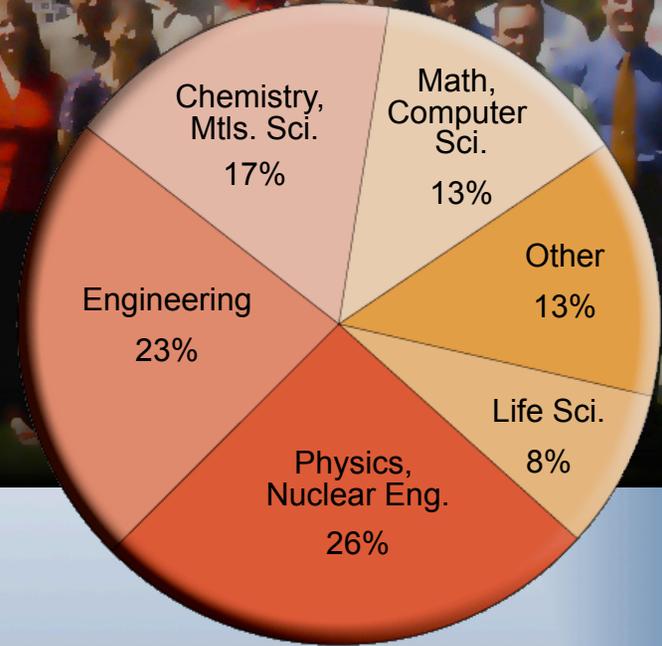
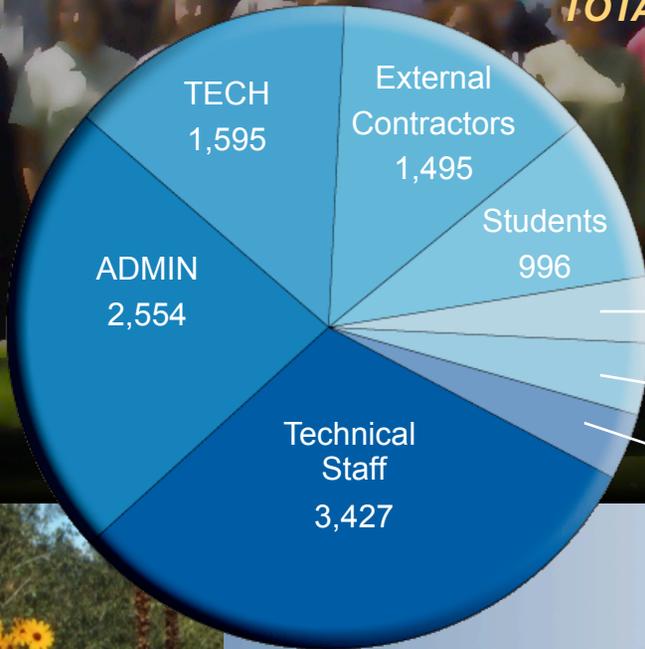
Los Alamos Computer Science Symposium (LACSS)

- ✦ LANL is delighted welcome you to the **Los Alamos Computer Science Symposium**

- ✦ **Motivation** for the Symposium:
 - serve as a premier international event showcasing research and development in high-performance computing
 - foster collaborations between national labs, academia and industry in the HPC arena
 - promote computer science research that will advance HPC programs at LANL and elsewhere
 - encourage a strong focus on HPC in the academic computer science community

- ✦ Symposium **theme this year**: Data Intensive Architectures and Applications.

**Current Work Force
TOTAL 11,174**



Technical Staff

LANL S&T base is Broad and Deep

- Drawn from across the nation
- 2,130 PhDs
- One quarter of workforce started as students or postdocs

**Outreach
is Essential
to LANL**



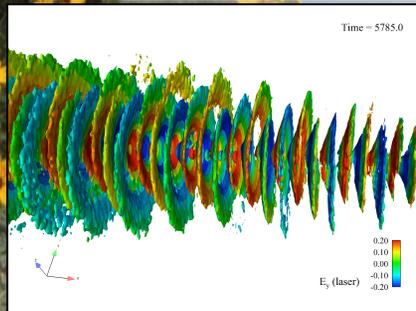
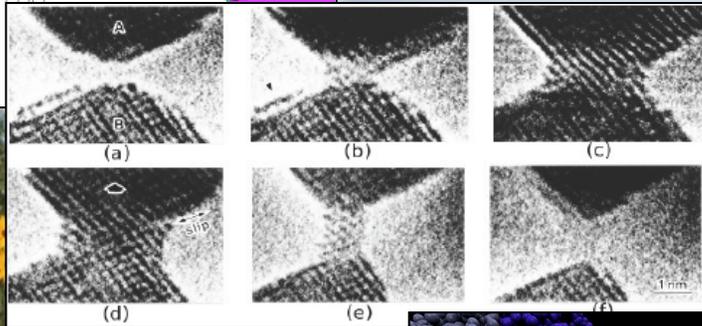
A time of transition and new opportunity for HPC nationally:

Los Alamos is committed to excellence in computer and computational sciences

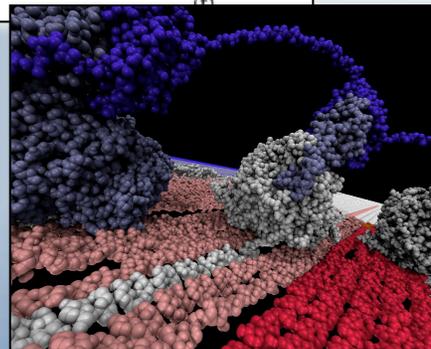


HIV epidemiology

Formation of nanomaterials



Laser plasma interactions



Breakdown of cellulose

■ Nuclear weapons program

- Support for enhanced Predictive/Control Capability

■ Open science

- Reliable and rich capability base for weapons programs
- Enabling new science and mission frontiers

■ Institutional computing

- Supporting scientific innovation and technology development
- Partnership with DOE-SC and ASC programs

■ Investing in the future

- Centers/Institutes: CAAUS, IS&T...
- Exascale planning! (Joint DOE-SC/NNSA)
 - “Codesigning” applications, codes, architectures

World-Class LANL facilities to support high performance computing systems



Secure Computing (Peak Performance)

- Roadrunner, IBM (sustained-1.105 PFlop, Peak 1.456 PFlop)
- Redtail, IBM (71 TFlop)
- Hurricane, APPRO (~50 TFlop)
- Lightning/Bolt, LNXI (34 TFlop)



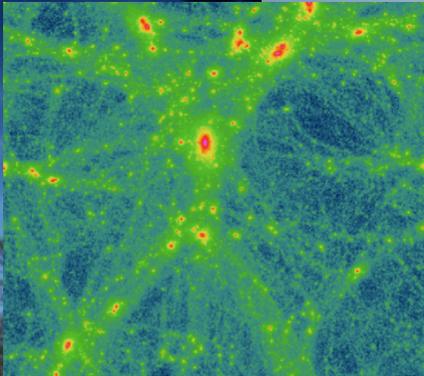
Open Computing (Peak Performance)

- Yellowrail, IBM (5 TFlop)
- Cerrillos, IBM (162 TFlop)
- Lobo, Appro (~40 TFlop)
- Coyote, LNXI (13.4 TFlop)
- Flash/Gordon, LNXI (8.6 TFlop)

Center for Advanced Architectures and Usable Supercomputing (CAAUS)

- The focal point for R&D in High-Performance Computing at the Lab
- Tasked to design the next generation architectures that maximize the performance and productivity of important national security applications
- The interface between the CS for HPC R&D efforts at the Lab with those in the community
- Specific thrust areas: performance of systems and applications under power and architectures, file systems and storage.



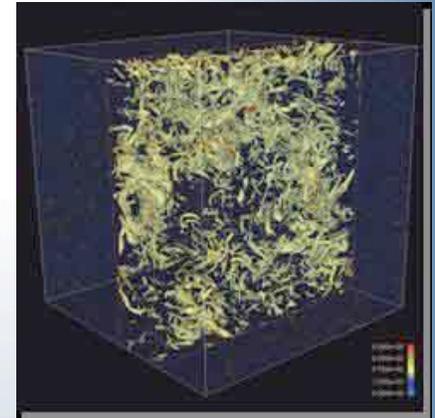


Cosmology: Filaments, Clusters, and Voids

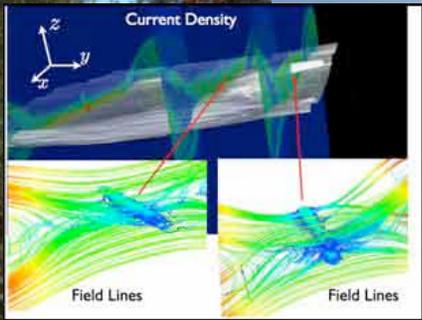
“The Century of Complexity”
(Systems of connected functional scales space time; Emergent functions)

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

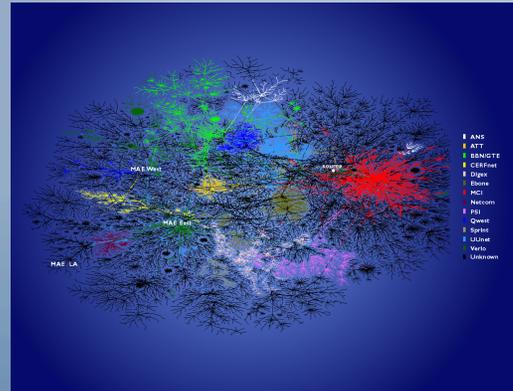
? Origins, Measures, Consequences ?



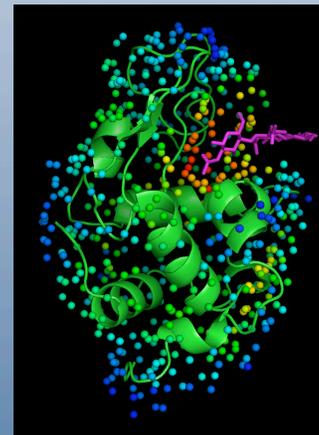
Fluid Turbulence



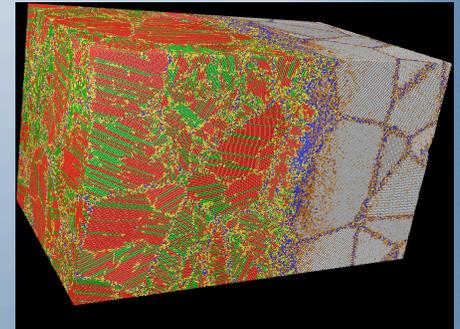
Magnetic Reconnection



Communication Networks



Protein Dynamics



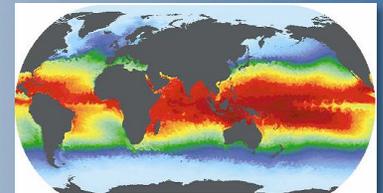
Shocked Metals

The Promise and Challenge of Science in the 21st Century

- ★ Isolating complicated phenomena to “understand” them necessary, but not sufficient

science of prediction & uncertainty quantification

for complex systems/networks



- ★ Quantitative tools for decision makers/risk assessment
 - (coupled) socio, economic, humanities, physical sciences, ...
 - from observation to prediction and uncertainty quantification



Computer and computational sciences at LANL

Today

Support the nuclear weapons mission

Directed Stockpile Work
Significant Finding Investigations
Life Extension Program
Annual Certification

Provide evolutionary technology

Tri-Lab Linux Capacity Clusters
Next ASC Capability Platform
High Performance Storage System
Common Computing Environment

Tomorrow

Support national security mission

Nuclear weapons
Materials-radiation interactions in
extremes (MaRIE)
Energy and climate impact

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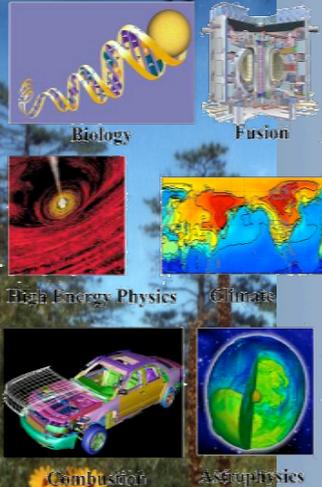
Prepare for revolutionary technology

Advanced architectures
New programming models
Resilient computing systems
Exascale << file systems

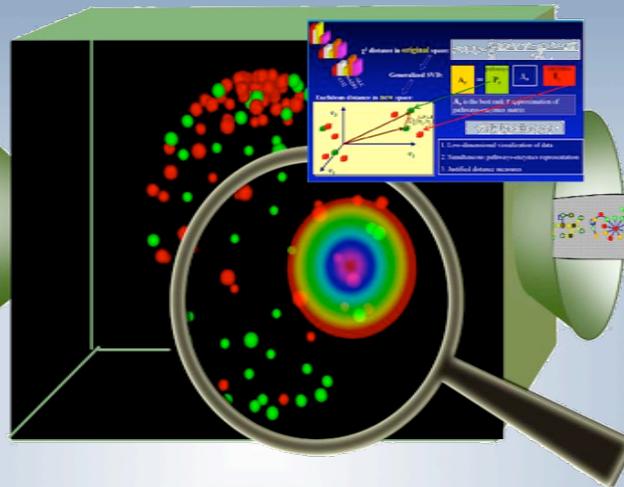
Information Science & Technology is the Infrastructure for Connecting the Dots in Science & Co-Designing National Assets

Finding the Dots

Raw Scientific Data



Connecting the Dots



Understanding the Dots

Payoffs for the Nation



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 computers
- Huge dimensional space
- Combinatorial challenge
- Complicated by noisy data

Providing Predictive Understanding

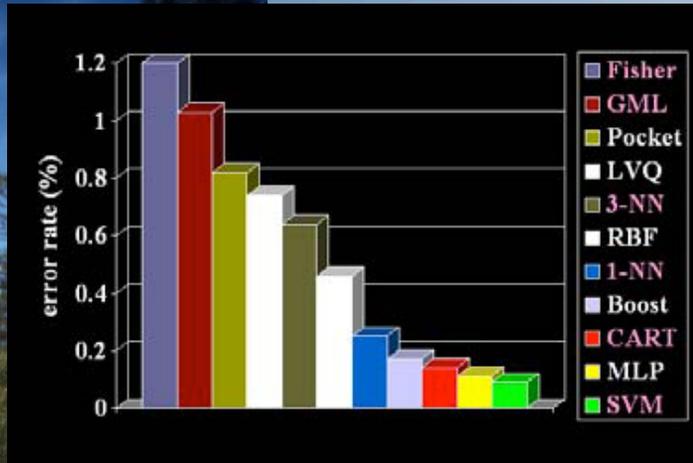
- Produce hydrogen-based energy
- Stabilize carbon dioxide
- Clean and dispose toxic waste



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

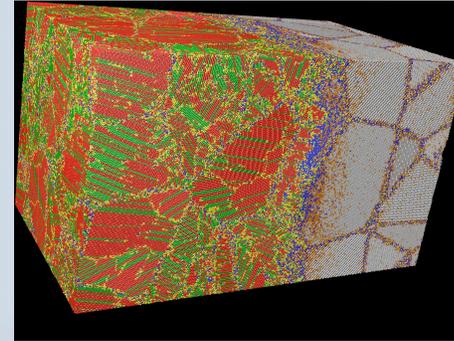


Applying IS&T to Accelerate Predictive Capability



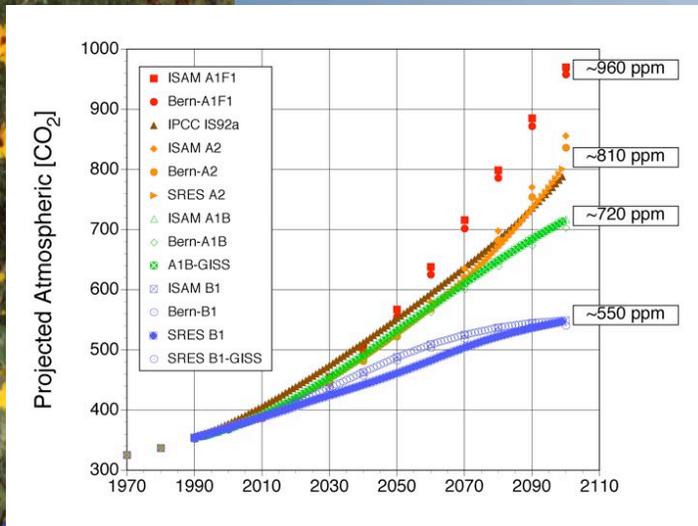
False Alarm rate for cybersecurity applications

IS&T developments are needed to identify “significant” events in real time and extract information-rich data for statistical interrogation, anomaly detection, and classification.



Molecular dynamics simulation of phase transformations in shocked metal

IS&T provides the framework to efficiently integrate information from experiment and theory, & accelerate model development

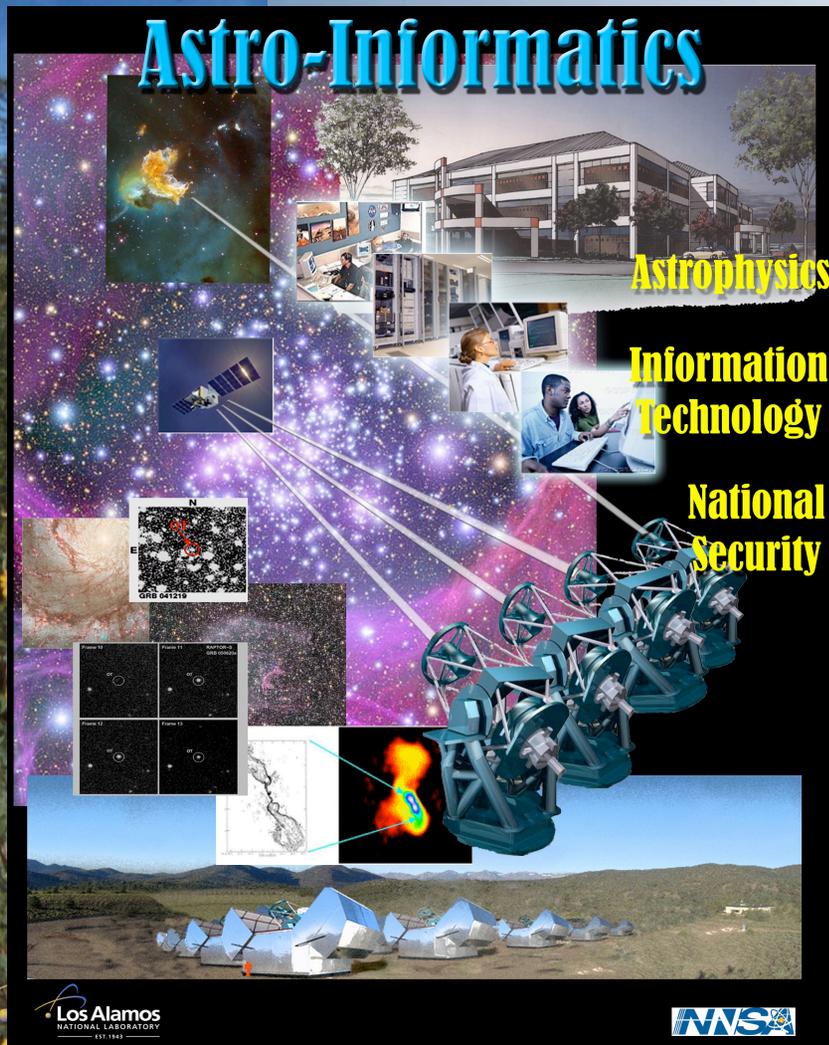


Uncertainty quantification for climate predictions



Change Detection in Images

IS&T for Global multi-bandpass coverage of the cosmos



- Space situational awareness impacts (Advanced IS&T is the driver for both science and intelligence work)
- Building the information science infrastructure for intelligence community applications
- LANL leadership autonomous robotic telescope networks
- LANL has proven the capability of autonomous systems being able to detect, track, and analyze LEO satellites
- Optical and radio systems working together with advanced IS&T and technology can discover, analyze, and characterize astronomical events and satellite detections in real time

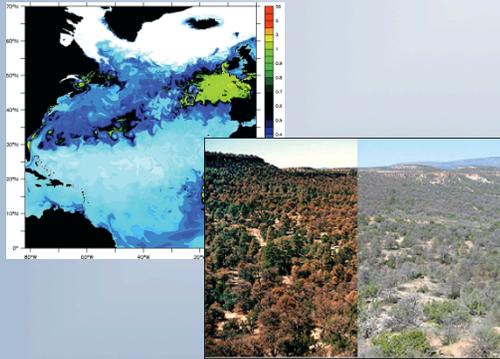
Energy Climate Impacts Project (ECI) –Multi-Lab

GHGIS – Measurements & Uncertainty Quantification



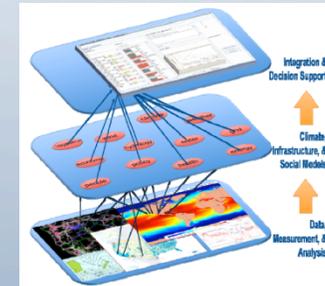
LANL ECI scientists contribute to the new GHGIS through estimating uncertainties, designing new instruments to measure GHGs, and using modeling to design the placement of new instruments.

Climate & Natural Systems Modeling



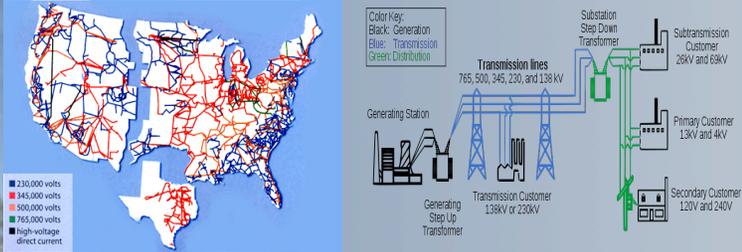
LANL ECI scientists participate in developing some of the most advanced climate models in the world: an ocean model, a sea ice model, physiology-based models for vegetation mortality, and a land ice model.

Social, Energy & Infrastructure Modeling for Climate Treaty support solutions



LANL ECI scientists can develop and apply Decision Support Systems to model the impacts of climate change and GHG emissions on regional and local scales and model its impacts on energy, social dynamics, and Infrastructure.

Smart Grid: a National Grand Challenge



R&D Problems for Smart Grids

A future grid, in which modern sensors, communication links, and computational power are used to improve efficiency, stability, and flexibility, has become known as the “smart grid.”

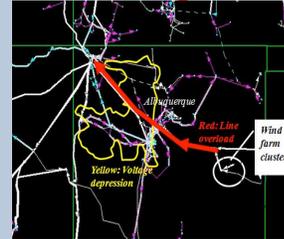
R&D Methodology: Road Map for Smart Grids

Driven by emerging technologies such as renewables, storage, and meters, specifies the technical challenges in *Grid Design*, *Grid Control* and *Grid Stability*.

All of the above require scientific advances in

- Analysis & Control
- Scalability/Reliability Mosaics
- State Estimation
- Data Aggregation & Assimilation
- Middleware for the Grid
- Modeling Consumer Response

Grid Designs

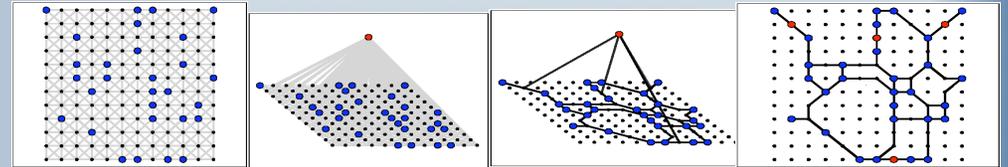


Generators – red dots
Loads – blue dots

NREL solution included

- Cost dispatch only
- Power flows highly approximate
- Unstable solutions
- Intermittency in Renewables not accounted

Toole, Fair, Berscheid, Bent '09
go beyond NREL
“20% renewables incorporated by 2030”



original graph for generation placement

“master generator” connected to possible sites.

Resulting Sparse Network

Minimize under constraints

Johnson, Cherkov '09
Network Optimization

Impact to LANL, NNSA & the Nation

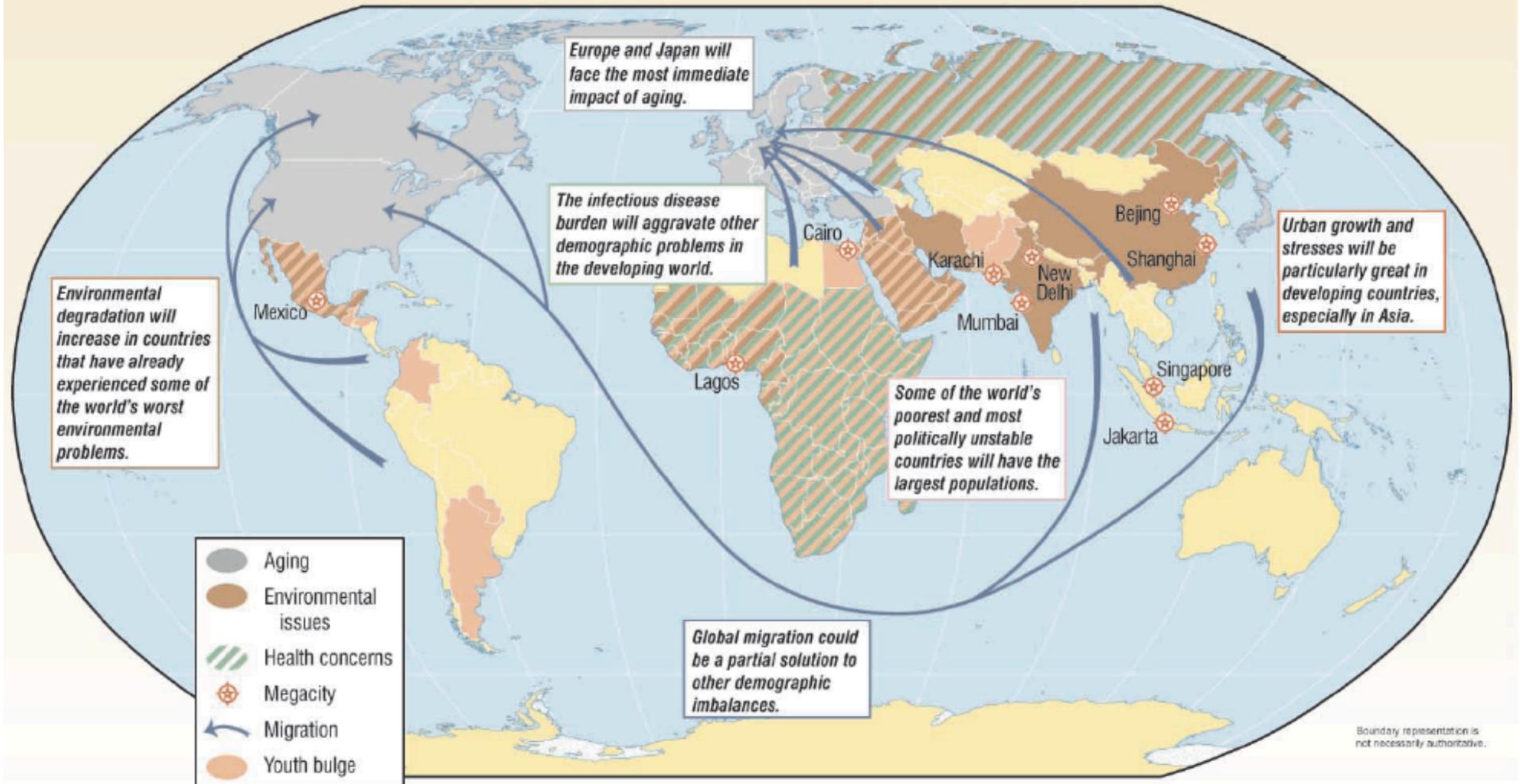
- Reduce consumer energy costs
- Promote energy independence
- Support national renewable penetration goals
- Address strategic problems at the intersection of energy, climate, and infrastructure
- Support LANL’s Energy Security Center and LANL’s Information Science and Technology Center

Coupled Complex systems: the need for system-level predictions

(Multi-scale Geo-Spatial Temporal Models)

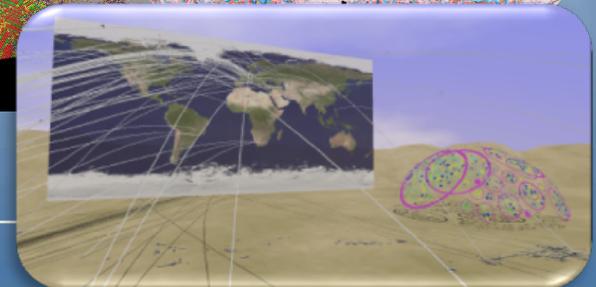
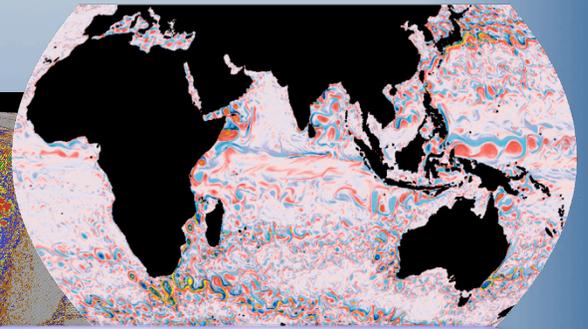
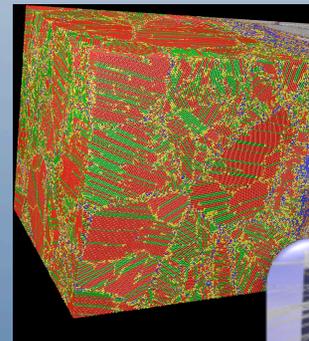
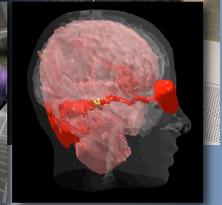
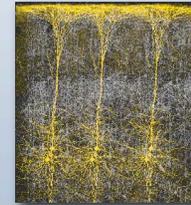
Population Dynamics, Environment and Water, Energy, Health, Megacities, Agriculture, Radicalization dynamics, Political Instabilities

A Snapshot of Global Demographic Trends



IS&T provides the frame-work to efficiently integrate information from experiment and theory, and accelerate model development

- Capabilities
 - Quantum Information Science
 - Inference/Learning/Prediction
 - Data Intensive Supercomputing
 - Synthetic Cognition
- Application Areas
 - Predicting Materials Performance
 - Energy – Climate
 - Situational Awareness
 - Space SA
 - Wide area persistent surveillance
 - Cyber SA
 - Bio SA
 - Structural Health Monitoring (bridges, infrastructure...)



Visualization and Analysis of Massive (Streaming) Data

- Exploring “Middle Ways” between numerically-intensive and data-intensive supercomputing
 - Need for interactive scientific visualization of massive (HPC) data
- 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 . . .
- Will enable a system that provides real-time:
 - Processing (correlation) of incoming measurements
 - Analysis of correlated data to identify events of interest and their storage



Information Science and Technology at LANL

Building toward a data-rich predictive capability

