SAND2008-3315P

Modeling and Simulation at Sandia: An Overview

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Sandia National Laboratories
April 23, 2008

*With thanks to Art Ratzel, Director, Engineering Sciences Center

Sandia National Laboratories: Approaching 60 Years of National Service

- Born of the atomic age.
- Heritage of engineering and production.
- Science mobilized for national security.
- A legacy of industrial management.
- Six key mission areas:
  - Nuclear weapons
  - Nonproliferation
  - Assessments
  - Military technologies and applications
  - Homeland security
  - Energy and infrastructure assurance

"you have …an opportunity to render an exceptional service in the national interest."
May 13, 1949 Letter from President Truman to Mr. Wilson, President of AT&T

AT&T | LOCKHEED MARTIN

1949-1993 **1993-Present**

Our Highest Goal: become the laboratory that the United States turns to first for technology solutions to the most challenging problems that threaten peace and freedom.

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Presentation outline

- **"Drivers" for modeling and simulation**
  - weapon engineering
  - science for materials, energy, and biology
  - system analysis
- **Enabling capability: computing**
- **Engineering-focused M&S**
- **Enabling capability: experiment & test**
- **Science-focused M&S**
- **System and enterprise M&S**
- **Path forward**

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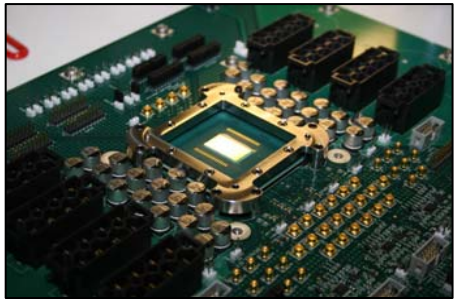
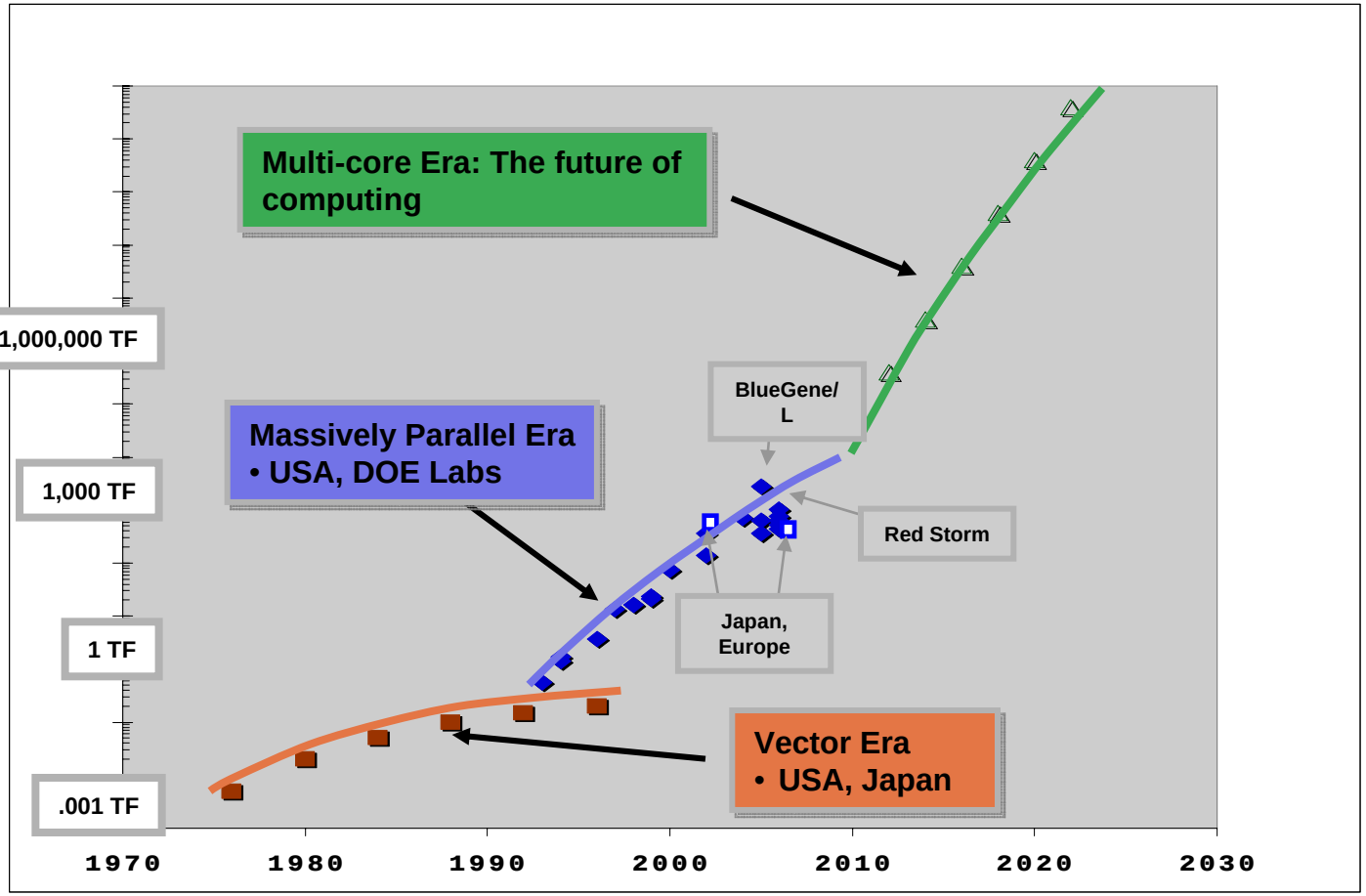
We are entering the 3rd era of supercomputing

1997: Janus Red
1 TeraFLOPs in a room
(2,500 ft² & 500,000 W)



2007: Microtechnology
1 TeraFLOPs on a chip
(275 mm² & 62 W)



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Sandia has made key contributions to the development of MP computing technology


CM-2


nCUBE-2


iPSC-860


Paragon


ASCI Red


Cplant


Red Storm

1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997 1998 1999 2000 2001 2002 2003 2004 2005 2006

Gordon Bell Prize

R&D 100
Parallel Software

Patent
Meshing

R&D 100
Dense Solvers

R&D 100
Storage

Gordon Bell Prize

World Record
Teraflops

Gordon Bell Prize

R&D 100
Allocator

R&D 100
Trilinos

SC96 Gold Medal
Networking

Mannheim
SuParCup

R&D 100
Signal Processing

Karp Challenge

World Record
281 GFlops

R&D 100
Aztec

Patent
Data Mining

R&D 100
Salvo

Fernbach
Award

R&D 100
Meshing

World Record
143 GFlops

Patent
Parallel Software

Patent
Paving

Patent
Decomposition

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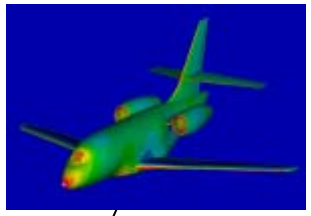
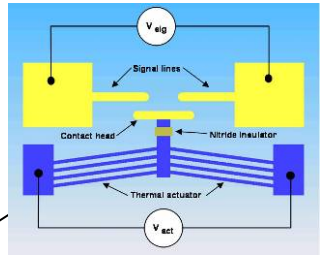
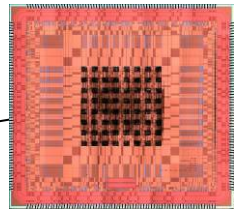
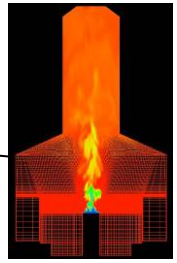
Trilinos solver architecture

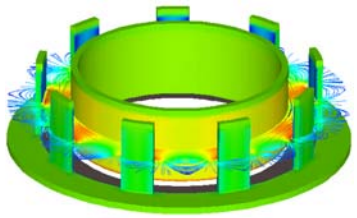
- **Recent Work**
  - **Trilinos 5.0 released; >1000 downloads**
  - **Focus on continued package development and software engineering**
- **Awards**
  - **R&D 100 (in 2004)**
  - **IEEE HPC Software Challenge Award**
  - **Sandia ERA team award and NOVA nomination**
- **First software architecture to allow community development**
  - **Two-level design:**
    - **Self-contained packages**
    - **Leveraged common tools.**
  - **Allows rapid algorithmic development and delivery**
- **Leveraging investments in software infrastructure without compromising individual package autonomy**











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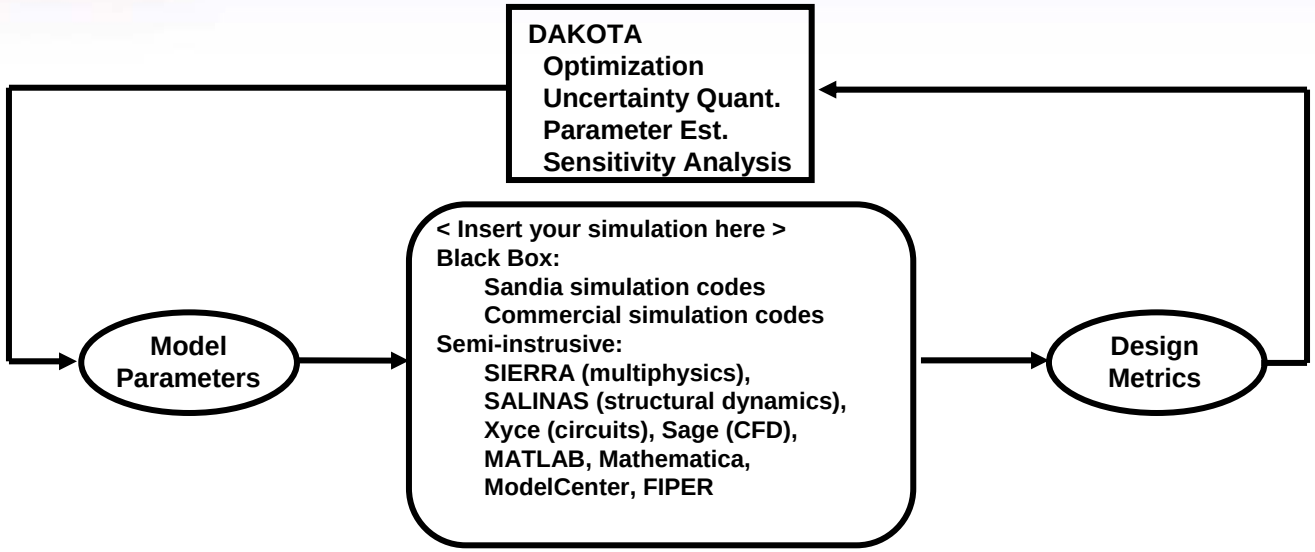
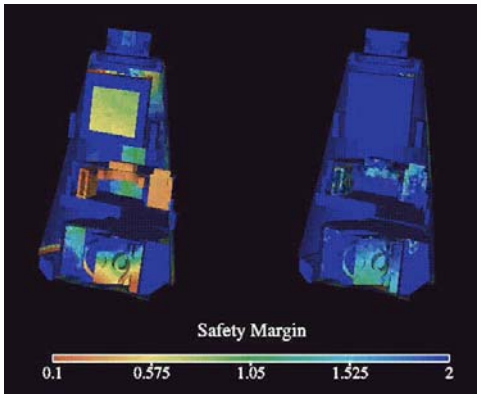
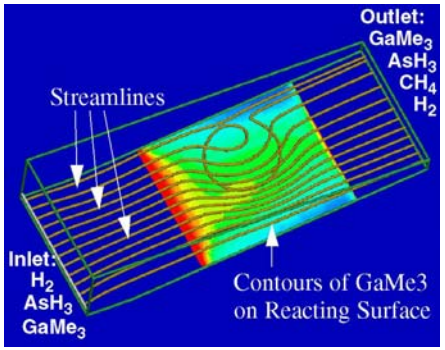
DAKOTA optimization toolkit





Nominal Optimized



***Goal:* answer fundamental engineering questions**

- What is the best design?
- How safe is it?
- How much confidence in my answer?

Challenges

- Reuse tools and interfaces, leverage commonalities → software
- Nonsmooth/discontinuous/multimodal, expensive, mixed variables, unreliable gradients, simulation failures → algorithm R&D
- ASCI-scale applications & architectures → scalable parallelism

Impact

- DOE: Tri-lab tool, broad application deployment
- External: WFO partners, GNU GPL (>3000 download registrations)

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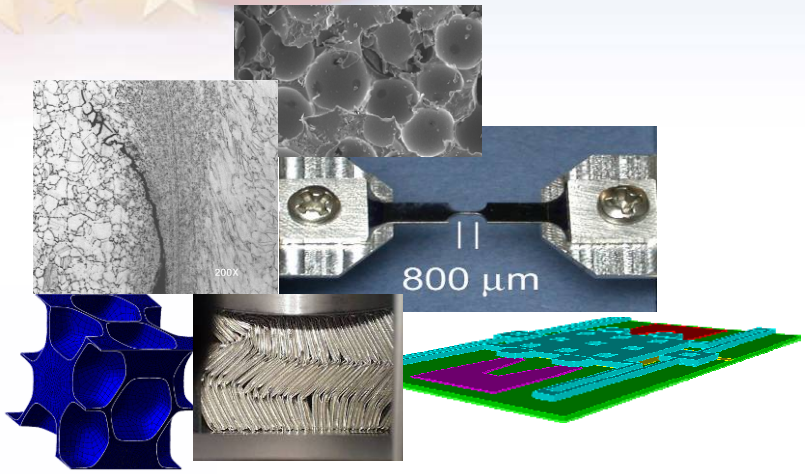
Engineering M&S at Sandia spans the physical sciences

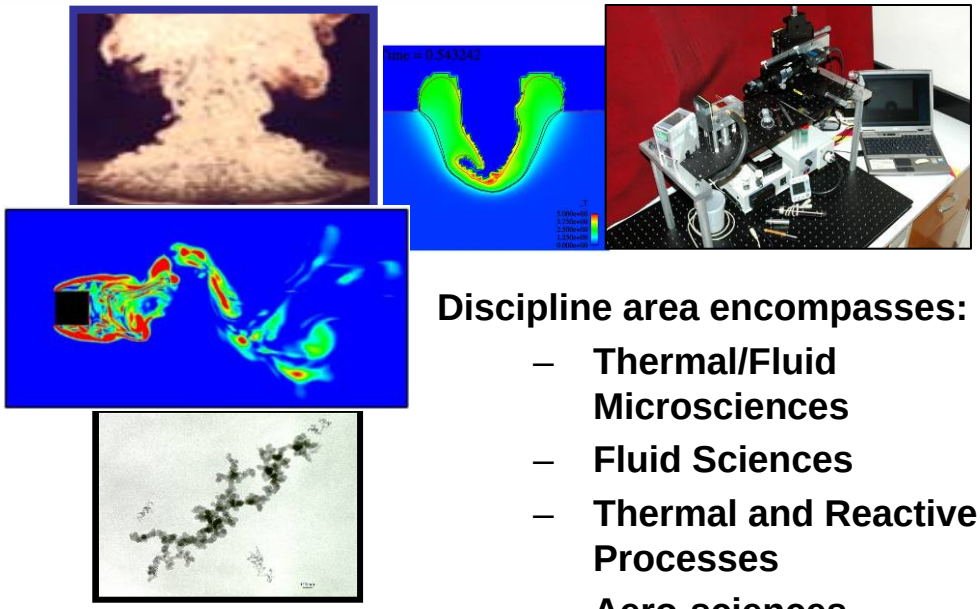


Solid/Material Mechanics & Structural Dynamics

Discipline area encompasses:

- Solid Mechanics
- Structural Dynamics
- Material Mechanics

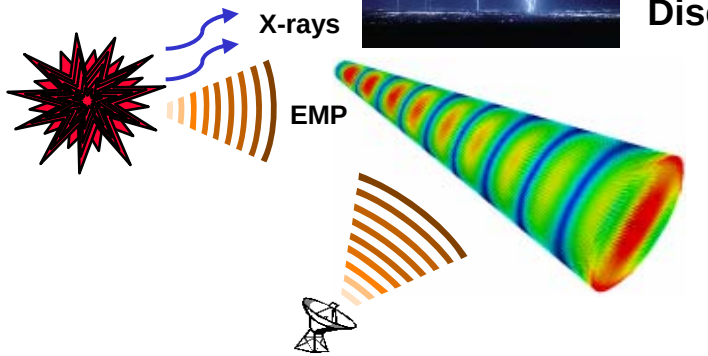
Thermal, Fluids & Aero-sciences



Discipline area encompasses:

- Thermal/Fluid Microsciences
- Fluid Sciences
- Thermal and Reactive Processes
- Aero-sciences

Electrical Sciences*



Discipline area encompasses:

- Electromagnetics, electrical effects, electrical devices, components & systems

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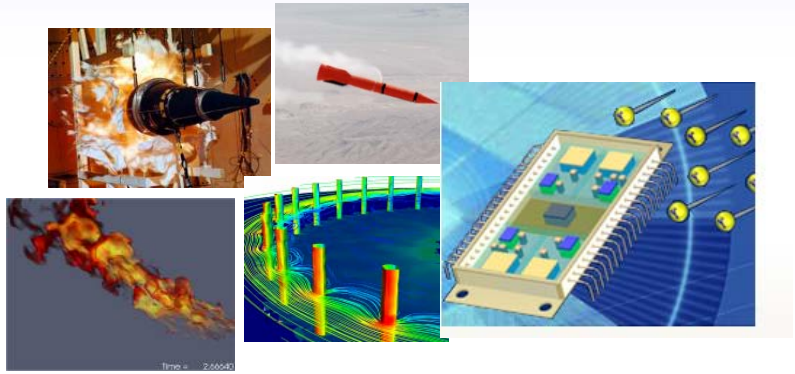
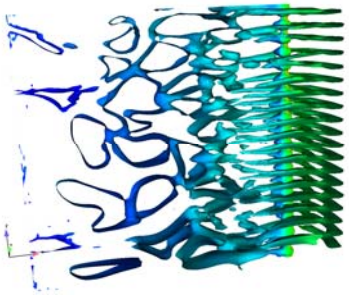
ASC's investment in Engineering Codes at Sandia is enabling simulation of a broad & diverse set of weapons applications

Complex Systems, Components, and Physics



Diverse Applications



ALEGRA

Radiation Analysis, Modeling and Simulation of Electrical Systems

- Electron & Photon Radiation Transport (ITS/CEPTRE)
- Neutron & Gamma Radiation Transport (NuGET)
- Electromagetics (EMPHASIS)
- Electrical Response (XYCE)

RAMSES

SIERRA Mechanics

Sandia is the Engineering Code Provider for the NW Complex

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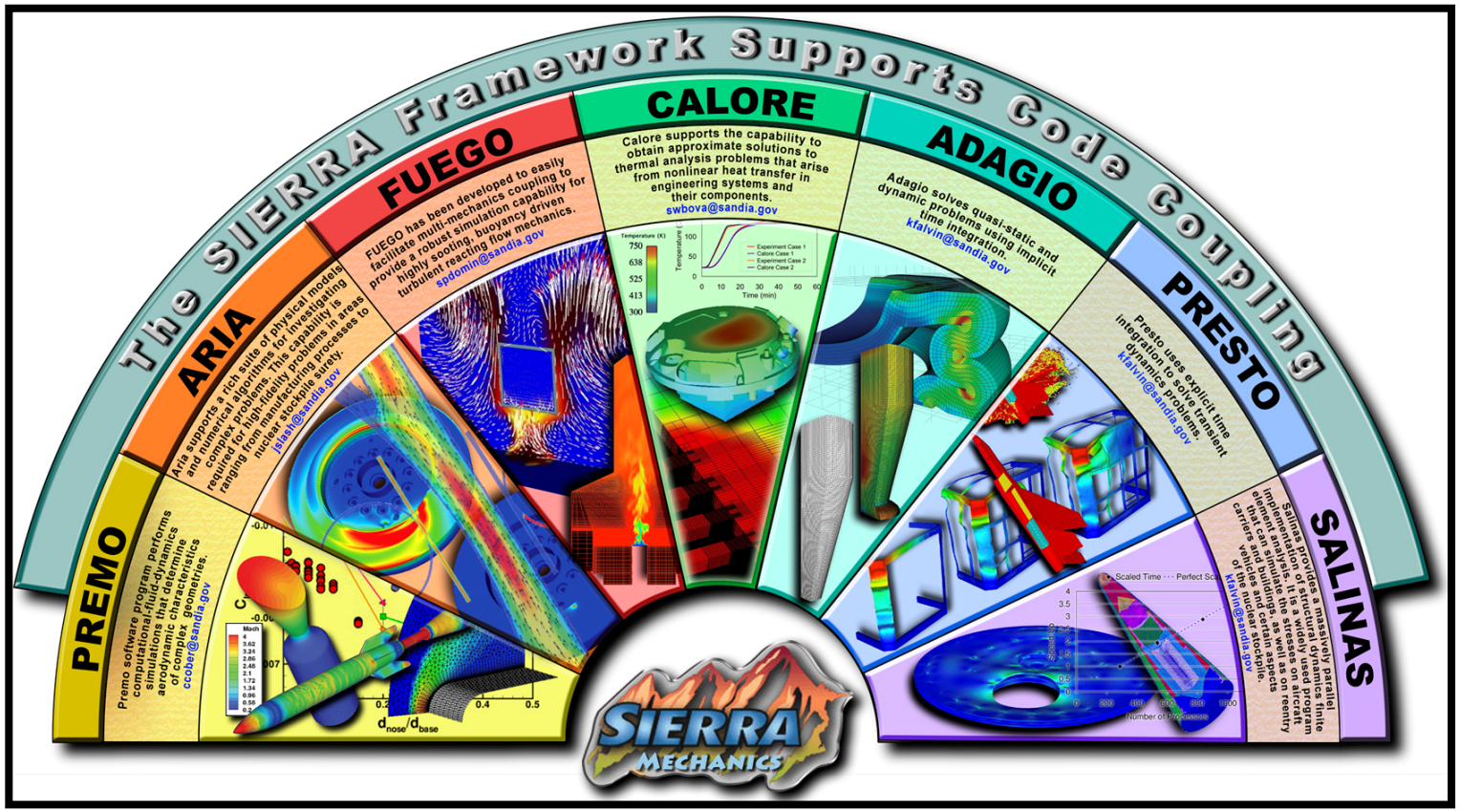
The SIERRA framework covers thermal, fluid, solid and structural mechanics



Q: Why frameworks?

A: parallel computing, adaptivity, multi-physics, V&V

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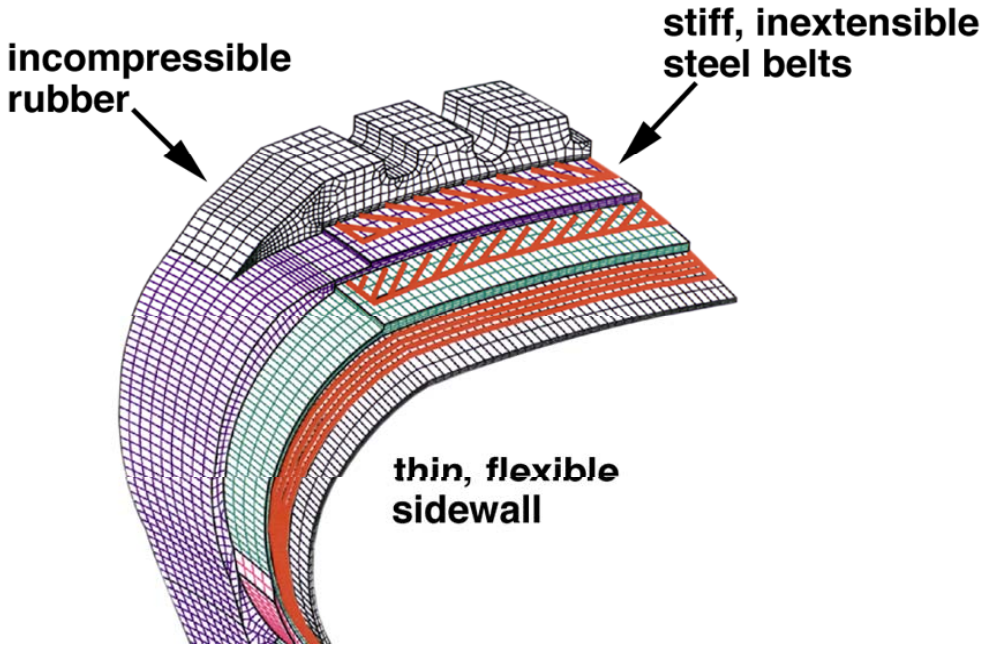
Sandia's Computational Mechanics Capabilities and Their Application at Goodyear

Goodyear and Sandia have been sharing technology through CRADAs for more than ten years. This long-term investment in scientific knowledge is paying off in technology breakthroughs behind some major new tire products by Goodyear. These same technology breakthroughs are helping Sandia fulfill its mission.



The Challenge: Facile Tire Design and Performance Quantification

A unique partnership with a history of developing technology critical to weapons systems and to tire design & manufacturing.

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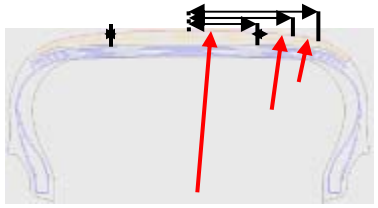
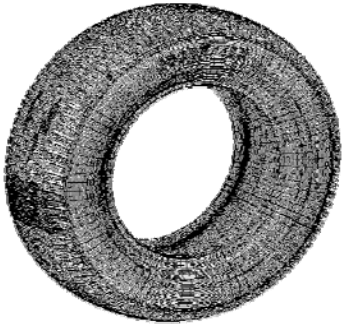
Teaming with Sandia, Goodyear Has Revolutionized Design-to-Production of Tires Through Mod-Sim

Then



Test-based Iterations

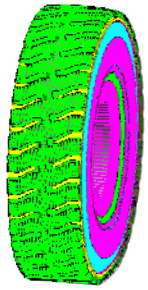
Multiple Builds!

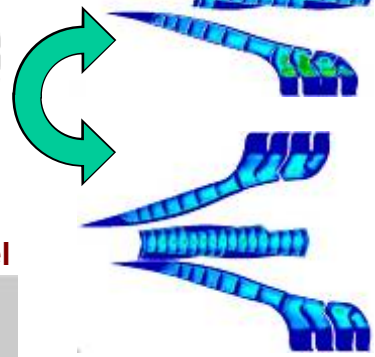


2-3 Years

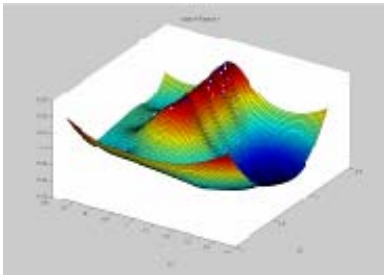
Now & Future

Computational-based Iterations





Solid Model **FE Model**



Optimization

Footprint Prediction

One Build!

Less than 1 Year

Sandia Enabled Computational Technology

Goodyear Assurance™ Featuring TripleTred Technology™

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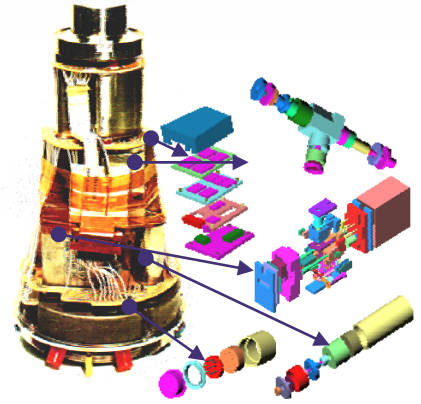
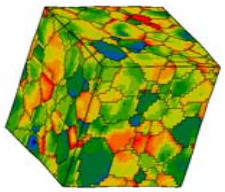
Enabling capability: test and experiment for discovery

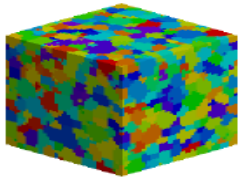
- Development of new tools/ computational capabilities for probing atomistic and molecular scales
- New computational methodologies for integrating atomistic and meso-scale data into continuum analysis
- A strong experimental component for discovery and model validation

Quantifying critical component response at the continuum

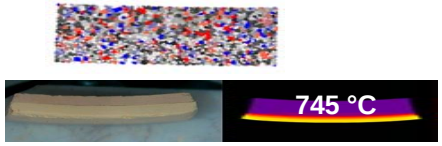




Crystal Plasticity

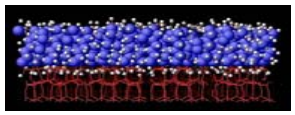


Quantifying response at the Micro-scale

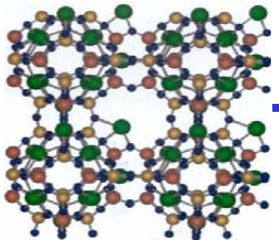


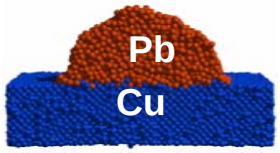
Experiment FEA

Ceramic Sintering



Polymer Coating





Reactive Wetting

Quantum & atomistic material models for properties

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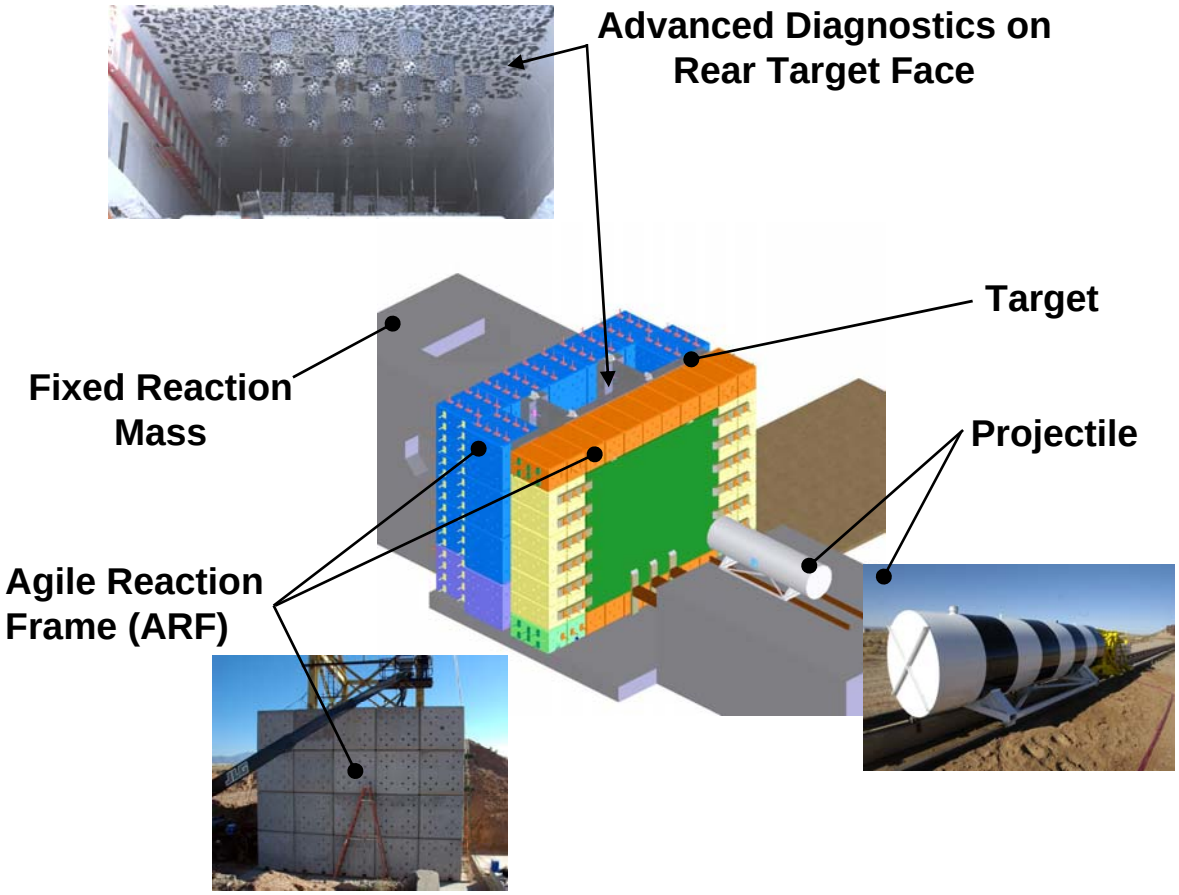
Enabling capability: test and experiment for validation

Program Goal: Capture critical validation data for numerical simulations of the structural collapse and failure of a heavily reinforced concrete structure.



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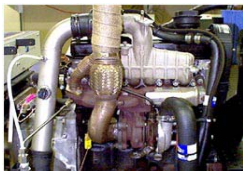
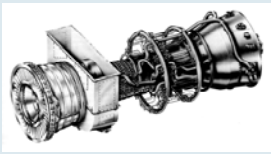
DOE Office of Science sponsors the Combustion Research Facility

Device Validation Experiments

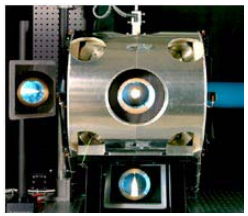


Detailed Device Models
• e.g. IC Engine, Gas Turbine, Boiler



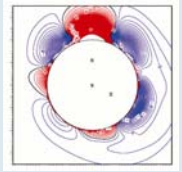
Device Engineering Models and Optimization Tools

Sub-Model Validation Experiments

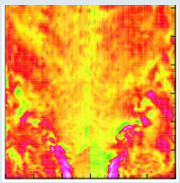


Detailed Device Sub-Models
• e.g. Atomization, Ignition, Soot

Chemical Dynamics (Theory)

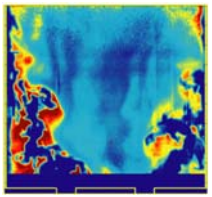


LES: Complex Geometry, High Reynolds Number

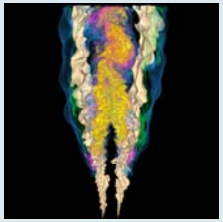


Basic Science Foundation for Predictive Combustion Models

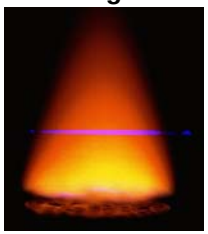
Turbulent Experiments



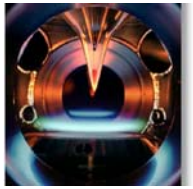
3D DNS of turbulent flames



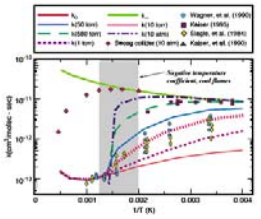
Laser Diagnostics



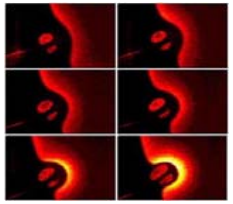
Kinetic Experiments
Mechanistic Experiments



Mechanism Development



Laminar Experiments



Mechanism Reduction

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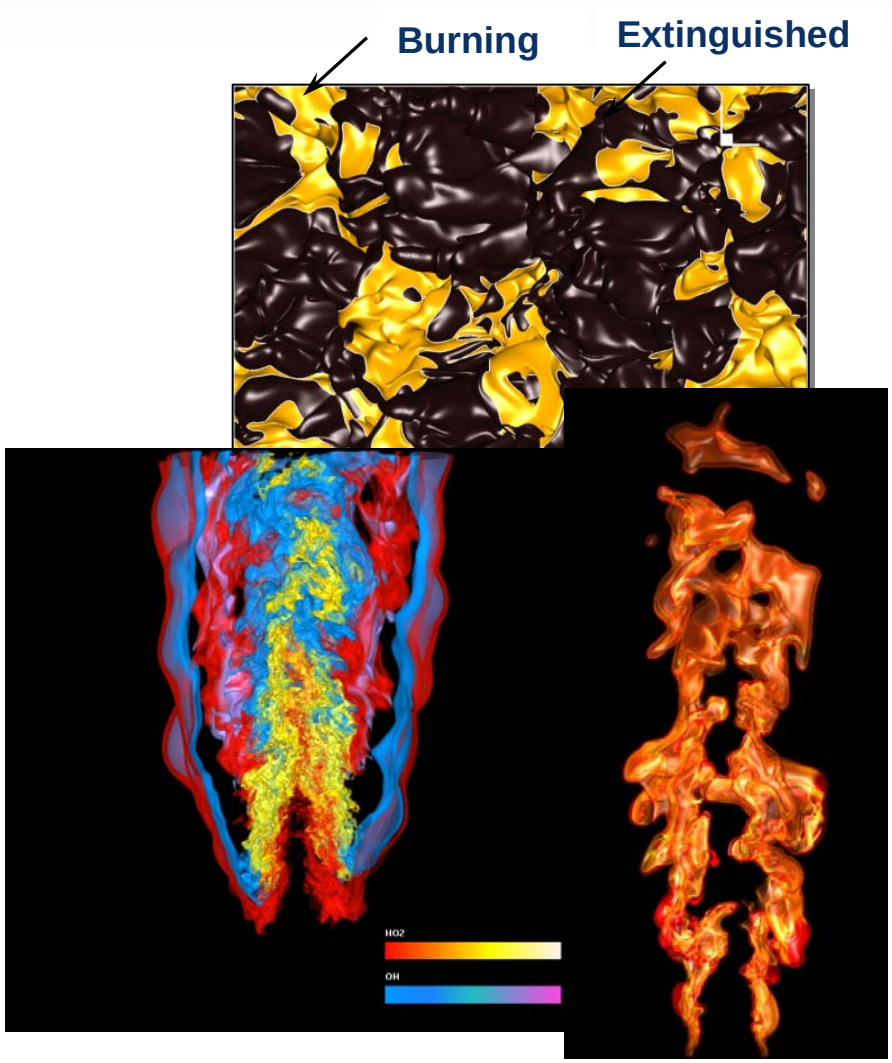
DNS (direct numerical simulation) of turbulent combustion

- Petascale DNS of turbulent combustion
- World's largest direct simulations of turbulent combustion
  - INCITE Awards (2.5 and 6M hrs)
  - 1 billion gridpoints, 14,000 processors
  - 50 TB data
- Study chemistry/turbulence interactions:
  - Extinction/reignition
  - Turbulent transport of soot
  - HCCI combustion
  - Premixed flame
  - Stabilization and autoignition
- A priori model validation



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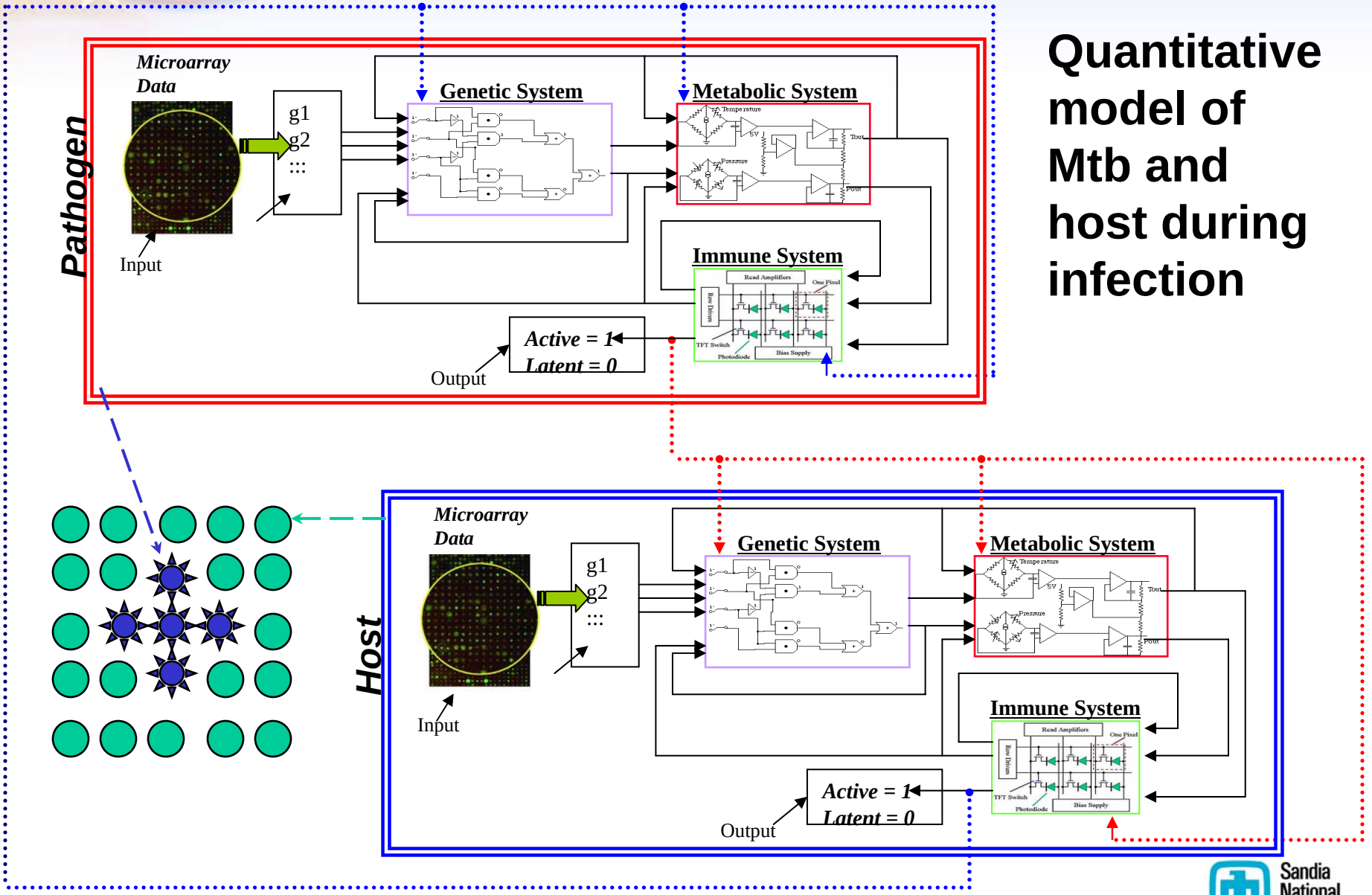
NIH sponsors bioscience M&S



Quantitative model of Mtb and host during infection

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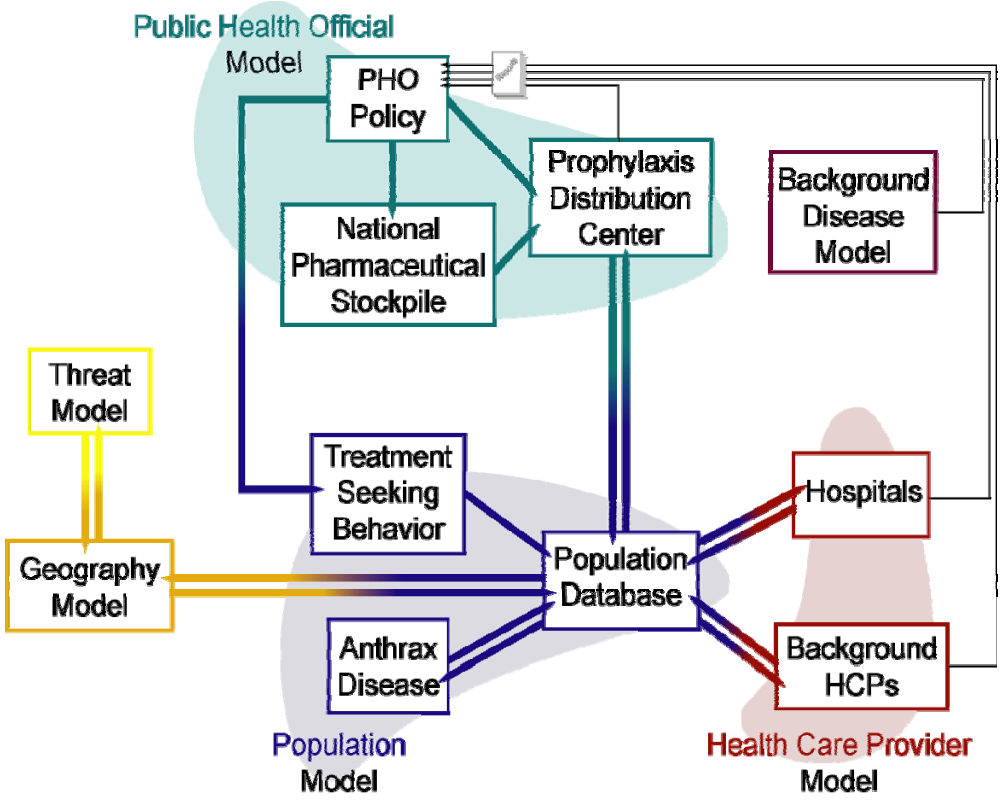
System models capture key aspects and relationships of a problem in an integrated software environment



Enterprise Modeling is a method used to capture the pertinent attributes of situations, behaviors, and business or institutional entities and express those attributes in an integrated environment.

Large-scale distributed enterprise models are used to represent complex, non-linear relationships between **technologies**, **resources**, and **policies**.

Interactive enterprise models add **human factors** (decisions).

For the last 10 years, Sandia has developed submodels of threats, technologies, resources, and policies applicable across many of the DHS national planning scenarios.

Approaches: discrete-event, agent-based, immersive environments, gaming

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The parts of a system model (one example)

- Population
  - Moving population of ~3 million
  - Military, civilian, tourist
  - Treatment-seeking behavior
- Health care providers
  - Hospital beds: normal or surge capacity
  - Case reports, clinical samples
  - Astute clinician diagnoses
  - Epidemiological investigations
- Civilian assets
  - Special events/tourist attractions
- Naval assets
  - Vessels and bases
  - Deployment schedules
- Prophylaxis
  - Distribution strategies
  - Points of distribution
  - Distribution rate
  - Strategic National Stockpile
- Laboratory
  - Sample processing
  - Processing rate
  - Normal, surge or halt operations
- Environmental monitoring
  - Sensors
  - Regular monitoring
  - Secondary sampling
  - Collection team management
- Health surveillance
  - ER visits, OTC drug sales, 911 calls
  - Simulated data superimposed on background data
  - Alarms
- Threat
  - Agent dispersion
- Disease
  - Evolving state-of-health distribution
  - Dose-dependent

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Sandia has developed M&S based tools for multiple homeland security applications

- **NISAC**
  - critical infrastructure and cascading effects
- **Borders point of entry**
  - tradeoff between detection thresholds, vehicle handling and throughput at points of entry
- **Public facility biological and chemical attacks**
  - simulation and analysis toolkit for indoor facilities (reachback)
- **BIONET system modeling**
  - integrated civilian-military response to a biological attack
- **TELL (Training, Exercise and Lessons Learned)**
  - NIMS-based response to multi-jurisdictional catastrophic events
- **Groundtruth**
  - “serious game” aimed at incident command team members
- **Biological warning and incident characterization**
  - test and evaluation of BWIC system
- **Investment planning**
  - DTRA tradeoff studies for DoD base protection
- **Pandemic flu surge response**
  - regional health care response to pandemic flu

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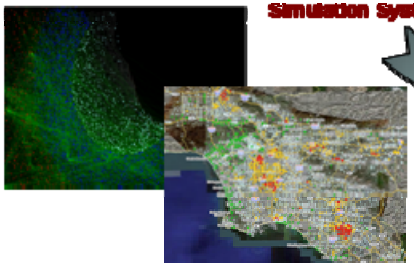
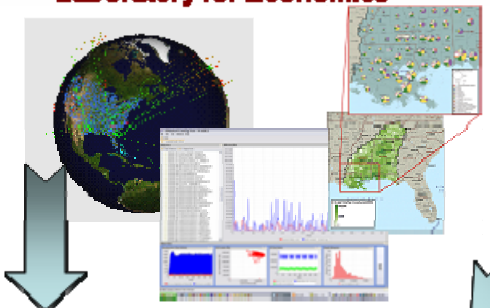
NISAC is focused on M&S of critical infrastructure

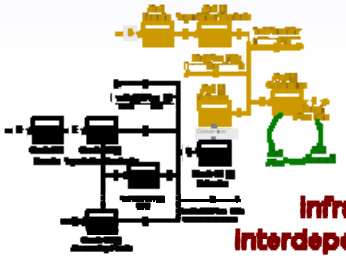
The Urban Infrastructure Suite

- Urban Population Mobility Simulation Technologies
- Epidemiological Simulation Systems
- Telecommunications Sector
- Transportation Analysis Simulation System



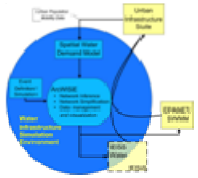
NISAC Agent-Based Laboratory for Economics



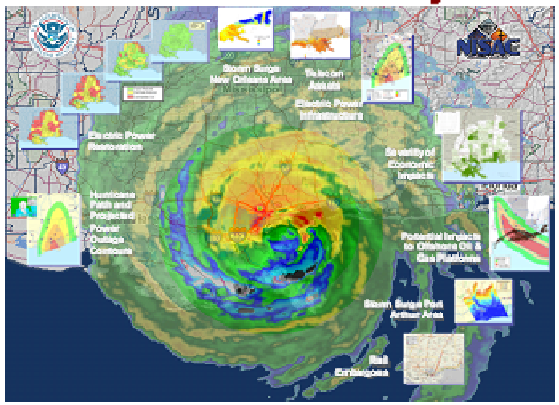


Dynamic Infrastructure Interdependencies Simulation & Analysis

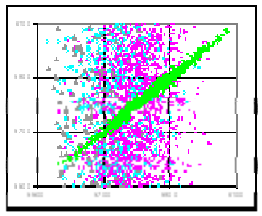
Water Infrastructure Simulation Environment

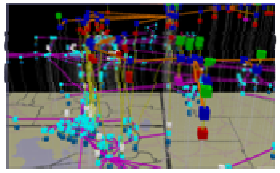


FAST Turnaround Analyses



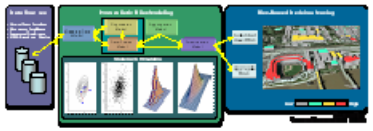
Advanced Modeling & Techniques Investigation



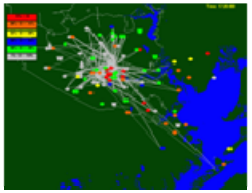


Interdependent Energy Infrastructure Simulation System

Methodologies for Asset Prioritization



Telecommunication Network Simulation Modeling and Analysis Tools



Transportation Network Optimization Models

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  - regional health care response to pandemic flu

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Presentation outline

- **“Drivers” for modeling and simulation**
  - **weapon engineering**
  - **science for materials, energy, and biology**
  - **system analysis**
- **Enabling capability: computing**
- **Engineering-focused M&S**
- **Enabling capability: experiment & test**
- **Science-focused M&S**
- **System and enterprise M&S**
- **Path forward**

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"Science of Prediction"

Intellectual Characteristics

"Information"
Science push
Less ambiguity
Capability-centered
"Analytic" judgment

Intellectual Characteristics

"Knowledge"
Decision pull
More ambiguity
Confidence-centered
"Intuitive" judgment

Predictive Science

Transformation

Science of Prediction

Transformation elements:

- V&V
- UQ
- Optimization
- Inference technologies
- Informatics technologies

How to do it:

- Physics
- Math
- Algorithms
- Software (Hardware, Infrastructure, etc)

How to use it:

- Complex decisions e.g. QMU
- Factors:
  - Communication
  - Clarity
  - Relevance
  - Trade-offs

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Extra slides

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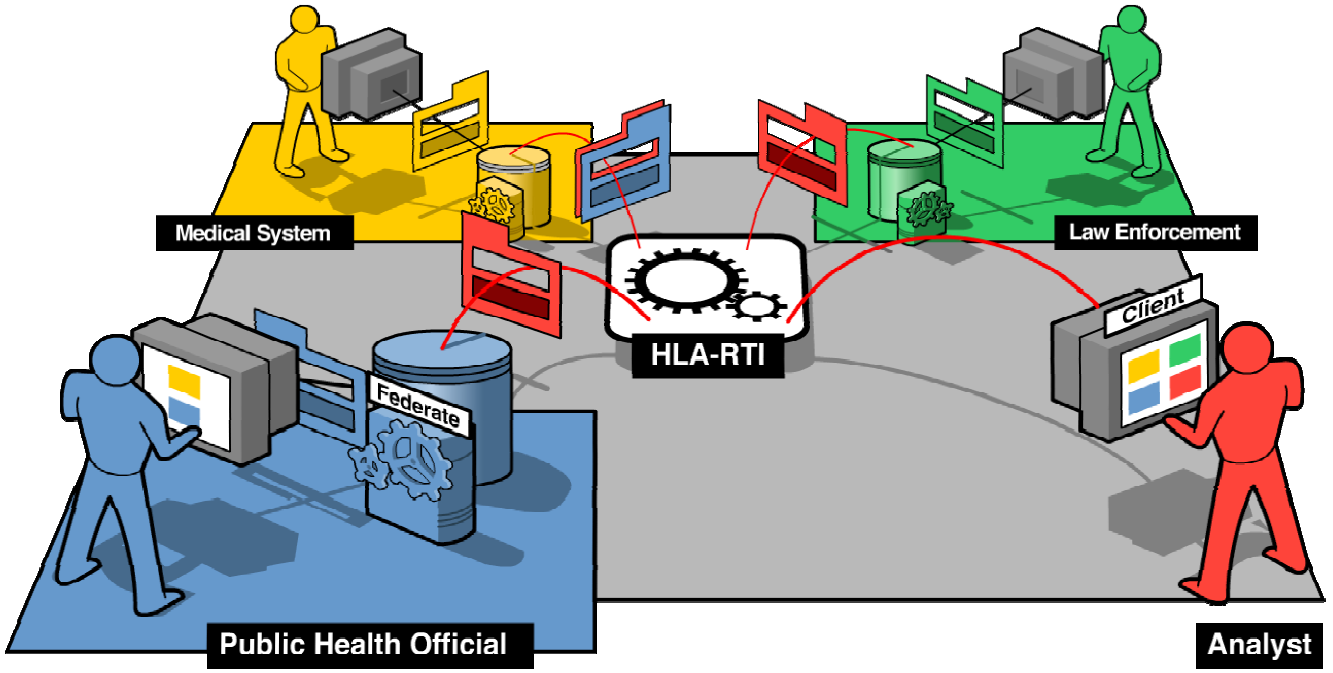
Sandia has developed a system modeling framework based on DoD/IEEE standards

The Enterprise Modeling Architecture (EMA) integrates the High Level Architecture (HLA), a standardized, DoD-sponsored simulation architecture, with Sandia's Enterprise Modeling Framework (EMF).



The Enterprise Modeling Framework (EMF) is a distributed software architecture designed to support open and secure communication protocols, integrated NTK mechanisms, and seamless integration of COTS applications.

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Enterprise Modeling Modes of Use

- **Simulation-based Systems Analysis**
  - **Architecture Definition**
    - Evaluate and optimize architecture performance
    - Develop and test threat tracking algorithms
  - **Technology Evaluation**
    - Explore impact of new sensor technologies for threat detection and response
    - Perform cost/benefit trade-off studies
  - **Concepts of Operation (CONOPS) Development**
    - Define and analyze system CONOPS (e.g.countermeasures)
    - Explore impact of policy changes to existing systems (e.g. detector siting)
- **Simulation-based Multi-Participant Exercises**
  - **Multi-jurisdictional planning and training**
    - Planning and training against unfamiliar threats and scenarios
    - Planning and training under realistic resource constraints and consequences
    - Knowledge elicitation
    - If real-time, then decision-making under pressure
- **Highly-interactive virtual environments (”serious games”)**
  - Individual training against unfamiliar threats and scenarios
- **Operational Deployments**
  - Allow switchover between operational monitoring and systems test
  - Real-time monitoring of deployed sensor systems

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Dealing with M&S in decision environments:

- "Predictive Science" consists of:
  - The physical theory
  - Algorithms
  - Software
  - Technologies for processing and summarizing computed information.
- "Transformation" consists of:
  - Technical means of assessing the accuracy and uncertainty in computed information resulting from the combination of theory, algorithms, and software
  - Technologies for processing and summarizing the assessment information.
    - One form of this summary is "Best Estimate Plus Uncertainty"
  - Methods for measuring the confidence we have in the generated information
- "Science of Prediction" consists of:
  - Shaping the information generated in Predictive Science and Transformation into the precise form required by the decision environment (i.e. decision makers and their processes, which typically include legal, economic, and political drivers, NOT just technical drivers)
    - We call this generically "risk-informed decision making"
  - Optimal communication of that information to the decision environment
  - Optimal application of that information in the decision environment

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