SAND2009-3129C

Energy Modeling and HPC

Salishan Conference

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Computational Sciences R&D Group

Sandia National Laboratories

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Sandia is a multiprogram laboratory laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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National Nuclear Security Administration

My Question: Can you talk about Energy and HPC?

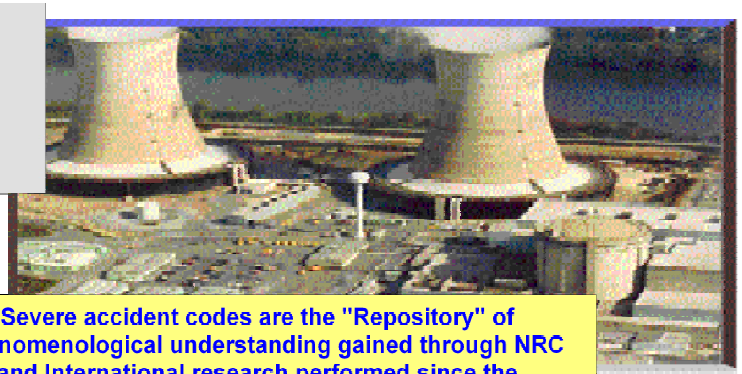
- What has been the role of HPC in energy research and development?
- What is driving the use (or lack of use) of HPC in energy research and development?
- What does the future look like?

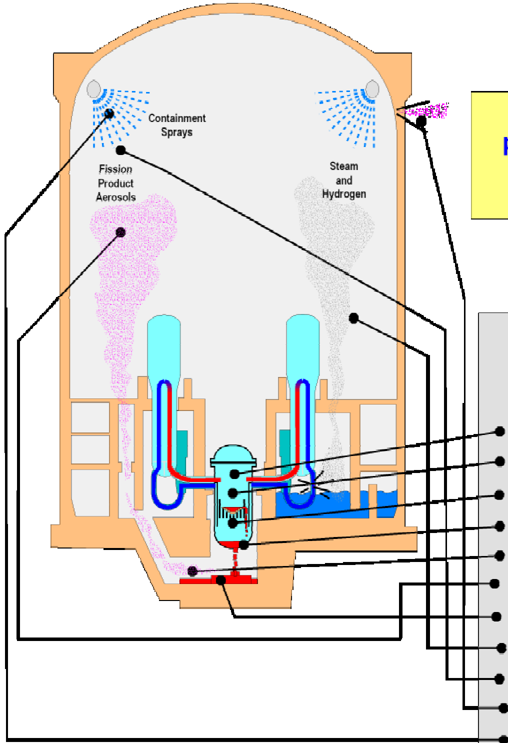
Sandia Energy Program Areas

- **Nuclear**
  - Nuclear Regulatory Commission Safety Analysis
  - Burner Reactor Integrated Safety Code
  - Nuclear Energy Advanced Modeling and Simulation Program
- **National Infrastructure Simulation and Analysis Center**
- **Concepts for Designing and Controlling the Energy Grid dominated by Intermittent, Non-Dispatchable Sources**
- Concentrating Solar Power
- Photovoltaic’s Analysis
- Geologic Storage of Waste and CO_2

MELCOR Severe Accident Analysis Code

Modeling and Analysis of Severe Accidents in Nuclear Power Plants





Severe accident codes are the "Repository" of phenomenological understanding gained through NRC and International research performed since the TMI-2 accident in 1979

Integrated models required for self consistent analysis

Important Severe Accident Phenomena

Phenomenon	MELCOR	CONTAIN	VICTORIA	SCDAP RELAP 5
Accident initiation	■	□	□	■
Reactor coolant thermal hydraulics	■	□	□	■
Loss of core coolant	■	□	□	■
Core meltdown and fission product release	■	□	◪	■
Reactor vessel failure	■	□	□	■
Transport of fission products in RCS and Containment	■	■	■	□
Fission product aerosol dynamics	■	■	■	□
Molten core/basemat interactions	■	■	□	□
Containment thermal hydraulics	■	■	□	□
Fission product removal processes	■	■	■	□
Release of fission products to environment	■	■	■	□
Engineered safety systems - sprays, fan coolers, etc	■	■	□	□
Iodine chemistry, and more	■	□	□	□

MELCOR Development began in 1983

- Targeted for HPC systems at that time (Cray vector machines)
- Now runs on single-processor workstations & PCs

MELCOR Has A Worldwide Usership

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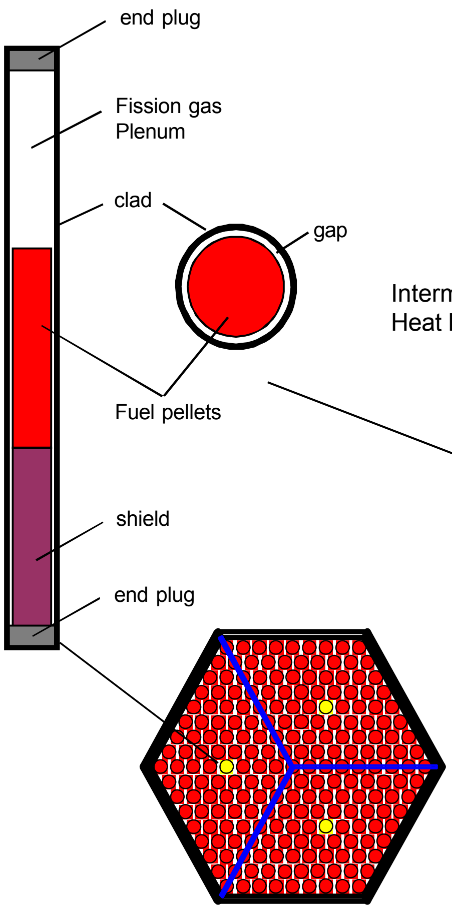
Advanced Modeling & Simulation for Nuclear Energy Requires Addressing Four Fundamental Challenges

- The "multi-scale" issue
  - Length-scales
  - Time-scales
  - Energy groups
- The "coupled multi-physics" issue
  - Fluid flow and heat transfer
  - Neutronics
  - Thermal mechanics
- The "complex geometry" issue
  - Nuclear reactors are not simple devices
- The "uncertainty quantification" issue
  - "without UQ (with requires V&V), results are no better than speculation, and often worse"

BRISC (Burner Reactor Integrated Safety Code) 3-Tiered Multi-Scale Modeling Strategy

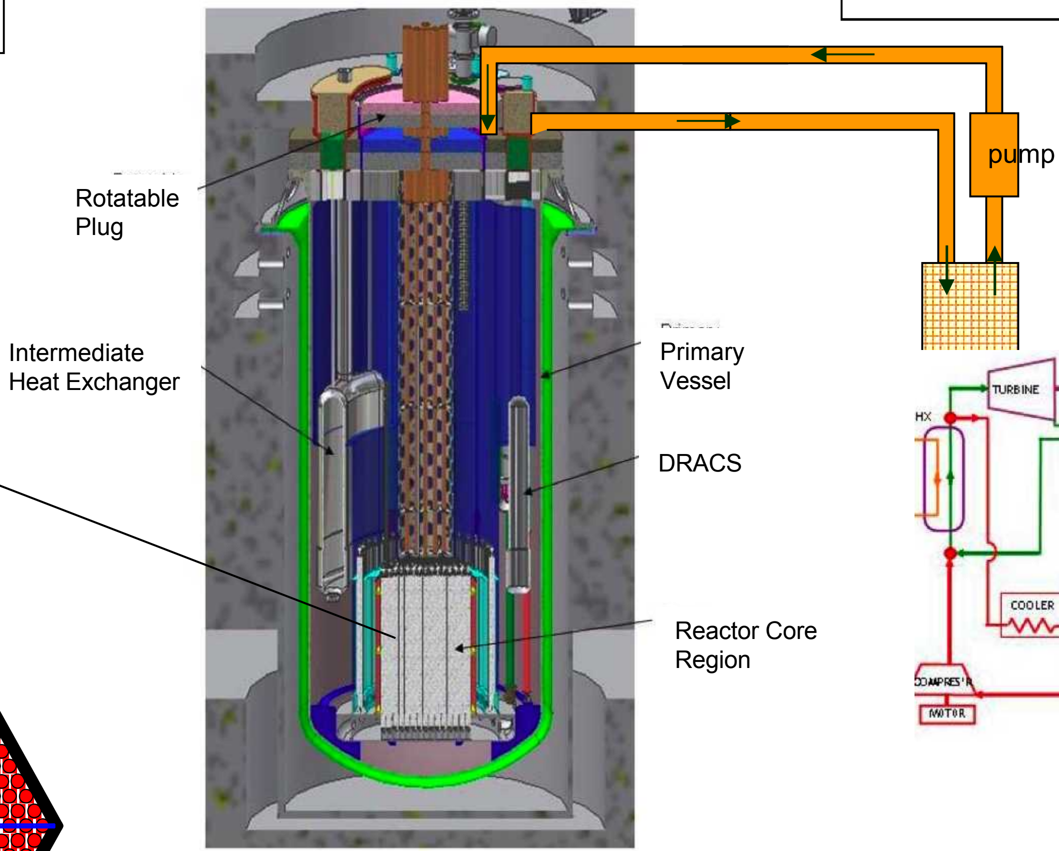
Structures and physics whose features are too small for resolution on 3D grid

Fuel-pins and control rods
- 0.5 - 10 mm-scale features
- conduction, fission heating …
- 2D or 3D representative models



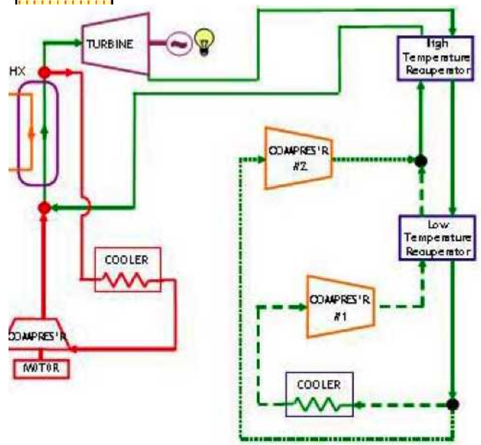
"Meso-scale" resolved by 3D grid

In-vessel Reactor Components
- 10 cm to 10 m scale geomtry
- Neutronics, Turb flow & heat transfer, thermal-mechanics, conduction, …
- 3D Modeling Framework

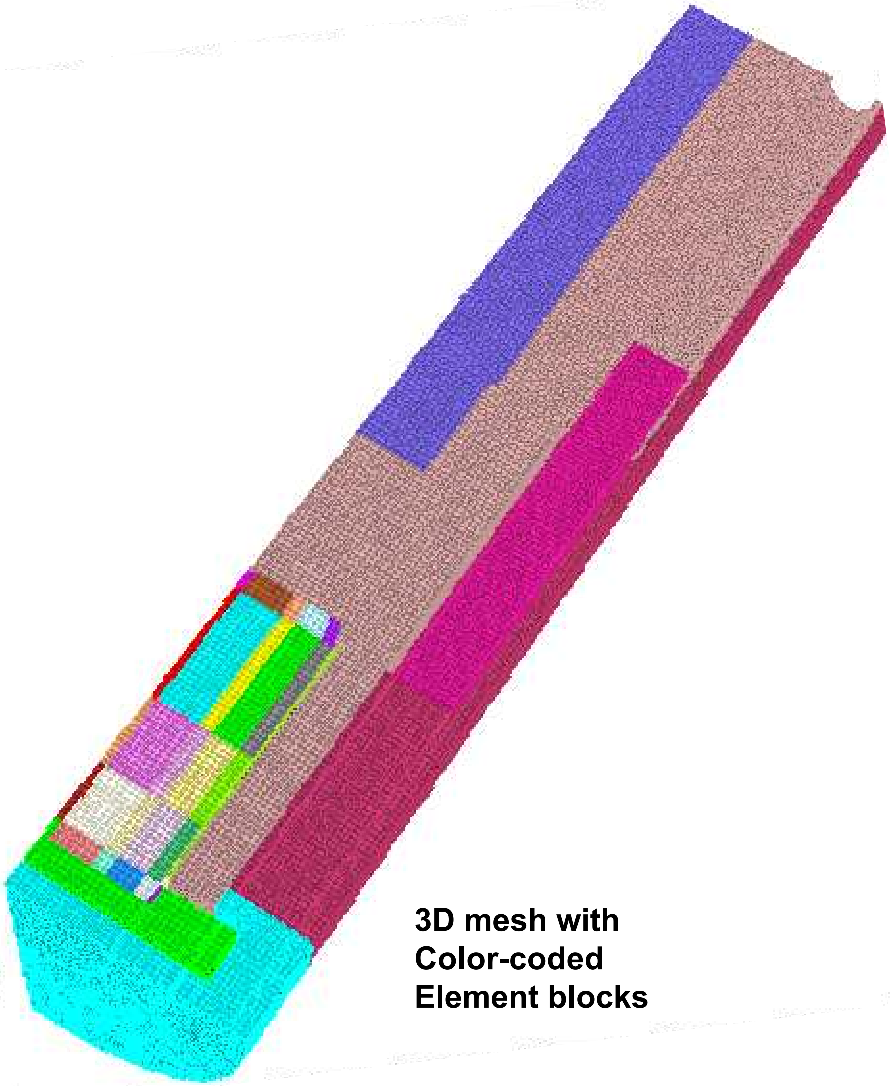


Balance of Plant Reactor System Components (& Containment)
- 1 - 50 m scale
- Pipes, pumps, valves, heat exchangers, turbines, rooms,
- 0D MELCOR models
- 3D Fire Modeling with RIO

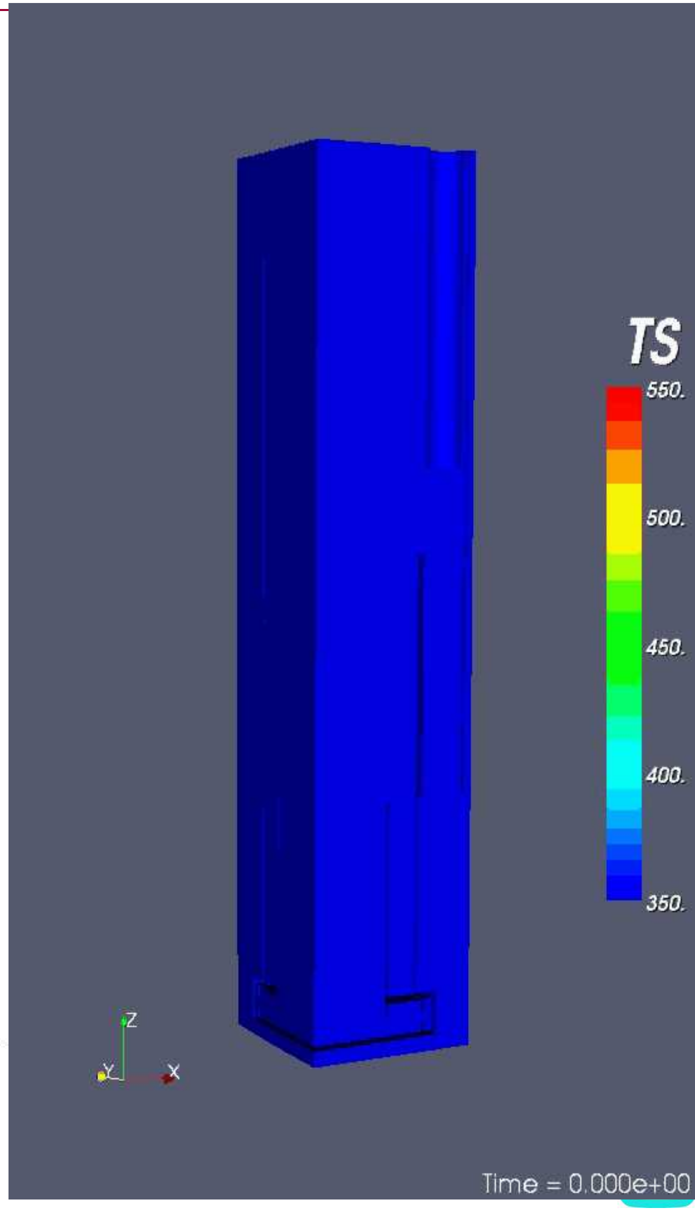
Structures and physics whose features are too large for resolution on 3D grid



Demo 3D Model Simulation - Fluid Temperature Initial 30 sec. start-up transient



3D mesh with
Color-coded
Element blocks



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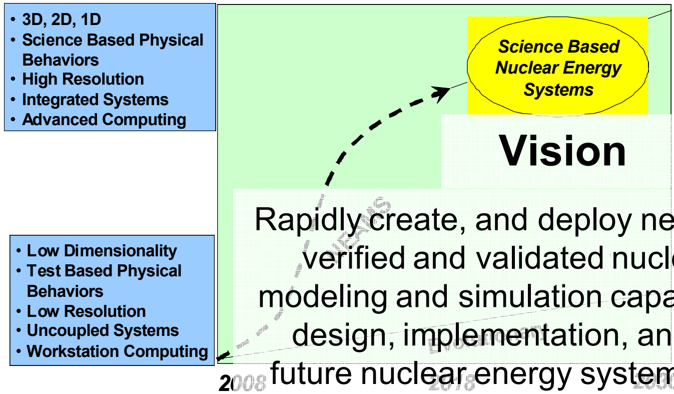
Nuclear Energy Advanced Modeling and Simulation (NEAMS) FY-10 Proposed Program Overview



Vision

Rapidly create, and deploy next generation, verified and validated nuclear energy modeling and simulation capabilities for the design, implementation, and operation future nuclear energy systems to improve the U.S. energy security future

Strategies

- **Integrated Performance & Safety Codes (IPSC) –** High resolution, 3D, integrated systems codes to predict performance
- **Fundamental Methods and Models (FMM) –** Lower length scale performance understanding
- **Verification, Validation & Uncertainty Quantification (VU) –** Understanding the “believability” of simulation results
- **Capability Transfer (CT) –** Moving modeling and simulation tools out of the research environment
- **Enabling Computational Technologies (ECT) –** Computer science resources needed to make the vision a reality

Major Milestones

- **Year 1**
  - Create product requirement documents for integrated codes
  - Initiate robust interaction with NRC on V&V and UQ
  - Establish overall plans and processes for FMM, CT and ECT el
- **Year 3**
  - Deliver initial versions of integrated codes and modeling and simulation interoperability framework
- **Year 5**
  - Deliver integrated codes with proper V&V and UQ pedigrees
- **Year 7**
  - Deliver codes with empirical “knobs” removed
- **Year 10**
  - Deliver predictive, science based modeling and simulation capabilities for new nuclear energy systems

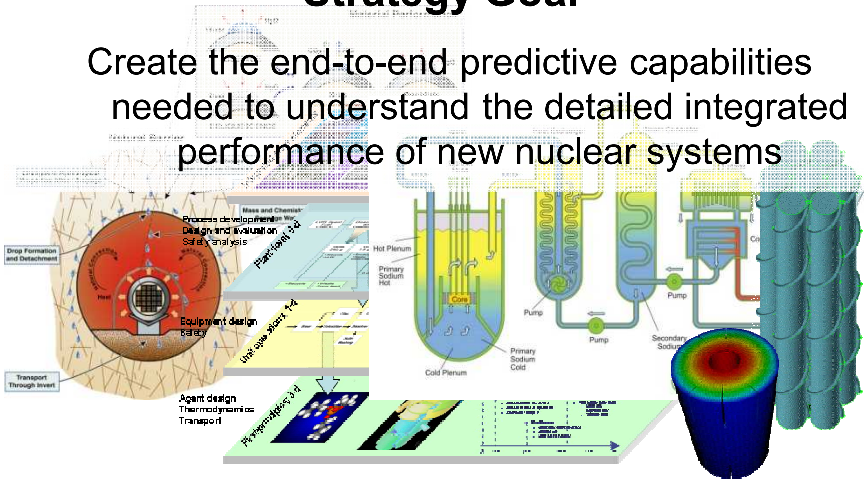
Approach

- Built on a **robust experimental program** for model development and V&V
- **Appropriate flexibility** so that the simulation tools are applicable to a variety of nuclear energy system options and fuel cycles
- **Continuously deliver** improved modeling and simulation capabilities relevant to existing and future nuclear systems (in the near, mid, and long term)

NEAMS Program Strategy – Integrated Performance and Safety Codes

Strategy Goal

Create the end-to-end predictive capabilities needed to understand the detailed integrated performance of new nuclear systems



Deliverables

- **Nuclear Fuels** – predict the performance of fuels in a reactor environment in steady state, transient and accident conditions
- **Reactor Core and Safety Systems** – end to end performance predictions for the life of the reactor
- **Safeguards and Separations** – understand the quantity and location of materials in an operational separations environment
- **Waste Forms and Systems** – predict the performance of a waste form in a repository environment

Approach

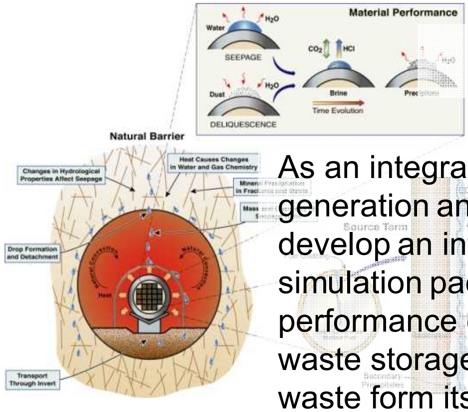
- Create large code teams with a centrally located "critical mass"
- Use additional individual or small teams to focus on particular code aspects
- Rough Composition
  - 1/3 Application specific expertise
  - 1/3 Advanced computing expertise
  - 1/3 Team support (V&V, SE and SQA, Support)
- Interface with application users and if not available create teams of "ghost users" to assess usability of applications

Risks & Issues

- Challenging and very aggressive milestones.
- Need to quickly create integrated code teams at laboratories that may not have experience with large code development.
- Finding the right talent to populate teams.
- Dependence on other NEAMS strategies (FMM, VU, CT, ECT) for success.
- Dependability of funding.

NEAMS Program Strategy –
Waste Forms & Systems IPSC

Strategy Vision



As an integral part of nuclear energy generation and management, we will develop an integrated, science-based simulation package for assessing performance of potential nuclear reactor waste storage or disposal options, from the waste form itself through the entire surrounding engineered environment and representing the range of important multi-scale effects.

Approach

- *Sub-continuum Scale Investigations*
- *Discovery Experiments*

Upscaling

THCM* Hi-Fi Analysis Code
Constitutive Models

UQ +SA

V&V

THCM* Assessment Code
Surrogate Models

Model Reduction

Infrastructure Tools (Software Engineering – Viz – V&V – Data Analysis)

** THCM: Thermal/Hydrological/Chemical/Mechanical*

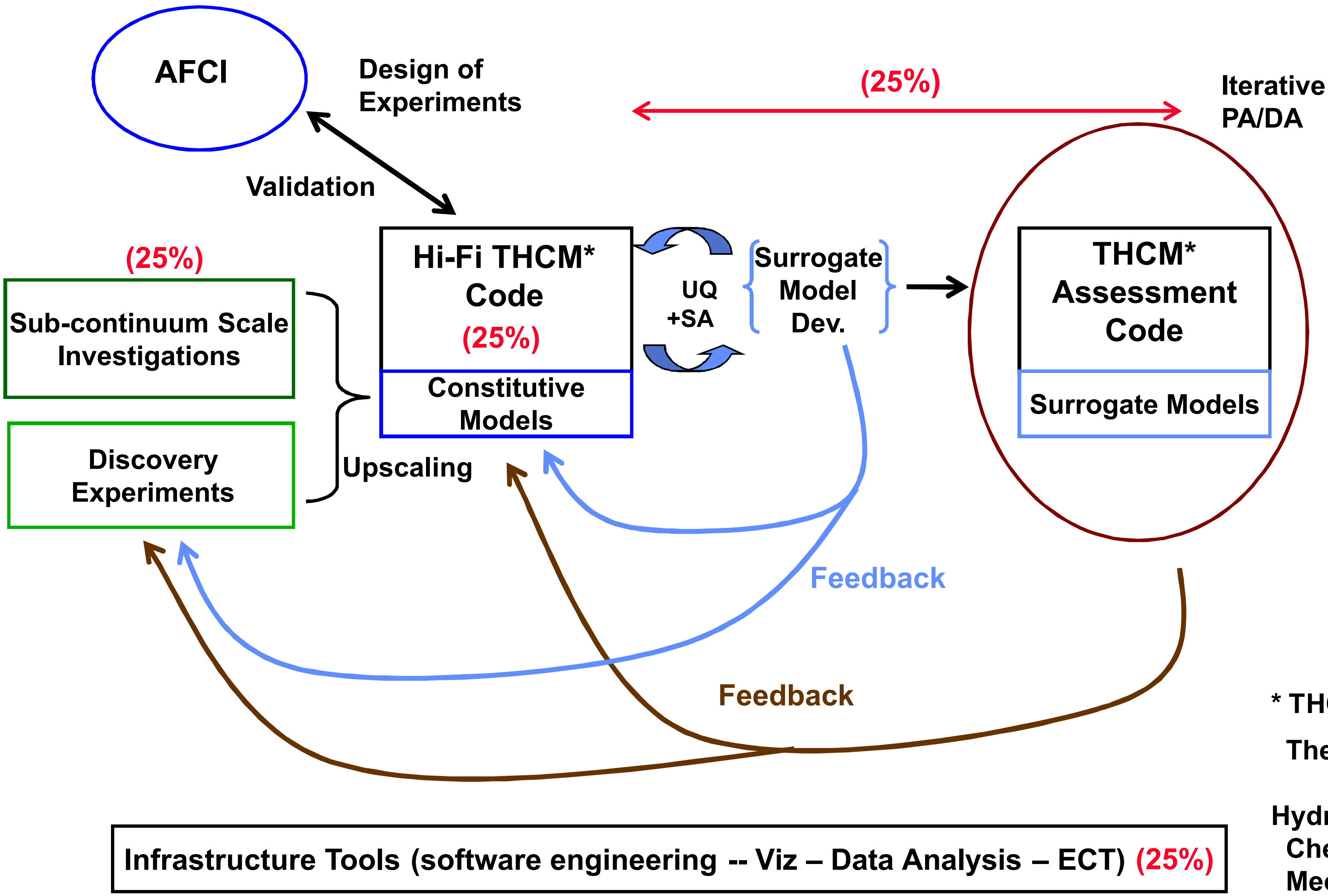
Milestones

- **Years 0-3:**
  - IPSC Design Specifications
  - PIRT & V&V Plan
  - THCM Architecture and Prototype
  - High priority sub-continuum studies
  - Generation of constitutive models
  - Initial Demonstration to WF/Environment Reference Case
- **Years 4-10**
  - High-fidelity continuum and surrogate models
  - Initial release of THCM and Assessment Codes
  - Full application to WF/repository environment

Risks & Issues

- Success depends on support from other NEAMS Strategies (FMM, VU, CT & ECT)
- Need to coordinate modeling activities with RW and AFCI Separations and Waste Forms Campaign
- Need to include waste form consideration as part of fuels, reactors, separations
- Availability of appropriate experimental data
- Lack of existing performance codes in this area (unlike other areas where existing codes are insufficient, but exist)

WF IPSC Relationships



* THCM:

Thermal

Hydrological
Chemical
Mechanical

Office of Infrastructure Protection (IP)

National Infrastructure Simulation and Analysis Center (NISAC)

Complex Adaptive Systems of Systems (CASoS) Engineering

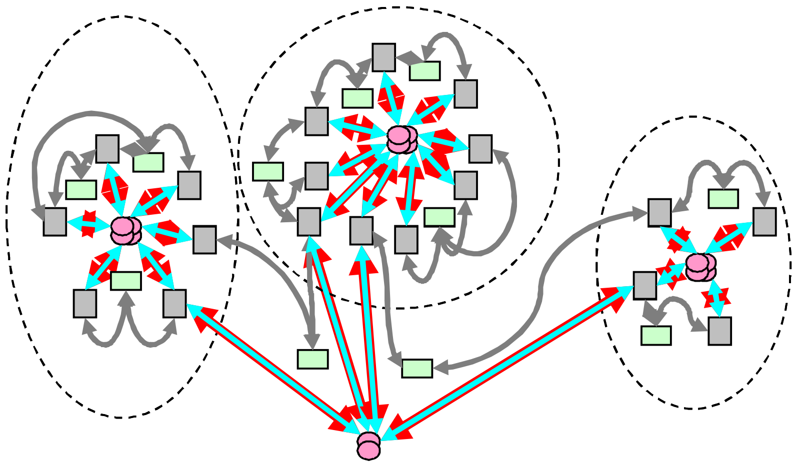
March 21, 2009

Homeland Security

UNCLASSIFIED

Outline – Bob Glass, lead

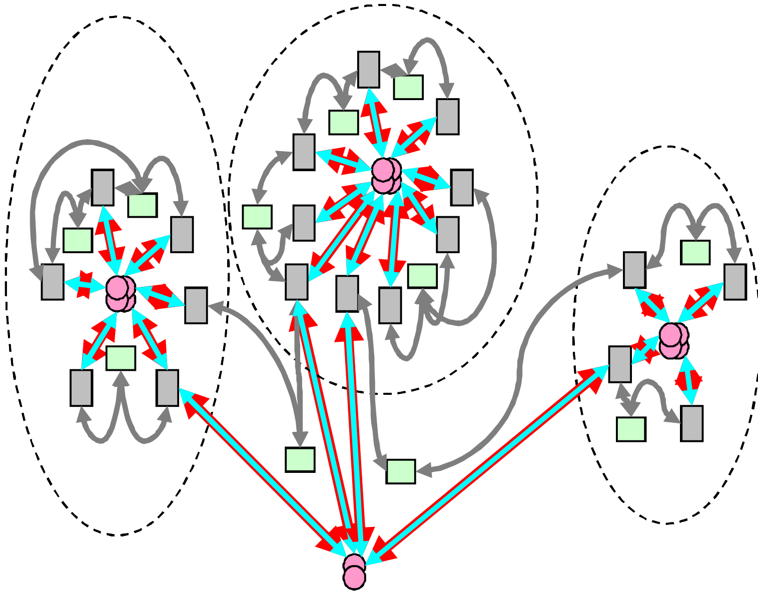
- CASoS Definition and Sandia's CASoS Engineering Initiative
- CASoS Engineering Framework
- CASoS Workbench
- Model Example: Global Energy System
- Past and Current CASoS Applications



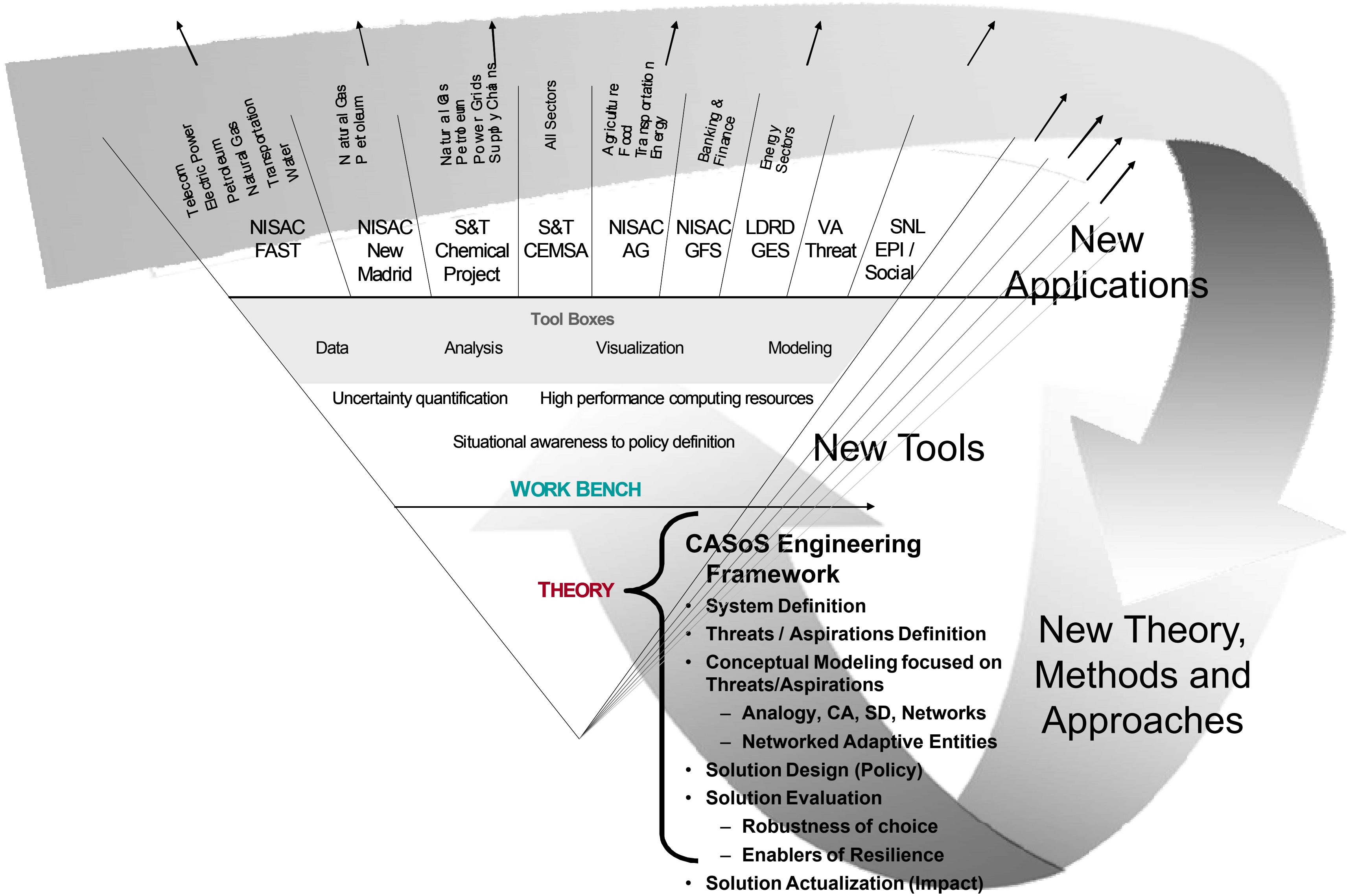
Complex Adaptive System of Systems (CASoS)

- **CASoS:**
  - Vastly complex physical-socio-technical-systems
  - Ubiquitous systems that include people, organizations, cities, infrastructures, government, ecosystems and the Planet
  - Must be understood to design a secure future for the nation
  - Examples encompass humanity’s largest problems including Global Climate Change
  - Theories, technologies, tools, and approaches to enable effective solutions to CASoS problems are the same across all contexts

- **Sandia’s CASoS Engineering Initiative:**
  - Harnesses the tools and understanding of Complex Systems, Complex Adaptive Systems, and Systems of Systems to engineer solutions for some of the worlds biggest, toughest problems



CASoS Engineering Framework



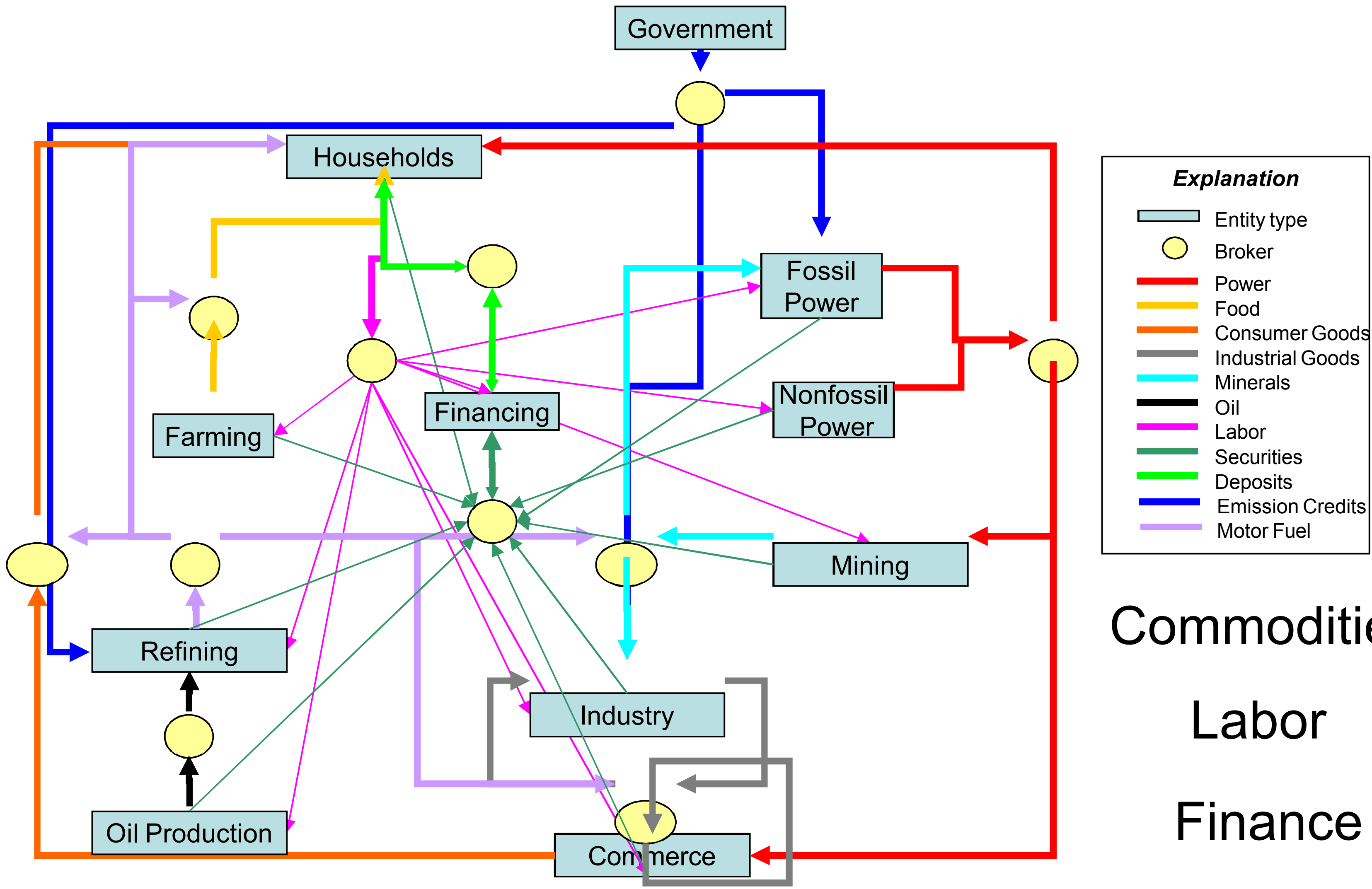
CASoS Workbench

- A platform for describing networks and processes in a consistent way
- Integrates existing network tools and agent-based models
- Allows models and tools to be chained together
- Provides large scale simulations on HPC machines
- Provides visualization and analysis tools
- Allows analysts to investigate adaptations and emergent behavior
  - Understand how interactions among many agents might generate system-level behavior
  - Understand how changes in agent's rules and interactions can shape system-level behavior

Global Energy System Example

- **Goal : understand the possible reactions of the global energy production system to a set of policies designed to reduce carbon emissions:**
  - Creation of carbon markets in individual nations or treaty blocs
  - Creation of a global carbon market
  - Imposition of a national/treaty bloc carbon tax
  - Imposition of a global carbon tax
- **Structure:**
  - Entities: Individual instances of basic macro-economic types (households, government, industries of various sorts)
  - State variables: Material resources of various kinds
  - Dynamics: First-order transformations modeled on chemical reactions

Global Energy System Example: Core Economy

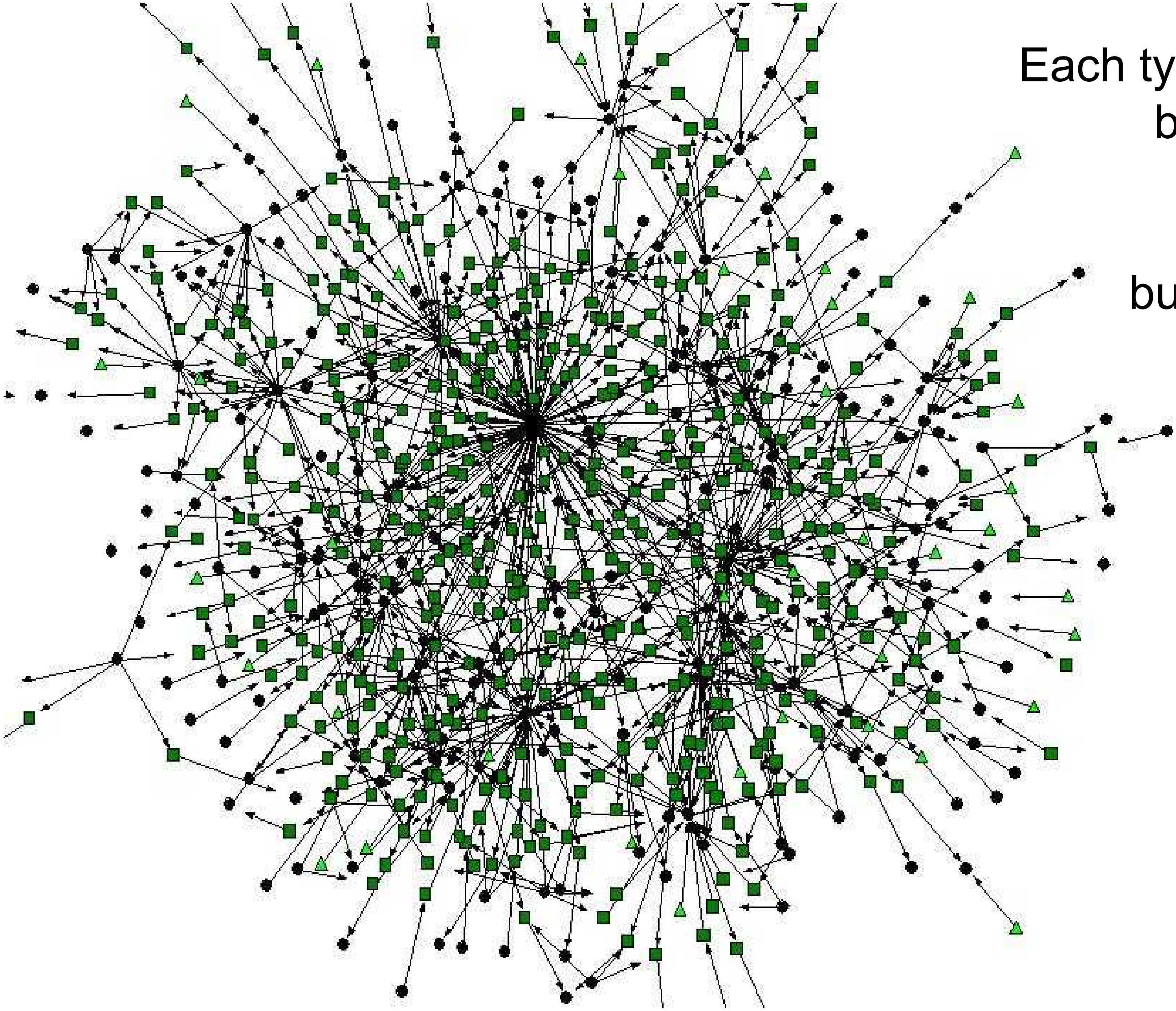


Commodities

Labor

Finance

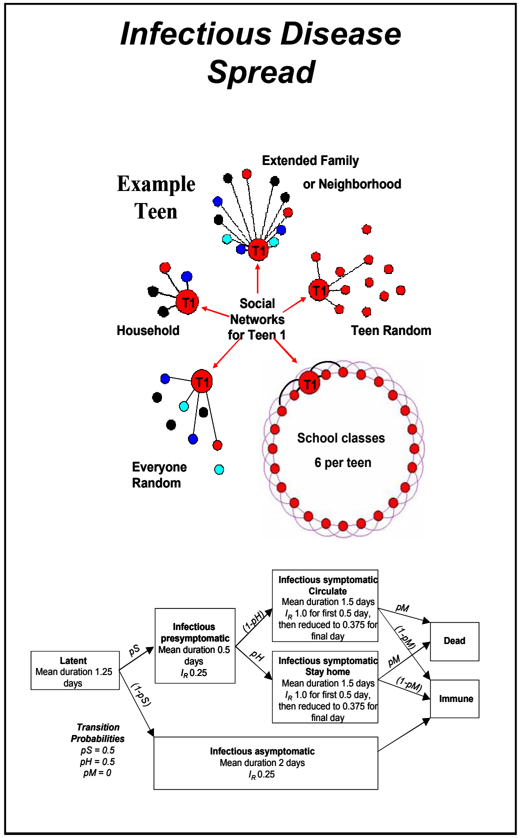
Within a sector type…



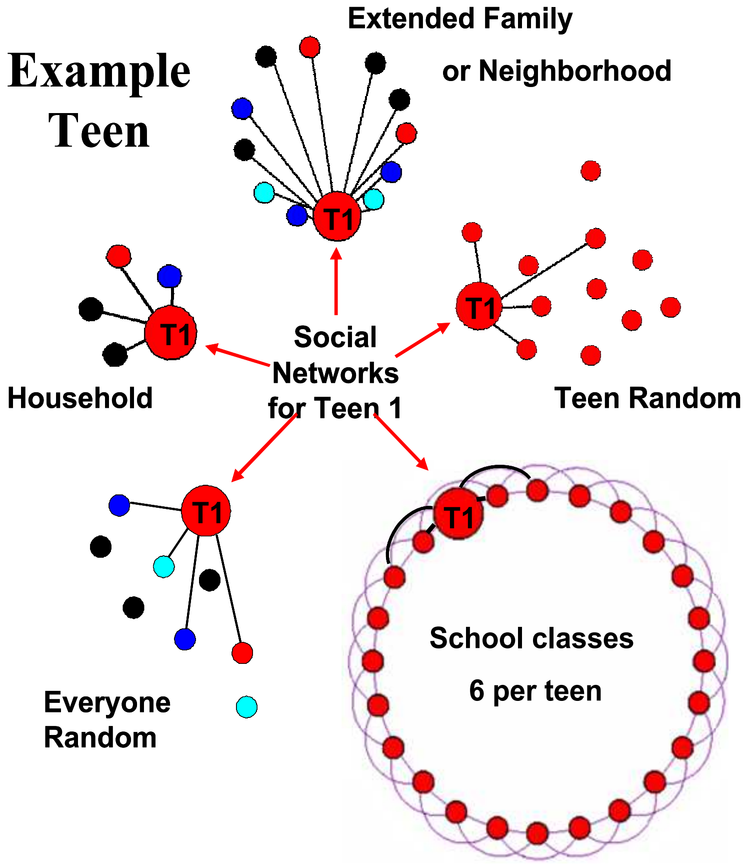
Each type is represented by many individual instances in a network of business and social relationships

CASoS Engineering Modeling and Analysis Applications

- **Past Applications:**
  - Pandemic Influenza Containment Strategy (NISAC, 2005)
    - Eight containment strategies and numerous disease manifestations were analyzed
    - NISAC proposed strategy incorporated in National policy by Center for Disease Control
  - Congestion and Cascades in Payment Systems (NISAC, 2004 - 8)
    - Results identified unexpected interdependencies arising from foreign exchange transactions
    - Collaboration with the Federal Reserve, European Central Bank, and international researchers
  - Critical National Infrastructures (NISAC – 2008, 2009)
    - Natural Gas Model (applied in New Madrid Earthquake Study)
    - Petrochemical Model findings used in chemical supply chain analysis
    - Global Financial System (goal is to identify origin of instabilities and determine how to control or mitigate them)



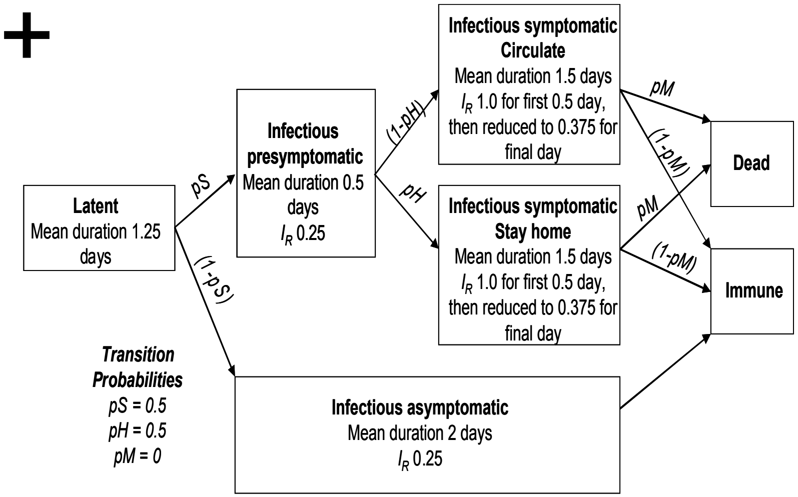
Application of Networked Agent Method



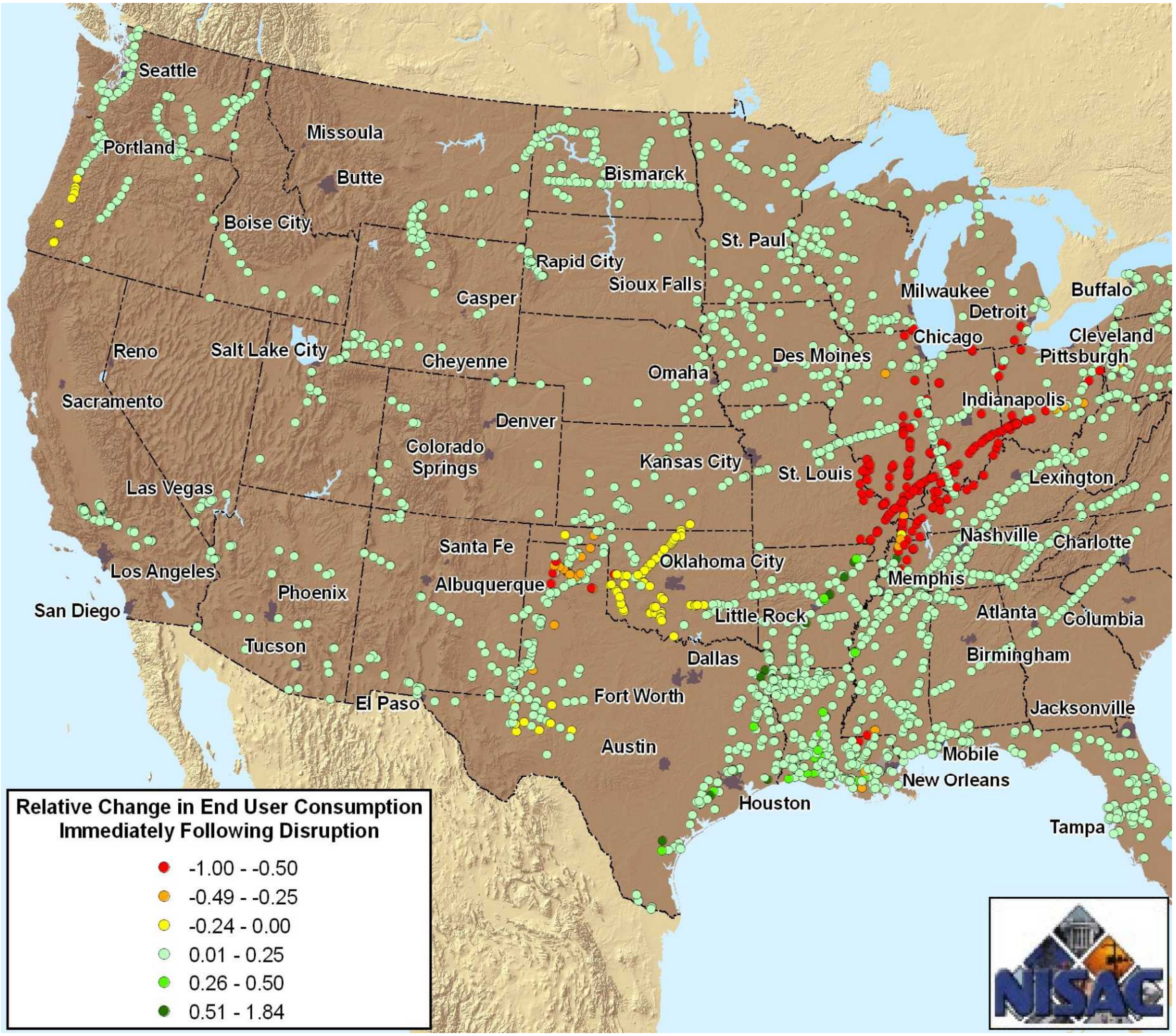
Stylized Social Network
(nodes, links, frequency of interaction)

+

Disease manifestation
(node and link behavior)



New Madrid Earthquake Study: Relative Change in End User Consumption of Natural Gas



Homeland Security

National "Green" Power Grid

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Challenge for Reducing Fossil Fuels in Electricity Production

- **Problem:** Accelerated Climate Change and a desire to reduce dependence on foreign oil
  - Electricity is the largest contributor and the easiest one to do something about.
- **Answer:** Incorporate renewable energy sources (Nuclear?)
- **Goal:** 20% of electrical power by 2020
- **Question:** Is this fast enough? Is this deep enough?

Inadequate Grid is a Barrier

- **Intermittent Renewable Sources destabilize current Grid**
  - Dominated by Stabile Large Generation (Coal, Gas, Nuclear)
  - No Storage to Damp System
- **Little Active Control and Sensing in System**
- **Bi-directional power flow control almost non-existent**
- **Vulnerable to attack (cyber, physical, weather)**

Future Grid

- Information-centric, actively controlled dynamic grid, information centric
- High penetration of renewables and storage
- Predictive scalable models of physical, economic, and policy scopes
- Integration with national energy and water resource planning

My Question: Can you talk about Energy and HPC?

- **What has been the role of HPC in energy research and development?**
  - Substantial in NE during the eighties, but low refresh rate from the point-of-view of keeping up with HPC capability
  - Low in Renewables (at least at Sandia)
  - Low in infrastructural impacts and socio-economic modeling (until recently)
- **What is driving the use (or lack of use) of HPC in energy research and development?**
  - Funding/commitment to energy research and development
  - Readiness to address more complex problems
- **What does the future look like?**
  - Energy/Climate interest is increasing dramatically
  - The communities are more ready and able to address issues that require HPC
  - Future barriers are primarily lack of experience with HPC