Sustainability

- PNNL is developing capabilities that will enable us to solve the nation’s challenges in climate, sustainability, energy smart data centers, and power grid stability.

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Climate and Sustainability

- Providing a better understanding of how human and natural components of the Earth system interact, and how those components affect overall evolution of the climate system

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Climate Science Program: Focusing on fundamental understanding of the climate system

- How the combination of human decisions and natural processes control evolution of climate system
  - Characterize and improve representation of aerosols and cloud processes in climate models
  - Understand effects of societal decisions and resultant impacts on climate, <u>and</u> how climate change will affect future decisions
- Informing near-term decision making within the context of a long-term strategic understanding

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Climate Science Themes and Resources

- Understanding the fundamental science of earth system processes and human systems
- Insights on interactions between climate systems and impacts
- Measurements to models – an integrated approach
- Decision-relevant insights and understanding
- Stewards for the Atmospheric Radiation Measurement (ARM) Climate Research Facility (ACRF) and the DOE Research Aircraft Facility
- Established the Atmospheric Measurements Laboratory (AML)
- Building strategic partnerships

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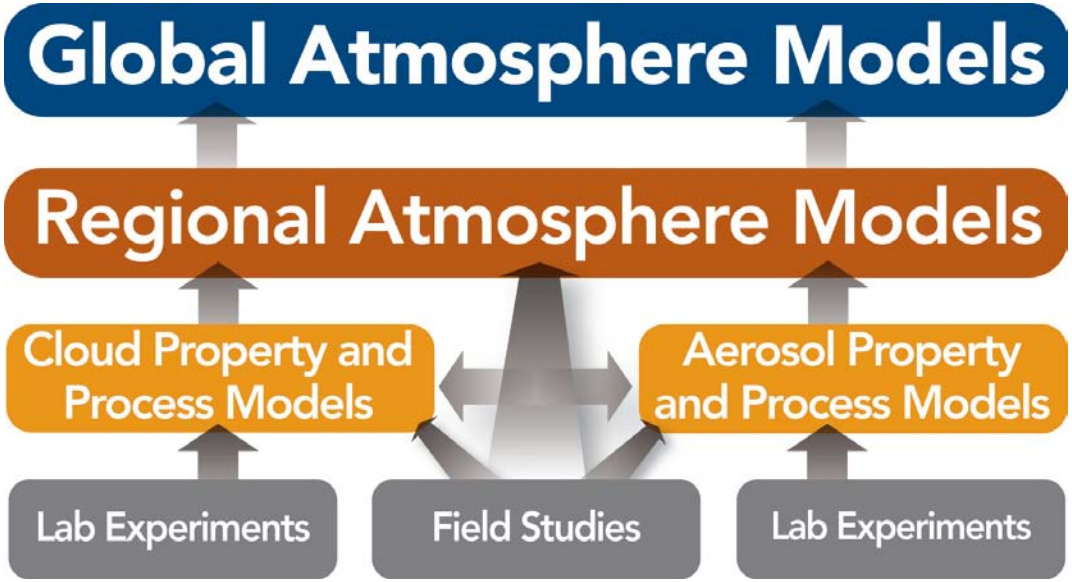
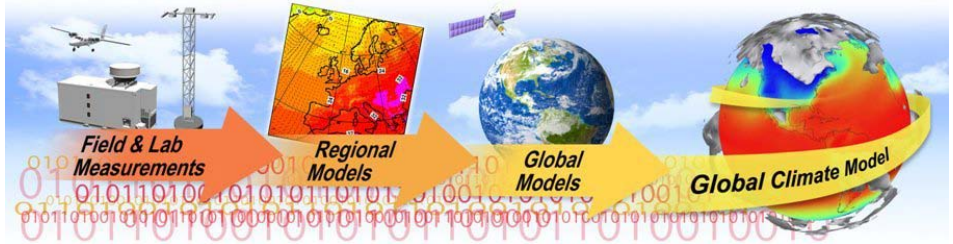
From Measurements to Models





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Scientific Leadership in Climate Science

- Leadership roles in every major assessment of the Intergovernmental Panel on Climate Change
  - (Nobel prize 20007)
- Leadership roles in National Academies' studies
- Co-chair of Community Climate System Model Atmosphere Model Working Group, Science Steering Committee member
- Member of NASA Global Modeling Initiative Science Steering Committee
- Leader, Regional Climate Modeling and Climate Change Impacts tasks, bilateral climate change agreement between DOE and China since 1996
- Affiliate scientists, National Center for Atmospheric Research

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PNNL Aerosol Climate Initiative

- B**uilding capabilities** in measurement, understanding, and modeling of aerosol lifecycle and indirect effects on climate
- Goal: **Improve climate models and inform policy decisions**
- Focus areas
  - Aerosol formation, aging, and transport
  - Aerosol indirect effects
  - Measurements and instrumentation
- Enabling new capabilities
  - Aerosol Model Testbed
  - Advanced Counterflow Virtual Impactor
  - Atmospheric Measurement Laboratory
  - Compact Ice Chamber
  - Dual-Sided Temperature-Controlled Continuous-Flow Environmental Chamber
  - Particle-resolved aging model
  - Cloud model with size-resolved microphysics

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A New Generation of High-Resolution, Regional Integrated Models

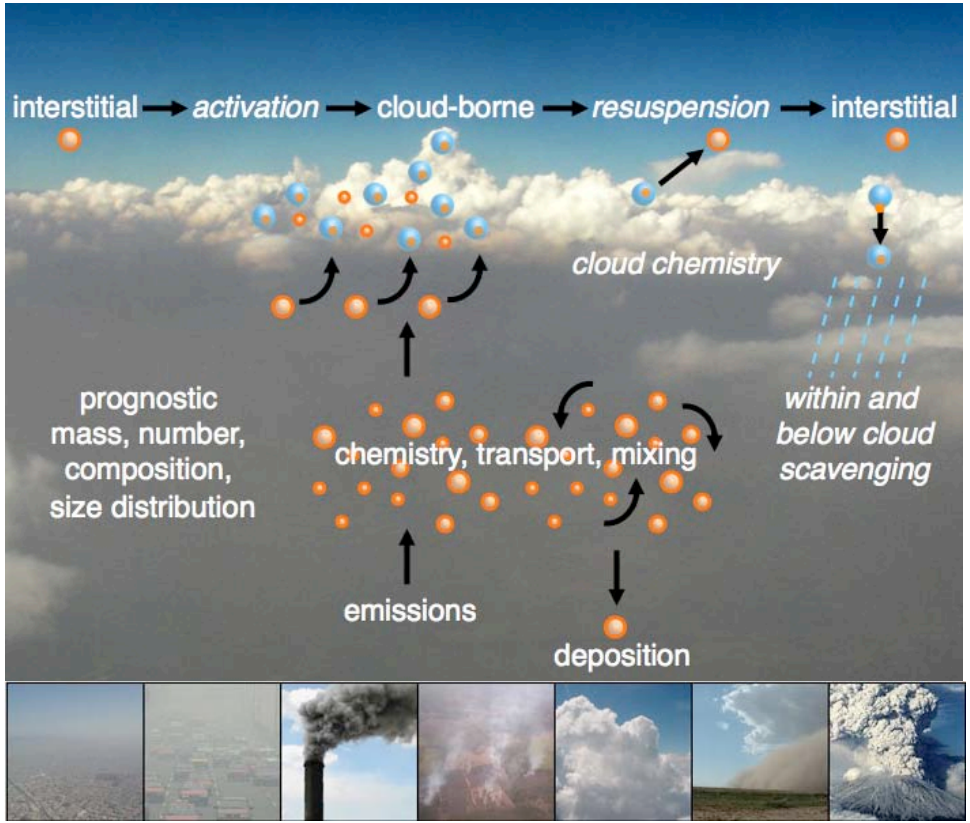
- Strengthening the scientific understanding of human/natural climate system interactions
- Enabling assessments at scales relevant to decision makers
- Research approach
  - Understand and model the dynamic interactions among climate, ecosystems and energy/economics over a range of temporal and spatial scales
  - Capitalize on our strengths in regional modeling and integrated assessment
  - Enable effective partnership between Richland and College Park
- Result: More accurate predictions of climate change/timing and impacts for decision-makers

High-Performance Computing in Climate Science

- Used for
  - Developing and testing treatments of climate-relevant aerosol and cloud processes
  - Performing climate simulations and analysis
  - Exploring the effect of climate consequences and decisions to cope with them
- Computing resources
  - Developmental Linux clusters (PNNL)
  - Northwest International Cloud Experiment (NW-ICE – IBM System Cluster 1350) and Chinook (HP supercomputer) (EMSL)
  - National Energy Research Scientific Computing Center (LBNL)
  - National Center for Computational Sciences (ORNL)
  - In 2010: New supercomputer will accelerate and expand modeling for coupling Earth and human dimensions of climate change (PNNL)

Modeling Aerosol Impact on Climate

Schematic Diagram Depicting Various Processes Affecting Aerosols



Global Climate Models
Simple Treatments
Computationally Efficient

Parameterizations

Research Models
Complex Treatments
Computationally Expensive

Next Generation of Global Climate Models

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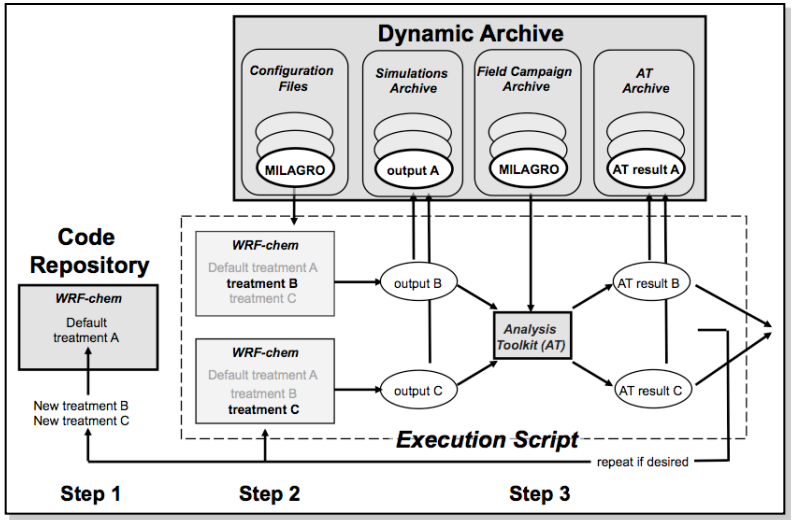
The Aerosol Modeling Testbed

- PNNL's Aerosol Modeling Testbed is a software suite designed to expedite development of aerosol modules
- "The best way to validate the strengths and weaknesses of candidate aerosol modules and their components is the Aerosol Modeling Testbed that you are working on. **I know of no other effort like this, worldwide.**" – University Professor



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Multi-Scale Atmospheric Modeling

Laboratory & Field Measurements

PNNL Models

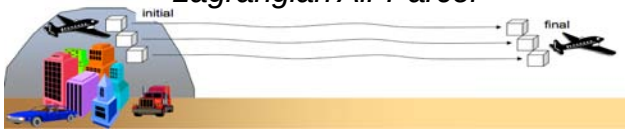
0-D Aerosol Process and Property (MOSAIC)
Δx ~ 1 m

Cloud-Resolving Aerosol Processing
Δx ~ 10 – 100 m

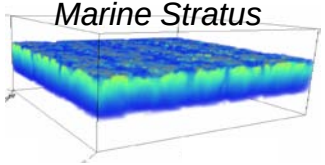
Regional Aging and Cloud Processing (WRF-Chem)
Δx ~ 1 – 100 km

Example Applications

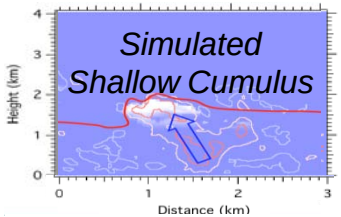
Lagrangian Air Parcel



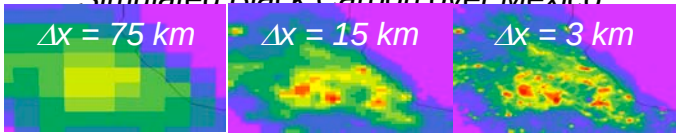
Simulated Marine Stratus



Simulated Shallow Cumulus



Simulated Black Carbon over Mexico



Community

WRF-chem
CCSM (SciDAC)
RegCM (NSF)

Cloud Parameterization

Air Quality Forecasts (NOAA)
Fundamental Aerosol Research
Regional Climate Studies

Employ models to make treatment of aerosol processes more consistent with observations before implementation in global models

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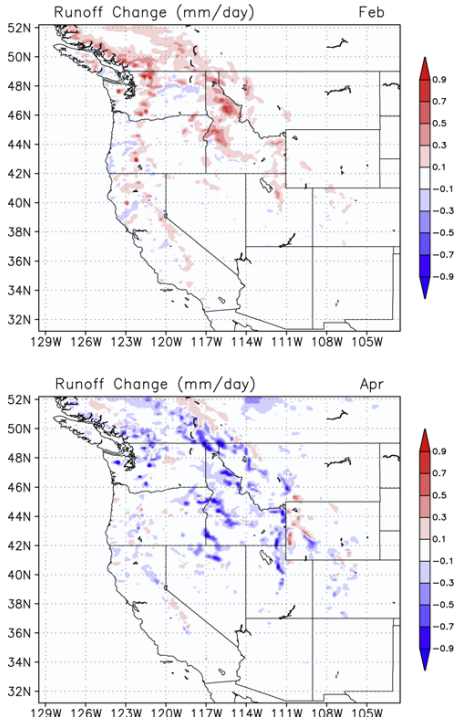
Research Highlight

Soot on Snow Causes Early Runoff in Western U.S.

- Snow polluted by soot absorbs more solar radiation, accelerating snowmelt
  - Potential impacts: water supply, winter flooding, reduced snowpack
  - Featured by *Associated Press, C&E News, National Public Radio , ABC news*
- Team: Qian, Y, W. I. Gustafson, L. R. Leung, and S. Ghan, 2009, *J. Geophys. Res*.
- Citation: Qian, Y., W. I. Gustafson Jr., L. R. Leung, and S. J. Ghan (2009), Effects of soot-induced snow albedo change on snowpack and hydrological cycle in western United States based on Weather Research and Forecasting chemistry and regional climate simulations, *J. Geophys. Res.*, 114, D03108, doi:10.1029/2008JD011039.



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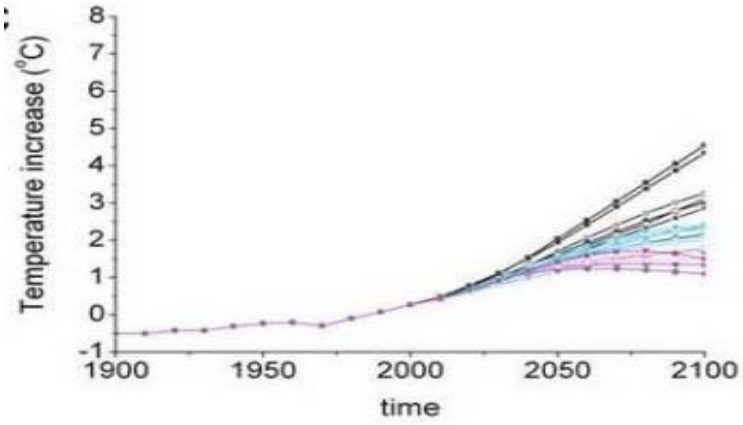
Research Highlight:

Residual Global Warming Will Occur Even with Cutbacks

- Analysis: Global warming can be slowed but not stopped
- Global surface temperature increases of 0.5 to 4.4 degrees Celsius relative to 1990 by end of century
  - Based on a wide range of climate policy scenarios, using MiniCAM
- Message: Mitigation important, but the world must also adapt to climate change now to reduce the impact of residual warming
- Published in the *Proceedings of the National Academy of Sciences*, 2008



Average minimum warming of 1.4 degrees Celsius by end of century

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Energy Grid

PNNL provides the science, technologies and leadership to:

- Move grid control and operation timeframes from minutes to seconds
- Integrate demand response into grid/power markets for efficiency, reliability, PHEVs and carbon offsets
- Enable real-time, wide-area situational awareness for increased reliability
- Innovations to enable renewable generation integration
- Cyber secure grid networks

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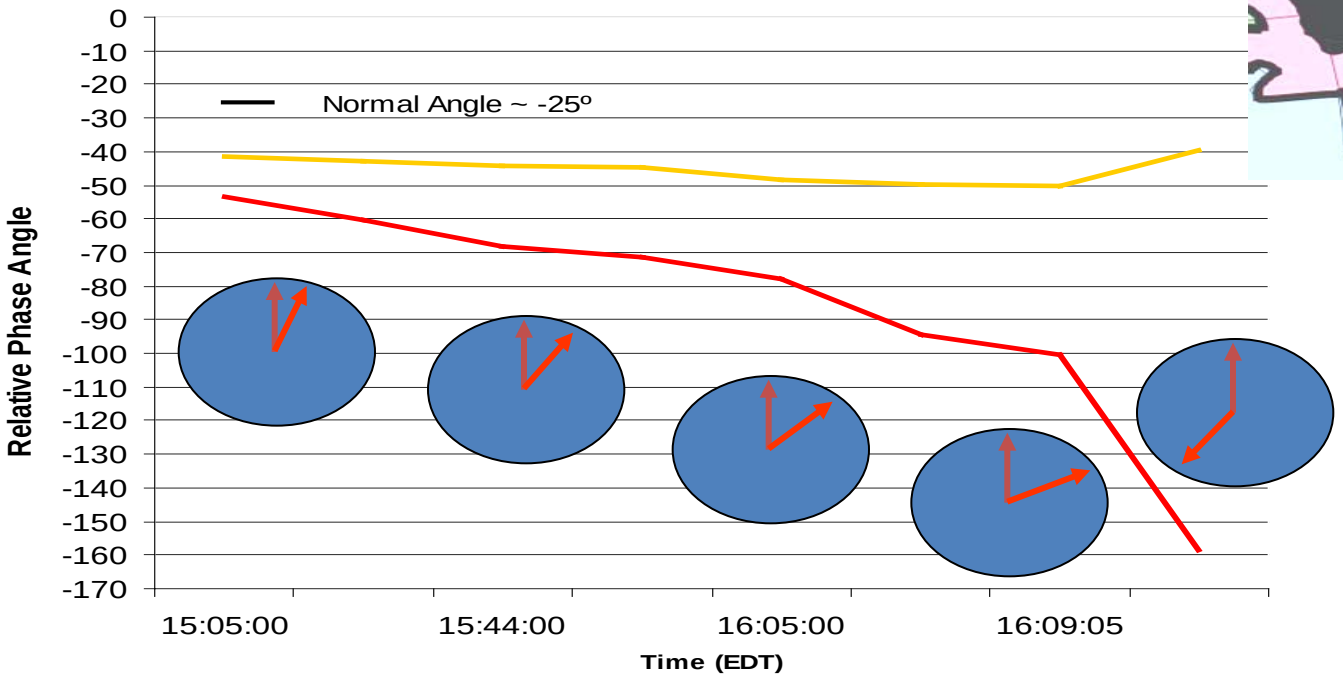
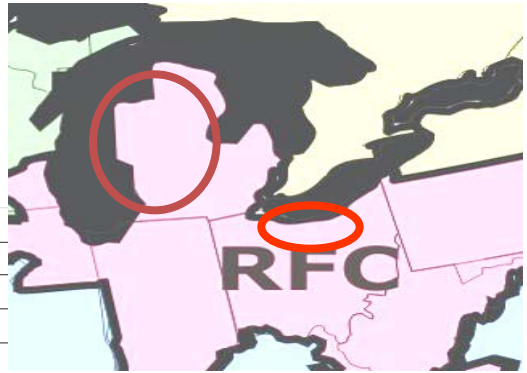
If we knew then…
August 14, 2003 Blackout





Slide Credit:
North American Electric Reliability Corporation (NERC)

Reference:
Browns Ferry

Cleveland West MI

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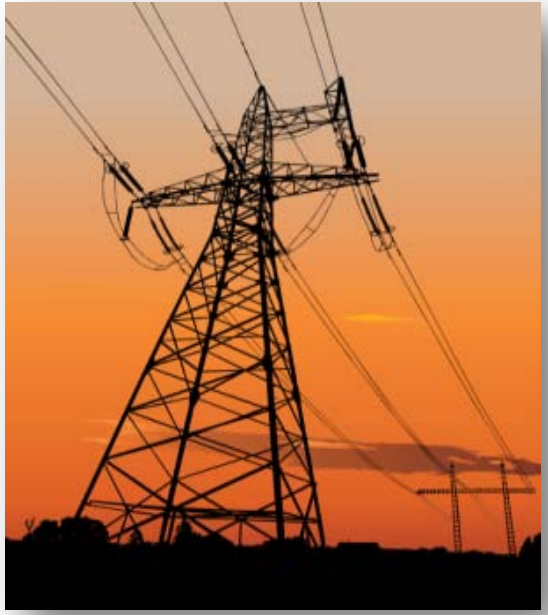
Creating a Smart Grid

- Creation of a Smart Grid requires:
- Consumer participation with distribution equipment in system operation
- The transmission and bulk generation resources get smarter too
  - Improve the timeliness, quality, and geographic scope of the operator's situational awareness and control
  - Better coordinate generation, balancing, reliability, and emergencies
  - Utilizing high-performance computing, sophisticated sensors, and advanced coordination strategies



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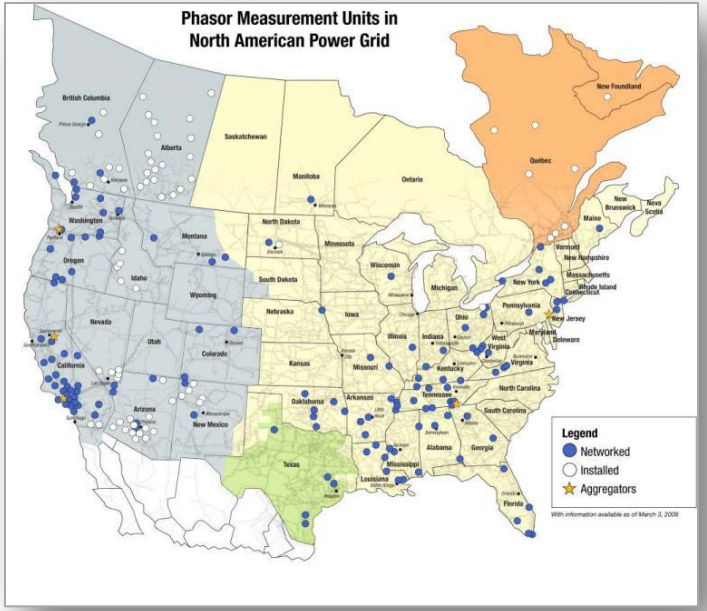
Wide-Area Awareness of Grid Status

North American SynchroPhasor Initiative (NASPI)

- New metering technology takes sampling window from six seconds to 60 times per second …. and a GPS time stamp!
- August 14, 2003 blackout reinforced the value of synchronous measurements for enhanced situational awareness
- Phasor data will drive a new generation of monitoring, operator decision support and, ultimately, fast real-time controls to improve grid performance



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Contingency Analysis and Emergency Management

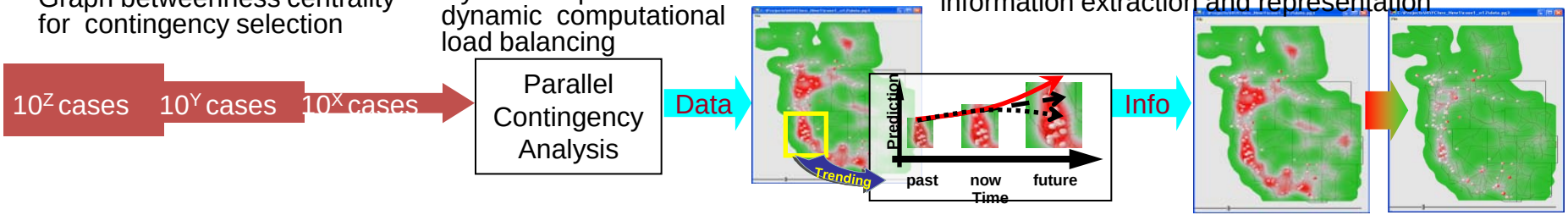
- **Today**: Number of simulations limited by sheer number of them to address. Contingency, analysis, no decision support
- **Tomorrow:** parallel processing to analyze more contingency cases
- **Future:** parallel massive “N-x” contingency analysis with real-time decision support

Contingency Analysis	Number of cases	Serial Computing on single processor	Parallel Computing on 512 processors	Speedup
WECC N-1 (full)	20,000	4.0 hours	0.5 minutes	469
WECC N-2 (partial)	153,600	25.8 hours	3.1 minutes	492
WECC N-2 (full)	~10^8	Not possible		
WECC N-3 (full)	~10^{12}			

Graph betweenness centrality for contingency selection

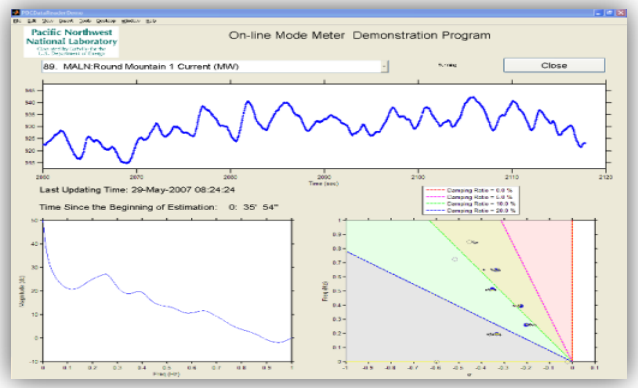
Hybrid computation with dynamic computational load balancing

Visual analytics techniques for information extraction and representation

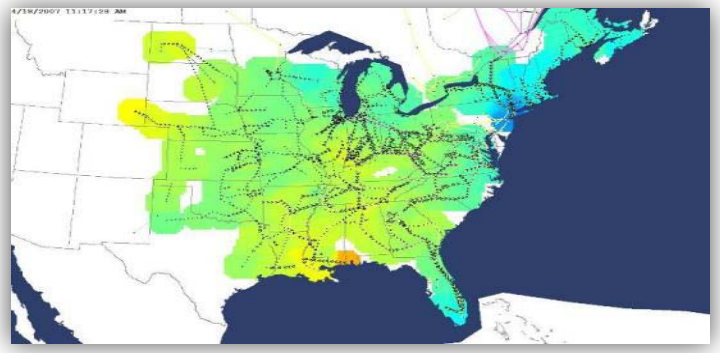


Multi-Threaded Parallel Machine | Cluster Machine | Multi-Threaded Parallel Machine

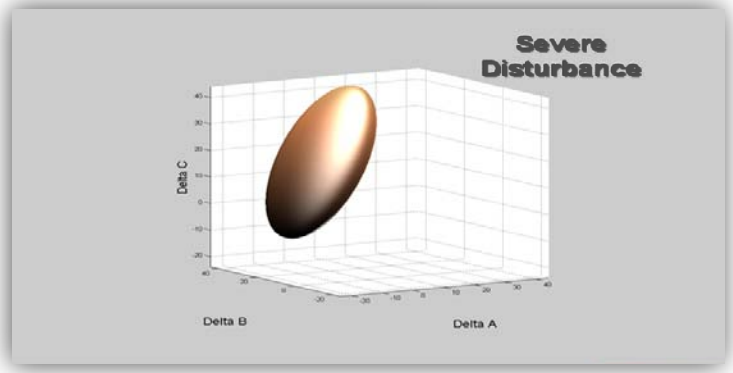
Advanced Tools Highlights



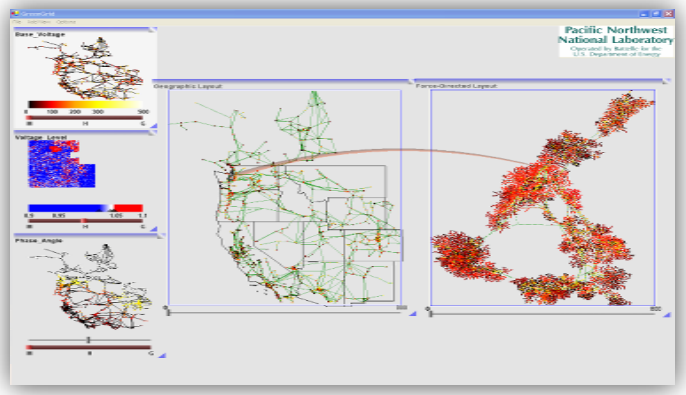
Small Signal Analysis Tool



Wide Area Hybrid Grid Health Tool



Visual views of RT Grid Security



NVAC Power System View

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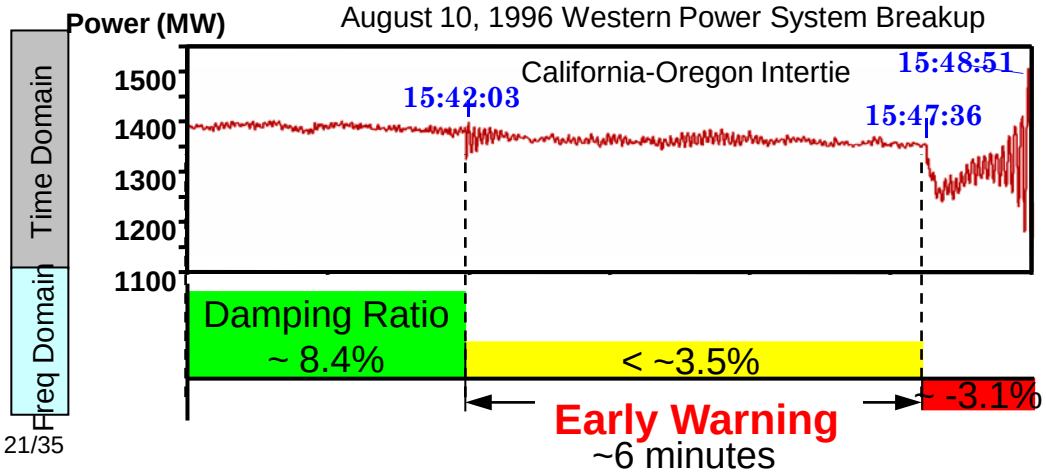
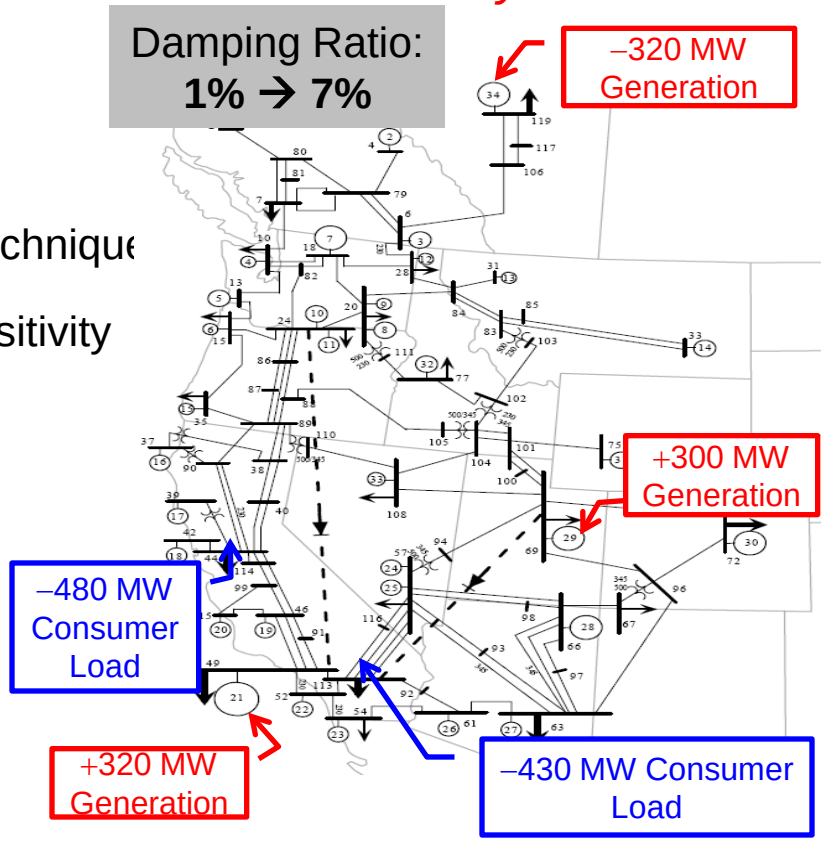
Stability Assessment and Blackout Prevention

- **Today:** no real-time monitoring of oscillatory stability
- **Tomorrow:** real-time monitoring of oscillatory signatures – frequency and damping ratio –using advanced signal processing technique
- **Long term:** real-time wide-area decision support to prevent oscillations using eigenvalue sensitivity analysis



Analytic Innovation?

Damping Ratio:
1% → 7%



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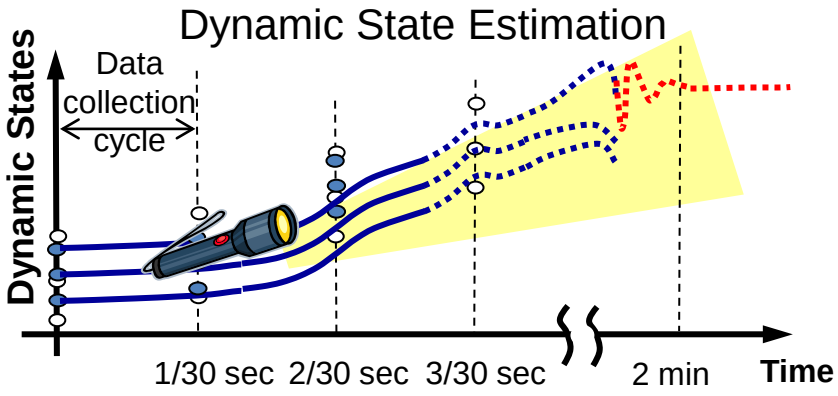
State Estimation for Real-Time Situational Awareness and Responsiveness

- **Today:** static, slow, and local view
  - 2-4 minutes to solve nonlinear equations on single Itanium processor with LU linear solver
- **Tomorrow:** static, but fast and global view
  - 2-4 seconds on parallel computers using parallelized Conjugate Gradient solver
- **Long term:** dynamic, fast, global, and predictive view
  - 1/30 second with predictive ability through solving a set of differential algebraic equations using Kalman filter techniques



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Energy Efficient Data Centers

- Advanced Cooling Solutions
- Meaningful Metrics
- Power Aware Computing

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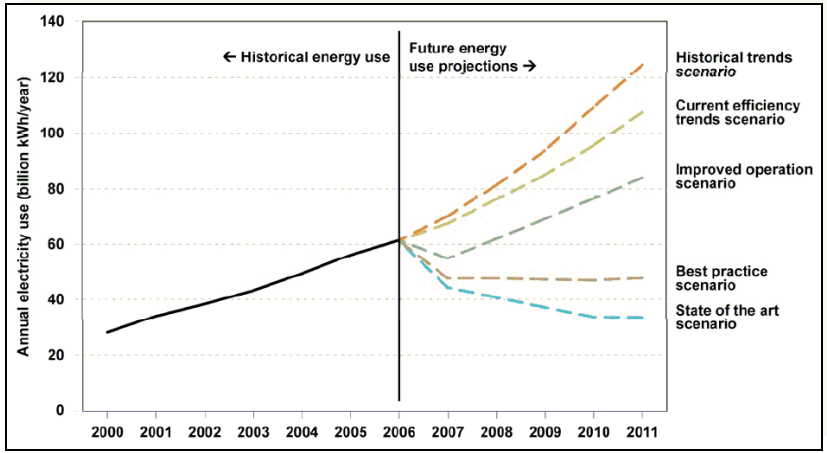
Energy Efficient Data Centers – A national challenge

- Current efficiency trends estimate energy use in data centers could double by 2011 from a 2006 baseline
- A combination of improved operations, best practices and state of the art technologies could reduce electricity use by up to 55% compared to 2006 efficiency trends



EPA Report to Congress on Server and Data Center Energy Efficiency
Released On August 2, 2007 and in response to Public Law 109-431

- PNNL Energy Smart Data Center testbed and metrics find the path

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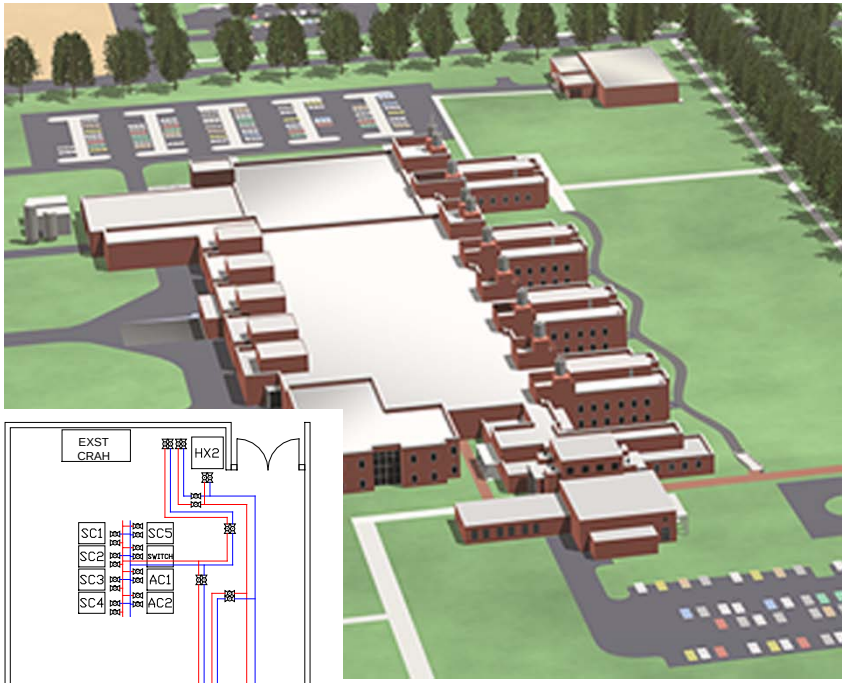
Energy Efficient Data Centers – Leadership

- Fully observable, almost fully controllable 700 sq.ft. data center
- Integrated in a mixed used facility, sharing power distribution and cooling provisioning
- Over 1000 sensors providing data at the chip, server, rack, room and facility level
- Unique, unbiased, real-world

http://esdc.pnl.gov



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Energy Efficient Data Center– Advanced solutions and solid collaborations

- Strong environment
  - Real world testbed of advanced cooling solutions
  - Real world evaluation and design of metrics
- Strong background
  - Computer and computational science
  - Facilities engineers
  - Statistical sciences
- Strong Partners
  - Industry: HP, IBM, Intel
  - Government: DOE, NNSA
  - Academic: Portland State

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Advanced Cooling Solutions

- Challenges: Evaluating existing cooling solutions for HPC
  - Are existing cooling solutions energy efficient?
  - Are best practices applied?
  - Do existing cooling solutions scale with high density racks?
- Our approach:
  - Evaluate advanced cooling solutions that act close to heat sources
  - Explore hybrid cooling solutions, e.g., air and spray

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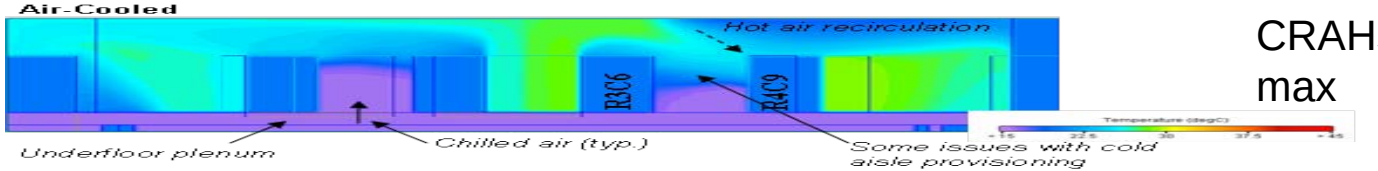
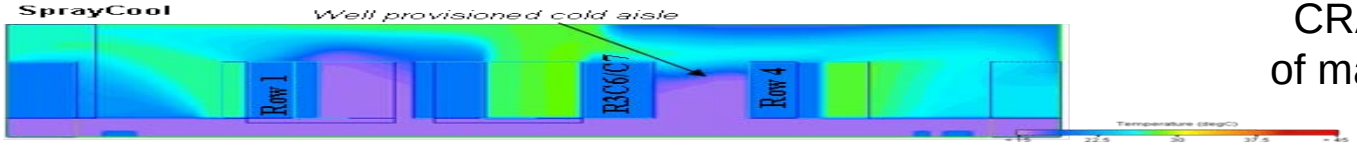
Replacing Processor Air-Cooling with Spraycooling (study conducted with HP)

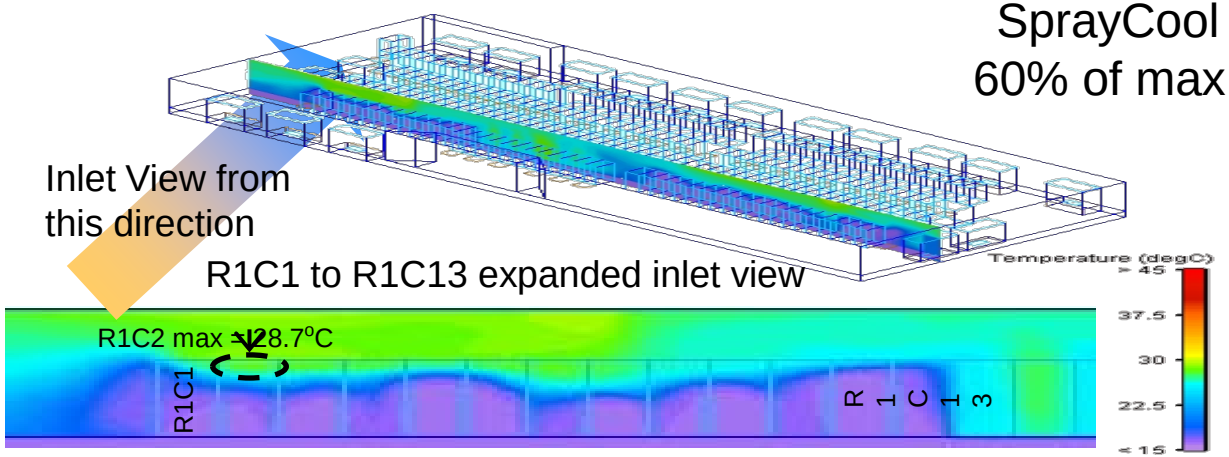


CRAHs at 100% of max



CRAHs at 80% of max

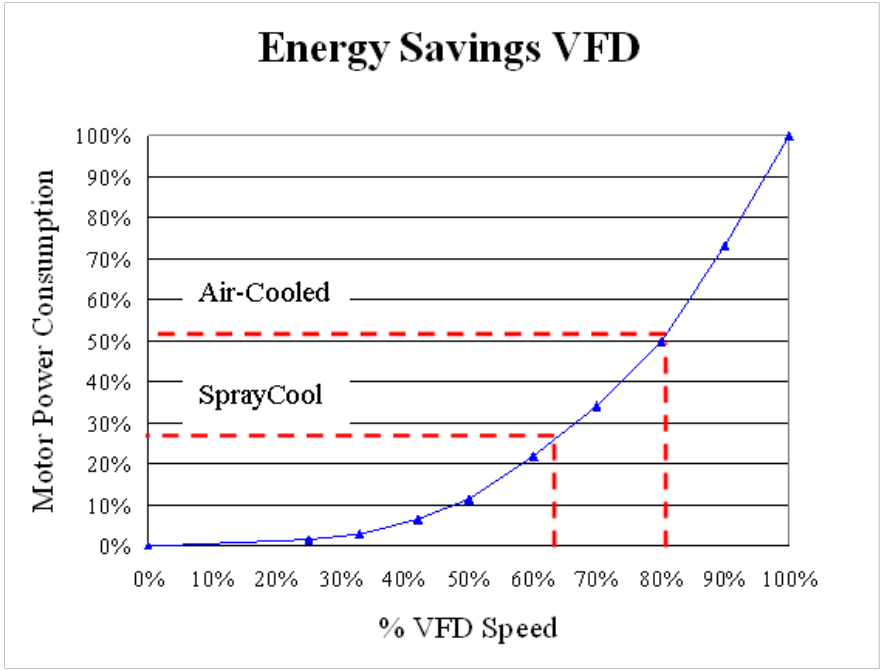
SprayCool - CRAHs at 60% of max



- Poor cold aisle provisioning at this CRAH setting
- Ideal CRAH setting for SprayCool is approx 70% of max

Energy Savings VFD

- Air-cooled facility's blowers use 82% more power



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Meaningful Metrics

- Challenges: Evaluating usability of existing metrics for HPC
  - Do existing metrics penalize HPC?
    - Not considering space/density
    - Not considering output: product (as in time-to-solution).
- Our approach:
  - Introduce productivity metrics in conjunction with The Green Grid
    - Data Center Productivity (DCP) and Data Center energy Productivity (DCeP) family of metrics
  - Establish realistic test cases

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Experimental Plan: A PNNL HPC workload

Completely randomized block design with a 2^2 factorial treatment structure:

- **Treatment 1**: application's machine load:
  - 75% WRF, 25% WRF
- **Treatment 2**: number of cores per server:
  - full-core, half-core
- **Block**: day of the week and time of run:
  - weekday, weekend, day, night

Each treatment produces Useful Computational Units (UCU) extracted from a stable, ~1.5 hour long assessment window

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Summary of Experimental Results

- DCeP ***can*** be used to distinguish between different operational states in a data center and guide load balancing
- Full core implementations use more energy than half core, but are also more efficient (regardless of weighting scheme)
- Treatments with 25% WRF load are more efficient than 75% (given weighting scheme where each CP2K unit is with 10% of a WRF unit)

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Integrating Power/Cooling Into Application Performance Analysis

- **Challenges**: combining two disparate worlds of tools and data
  - Infrastructure for collecting, storing and analyzing data
    - Combine data from the application and room environment perspectives
    - Ex. “What was the rack temperature during this run?”
- **Our answers**:
  - PerfTrack performance database extended to hold room data
  - Job placement study currently being conducted at ESDC facility
    - “Can we save $ on cooling by changing job placement within the cluster?”
    - “Is it more efficient to use one rack, or use them all?”

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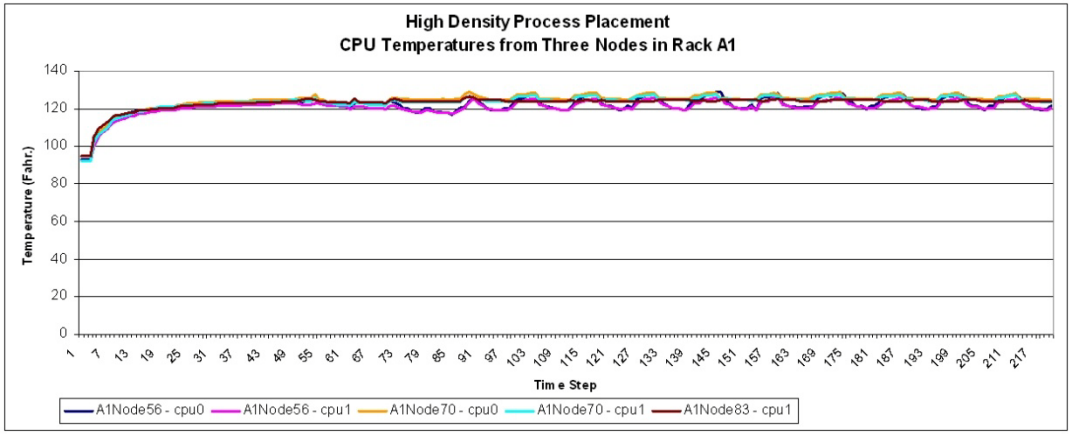
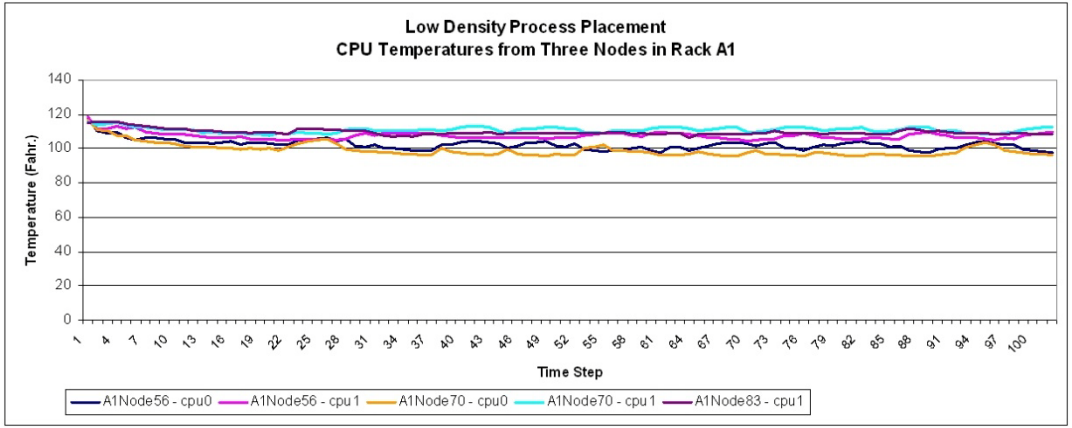
Thermal Profiles of Running Applications

- **“High Density” Placement**
- 224 processes on 1 rack
- (8 processes per node)
- CPU temperatures stay above 120ºF



- **“Low Density” Placement**
- 224 processes on 4 racks
- (2 processes per node)
- CPU temperatures stay below 110ºF



Energy Efficient Data Center Summary

- **Energy use is an increasingly acute problem**
  - At the national level
  - At the data center level
  - As HPC user
- **The Energy Smart Data Center (ESDC) at PNNL** provides the building blocks to conduct energy efficiency studies by providing monitoring and control tools
  - At the mechanical side
    - Advanced Cooling solutions
    - Advanced Power Distribution
  - At the software side
    - Sensible HPC Metrics
    - Power Aware Computing

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