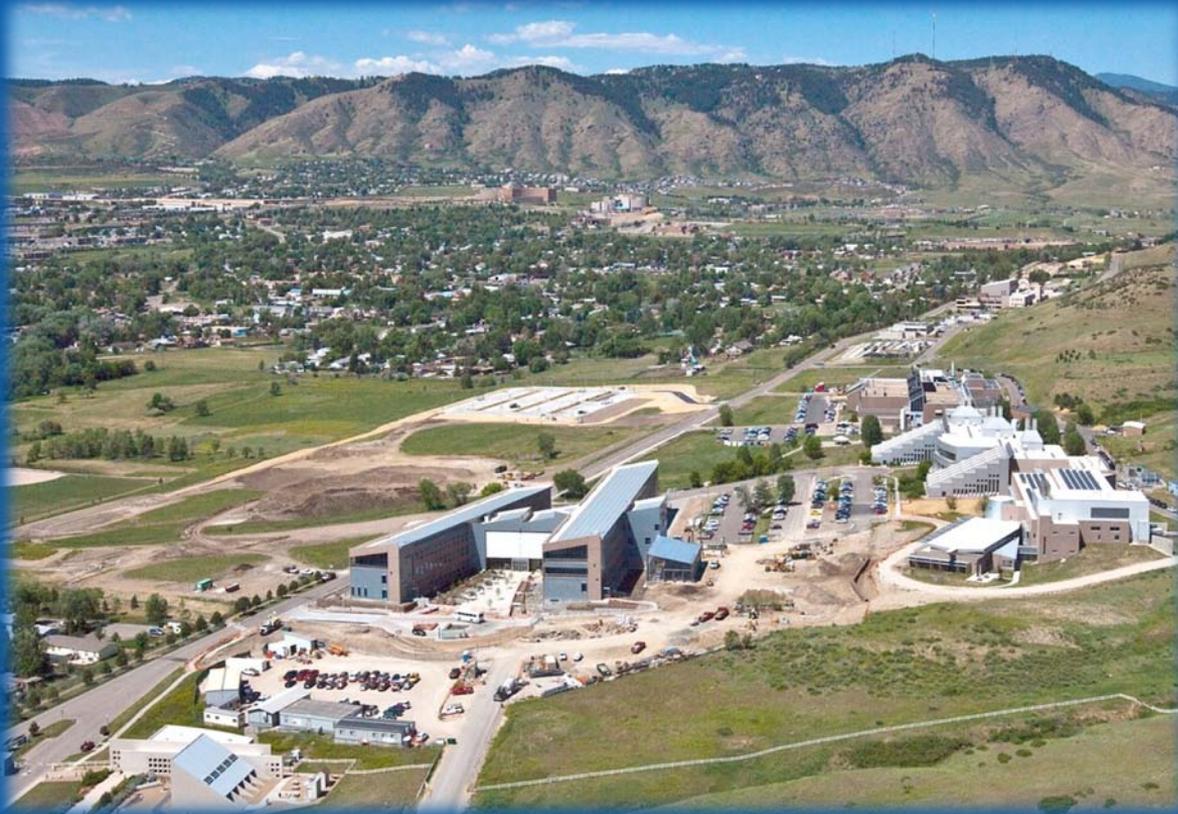


ESIF High Performance Computing

Steve Hammond
Director, Computational
Science Center

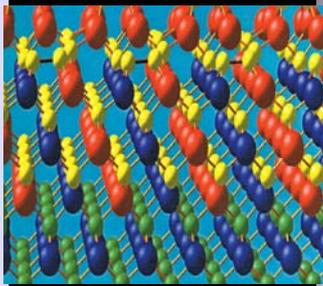
October 27, 2011

Disclaimer: The opinions expressed in this presentation are that of the presenter and do not necessarily reflect the views of NREL or the U.S. Dept of Energy.



NREL HPC: Vital to Meeting Energy Goals

Molecular & Nanoscale



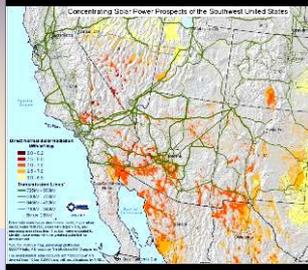
Simulation at scales that evade direct observation

Large Scale Systems



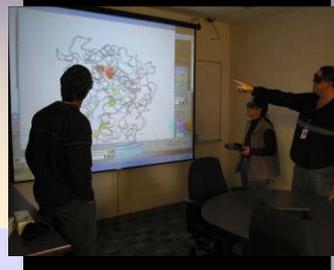
Simulation and modeling of fully integrated systems.

Analysis & Resource Assessment



Integration of data, resource assessments and analysis

Visualization & Insight



Display, convey and manage complex information

Collaboration, Involvement



Link NREL expertise with universities & industry

Data Mgmt

Computational Science Expertise, Math, Data Mining, Viz
High Performance Computing, Data Storage, Networking

LCFs

Capabilities anchored in a new facility, the ESIF

Current NREL HPC Capabilities

- RedRock - test & develop
 - Production use December 2009.
 - 1344 Processors, 15 TFlops peak



- RedMesa

- 15,360 Processor, 180 TFlops peak
- Production use April 2010.
- Significant impact on NREL/EERE mission.



RedMesa is fastest system in the world dedicated advancing energy efficiency and renewable energy technologies.

NREL HPC: FY11 Impact

- Biomass: World leaders in modeling biomass deconstruction
 - Gained new insights into biomass gasification process optimization
 - Developing new approaches to high fidelity process modeling and kinetics
- Solar: Developing OPV materials genomics database.
 - To date, material screening saved 7,000+ man-years of chemical synthesis time.
 - Concentrated Solar thermal materials modeling.
- Vehicles: Won VTP FOA with Cooper Tire, energy efficient tires.
 - Participant in CAEBAT effort.
- Wind: Rapid advances in coupled multi-turbine array efforts.
 - Substantial role in recent Wind-Water Program proposals.
 - Requests from outside NREL to use NREL HPC resources.
 - New effort in blade structural modeling.
- Combustion: part of combustion exascale winning team (SC).
- Buildings:
 - Decreased sensitivity analysis computation time 200-fold in EnergyPlus.

Energy System Integration Facility



ESIF HPC Data Center

- Showcase Facility
 - 10MW, 10,000 s.f.
 - Leverage favorable climate
 - Use evaporative rather mechanical cooling.
 - Waste heat captured and used to heat labs & offices.
 - World's most energy efficient data center, PUE 1.06!
 - Lower CapEx and OpEx.
- High Performance Computing
 - Petascale+ HPC Capability
 - New system delivered Q4 2012
 - 2-4x current capabilities.
 - 20 year planning horizon
 - 5 to 6 HPC generations.
 - Insight Center
 - Scientific data visualization
 - Collaboration and interaction.

Reduce Risk

*Accelerate Progress from
Inspiration To Installation*

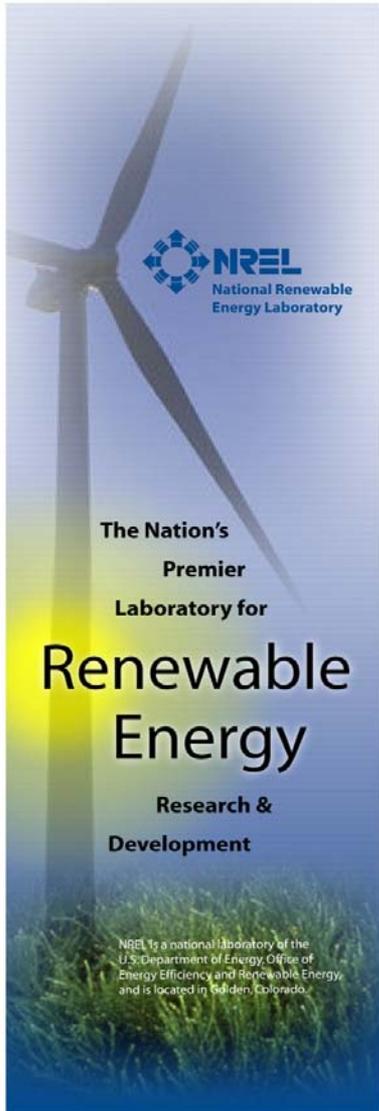
Eliminate Uncertainty



Optimizing ESIF's Data Center Performance

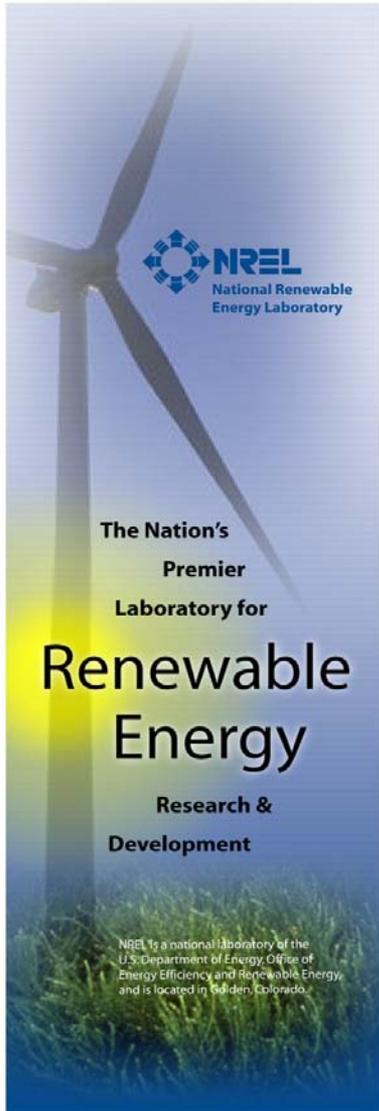
- Required: Annual PUE < 1.06
 - NO mechanical cooling or perimeter CRAC units.
 - Leverage favorable climate, evaporative cooling only.
 - “Cool” computing equipment with warm, indirect tower water.
 - Minimize power conversions and losses.
 - UPS exclusively for critical components.
 - Numerous waste heat utilization opportunities (pre-treat lab air, radiant heating in office space, snow melt, ...)
- Monitor PUE (power usage effectiveness).
 - $PUE = \text{Total Power} / \text{IT Equipment}$
 - Economizer hours, temperature profiles, allowable conditions.
- Dashboards to report instantaneous, seasonal and cumulative PUE values.

ESIF Data Center Electrical Power Systems



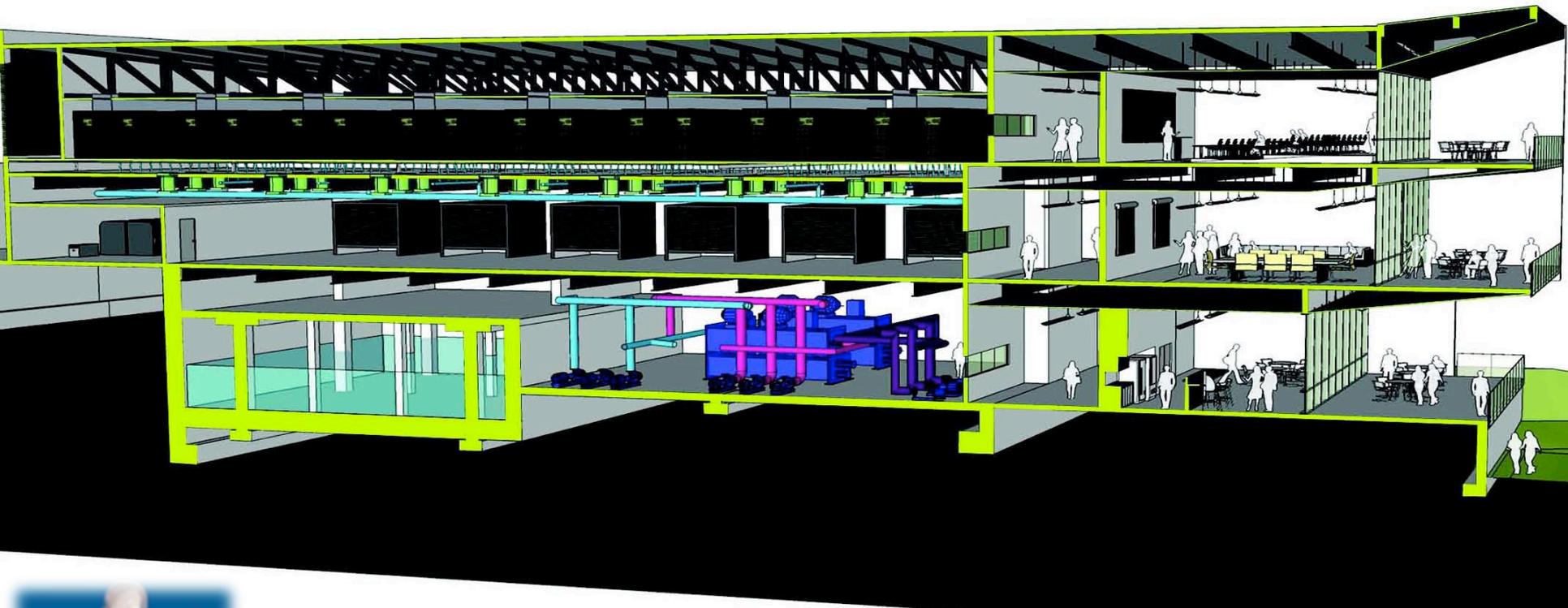
- Primary utilize 480V 3P distribution to enhance energy efficiency, eliminate the losses and heat associated with PDU's and step down transformers.
- Switchboards and distribution panels will include extensive power monitoring.
- UPS at 10% of peak load
 - 3 by 320kW UPS in parallel on common bus.
 - Provides N+1 configuration.
 - Sufficient duration to allow generator to spin up and protect critical components.

ESIF Data Center Mechanical System



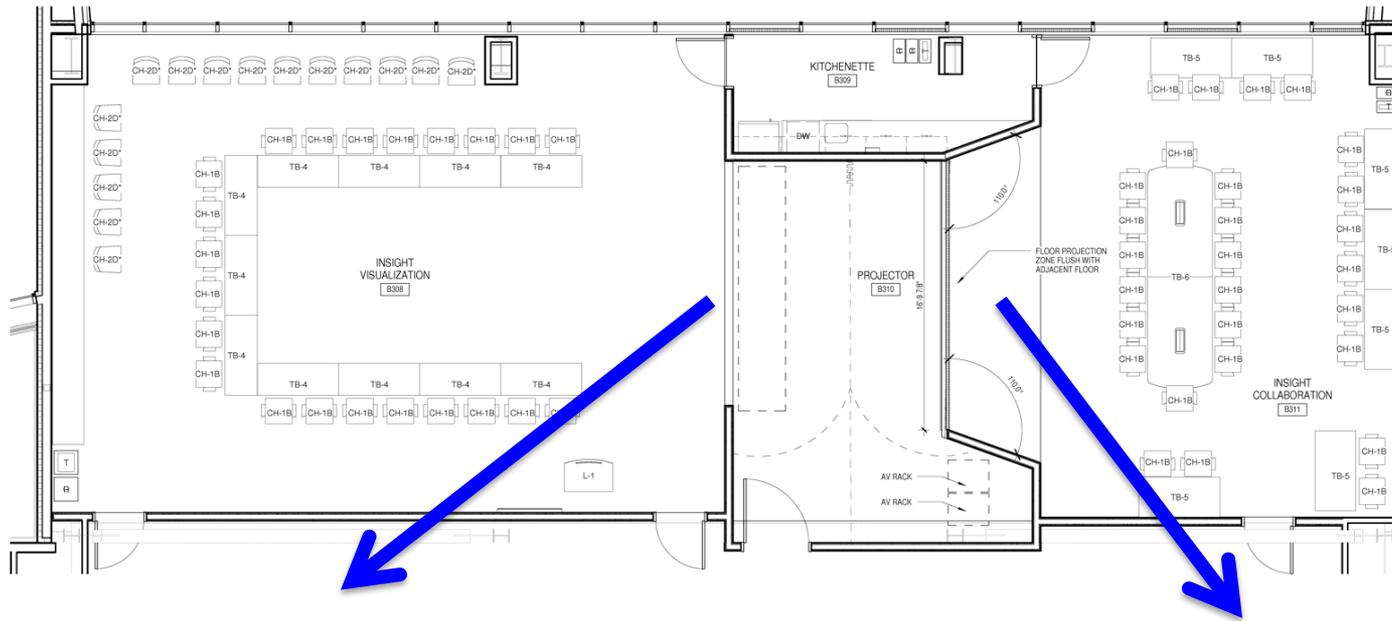
- Operate in ASHRAE TC 9.9 recommended range 99% of the time (~87 hours per year in allowable).
- HPC equipment cooled indirectly with tower water.
 - Able to manage 100% heat load dissipated to liquid
 - Able to manage up to 10% heat load to air.
 - Pumps/water more efficient fans/air.
- “Cooling” supply temp, 75F
- Return temp, 95F (20F delta T)
- Waste heat will be used in cold months to heat lab and office space, temper inlet air, or ejected directly outside when not needed.

NREL ESIF Data Center Cross Section



- Treat this as the data center equivalent of the “visible man”
 - Tour views into pump room and mechanical spaces
 - Color code pipes, LCD monitors

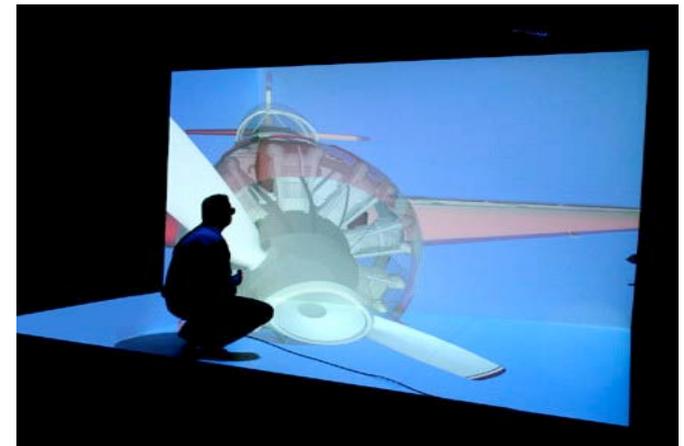
ESIF: Insight Center



High-resolution rear-projected display wall

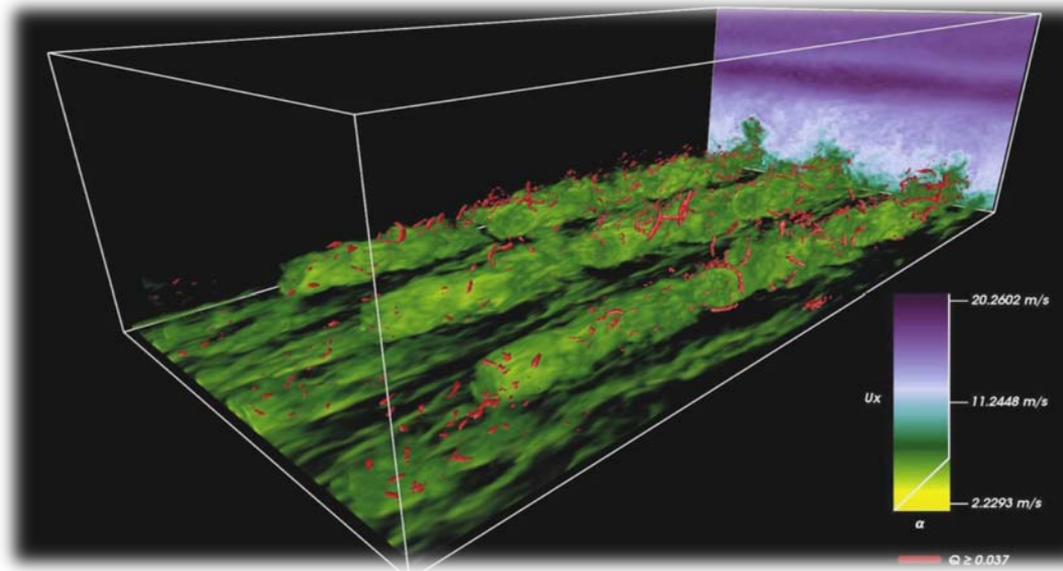
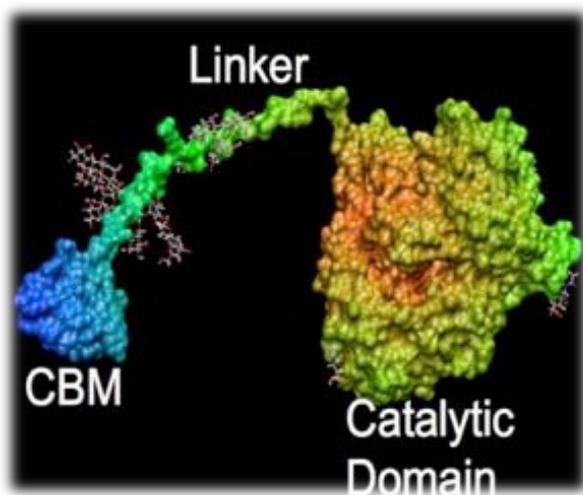


Immersive & Collaborative Displays



ESIF HPC Capabilities – An EERE Asset

- Lab-wide resource with associated expertise.
- Model and simulate phenomena and systems that are difficult to directly measure and manipulate.
- Historically supported R&D in PV materials, biofuels, reacting flows, and wind plant aerodynamics.
- Optimizing building energy use - large-scale parametric studies involving EnergyPlus.



ESIF HPC, future modeling possibilities ...

- Integration of high penetration renewables and the Grid: Make renewables a predictable resource.
 - Ramp events, detailed power production known 24 hrs+ in advance. *Improve confidence.* Reduce risk.
 - Reliable unit commitments, storage, & planning. *Reduce uncertainty.*
- Smart Grid: Model the dynamic behavior of 1 billion devices (appliances, roof top solar, EVs ...) on the grid? Predict demand response ...



Questions?



Discussion