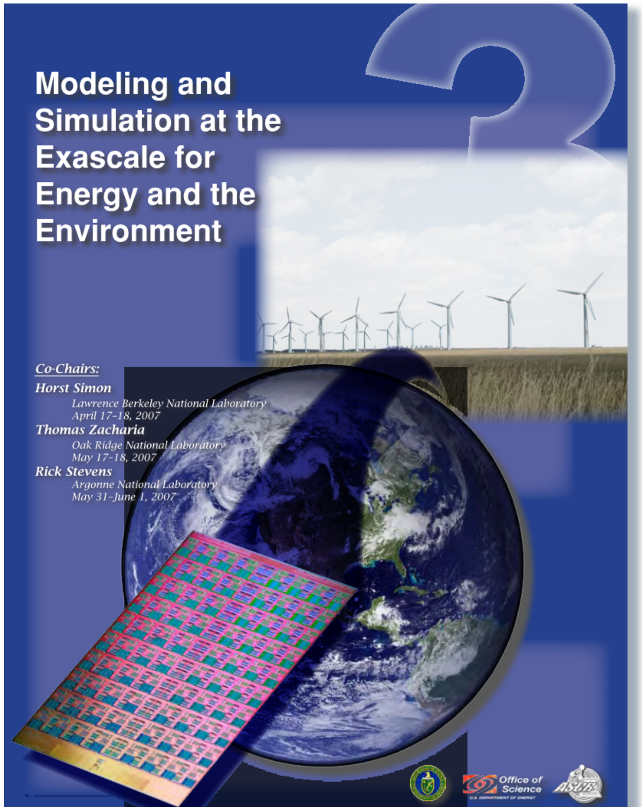


Exascale Town Hall Mtgs

Environment

Climate modeling:

- much higher resolution models -> local impacts of climate change;
- dramatic improvement of physical, chemical, & biological process,
- exploration of uncertainty in climate models via large-scale ensembles

Significant investments will be needed

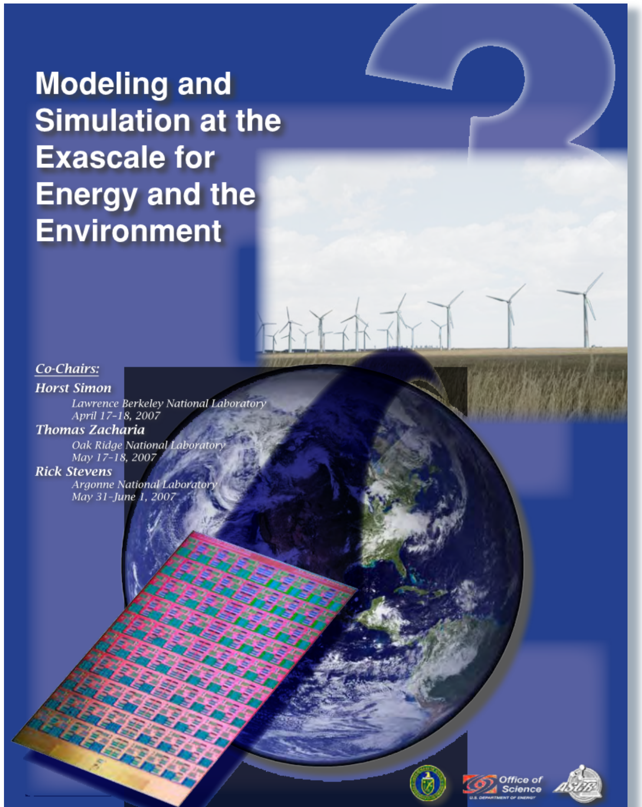
- to port and improve climate models for exascale architectures,
- explicit targeting of multicore in next-generation models
- development of an integrated climate research computing environment linking climate modelers with climate data sources, collaborators, and university and laboratory resources.

Integrating energy, socioeconomics, and environmental modeling.

- couple detailed models of Energy production/utilization with geospatialized socioeconomic models
- couple these to ESMs to capture feedbacks to and from the environment from human activities.
- This would enable fundamental research into strategies for sustainable global economic development
- Lead to exploration of alternative development paths and their impacts on global energy security.

Multiscale biological modeling. Exascale computing will enable computational biologists to

- build models bridging the space-time parameters that characterize important biological processes,
- model diverse microbial ecosystems (bioenergy, CS, environmental technology, and industrial processes).
- coupling research in high-throughput genomics, proteomics, and bioinformatics to applications, for example, accelerating the computing vision of programs such as DOE's Genomics:GTL initiative.



Computer Science and Applied Mathematics

To realize science at the exascale, advances req'd in

- algorithms, programming models, OS, filesystems, I/O , and data analysis tools.
- new working relationships between the physical, computer and mathematics science communities.

Specific challenges that need to be overcome include

- scalable OS services that can manage 10M to 100M cores,
- scalable programming models/tools w/orders of magnitude more concurrency
- Exabyte data storage & sustained TB/sec transfer speeds

Cyberinfrastructure and Cyber Security: HPC is only a part of the exascale computing env:

- high-performance networking, mid-range and smaller clusters, visualization engines, large-scale data archives, a variety of data sources and instrumentation including emerging sensor networks, and the tens of thousands of workstations that enable access to and are the primary development machines.
- A vast software ecosystem spanning networking software, databases, security, and hundreds of domain-specific tools.
- Additional investments in cyberinfrastructure and cyber security

"Rate Limiters" WS

Advanced Scientific Computing Advisory Committee and Biological and Environmental Advisory Committee

Report on Computational and Informational Technology Rate Limiters to the Advancement of Climate Change Science

March 17, 2008

Prepared by the Joint ASCAC-BERAC Subcommittee

James J. Hack, NCAR (Co-chair)
Eugene Bierly, AGU (Co-chair)
Dave Bader, LLNL
Phil Colella, LBL
William D. Collins, LBL
John B. Drake, ORNL
Ian Foster, ANL
Brian Gross, GFDL
Philip Jones, LANL
Edward S. Sarachik, University of Washington
Dean N. Williams, LLNL

Recognizing that computational and information technology solutions cannot be separated from the underlying science drivers; the committee recommends that ASCR and BER undertake joint ventures to:

- **Continue to invest in leadership class computational facilities**, data storage facilities, analysis environments, and collaborative tools and technologies. A significant fraction of these resources should be dedicated, configured and managed to support integrated and multi-faceted climate research and prediction across DOE and broader national and international efforts
- Invest in strategic collaborations to **develop computational algorithms and scalable software** to accelerate computational climate change science
- **Develop computational and theoretical foundations for new modes of climate simulation**, including ensemble short-range forecasts with regional fidelity and Earth system assimilation
- Focus the scientific effort to **pursue robust predictive capability of lower-probability/higher-risk impacts**, including climate extremes and abrupt climate change
- **Develop a strong scientific understanding of leading-order uncertainties** in the carbon cycle, in particular how the efficiency of natural carbon sinks will change with our changing climate

Report on the DOE/BERAC Workshop

Identifying Outstanding Grand Challenges in Climate Change Research: Guiding DOE's Strategic Planning

September 5, 2008

Grand Challenges WS (Dickenson & Meehl

1. *Characterize the Earth's current climate, and its evolution over the last century to its present state.*
2. *Predict regional climate change for the next several decades.*
3. *Simulate Earth System changes and their consequences over centuries*

ID'd Research initiatives where DOE already has program strengths:

- Characterization of impacts of radiatively active atm constituents, especially aerosols & clouds,
- Interactions between ecosystem processes and changes and the climate system.
- Interactions between changing climate, hydrological systems, and their management.
- Incorporation of knowledge from observational and modeling process studies into ESMs;
- Implications of climate change for energy systems, strategies for mitigation & adaptation

Although climate science intersects a broad range of physical, biological, and social sciences, the science community concurs on the major crossdisciplinary issues that need to be addressed through enhanced research. And that such research must now connect across disciplinary boundaries in a more integrated approach and more explicitly include human dimensions

Science (wmw)

1. **Model Development and Integrated Assessment**
    1. interaction of carbon, methane, and nitrogen cycles
    2. local and regional water, ice, and clouds change with global warming.
    3. regional climate change with global warming: Δ WX & extreme events
    4. Future sea-level and ocean circulation changes.
    5. Incorporate integrative assessment and economic model components

2. **Algorithms and Computational Environment:** <u>Becoming increasingly complex</u>,
    1. Scalable numerical algorithms to efficiently use peta & exascale archs.
    2. Parallel input/output, metadata, analysis and modeling tools
    3. Programming models, fault resilience, and software infrastructure..
    4. Training of scientists in the use of high performance computers

3. **Decadal Predictability and Prediction**
    1. Establish a multi-agency, multi-institutional partnership
    2. Predict changes in land plants, oceanic biology, and atm & ocn chemistry.
    3. Educate the next generation of climate scientists in extreme computing

4. **Extreme Scale Data Management, Analysis, Visualization, and Productivity**
    1. Production, management, and access for exascale data.
    2. Integration of diverse complex data, format-neutral data interfaces & effective methods for dealing with diverse grid structures and advanced metadata.
    3. Scalable analysis and viz infrastructure, exascale climate analysis facilities.
    4. Distributed governance for data policy, standards, and federation

1. A Scalable and Extensible Earth System Model for Climate Change Science
John Drake (ORNL), Michael Wehner(LBNL):

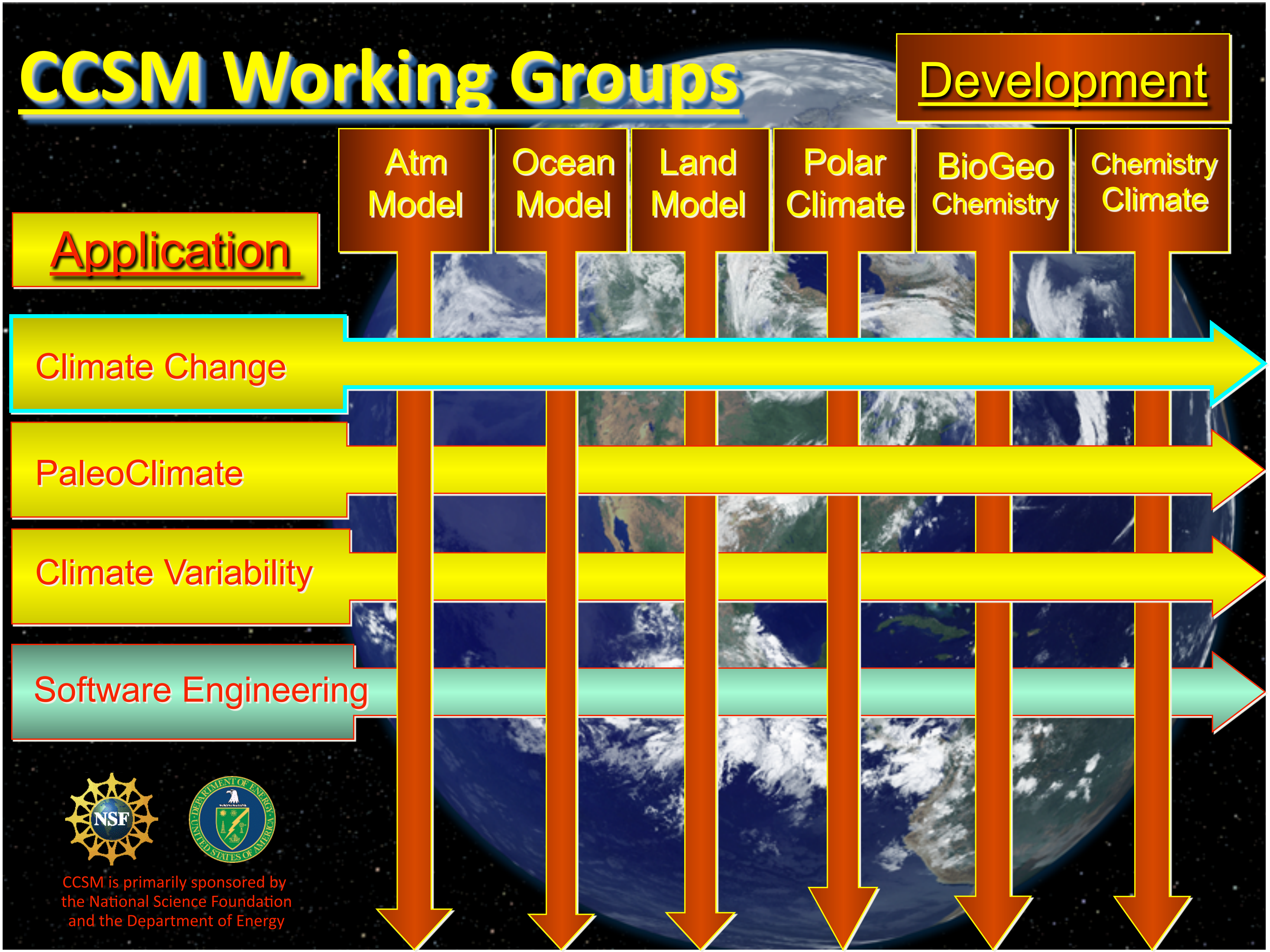
2. Climate Change Simulations with CCSM: Moderate and High Resolution Studies
Lawrence Buja, John Dennis (NCAR)

DOE's BER/ASCR partnership with NSF and NCAR to simulate the earth's climate and climate change based on first principles, physical modeling techniques using parallel, scalable computers extending the process models to a comprehensive earth system model that balances the global carbon and sulfur cycles.

The scientific objectives of the work are to assemble a first-generation Earth system model that allows us to understand the coupling between the physical, chemical, and biogeochemical processes in the climate system.

Immediate goal: development, release & use of the CCSM4 for use in upcoming IPCC Assessement and CMIP 5 studies.

- Low-res, 2 degree model for earth system modeling and mitigation studies
- High resolution 0.5 degree model for regional projection of climate change.


CCSM Working Groups
Development
Atm Model
Ocean Model
Land Model
Polar Climate
BioGeo Chemistry
Chemistry Climate
Application
Climate Change
PaleoClimate
Climate Variability
Software Engineering
NSF
CCSM is primarily sponsored by
the National Science Foundation
and the Department of Energy

2. Current HPC Requirements

(see slide notes)

- Architectures: **CRAY, IBM Power & Linux clusters**

  NERSC, NCCS, ACLF, NSF Centers, NCAR & universities
- Compute/memory load: **Typical run: 2288 Pes for 20 days, 1.7GB/core**
- Data read/written **1000GB, 2-10GB checkpoint files, Goal: 0 bytes moved.**

  Min throughput metric: 5 simulated years / wall-clock day
- Necessary software, services or infrastructure: **MPI + OpenMP**
- Current primary codes and their methods or algorithms:

  CCSM = CAM + POP + CLM + CICE + CPL

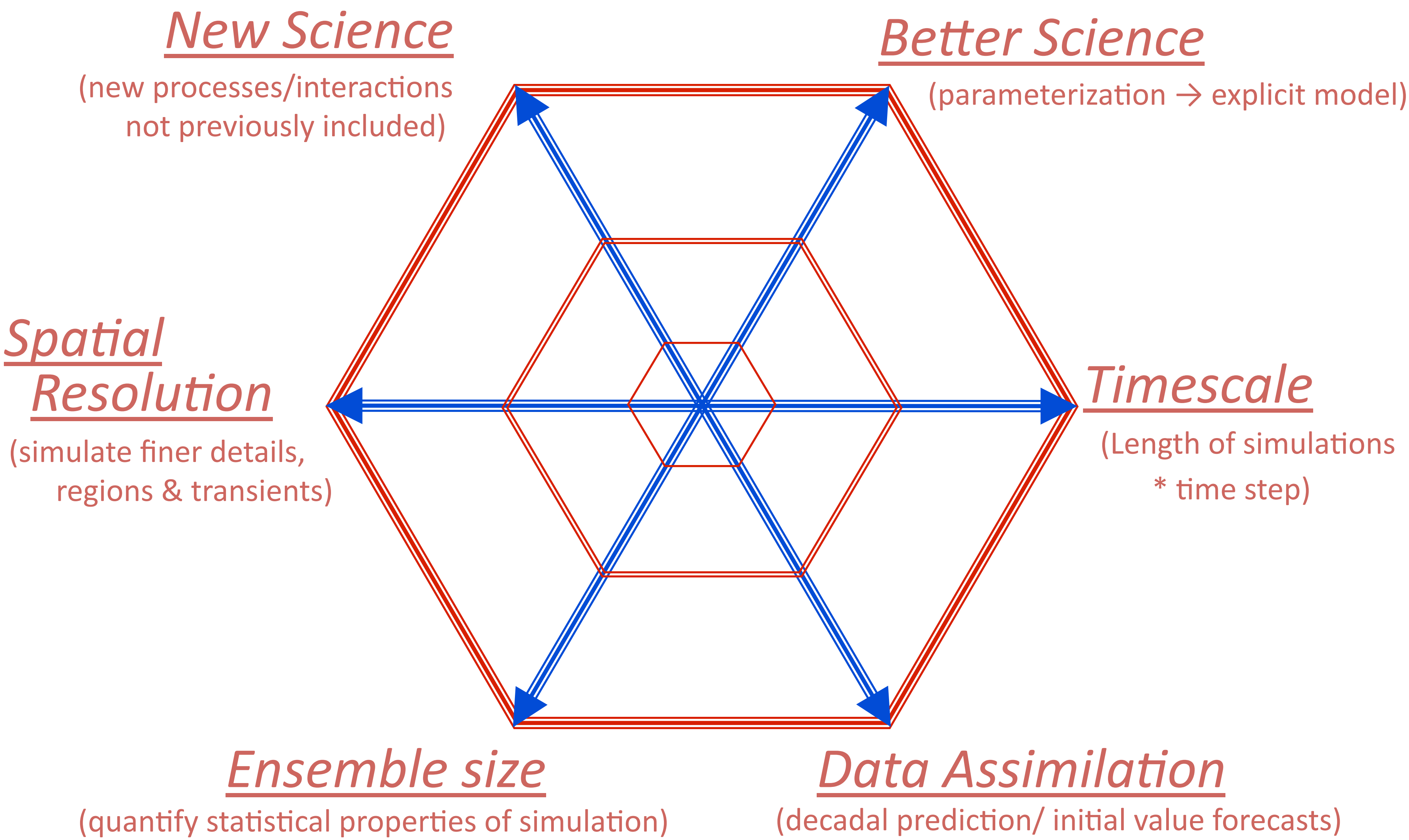
  CAM: Finite Volume dynamical core, lagrangian vertical, polar FFT filters

  POP: FV with semi-implicit elliptical solver for barotropic modes

  CICE: FV dynamics, incremental remapping advection
- Known limitations/obstacles/bottlenecks

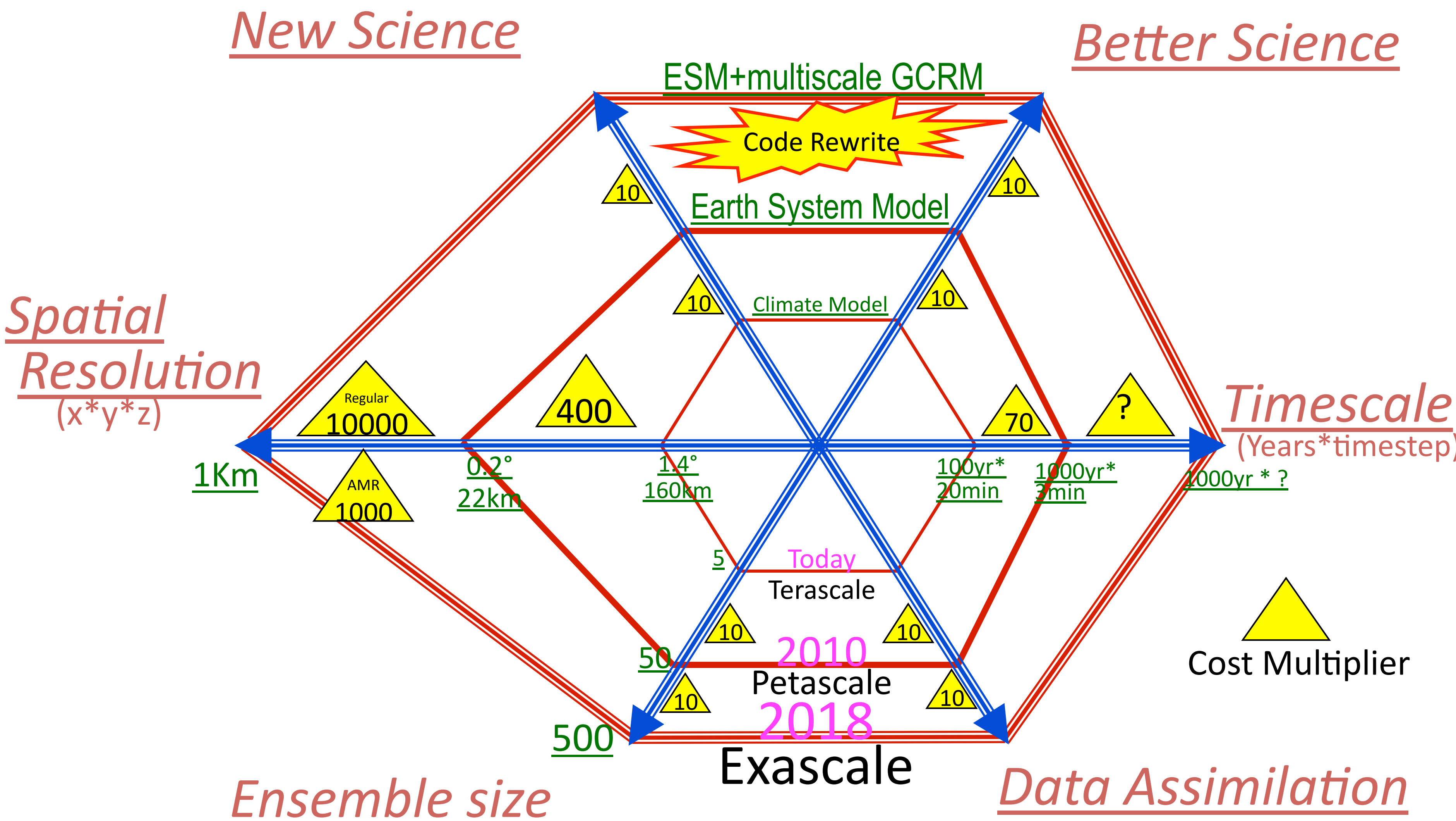
  Scalability of current component models, I/O
- Anything else? **System Stability and throughput**

HPC dimensions of Climate Prediction

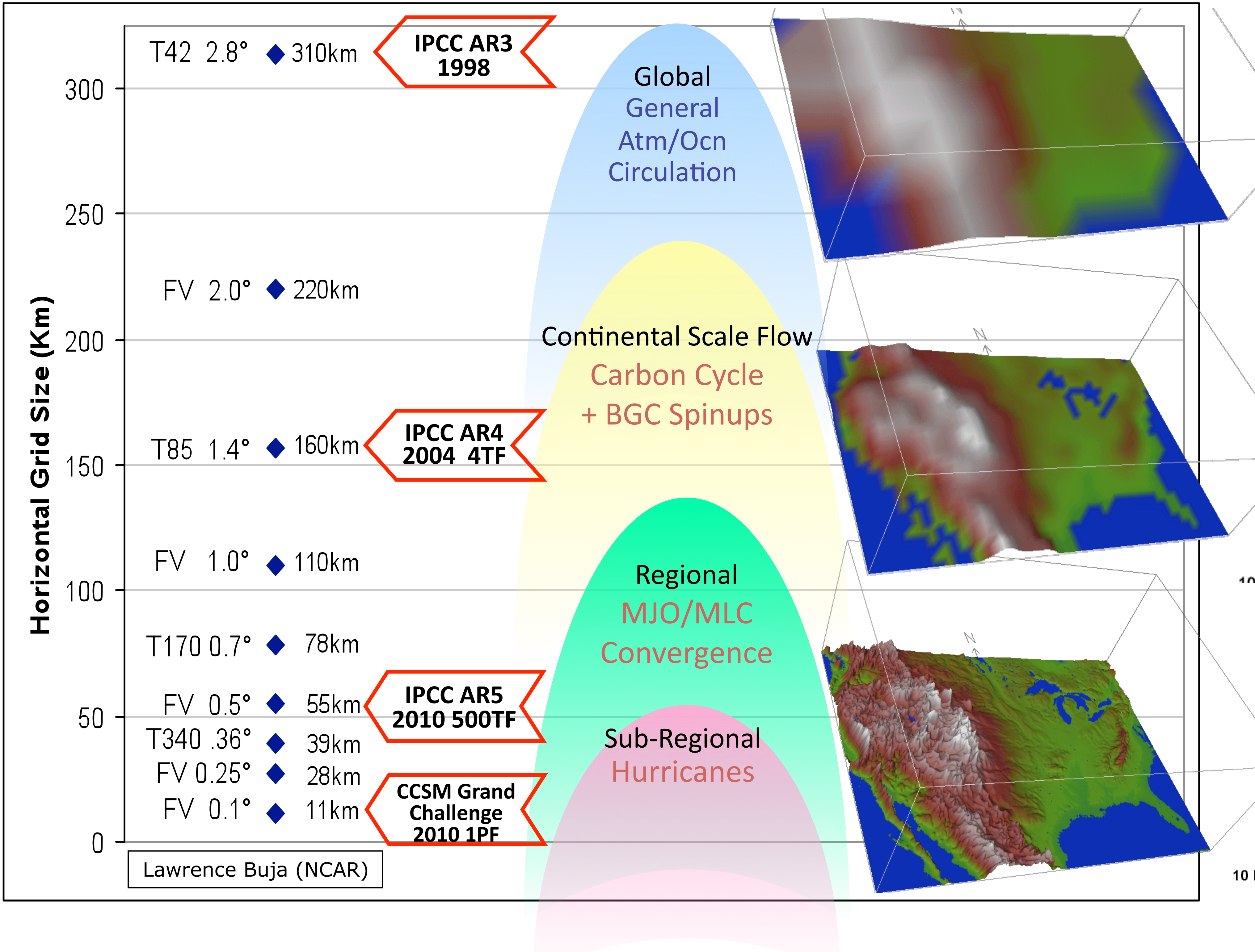


Lawrence Buja (NCAR) / Tim Palmer (ECMWF)

HPC dimensions of Climate Prediction



Lawrence Buja (NCAR)



Horizontal Grid Size (Km)
300
250
200
150
100
50
0
T42 2.8° 310km
FV 2.0° 220km
T85 1.4° 160km
FV 1.0° 110km
T170 0.7° 78km
FV 0.5° 55km
T340 .36° 39km
FV 0.25° 28km
FV 0.1° 11km
IPCC AR3 1998
IPCC AR4 2004 4TF
IPCC AR5 2010 500TF
CCSM Grand Challenge 2010 1PF
Global General Atm/Ocn Circulation
Continental Scale Flow Carbon Cycle + BGC Spinups
Regional MJO/MLC Convergence
Sub-Regional Hurricanes
Lawrence Buja (NCAR)

3. HPC Usage and Methods for the Next 3-5 Years

(see slide notes)

- Upcoming changes to codes/methods/approaches

  Cubed sphere grid & higher order spectral element methods

  Higher resolutions (Convection resolving in atm & ocn)

  More detailed physical processes (chem, bio, hydro etc)

- Changes to Compute/memory load

  John Dennis Presentation

- Changes to Data read/written

- Changes to necessary software, services or infrastructure

- Anticipated limitations/obstacles/bottlenecks on 10K-1000K PE system.

- Anything else?

4. Summary

- What new science results might be afforded by improvements in NERSC computing hardware, software and services?
  - Characterization of impacts of radiatively active atm constituents, especially aerosols & clouds,
  - Interactions between ecosystem processes and changes and the climate system.
  - Interactions between changing climate, hydrological systems, and their management.
  - **Incorporation of knowledge from observational and modeling process studies into ESMs;**
  - Implications of climate change for energy systems, strategies for mitigation & adaptation
  - Characterization of changes in regional and extremes to climate change
  - Understanding abrupt transitions
  - Bringing humans/technology/economics/health in via IAMs & other collaborations
- Recommendations on NERSC architecture, system configuration and the associated service requirements needed for your science?
  - A known development trajectory, the closer to other sites the better.
  - **A stable system! Use CCSM for benchmarking, not CAM**
  - **A balanced system! HPC + Data + Networks**
- General discussion
  - We view NERSC to be both a development and a production center
  - We are building the DOE data grids, what does a national computational grid look like
  - People: Can’t clone our heros, how to bring CS & Math expertise to bear ?