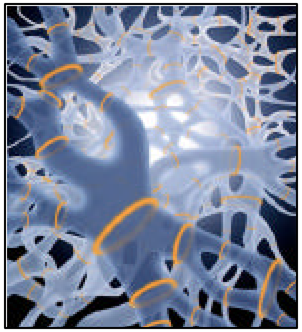
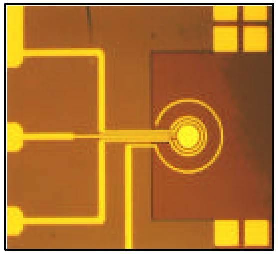
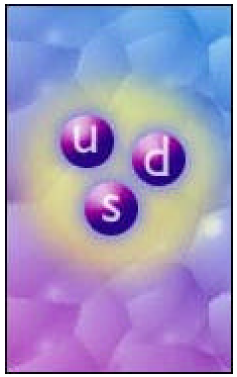
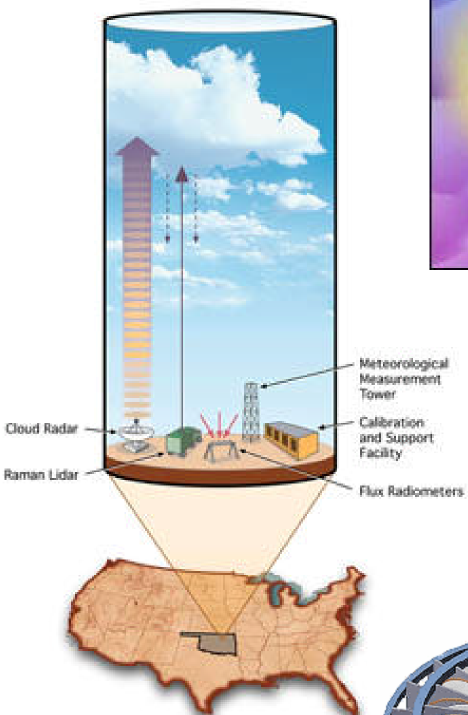


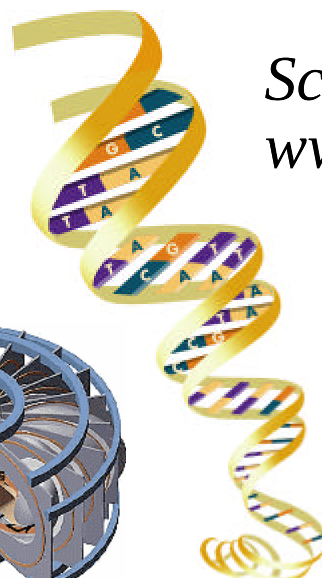






Computational Challenges and Directions in the Office of Science

Science for DOE and the Nation
www.science.doe.gov




NCSX

Dr. Fred Johnson
Program Manager
Advanced Scientific Computing Research

The Office of Science

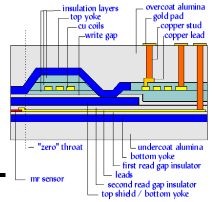
- **Supports basic research that underpins DOE missions.**
  - Provides over 40% of federal support to the physical sciences (including more than 90% of high energy and nuclear physics)
  - Provides sole support to select sub-fields (e.g. nuclear medicine, heavy element chemistry, magnetic fusion, etc.)
  - Supports the research of 15,000 PhDs and graduate students
- **Constructs and operates large scientific facilities for the U.S. scientific community.**
  - Accelerators, synchrotron light sources, neutron sources, etc.
  - Used by about 18,000 researchers every year
- **Provides infrastructure support for the ten SC laboratories.**

Advanced Computing and Networking is Critical to Office of Science Mission

Scientific problems of strategic importance typically:

- Involve physical scales that range over 5-50 orders of magnitude;
- Couple scientific disciplines, e.g., chemistry and fluid dynamics to understand combustion;
- Must be addressed by <u>teams</u> of mathematicians, computer scientists, and application scientists; and
- Utilize facilities that generate millions of gigabytes of data shared among scientists throughout the world.

The Scale of the Problem



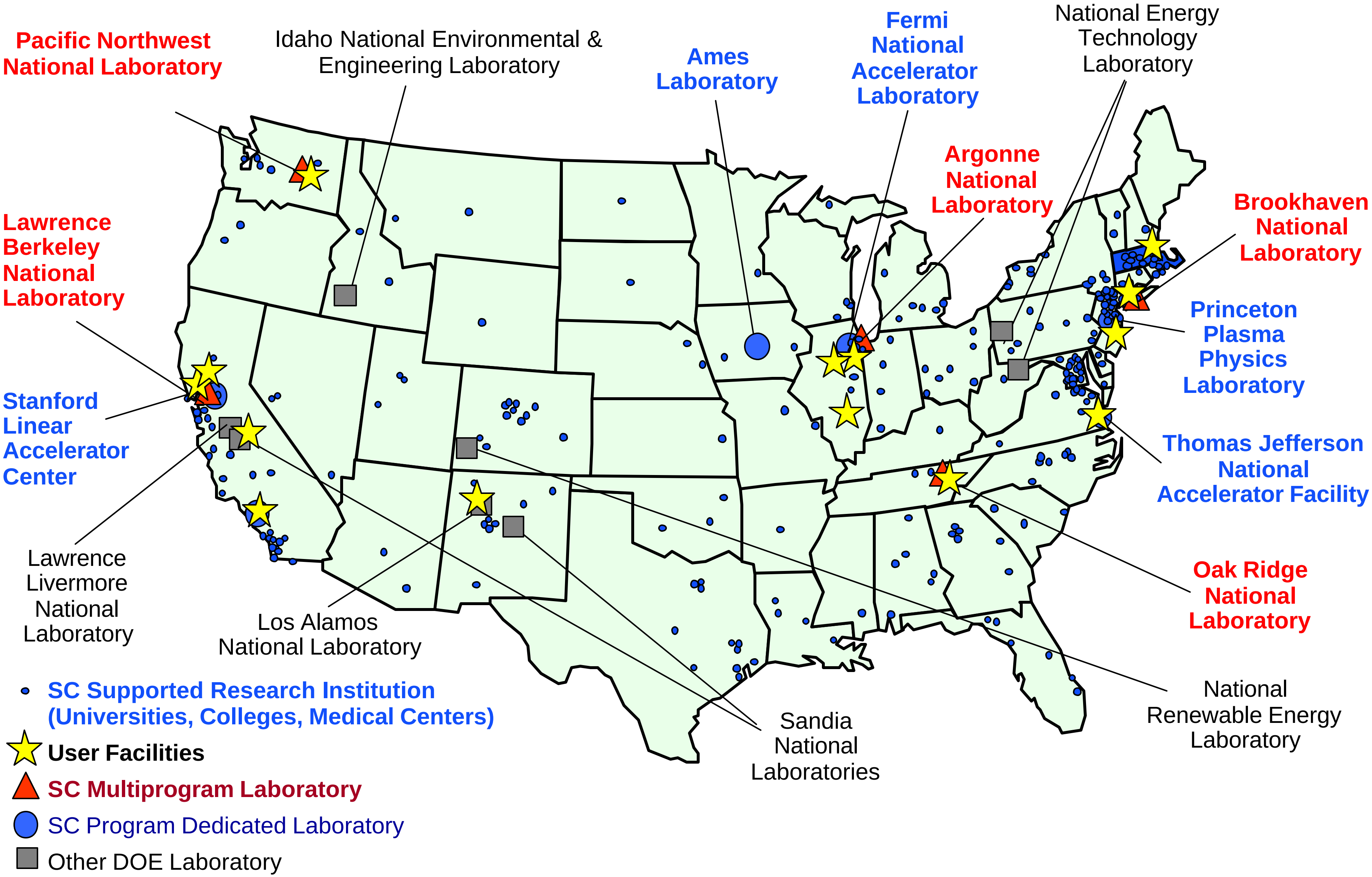
Two layers of Fe-Mn-Co containing 2,176 atoms corresponds to a wafer with dimensions approximately fifty nanometers ($50x\ 10^{-9}$m) on a side and five nanometers (5×10^{-9}m) thick. A simulation of the properties of this configuration was performed on the IBM SP at NERSC. The simulation lasted for 100 hrs. at a calculation rate of 2.46 Teraflops (one trillion floating point operations per second). To explore material imperfections, the simulation would need to be at least 10 times more compute intensive.

DOE Science Needs for Computing and Networking…

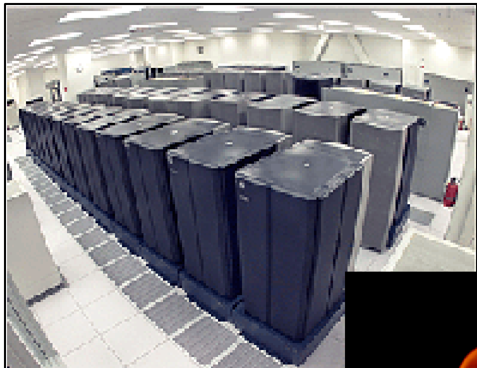
…far Exceed Commercial Market Capabilities

- Computing capabilities 10 to 100 times greater than those provided by commercial systems designed for business applications.
- Computing systems with more sophisticated architectures and higher performance components than current commercial systems.
- Mathematical and computer science techniques to enable a scientific application to effectively use 1,000s of processors simultaneously and effectively exploit sophisticated architectures.
- Networks and software to move hundreds to thousands of gigabytes of data between targeted science locations.
- Software “glue” to link computer and network components together with performance levels 1,000 to 1,000,000 times higher than commercial solutions.

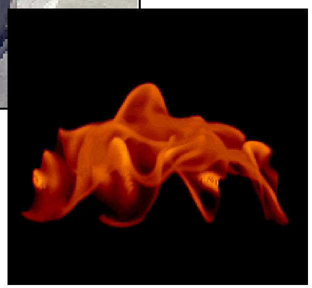
SC Laboratories, User Facilities and the Institutions That Use Them



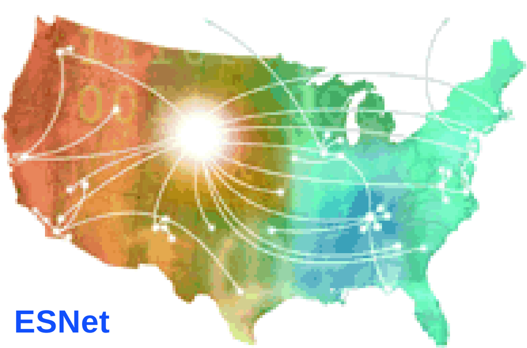
Advanced Scientific Computing Research



NERSC IBM SP RS/6000—"Seaborg"



modeling turbulent combustion



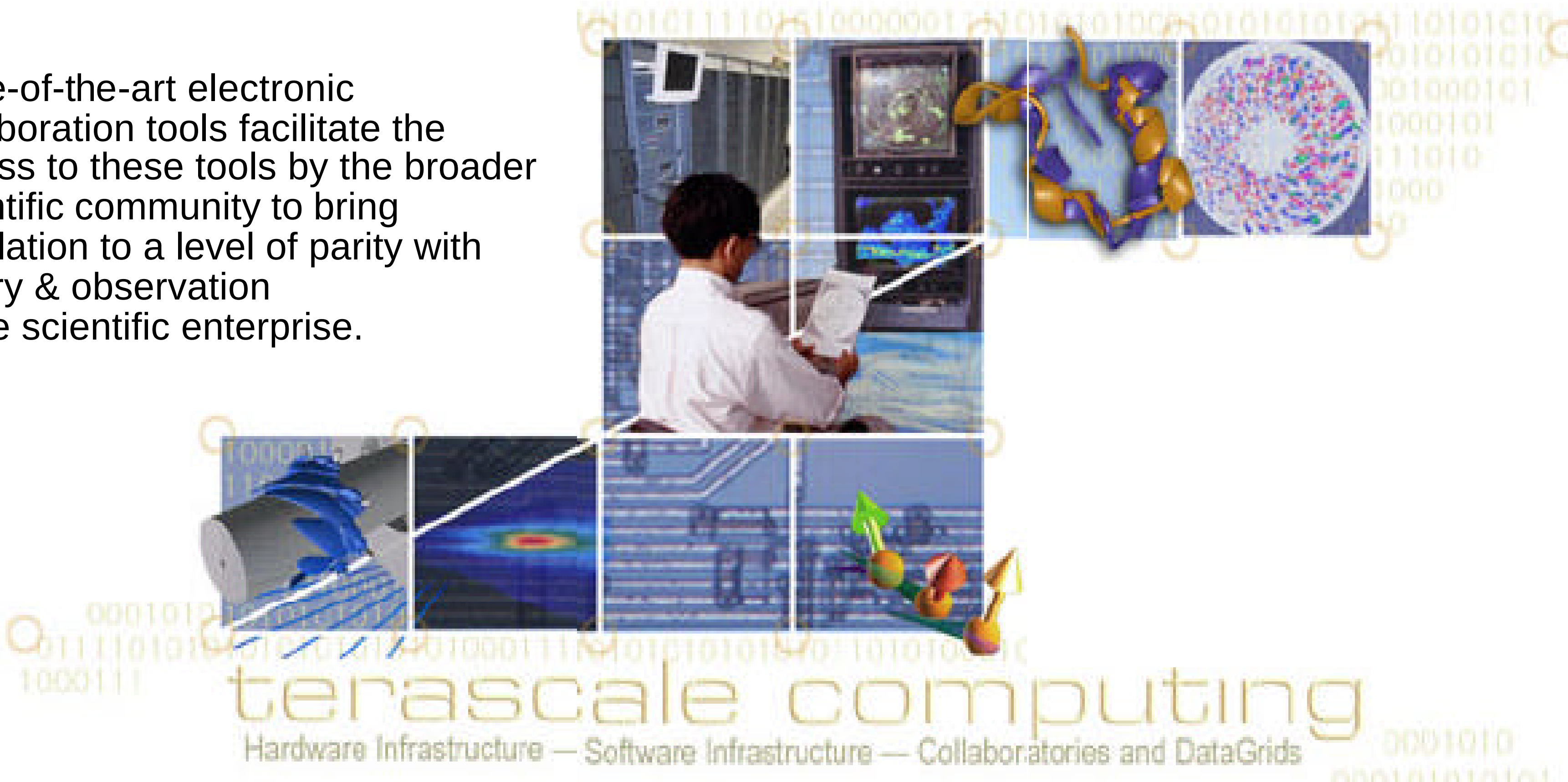
ESNet

- **Supports operation of supercomputer and network facilities available to researchers**
  - National Energy Research Scientific Computing Center (NERSC),
  - Advanced Computing Research Testbeds, and
  - Energy Sciences Network (ESNet).
- **Scientific Computing Research**
  - Applied Mathematics,
  - Computer Science, and
  - Advanced Computing Software Tools.
- **High Performance Networking, Middleware and Collaboratory Research**
  - Networking,
  - Collaboratory Tools, and
  - National Collaboratory Pilot Projects.

Scientific Discovery Through Advanced Computation (SciDAC)

- SciDAC brings the power of terascale computing and information technologies to several scientific areas -- breakthroughs through simulation.
- SciDAC is building community simulation models through collaborations among application scientists, mathematicians and computer scientists -- research tools for plasma physics, climate prediction, combustion, etc.

- State-of-the-art electronic collaboration tools facilitate the access to these tools by the broader scientific community to bring simulation to a level of parity with theory & observation in the scientific enterprise.



Ultrascale Simulation Capability Needs

FY2004-05 Timeframe

Application	Simulation Need	Sustained Computational Capability Needed (Tflops)	Significance
Climate Science	Calculate chemical balances in atmosphere, including clouds, rivers, and vegetation.	> 50	Provides U.S. policymakers with leadership data to support policy decisions. Properly represent and predict extreme weather conditions in changing climate.
Magnetic Fusion Energy	Optimize balance between self-heating of plasma and heat leakage caused by electromagnetic turbulence.	> 50	Underpins U.S. decisions about future international fusion collaborations. Integrated simulations of burning plasma crucial for quantifying prospects for commercial fusion.
Combustion Science	Understand interactions between combustion and turbulent fluctuations in burning fluid.	> 50	Understand detonation dynamics (e.g. engine knock) in combustion systems. Solve the "soot " problem in diesel engines.
Environmental Molecular Science	Reliably predict chemical and physical properties of radioactive substances.	> 100	Develop innovative technologies to remediate contaminated soils and groundwater.
Astrophysics	Realistically simulate the explosion of a supernova for first time.	>> 100	Measure size and age of Universe and rate of expansion of Universe. Gain insight into inertial fusion processes.

For More Information

Wednesday, 8:30	**Ray Orbach, "Ultrascale Computation and Scientific Discovery,"**
Thursday, 12:00	**Town Meeting on Ultrascale Simulation**
Exhibit Floor:	**Zone 5, DOE Science Group**
Web Sites:	http://www.sc.doe.gov/scidac
	http://www.ultrasim.info
	http://www.appsmatrix.info

Make no little plans; they have no magic to stir men's blood, and probably themselves will not be realized. Make big plans; aim high in hope and work, remembering that a noble logical diagram, once recorded, will never die, but long after we are gone will be a living thing, asserting itself with ever-growing insistency.

Daniel Burham, 1907, architect of the modern skyscraper.