Office of Science
Computational Science Graduate Fellowship

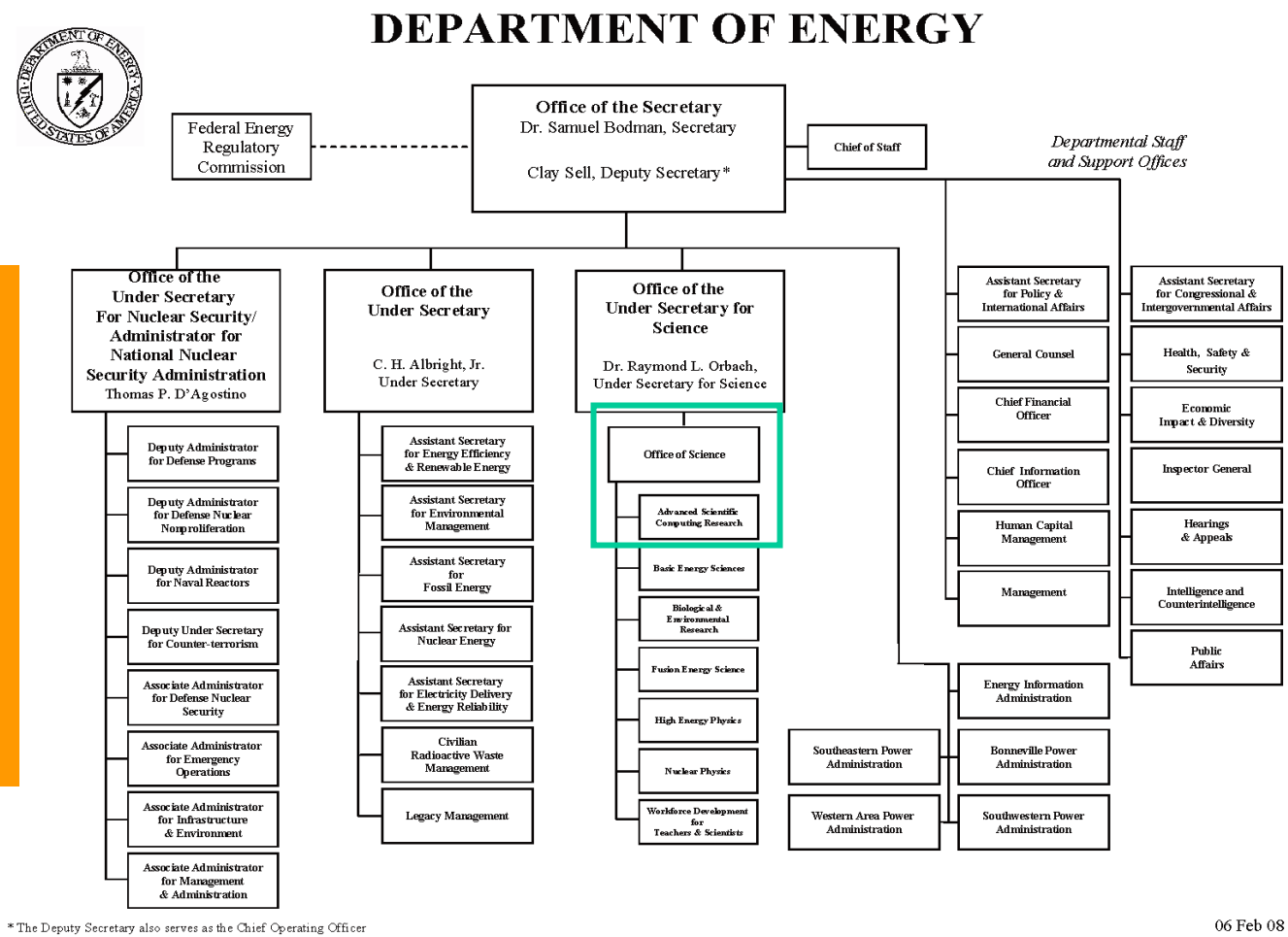
Barbara Helland

Advanced Scientific Computing Research

Department of Energy Organizational Structure

Advanced Scientific Computing Research Program

The Office of Science is the single largest supporter of basic research in the physical sciences in the United States.



U.S. Department of Energy

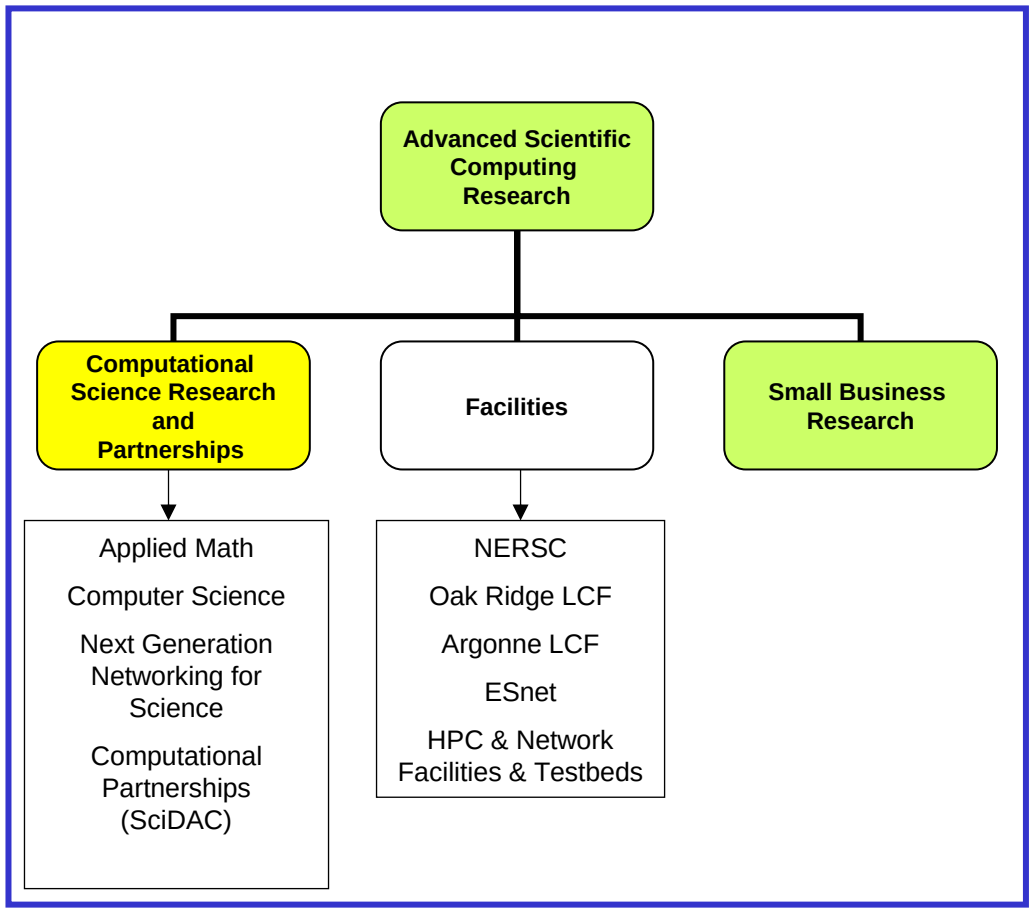
Office of Science

Advanced Scientific Computing Research

Advanced Scientific Computing Research Program

ASCR Mission: To deliver forefront computational and networking capabilities to scientists nationwide that enable them to extend the frontiers of science, answering critical questions that range from the function of living cells to the power of fusion energy.

ASCR Strategy: Bring together world-class researchers in applied mathematics, computer science and scientific disciplines across the Office of Science with world-class computing and network facilities to enable new scientific discovery.



http://www.science.doe.gov/ascr

The Plan for ASCR

- **Deliver Petascale Computing for Science Applications**
  - –Continue to make the Leadership Computing Facilities available to the very best science through INCITE.
  - –Continue to work with Pioneer Applications to deliver scientific results from day one.
- **Keep DOE Computational Science at the Forefront**
  - –Continue to nurture applications critical to DOE missions through SciDAC.
  - –Provide direct support for “bleeding-edge” research groups willing to take on the risk of working with emerging languages and operating systems.
  - –Foster innovative research at the ever blurring boundary between Applied Mathematics and Computer Science.
- **Realize the Promise of Exascale**
  - –Work with key science applications to identify opportunities for new research areas only possible through exascale computing.
  - –Support innovative research on advanced architectures and algorithms that accelerates the development of hardware and software that is well suited to exascale computational science.

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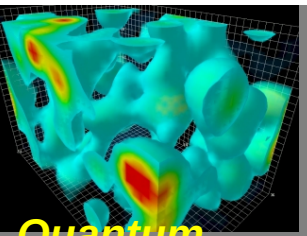
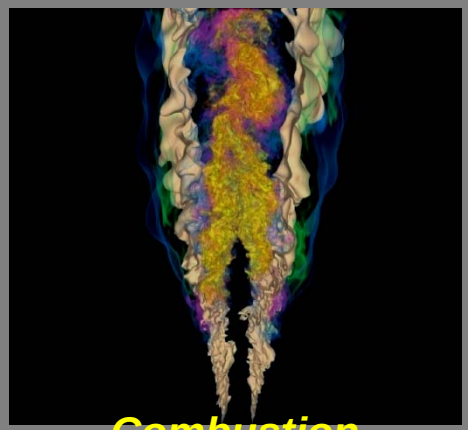
SciDAC: Keeping Computational Science at the Forefront

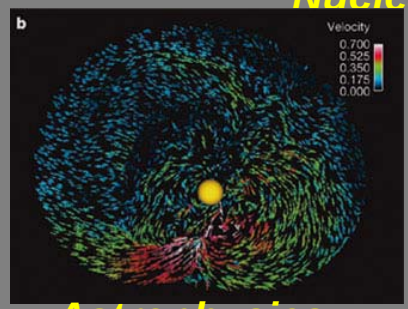
Advanced Scientific Computing Research Program



Quantum Chromodynamics

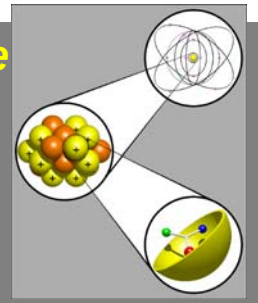


Combustion

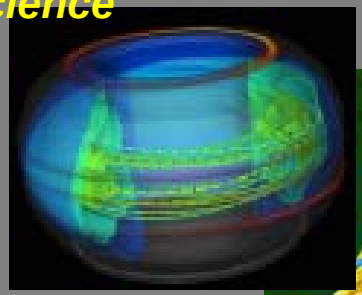


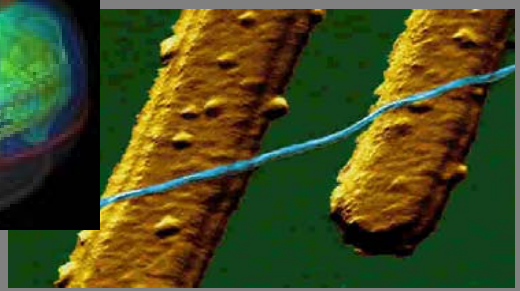
Astrophysics

Nuclear Structure



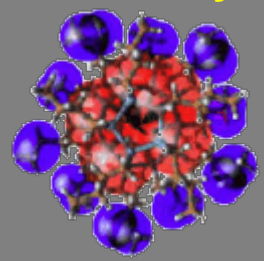
Fusion Energy Science



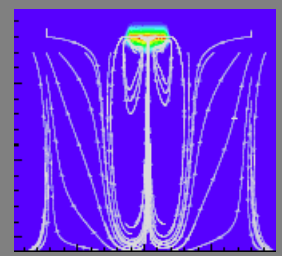


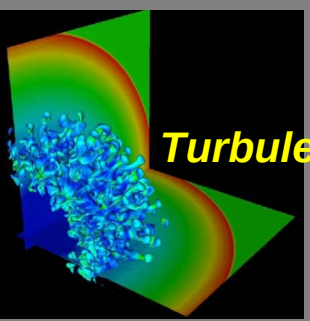
Materials Science

Chemistry

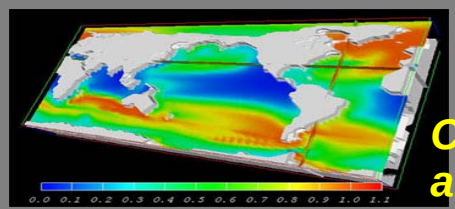


Groundwater Reactive Modeling and Simulation



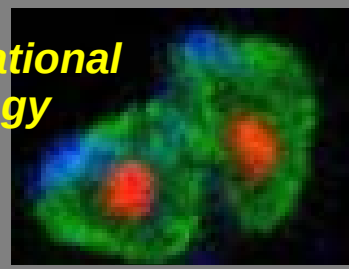


Turbulence



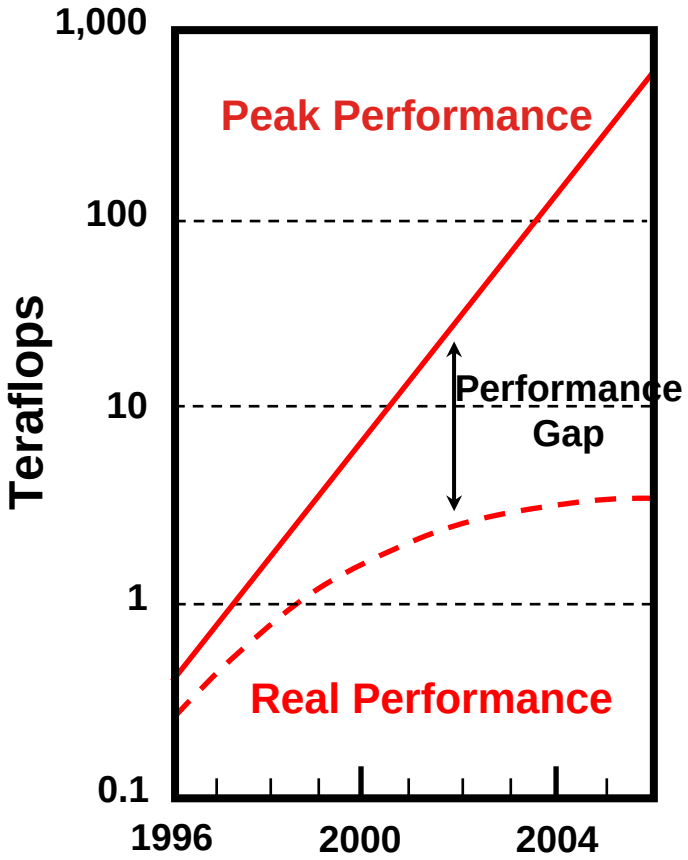
Climate Modeling and Simulation

Computational Biology



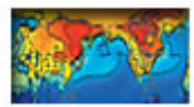
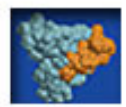
SciDAC: What We've Done

Advanced Scientific Computing Research Program



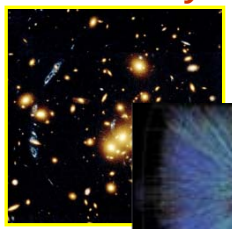
- Accelerating new tools and technologies for scientific computing through partnerships between science **application researchers, computer scientists and applied mathematicians**
- Improved effectiveness of scientific applications codes up to 10,000%
- Some key contributions of SciDAC teams
  - First laboratory-scale flame simulation in three dimensions
  - 3-D fusion plasma simulations, validated experimentally
  - Improved and integrated climate models
  - First ever 3-D Supernovae simulations deliver insights were no experiment is possible but validated by observational data.



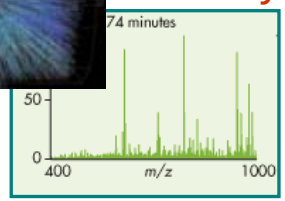
The Data Explosion

10Terabytes/day



2Petabytes/exp

1Petabyte/yr



Astro-physics

Nuclear Physics (Star)

Biology (Peptide data)

Two different kinds of very large data sets:

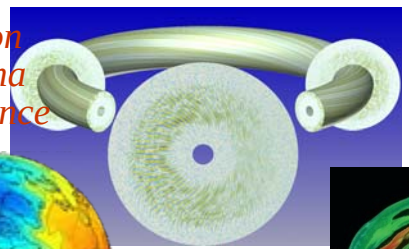
Experimental data (growing exponentially)

- High energy physics, power grids, environment and climate observation data, cosmology, biological mass-spectrometry.
- Data needs to be retained for long term.

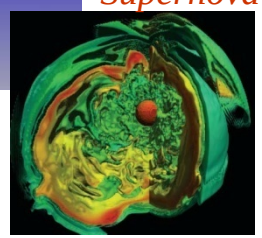
Simulation data (growing even faster)

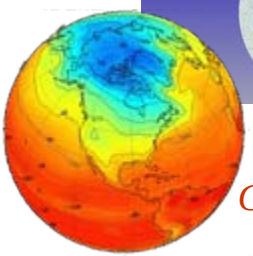
- Nuclear energy, astrophysics, climate, fusion, catalysis, Lattice Quantum Chromodynamics.
- Post processing of data using quantum Monte Carlo, clustering, Single Value Decomposition, perturbation theory, and molecular dynamics.

Fusion Plasma turbulence



Supernova





Climate

50-500TB/simulation

Where is the wisdom that is lost in knowledge? Where is the knowledge we have lost in information?" -T.S. Eliot

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Revolutionizing global challenges in energy and environment

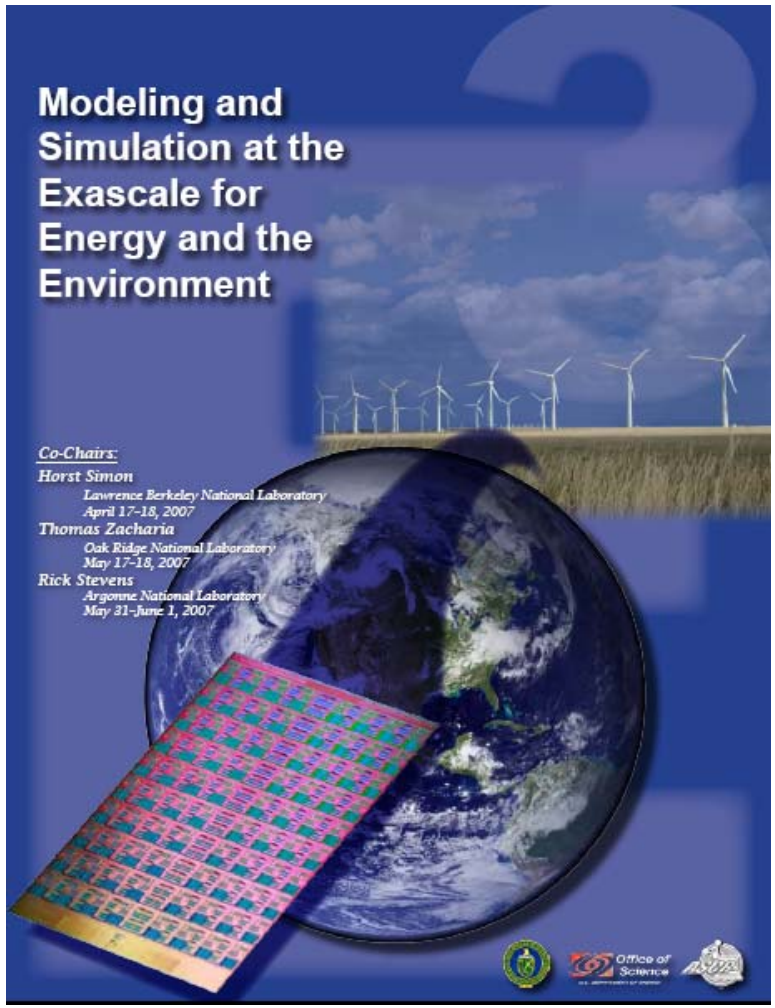
Advanced Scientific Computing Research Program

Climate, Combustion, Fusion, Fission Solar, Biology, Socioeconomic Modeling and Astrophysics

Mathematics, Computer Science Algorithms, Software infrastructure and Cyberinfrastructure

Integrated program- investments in hardware and software research and development

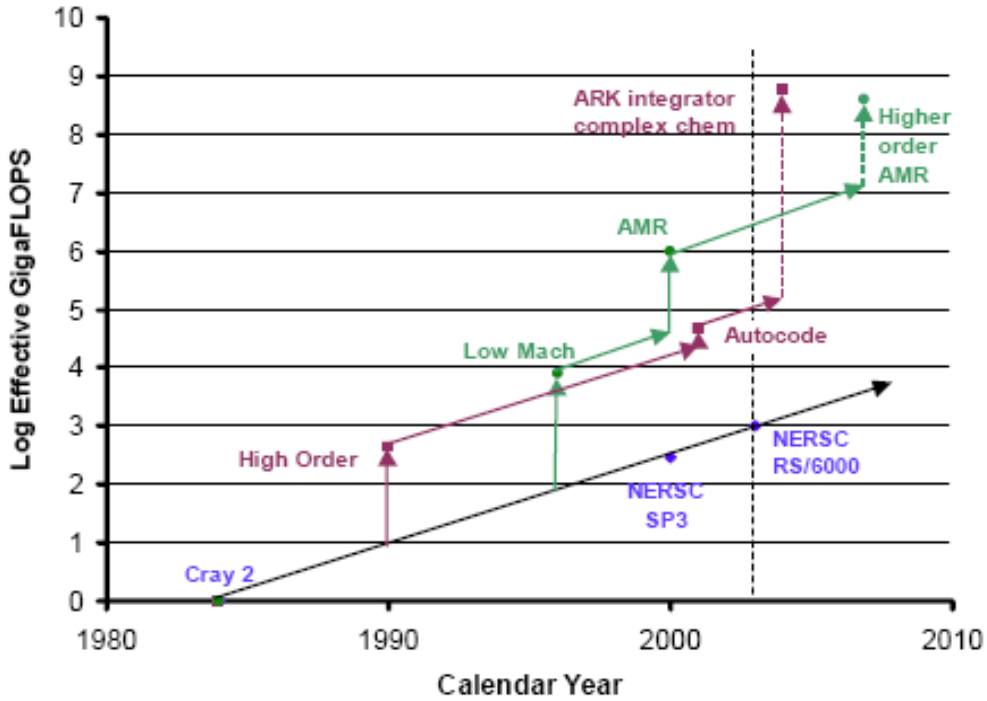
Tight coupling to a selected set of science communities and the associated applied mathematics R&D.



The Promise of Computational Science at the Exascale

- Today **(with ~10 TF sustained)** we can <u>almost</u> simulate the length scales of simple combustion
- Must address in the future:
  - More complex chemical networks and flames
  - Complex engine geometries
  - Cleaner and more efficient combustion
- This will require at least **3-300 exaflops, 6-8 orders of magnitude more than today**

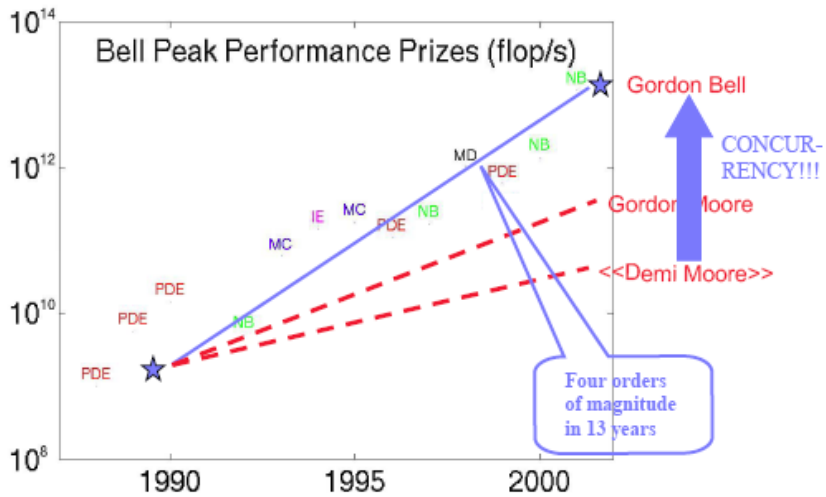
"Moore's Law" for combustion simulations



Math and CS improvements reduce the necessary compute power significantly.

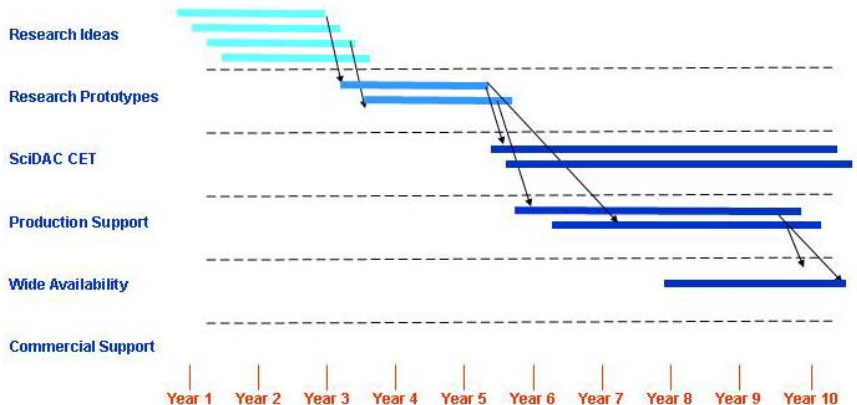
It's not just hardware!

Gordon Bell Prize outpaces Moore's Law



- Applied Math and Computer Science have contributed even more than Moore
  - Adaptive Mesh
  - MPI / MPICH / MVAPICH
  - Multiscale Math
  - Libraries
  - Tools

Timeline for ASCR Research Software Pipeline



- Much of these hard-earned gains won't work as well or at all on the new architectures.
- Building/re-building science application software takes time.

The Promise of the Future: *Computational Science Graduate Fellows*

"To keep America competitive into the future, we must trust in the skill of our scientists and engineers and empower them to pursue the breakthroughs of tomorrow..."

President George W. Bush
State of the Union Address
January 28, 2008