2009 Conference on High Speed Computing

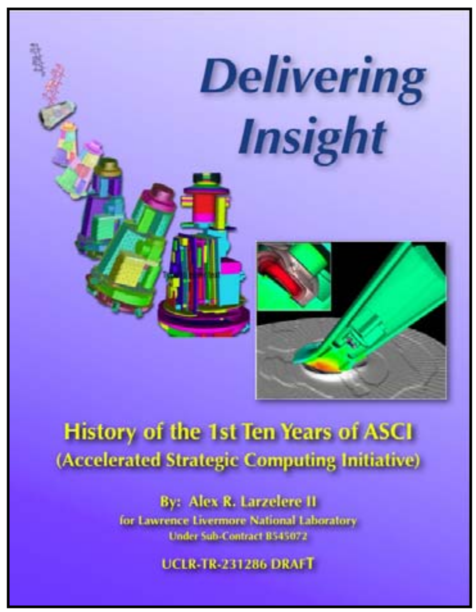
Potential Roles for High Performance Computing in the Obama Administration

With Specific Emphasis on DOE

Victor Reis
Senior Advisor
Department of Energy

&

Alex Larzelere
Lt. USCG(Ret)
Department of Energy



Outline

- The Obama Administration Views on HPC
  - From White House Website
- A very short history of U.S. High Performance Computing
  - The role of computer architecture
- A short history of ASCI
  - Lessons Learned
    - Problem & Partnership drives the platform
- Potential Future Problems
  - From short survey
- Discussion
  - Lively
- Summary
  - Problems & Partnerships drive the Platform
  - Lots of Problems
  - Lots of Opportunity

Obama Administration: Lots of Science & Technology stuff, but no mention of High Performance Computing

www.whitehouse.gov

Science

"Today, we face a new set of challenges, including energy security, HIV/AIDS, and climate change. President Obama and Vice President Biden believe federally funded scientific research should play an important role in advancing science and technology in the classroom and in the lab."

Technology

"President Obama and Vice President Biden understand the immense transformative power of technology and innovation and how they can improve the lives of Americans. They will encourage the deployment of modern communications infrastructure to improve America's competitiveness and employ technology to solve our nation's most pressing problems -- including improving clean energy, healthcare costs, and public safety."

Energy

"The energy challenges our country faces are severe and have gone unaddressed for far too long. Our addiction to foreign oil doesn't just undermine our national security and wreak havoc on our environment -- it cripples our economy and strains the budgets of working families all across America. President Obama and Vice President Biden have a comprehensive plan to invest in alternative and renewable energy, end our addiction to foreign oil, address the global climate crisis and create millions of new jobs."

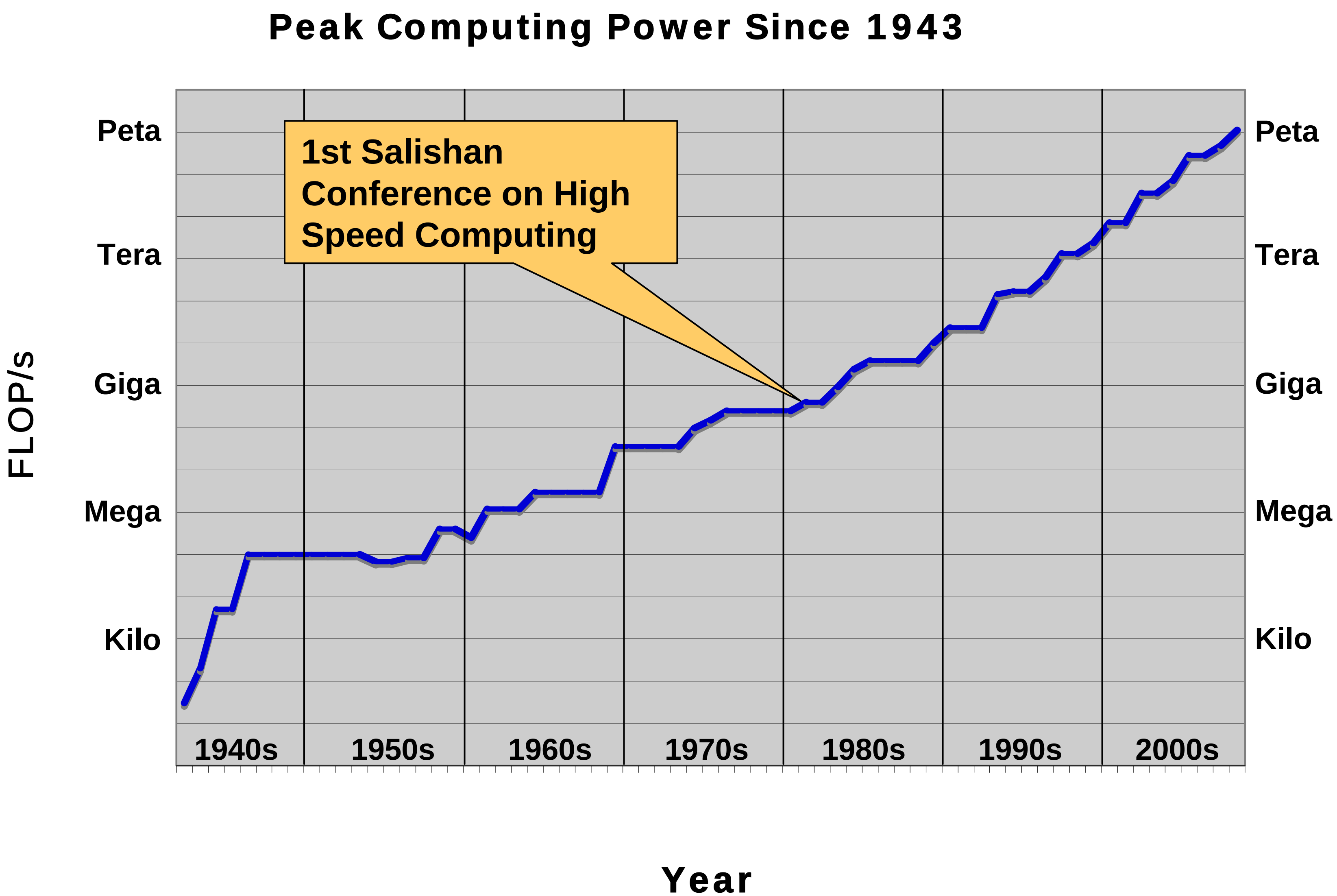
Climate

"Invest in Climate-Friendly Energy Development and Deployment: Invest $150 billion over the next ten years to enable American engineers, scientists and entrepreneurs to advance the next generation of biofuels and fuel infrastructure, accelerate the commercialization of plug-in hybrids, promote development of commercial-scale renewable energy, and begin the transition to a new digital electricity grid. This investment will transform the economy and create 5 million new jobs."

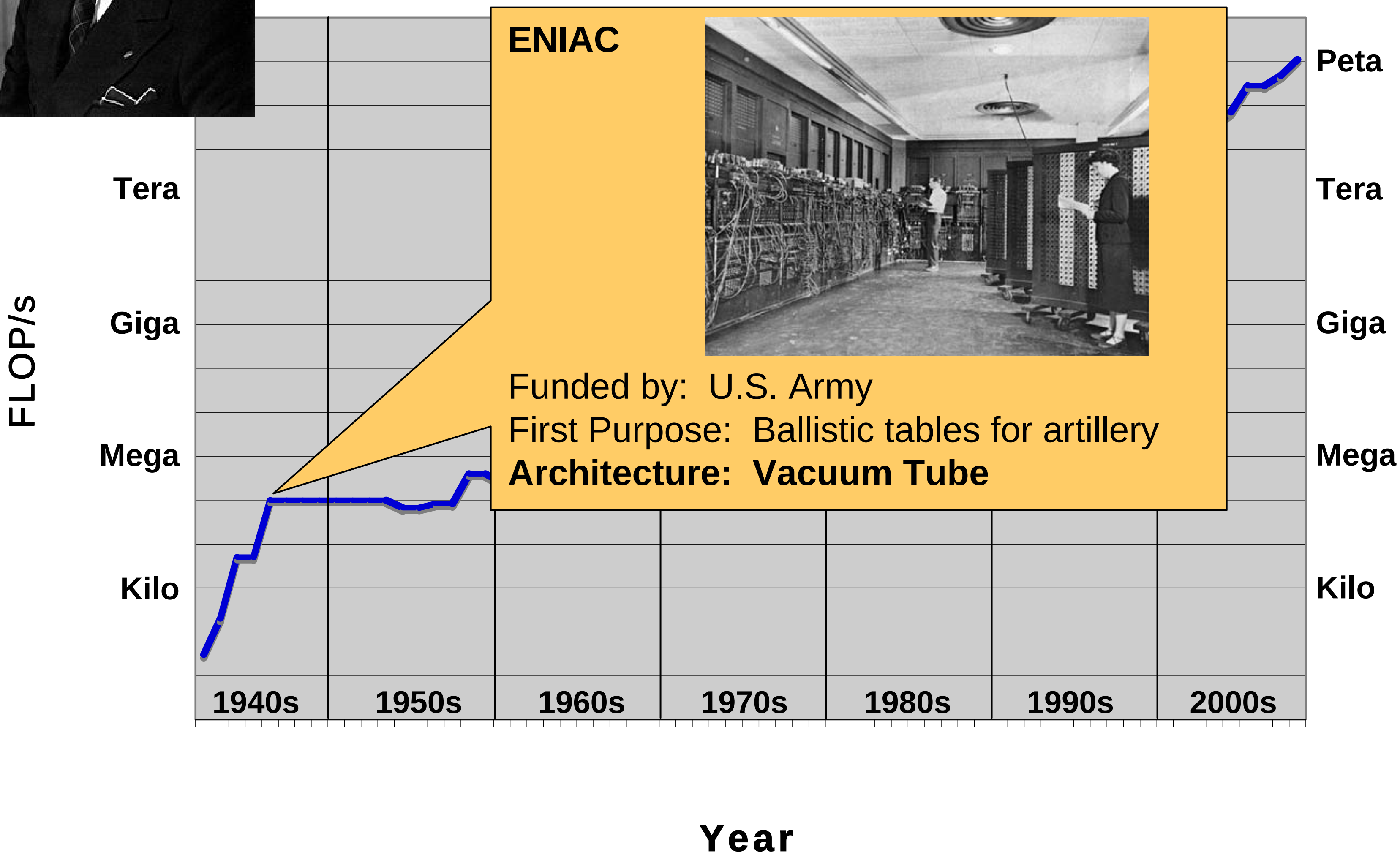
BioMedical

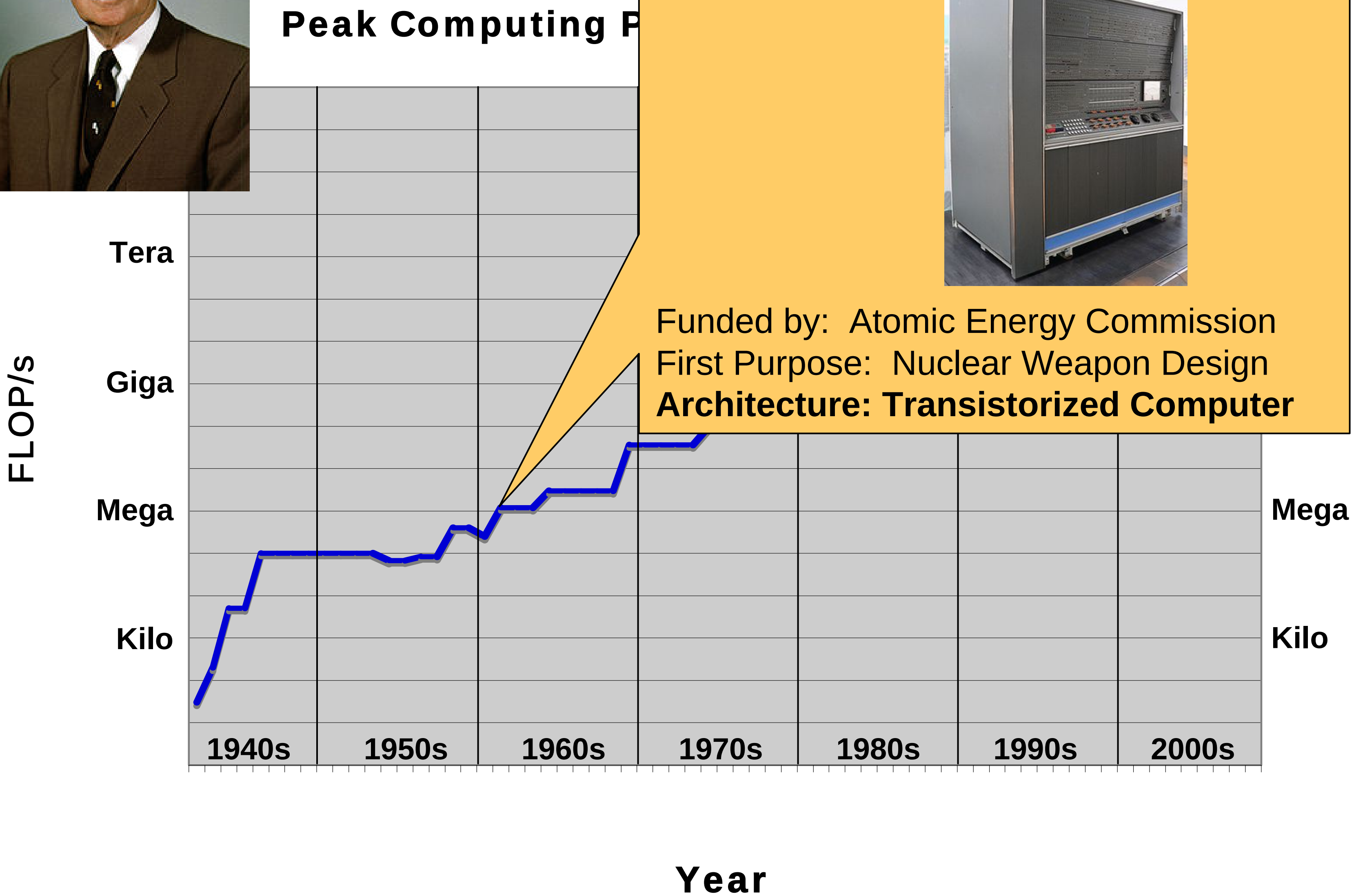
"Advance the Biomedical Research Field: Support investments in biomedical research, as well as medical education and training in health-related fields. Fund biomedical research, and make it more efficient by improving coordination both within government and across government/private/non-profit partnerships."

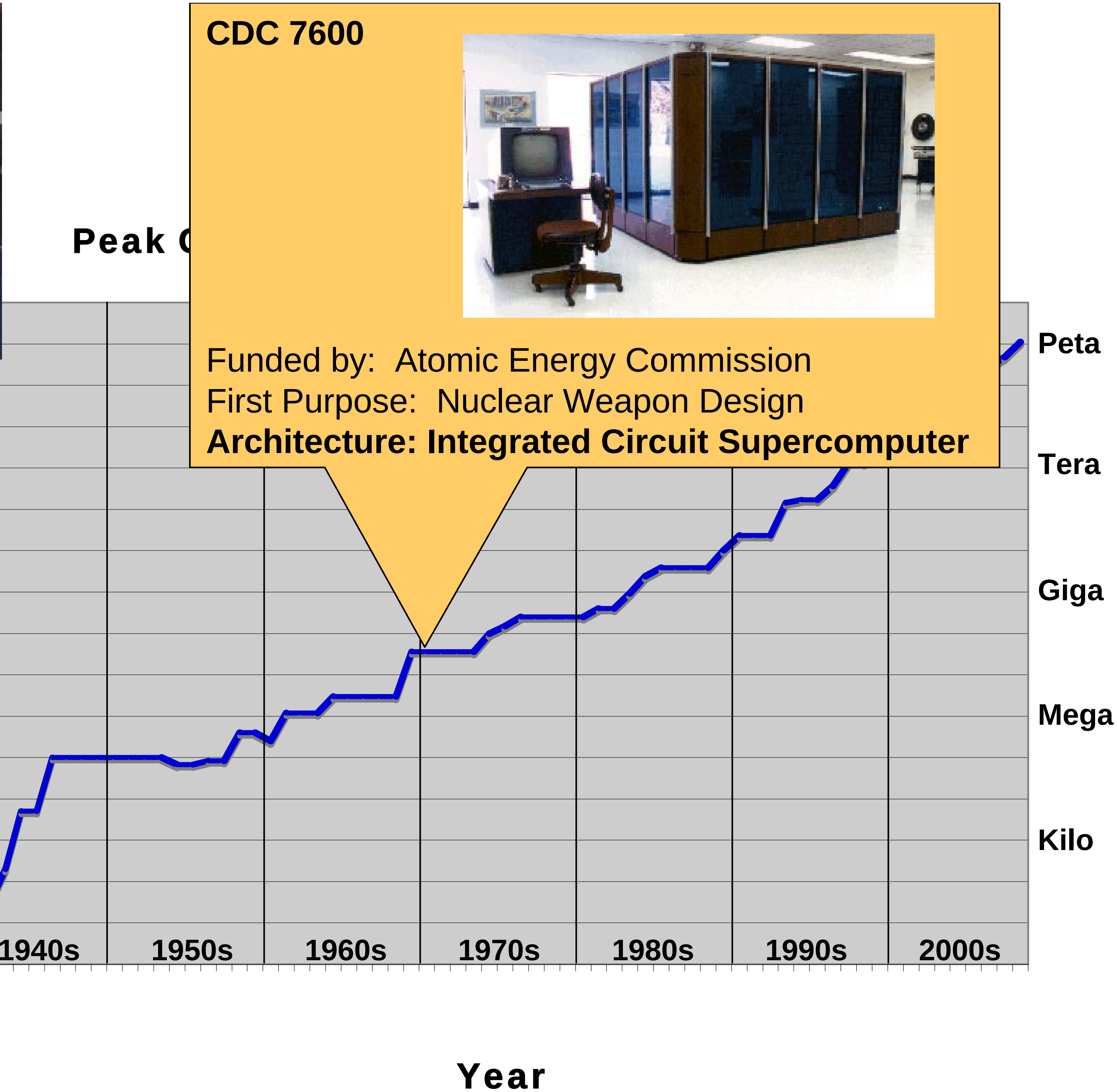
History of Peak Computing



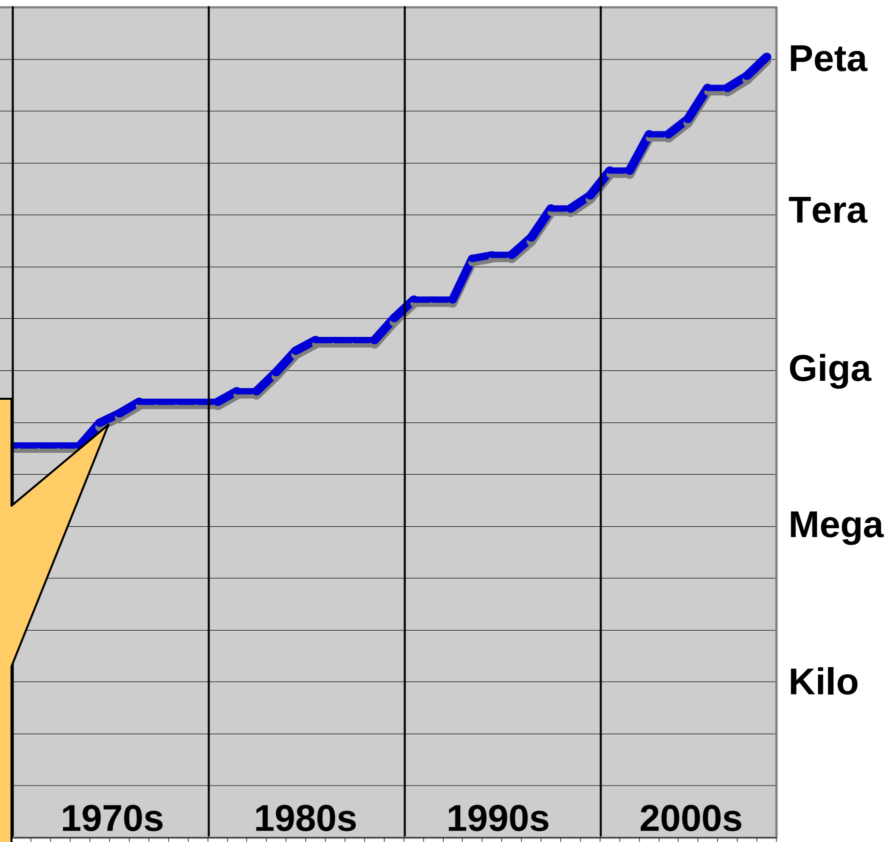
Peak Computing Power Since 1943




Peak Computing P
FLOP/s
Tera
Giga
Mega
Kilo
Mega
Kilo
1940s
1950s
1960s
1970s
1980s
1990s
2000s
Year
IBM 7300
Funded by: Atomic Energy Commission
First Purpose: Nuclear Weapon Design
Architecture: Transistorized Computer


CDC 7600
Funded by: Atomic Energy Commission
First Purpose: Nuclear Weapon Design
Architecture: Integrated Circuit Supercomputer
Peak C
FLOP/s
Peta
Tera
Giga
Mega
Kilo
1940s
1950s
1960s
1970s
1980s
1990s
2000s
Year

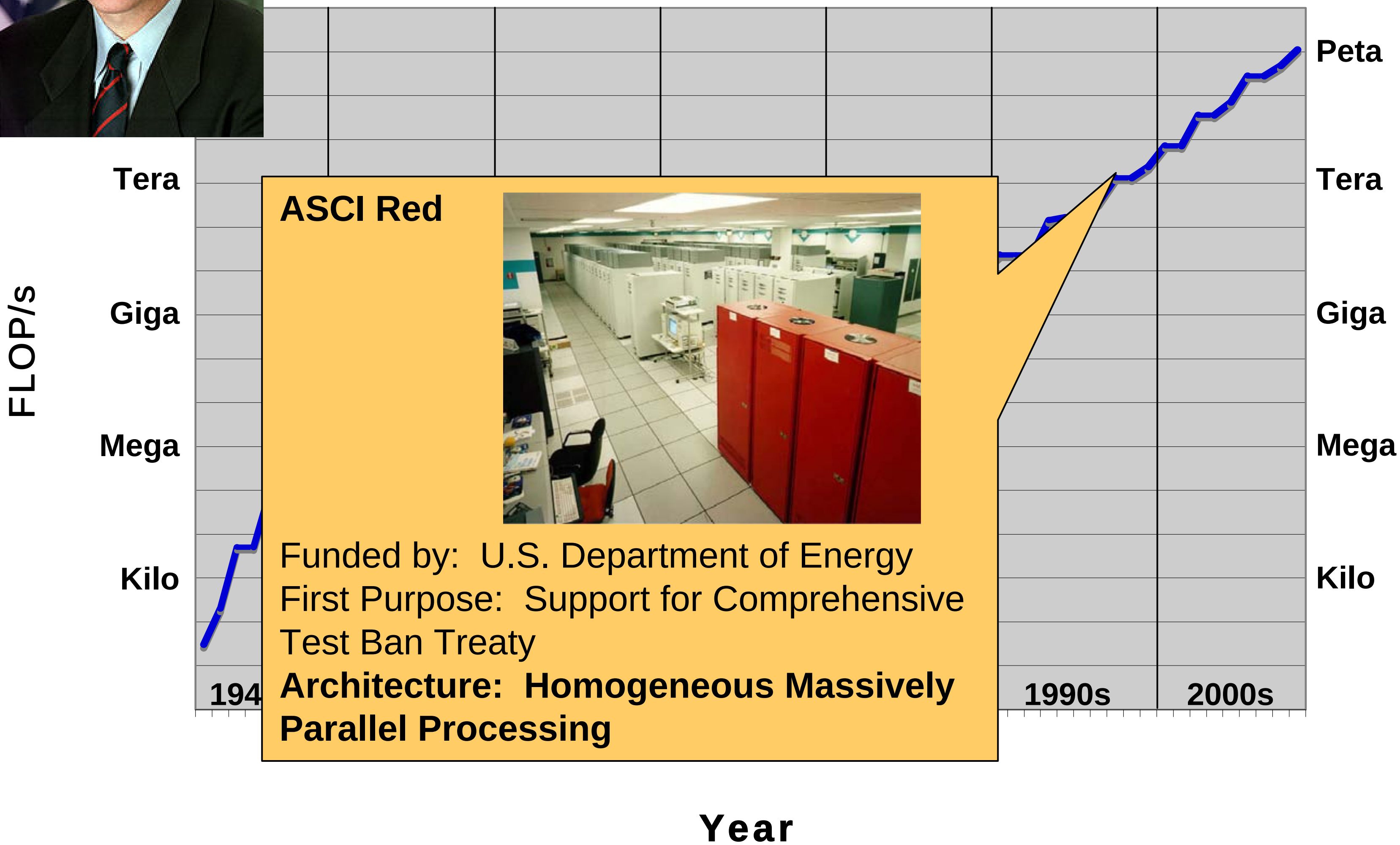
Peak Computing Power Since 1943



Cray 1

Funded by: Energy Research and Development Administration
First Purpose: Nuclear Weapon Design
Architecture: Vector

Peak Computing Power Since 1943



ASCI Red

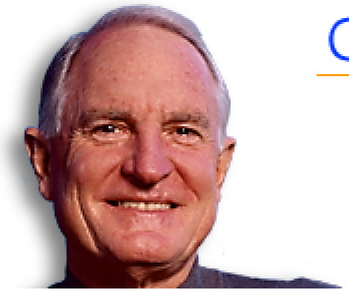
Funded by: U.S. Department of Energy
First Purpose: Support for Comprehensive Test Ban Treaty
Architecture: Homogeneous Massively Parallel Processing

12/16/96 NEWSFLASH - ONE TERAFLOPS BROKEN BY SANDIA/INTEL SYSTEM

The teraflops milestone was announced this morning by Energy Secretary Hazel O'Leary, who called it "an astonishing and extraordinary achievement."

"The nation has received an early holiday gift, and it was delivered online, on time, and on budget," said a jubilant O'Leary. "This milestone, once thought to be unachievable in this century, will help us deliver on our commitment to provide a safe, effective nuclear deterrent without the need for underground tests."

12/16/96 NEWSFLASH - ONE TERAFLOPS BROKEN BY SANDIA/INTEL SYSTEM



Craig R. Barrett

Chairman of the Board

"Today's accomplishment is computing's equivalent to breaking the sound barrier," said Craig R. Barrett, Intel executive vice president and chief operating officer. "Just a few years ago, a teraflop was an intellectual barrier that nature dared us to cross. Now that we've surpassed that barrier

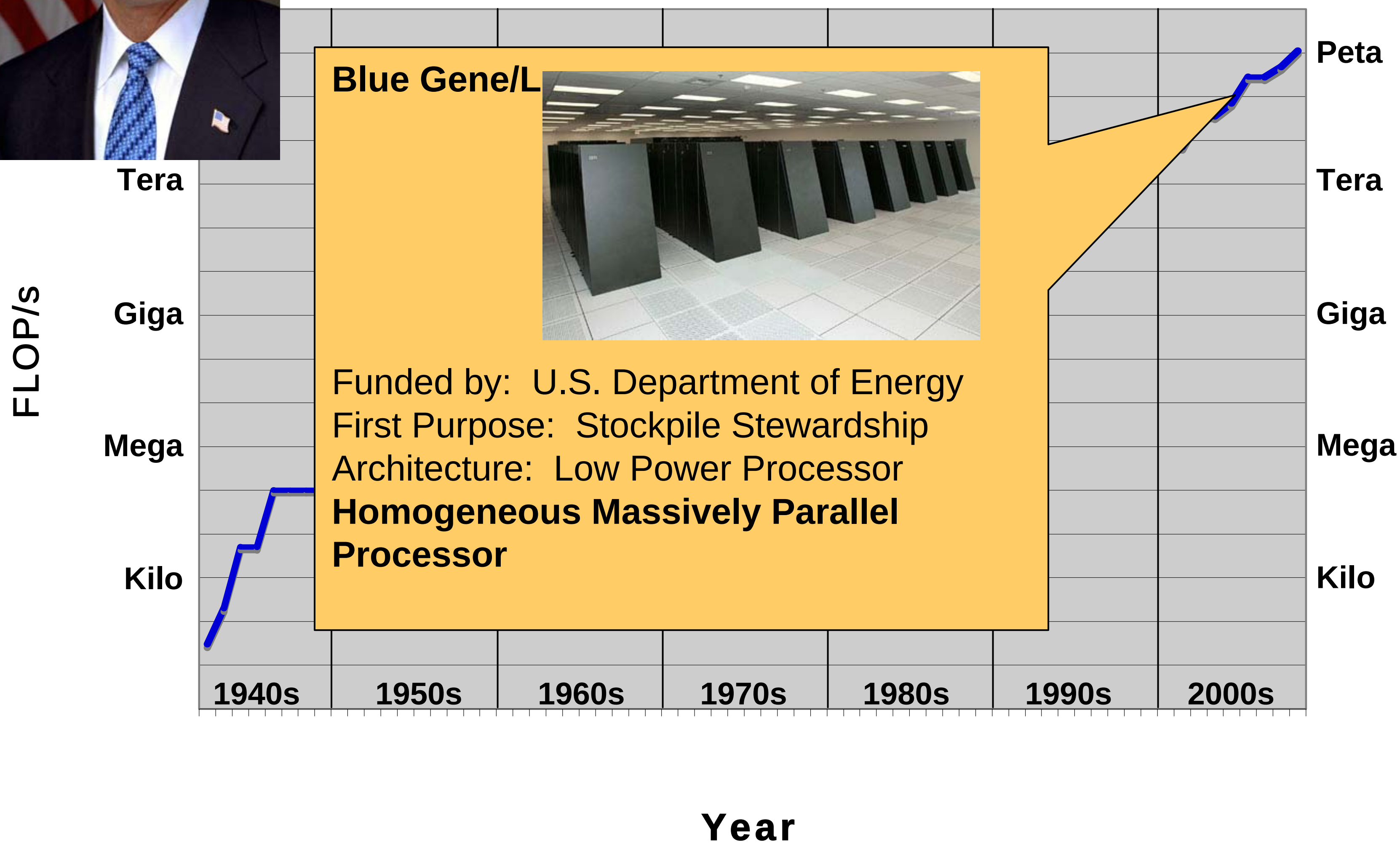
"The Intel/Sandia teraflop computer is built from commercial, off-the-shelf products and technologies including the same Pentium Pro processor in many of today's workstations and servers," said Ed Masi, general manager and vice president of Intel's Server Systems Products Division. "Using commercially available technology has enabled the government to utilize the R&D muscle of the marketplace, focusing tax dollars on combining these standard building blocks into the world's most powerful computer."

12/16/96 NEWSFLASH - ONE TERAFLOPS BROKEN BY SANDIA/INTEL SYSTEM

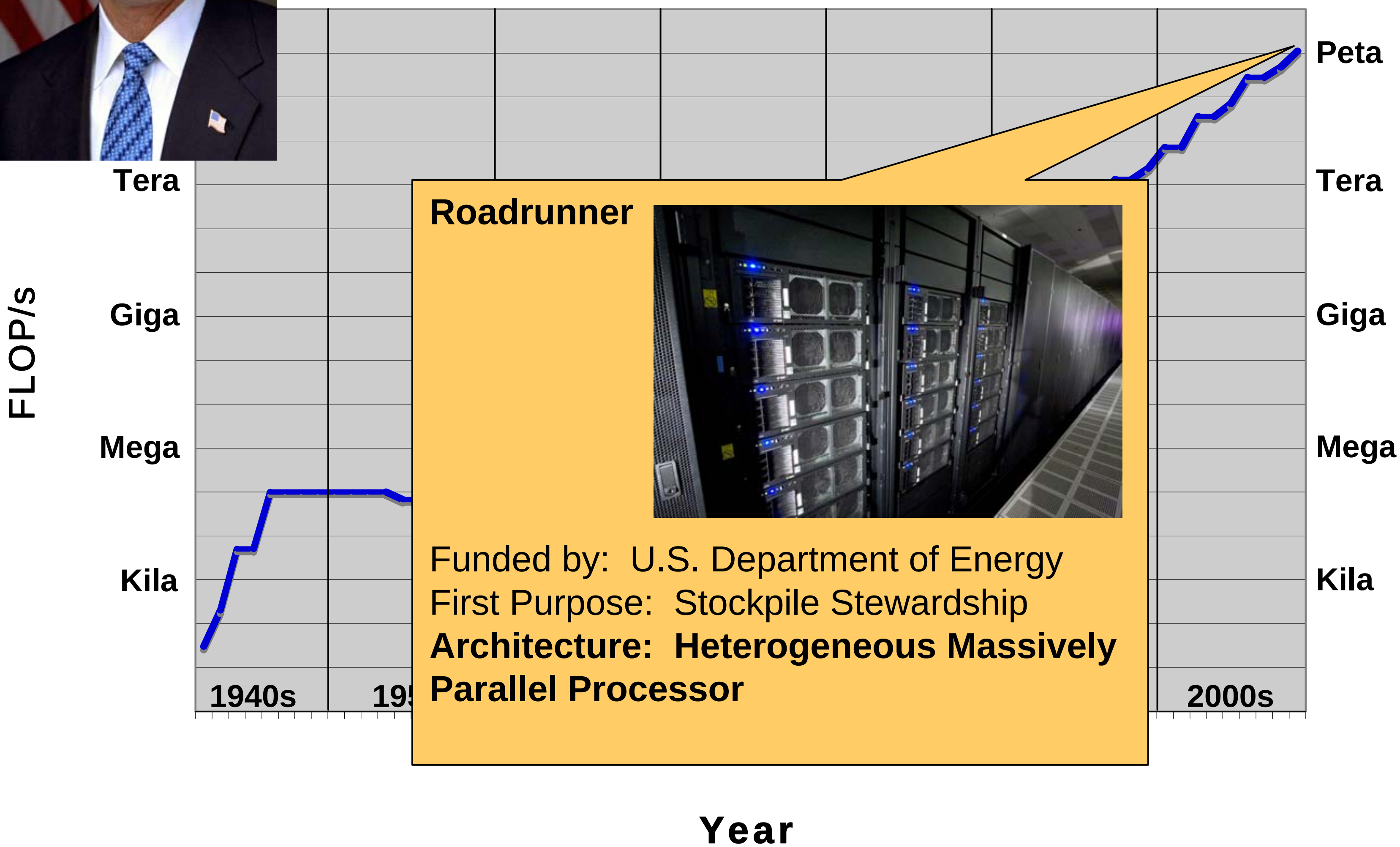
Vice President Al Gore issued a statement saying that the teraflops breakthrough "confirms the United States as the world's preeminent computer power, and maintains our national standard of global scientific and technological leadership."

"When I authored the High Performance Computing Act of 1991, this kind of computing power was a noble but distant dream," Gore commented. "We knew it would take more than bigger machines and better software. It would take an entirely new kind of computing technology. With the strong support of the Clinton Administration and the ingenuity of American industry, we have been able to bring about this achievement. I am proud of this Administration's role in making this new technology possible."

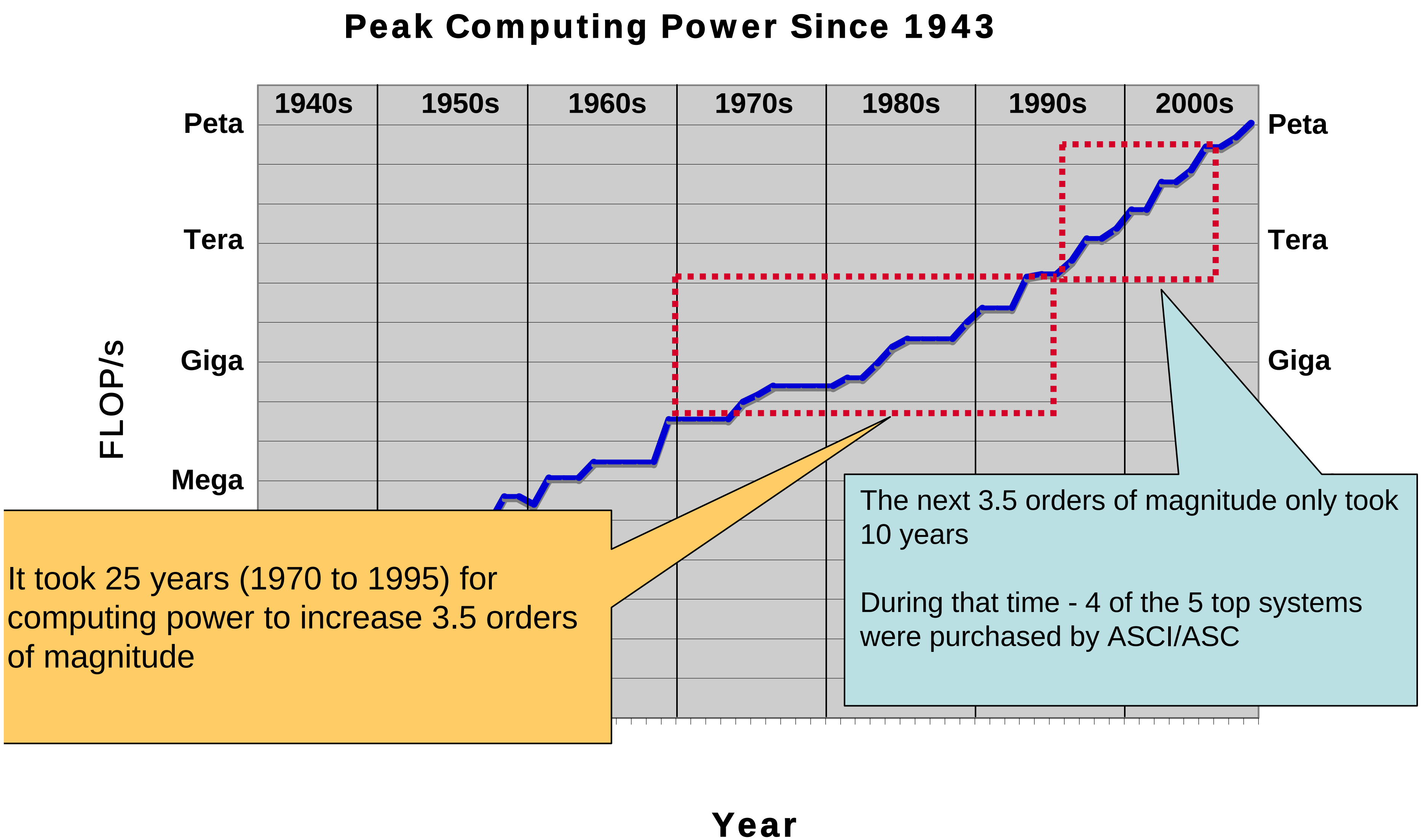
Peak Computing Power Since 1943



Peak Computing Power Since 1943



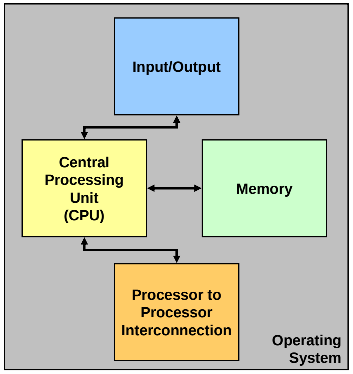
Changing the Rate of Peak Computing Power Growth



Some Observations

- All of the systems that appear on the "peak power" list were purchased by governments, for government purposes; vast majority by the U.S.

- Most of the time the shift in computer architecture appears to result in a (temporary) slowing of the growth rate. Shifts included:
  - Transistors
  - Microprocessors
  - Vectors
  - Homogeneous Massively Parallel
  - Low Powered Homogeneous Massively Parallel
  - Heterogeneous Massively Parallel



- Primarily due to the need to change programming models, develop tools, and to optimize programs.

- Accelerated Strategic Computing Initiative changed the model

How?
– Are the ASCI "lessons learned" applicable to the next generation?

ASCI was a response to the Stockpile Stewardship Challenge

July 3, 1993

President Clinton:

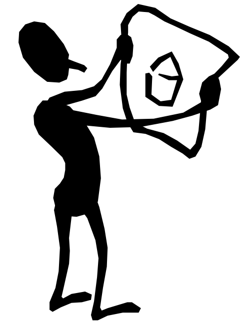
- Continue Moratorium on Nuclear Weapons Testing
- Seek a Comprehensive Test Ban Treaty

"to assure that our nuclear deterrent remains unquestioned under a test ban, we will explore other means of maintaining our confidence in the safety, the reliability, and performance of our own weapons."

November 1993, Direct DOE to:

"to establish a stewardship program to ensure the preservation of the core intellectual and technical competence of the U.S. in nuclear weapons."

Accelerated Strategic Computing Initiative



Talk to Designers First

- develop performance & time requirements

Multi-lab effort

- each lab gets one

Industry Lab Partnerships

Commercial Components

United States

Setting the ASCI Requirements – What do you need, When?

The complexity of modeling nuclear weapons performance defined the compute needs (100 teraFLOP/s)

JUSTIFICATION FOR THE NEED FOR 100 TFLOP COMPUTERS TO SOLVE NUCLEAR WEAPON SIMULATION PROBLEMS

- 1. To simulate a nuclear weapon primary boost with sufficient resolution (dimensions are classified), today's 2D codes require 500 Cray YMP hours.
- 2. Experiments have shown that primary boost is fundamentally 3D and to understand the effects of aging and/or changes in the weapons, they must be simulated in 3D. The move from 2D to 3D increases the compute time by a factor of 1000 to 500,000 Cray YMP hours.
- 3. Today's codes contain many empirical factors that are based on tests of existing weapons. As weapons age and changes are made, these empirical factors must be replaced by better physics. The calculation of the additional physics is expected to increase the compute time by a factor of ~100 to 50,000,000 Cray YMP hours. A reasonable run time for a weapons analysis code is about 100 hours (4 days). This allows the analyst to remember what they computed and provides enough iteration to support problem solving. Therefore, 500,000 Cray YMP equivalents (50,000,000 YMP hours/100 hours) are needed to support 3D, better physics simulations of primary boost.
- 5. The peak performance of a Cray YMP is 333 MFlops. Thus the Flops needed to support 3D, better physics simulations of primary boost is roughly 167 TFlops (500,000 Cray Equivalents * 333 MFlops/ Cray).
- NOTE: Please remember that the 167 TFlop figure is based on the problem and does not pre-suppose how the Flops will be delivered. It is also based on our current understanding of the problem and the compute power needed do the simulations. As the codes are developed we anticipate that research will provide additional understanding that will probably increase (physics issues) and decrease (algorithms efficiencies) the compute power needed. Hopefully they will balance each other out.2

By Randy Christensen and Charlie McMillan, LLNL

Before the final retirement of leading stockpile weapons designers ~ 2004.

Seymour Sack

A program - not just a goal

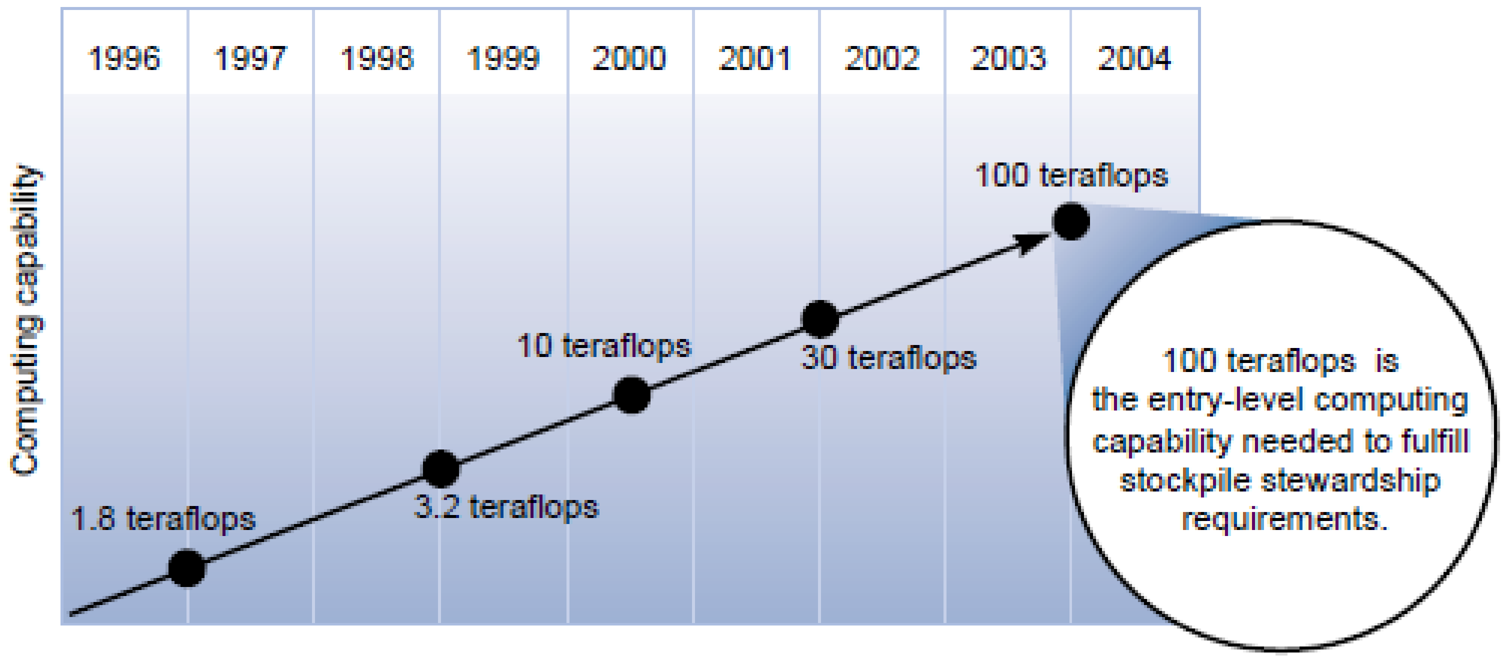
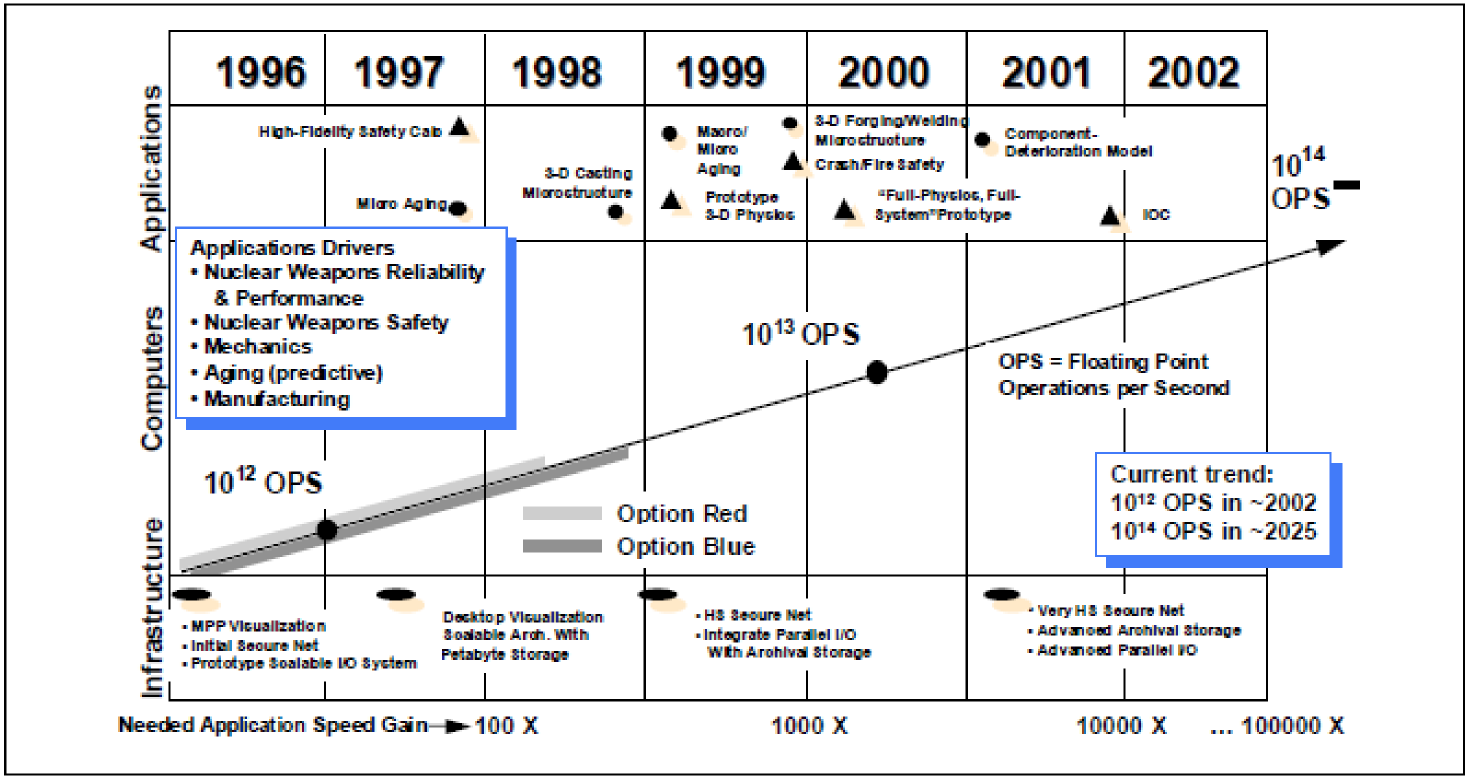


Figure 4. The ASCI goal is to achieve the 100-teraflops (trillion-floating-point-operations-per-second) threshold by 2004.

An integrated, Balanced Program



A comprehensive program to develop the applications, development tools, computers, networks, and visualization to create the simulation capabilities to enable a science based approach to stockpile stewardship.

ASCI was built upon Partnerships

Labs

Los Alamos National Laboratory

Sandia National Laboratories

Hardware

IBM

intel

CRAY

hp invent

COMPAQ

sgi

LINUX NETWORX

APPRO

Sun microsystems

Academia

California Institute of Technology 1891

Stanford University

Illinois

The University of Utah

The University of Chicago

Software

ParaView Parallel Visualization Application

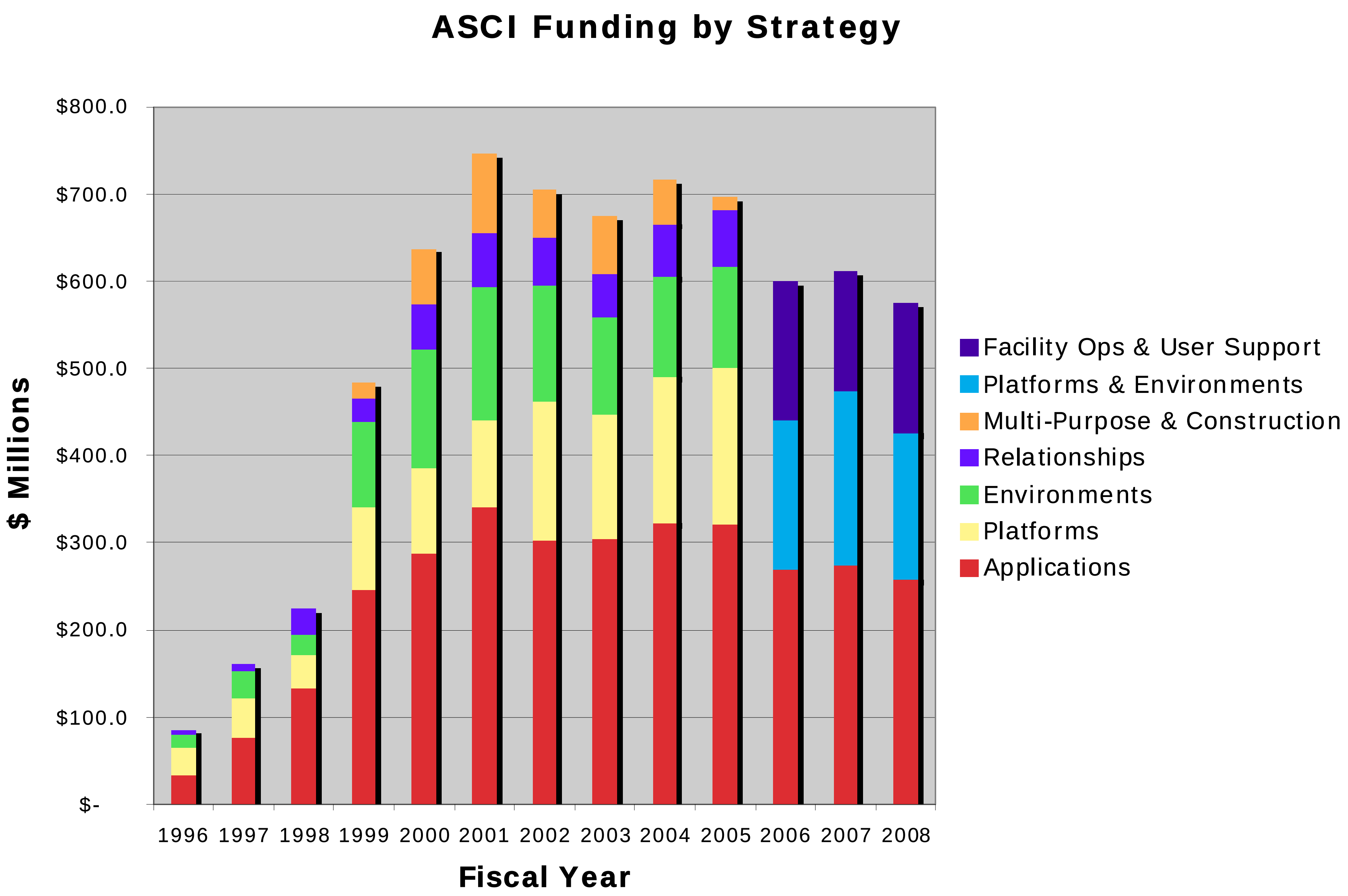
lustre

TotalView Technologies

CEI

panasas

Robust, Balanced and Long Term Funding



Result: US leadership in multi-physics simulation – (and High Performance Computing)

- Multi-physics:
  - Much more complex that simple mechanics or fluid dynamics codes
  - e.g.: radiation transport + hydrodynamics + nuclear processes; or, material transport + chemical kinetics.
- Examples:
  - Integrated weapons physics design codes for nuclear weapons
  - Structural mechanics codes
  - Physics codes for non-nuclear components.
  - Casting codes
  - Materials modeling codes (molecular dynamics, lattice defect dynamics).

Why did ASCI work?

- Focus on the high end.
  - Programming on 10,000 processors requires a different approach and different discipline
- Commercial partnerships for platforms
  - High end platforms are affordable only because costs can be amortized over commercial scale production rather than one-of production.
- Integrated Code teams
  - This is a strength of the national labs, because it requires focus, intercommunications and sustainability across a variety of disciplines, computation, experimental and theoretical.
- Focus on simulation solutions to well-posed problems
- – where ASC was most successful was where it has been directed toward "scientific" problems.
- Support environment matters
  - Data analysis and visualization, debugging, load balancing, etc.

Some hard lessons that had to be learned

- Put science in at the beginning
  - Simulation is not just a code writing exercise, and challenges physical models and algorithms as much as platforms.

- Validation and Verification is a scientific challenge that must be integrated with design and code
  - Must involve the users who own the problems to be solved.
  - More than a software QA problem - codes, methods and fundamental understanding undergo rapid evolution
  - Learning to work with uncertainty quantification (QMU)

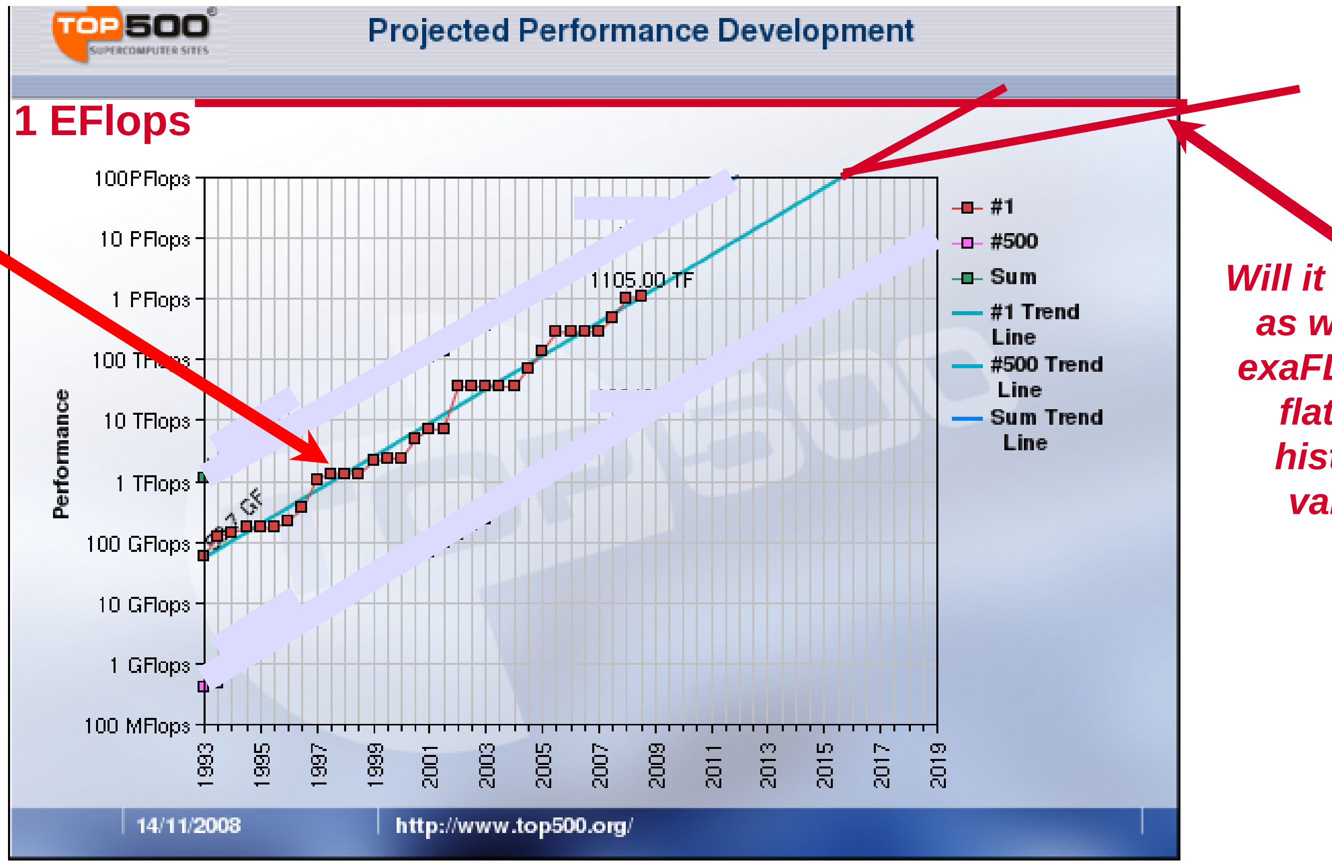
- Scalable algorithms are a key challenge
  - For every decade of hardware acceleration you need concurrent algorithm improvement.

- University partnerships important
  - ideas, algorithms, models, codes, and of course people.

- Most successful efforts aim at what can be achieved in about a 3-4 year time horizon.

Looking Forward - What are the current big problems?

This rate of growth was seen since the early 90s

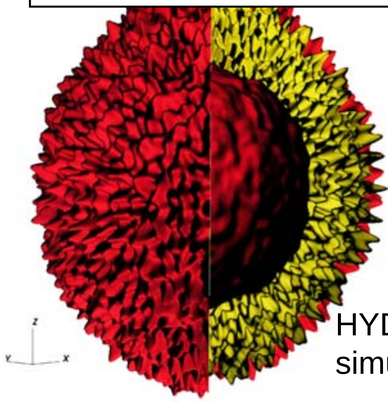


Will it continue as we go to exaFLOP/s or flatten to historical values?

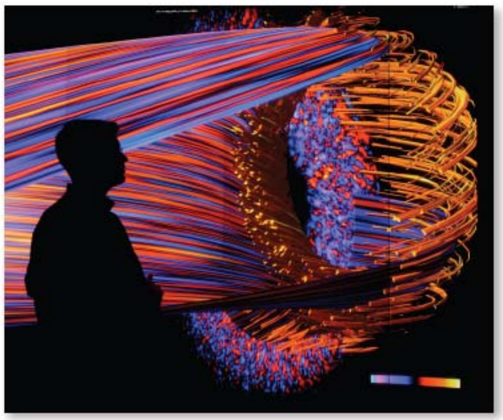
What are the PROBLEMS of "national importance" that would support a PROGRAM to power through the next architectural shift?

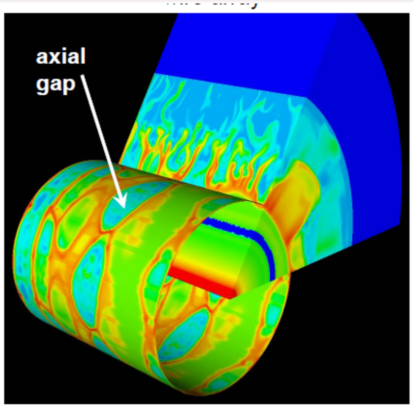
Fusion for Stewardship and Energy

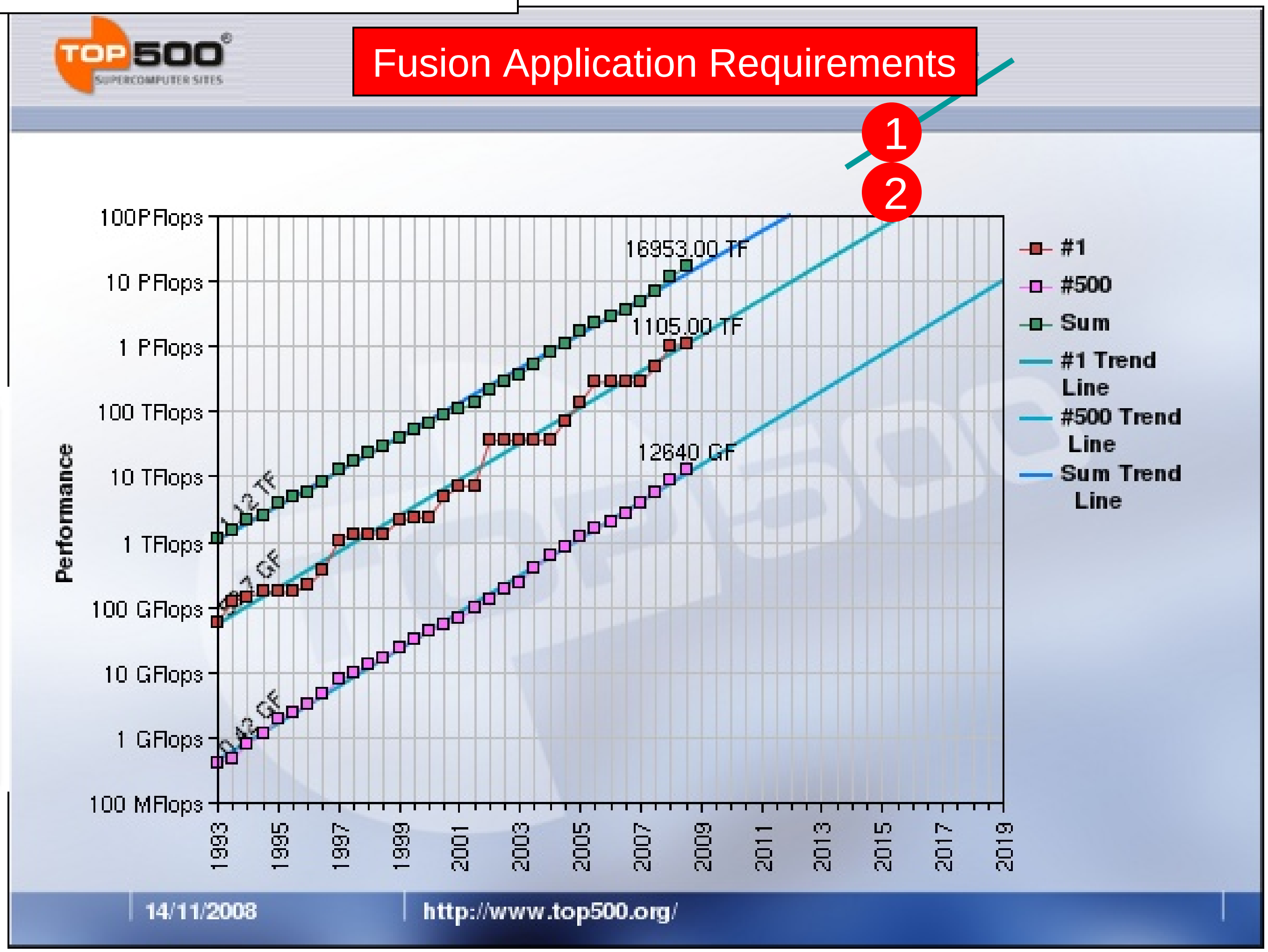
From: Brad Wallin, NNSA



HYDRA simulation



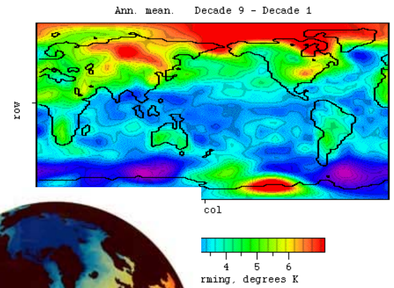


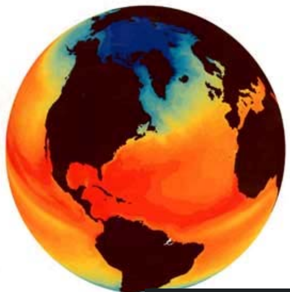


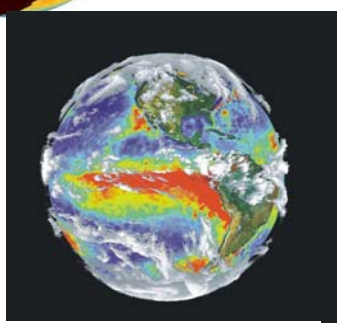
1. High resolution, discovery-level simulation of integrated physics for Boost and fundamental science
2. Uncertainty quantification

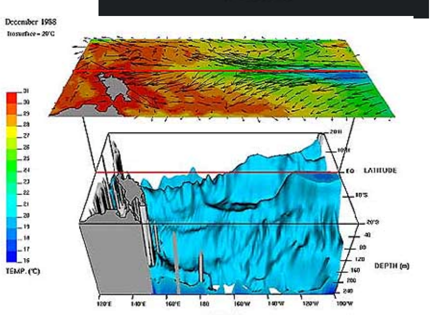
Climate

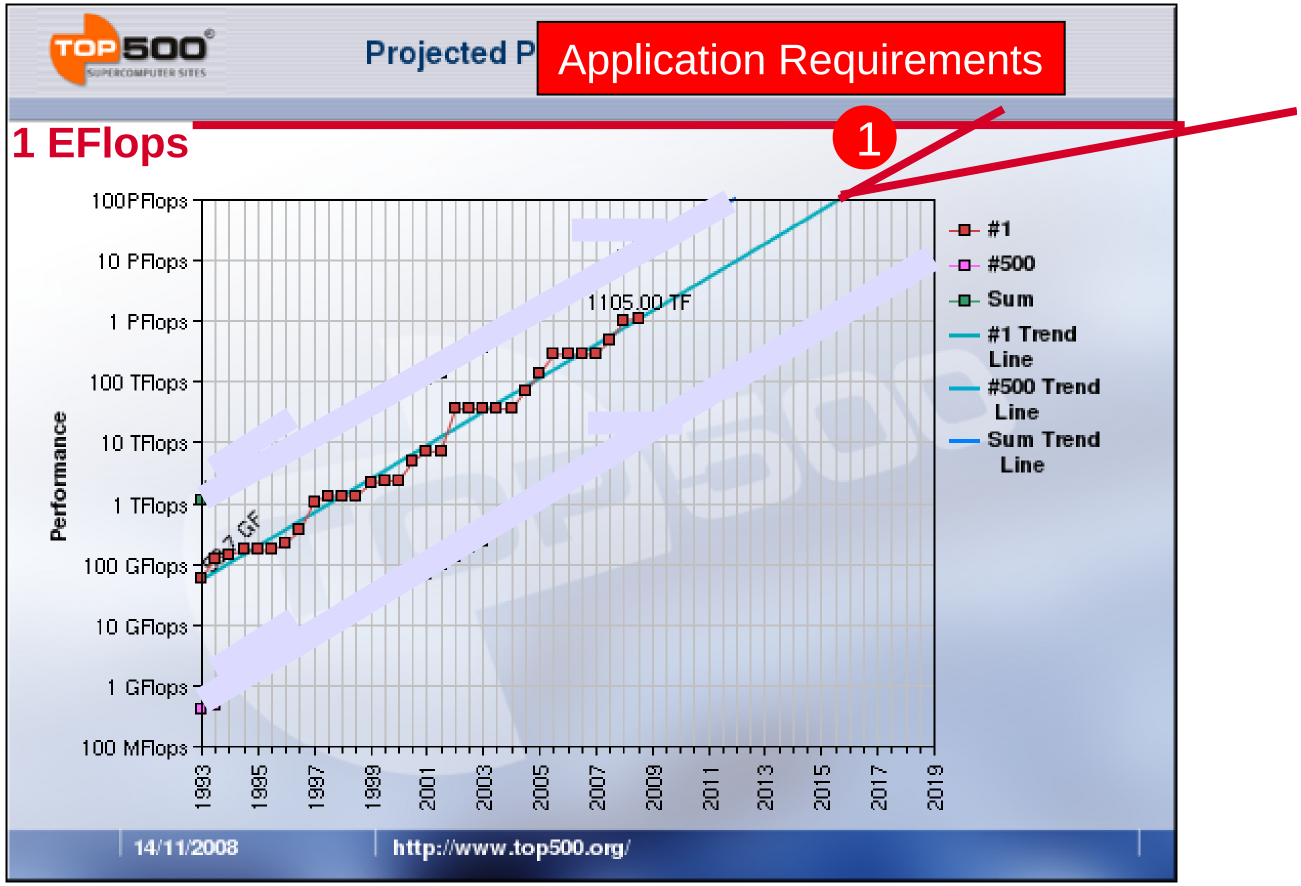
From: Doug Rotman, LLNL









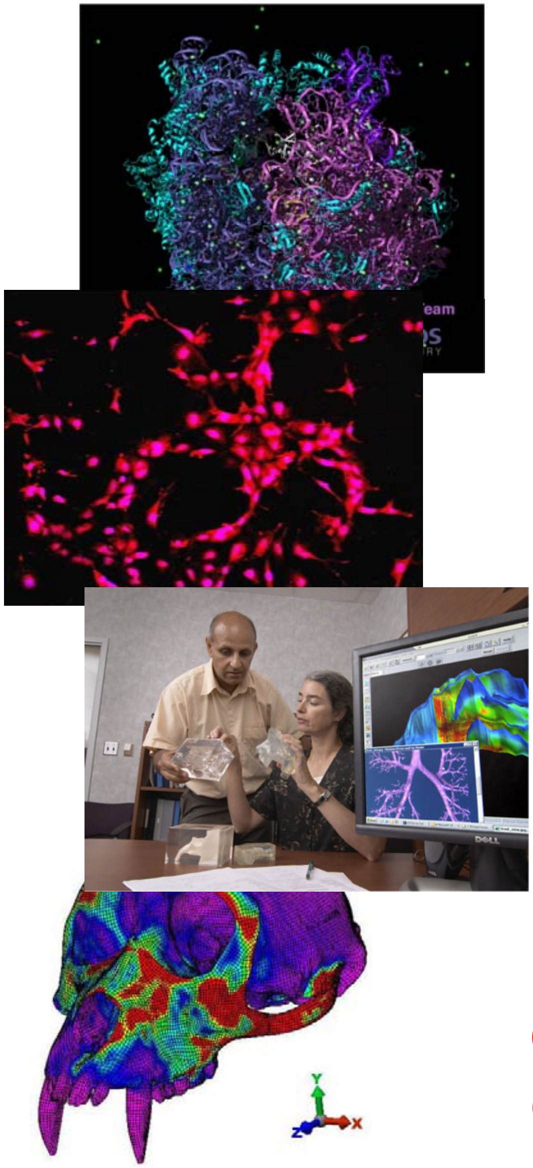


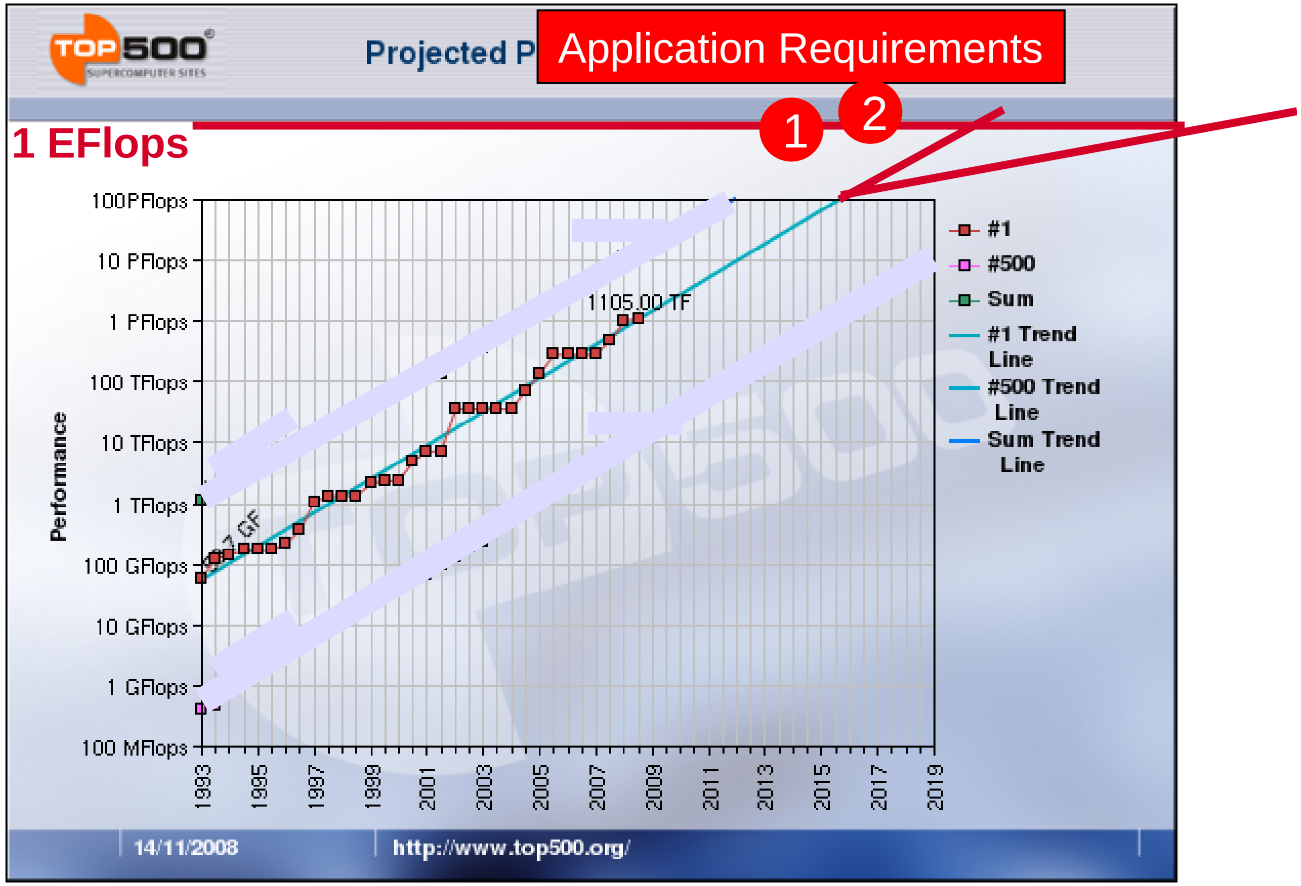
1

- Well understood, appropriate, and comprehensive chemistry and physics
- Fine resolution to enable local/regional analysis (think kilometer resolution in a global model)
- Ensembles of runs coupled with careful uncertainty quantification to understand uncertainties, risks, and probability distributions.

Bio-Medical

From: Dan Reed, Microsoft



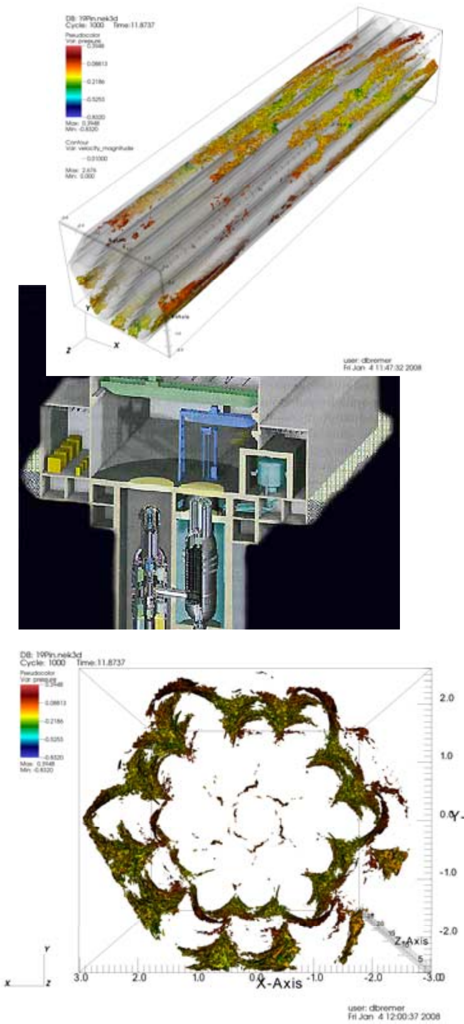


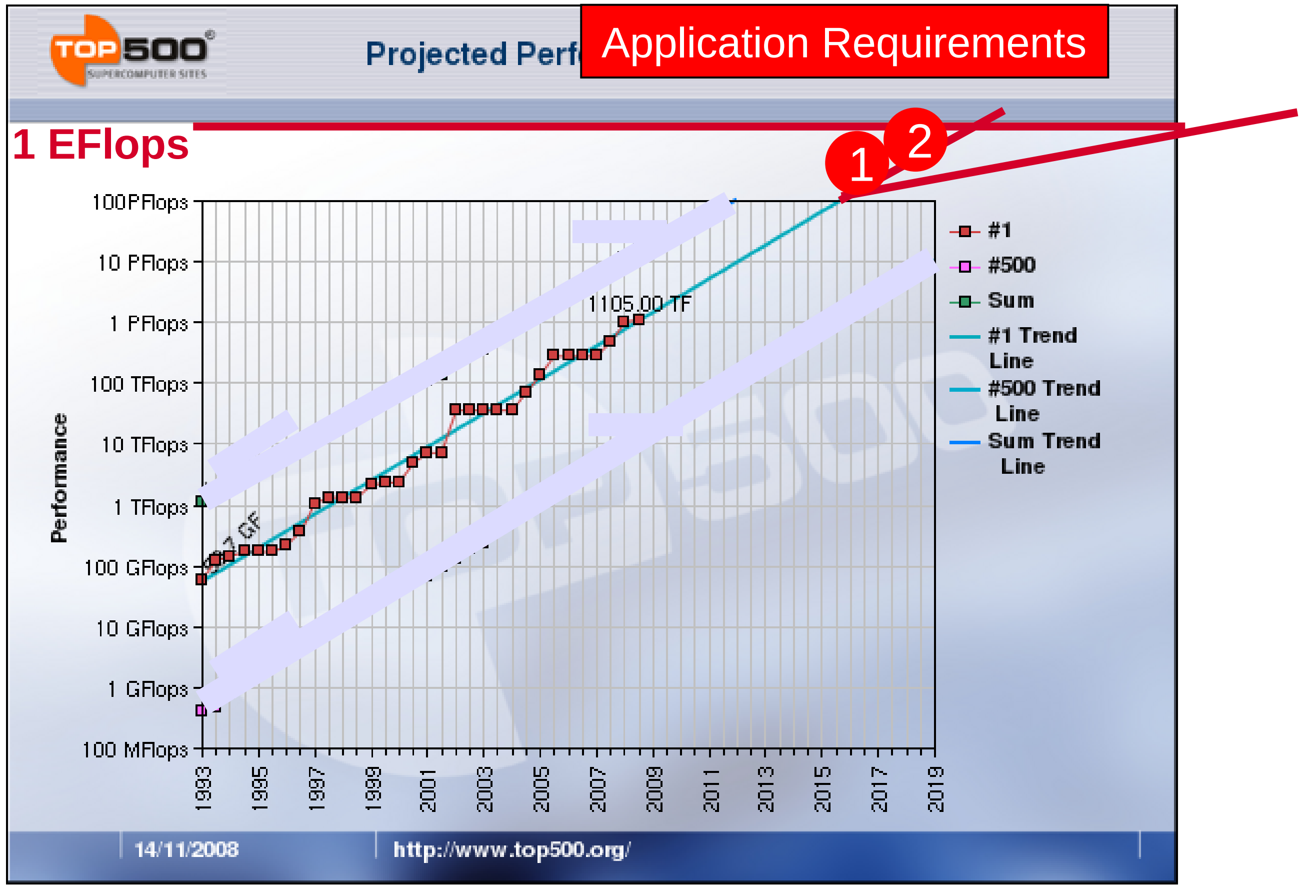
1 • Ab initio biological cell simulation

2 • Ab initio simulation of cell and drug interactions

Nuclear Energy

From: Phillip Finck, INL





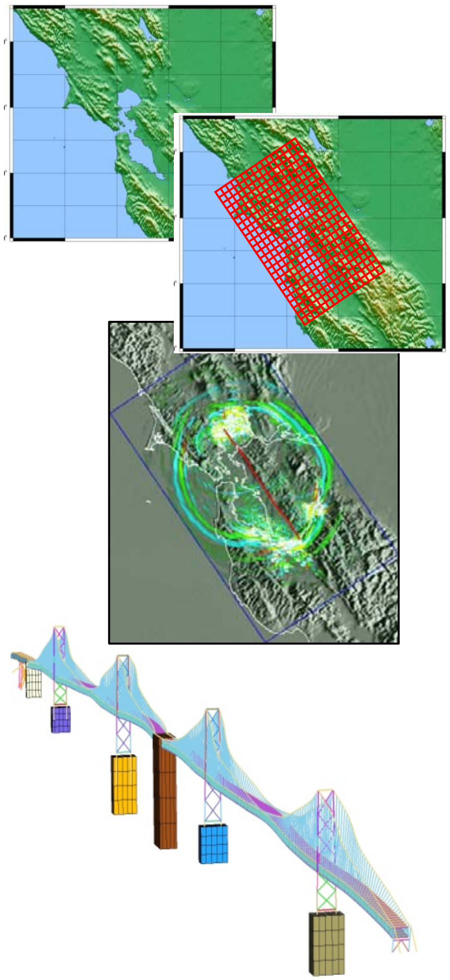
1 • High resolution, integrated system, science based behavior reactor simulation

2 • Science based simulation of nuclear waste form interactions with repository environment over 1 million year lifetime

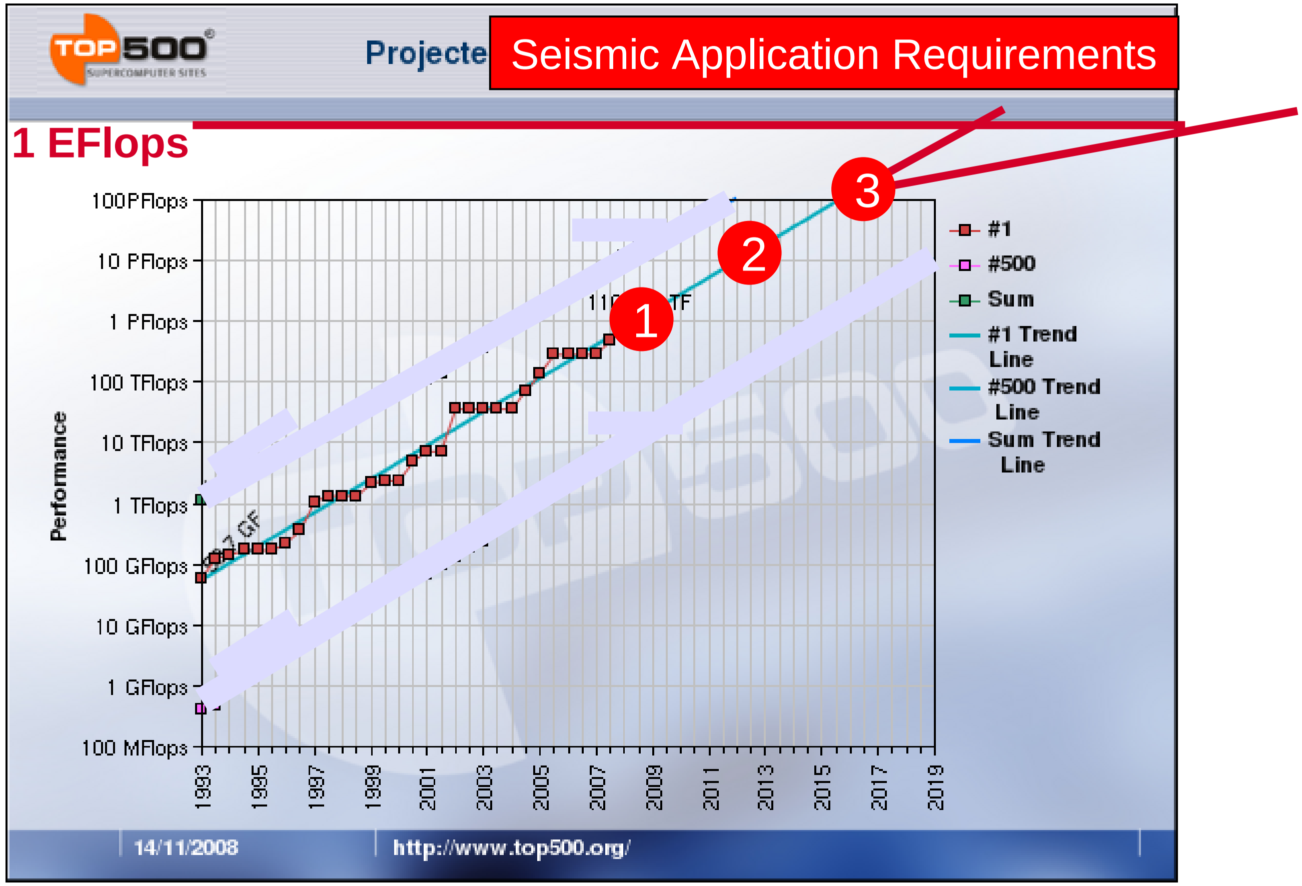
<u>Seismic</u>

From David McCallen, LBNL

Earth-to-structure response simulations



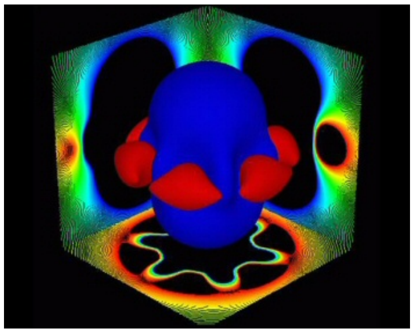
(Earthquake and infrastructure response)

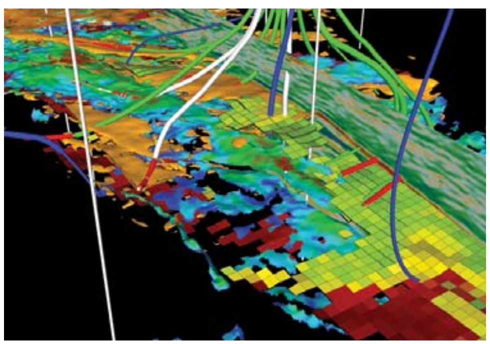


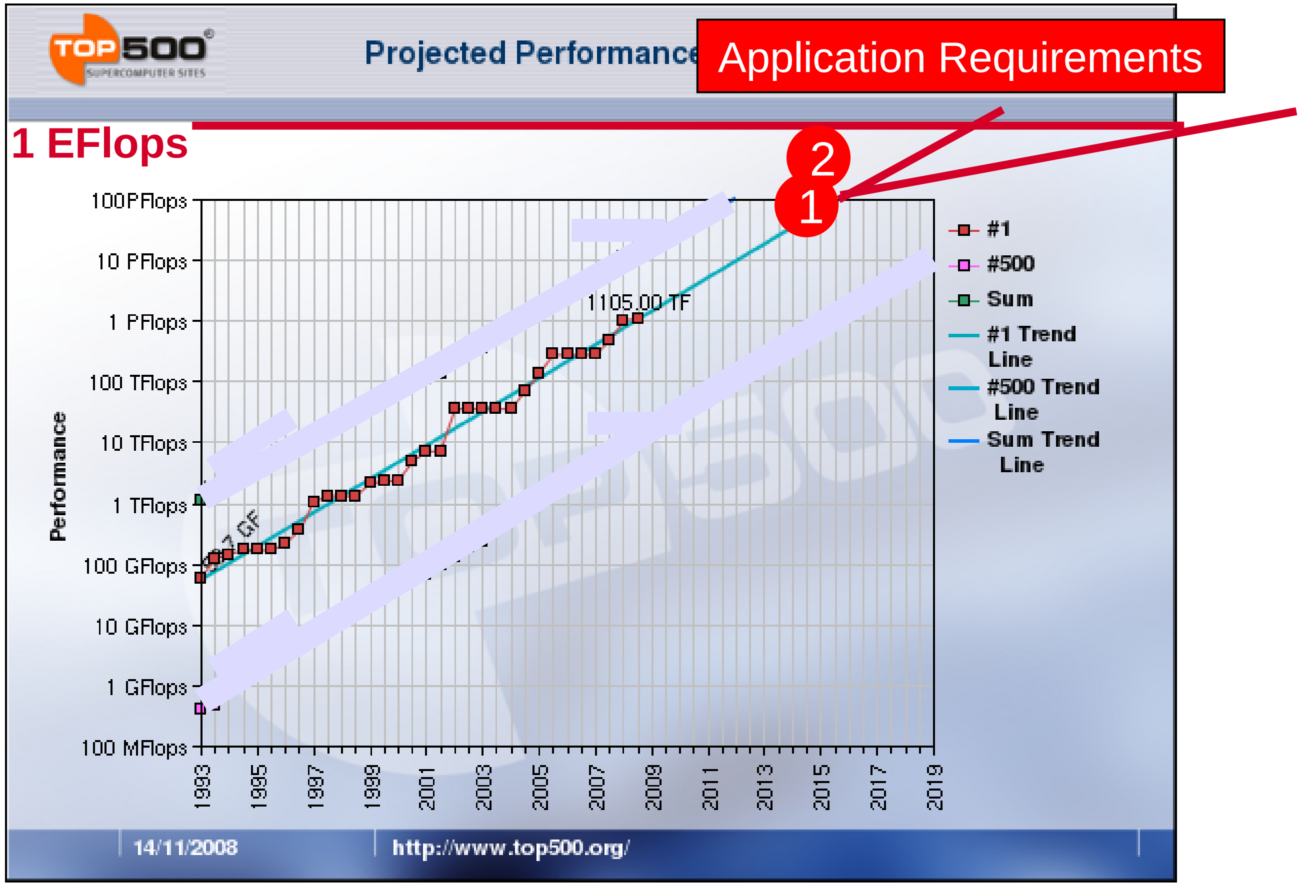
1. Weakly coupled ground and structure at ~ 1Hz (current) (or local ground model to higher frequencies)
2. Weakly coupled ground and structure at ~5Hz
3. End-to-end high frequency (~10Hz) coupled earth/structure

Domestic Fossil Fuel

From: Michael P. Perrone, IBM





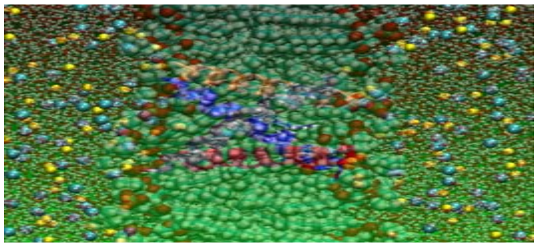


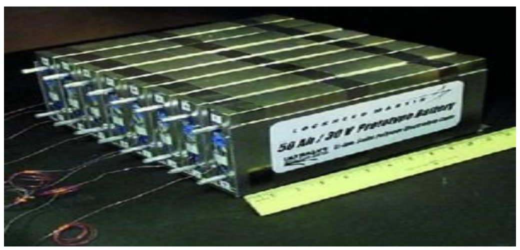
1 Rational catalyst design for improved chemical processes in a wide variety of areas

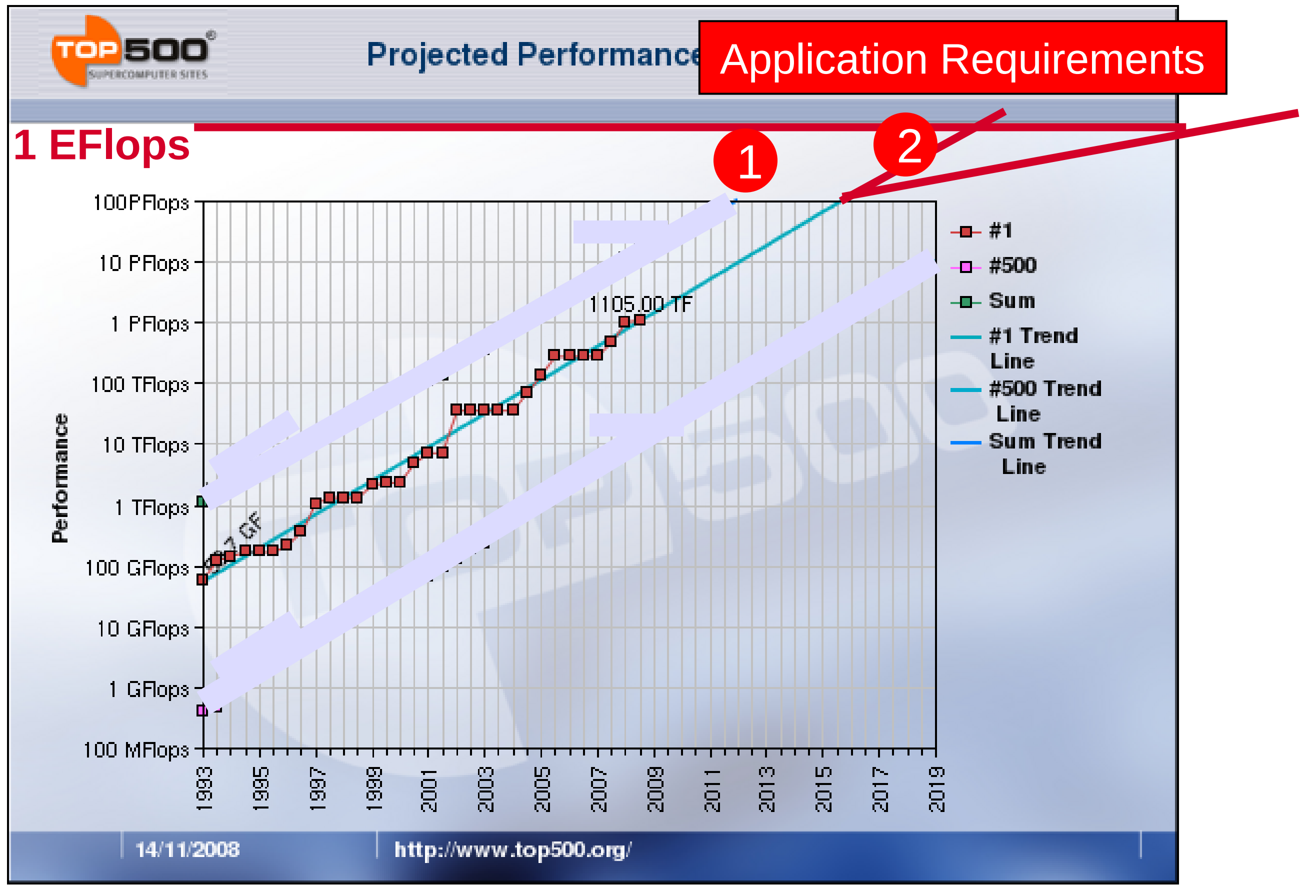
2 Improved seismic processing for oil exploration for continued supply

Advanced Energy Storage

From: Gil Weigand, ORNL



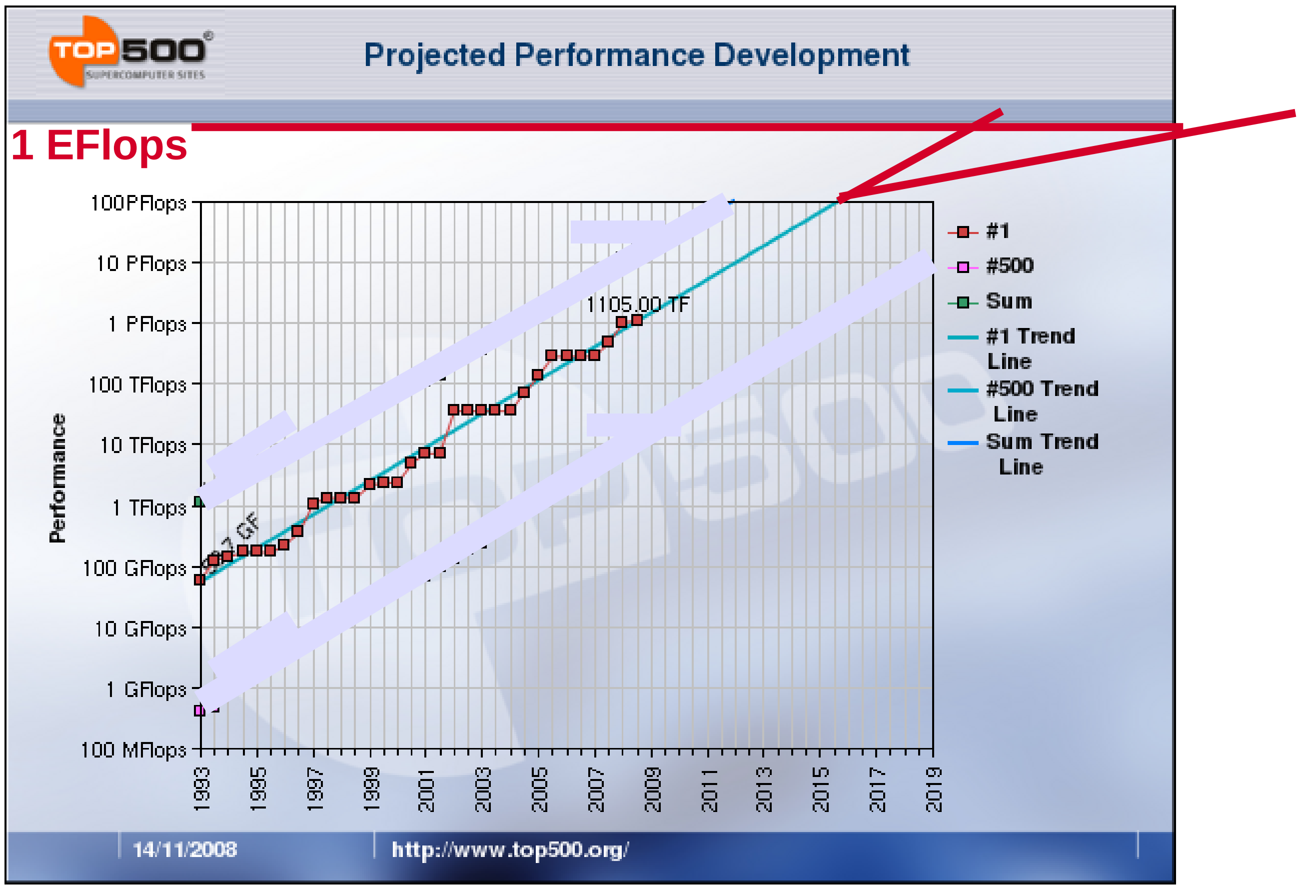




1 **Ab initio materials models to discover the behavior of advanced batteries capable of energy densities approaching gasoline and photovoltaics capable of efficiencies of at least 50%**

2 **Science-based safety and aging simulation, including cycling and environmental insult, for battery and photovoltaic systems**

Other Important Applications?



"Never, ever, think outside the box."

Summary

- Current Problems provide a major opportunity for High Performance Computing
  - Many important national problems
    - Energy, Health, National Security, Climate …..
  - Strong role for Government (DOE) as “problem owner”
  - But HPC not yet recognized by the Obama Administration
    - Who will be the “Al Gore”?
- Historically “Architecture” drives the rate of growth
  - Driven by Problems & Partnerships > Programs >Platforms
    - ASCI experience
- Will Government (DOE) be a partner or an HPC customer?
- Opportunity for Obama Administration – DOE
    - Role of DOE labs
    - Academia
    - Industry