



---

# **The Grand Challenge Question for Performance Evaluation of HPC Systems**

Horst D. Simon

Director, NERSC Center and Computational  
Research Divisions

Lawrence Berkeley National Laboratory

May 5, 2003

# The GC Question

---



What quantitative and objective measure of enabling scientific discovery can be used as the basis of evaluating computing facilities for basic science?

# NERSC 3 (Seaborg) Upgrade to 10 Tflop/s Completed



## ❖ System Characteristics:

- 416 16 way Power 3+ nodes with each CPU at 1.5 Gflop/s
  - 380 for computation
- 6,656 CPUs – 6,080 for computation
- Total Peak Performance of 10 Teraflop/s
- Total Aggregate Memory is 7.8 TB
- Total GPFS disk will be 44 TB
  - Local system disk is an additional 15 TB
- Combined SSP-2 measure is 1.238 Tflop/s
- In production now; largest unclassified system in the U.S.



# Goal of NERSC: Enabling Scientific Discoveries



Borrill (LBNL) + CalTech + others.  
April 27, 2000

- ❖ BOOMERANG Experiments – analyze cosmic microwave background radiation data to obtain a better understanding of the universe
- ❖ The data analysis provides strong evidence that the geometry of the universe is flat
- ❖ Computational capability provided on NERSC platforms
- ❖ MADCAP software developed at NERSC for general community

# Enabling Scientific Discoveries

---



- ❖ Many other examples available spanning entire history of NERSC
- ❖ What are the characteristics of NERSC that enabled this work to be done here?
- ❖ What type of measures could we have used to have predicted the enablers for these scientific discoveries?

# The Current Political Debate about Performance

---



The good news: the arrival of the Earth Simulator has made “Washington” realize that peak performance alone alone is not the answer

The bad news: “sustained to peak ratio” has replaced peak performance as the new single figure of merit

# How SciDAC was “sold”



## Peak Performance is skyrocketing

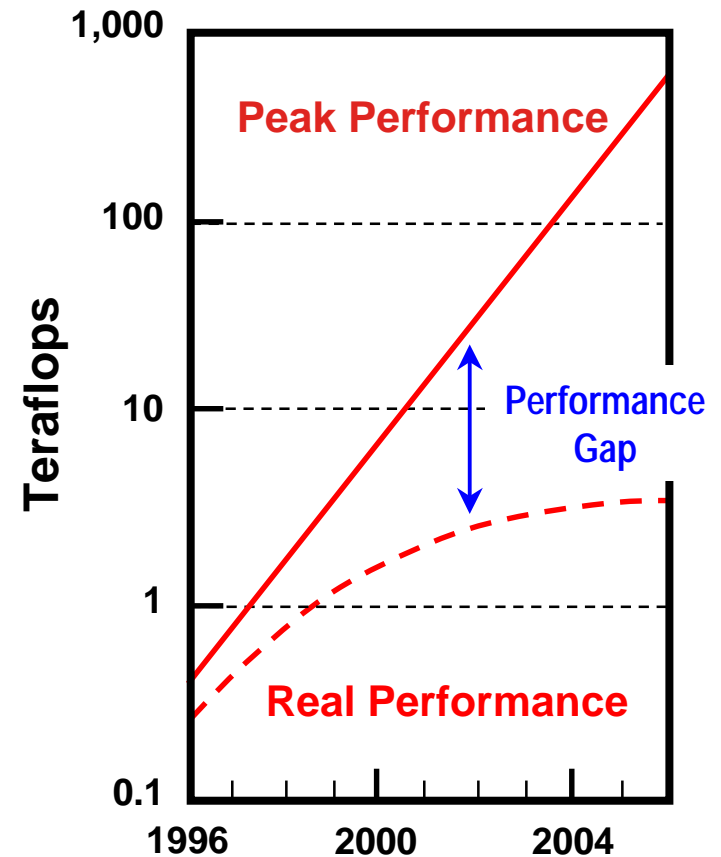
- In 1990's, peak performance increased 100x; in 2000's, it will increase 1000x

## But ...

- Efficiency declined from 40-50% on the vector supercomputers of 1990s to as little as 5-10% on parallel supercomputers of today

## Close the gap through ...

- Mathematical methods and algorithms that achieve high performance on a single processor and scale to thousands of processors
- More efficient programming models for massively parallel supercomputers
- Parallel Tools



Source: DOE presentation about SciDAC, 2000

**... two years later ...**

---



**... you get what you set out to measure**



# Science of Scale



<u>Project</u>	<u>Performance</u> (% of peak)
❖ Terascale Simulations of Supernovae	35%
❖ Accelerator Science and Simulation	25%
❖ Electromagnetic Wave-Plasma Interactions	68%
❖ Quantum Chromodynamics at High Temperatures	13%
❖ Cosmic Microwave Background Data Analysis	50%

Source: HDS' presentation to OMB examiner and to ASCAC advisory committee, 2003

# Science of Scale: Cosmic Microwave Background Data Analysis



- ❖ **PI:** Julian Borrill, LBNL & UC Berkeley
- ❖ **Allocation Category:** Class B
- ❖ **Code:** Maximum likelihood angular power spectrum estimation (MADCAP)
- ❖ **Kernel:** ScaLAPACK
- ❖ **Performance:** 750 Mflop/s per processor (50% of peak)
- ❖ **Scalability:**
  - ❖ 0.78 Tflop/s on 1024 proc
  - ❖ 1.57 Tflop/s on 2048 proc
  - ❖ 3.02 Tflop/s on 4096 proc
- ❖ **Allocation:** 1.1 million MPP hours; requested and needs 2 million

# Cosmic Microwave Background Data Analysis (cont.)

---



Recent accomplishments:

- ❖ MADCAP extended to enable simultaneous analysis of multiple datasets and CMB polarization – the new frontier.
- ❖ MADCAP was rewritten to exploit extremely large parallel systems, allowing near-perfect scaling from 256 to 4,096 processors.
- ❖ MADCAP++ is being developed using approximate methods to handle extremely large datasets for which matrix multiplications are impractical, such as will be generated by the PLANCK satellite.
- ❖ Recent results from NASA's WMAP satellite observations of the whole CMB sky confirm MADCAP analyses of previous partial-sky balloon datasets.

# Status today

---



- ❖ We still get excellent science at NERSC -- but I have to work harder to explain it
- ❖ This challenge is everywhere
  - ASCI needs to relate platform performance to mission milestones
  - NAS study on the Future of Supercomputing
- ❖ As a community HPC needs to be more sophisticated to report about performance
- ❖ As a community HPC needs to show more unity in our communications

# The Opportunity Today



National Coordination Office for  
Information Technology Research and Development



## The HECRTF seeks input about:

(3) Federal Procurement of HEC Systems: This subtask will produce findings and recommendations that include:

- Identification of a strategy for developing practical performance measures for system procurement that correlate well with realized performance of actual applications
- Recommended methods for deriving system performance targets from actual or projected application requirements or other user needs

see <http://www.hpcc.gov/hecrtf-outreach/>

# The GC Question for the Future

---



What quantitative and objective measure of enabling scientific discovery can be used as the basis of evaluating computing facilities for basic science?