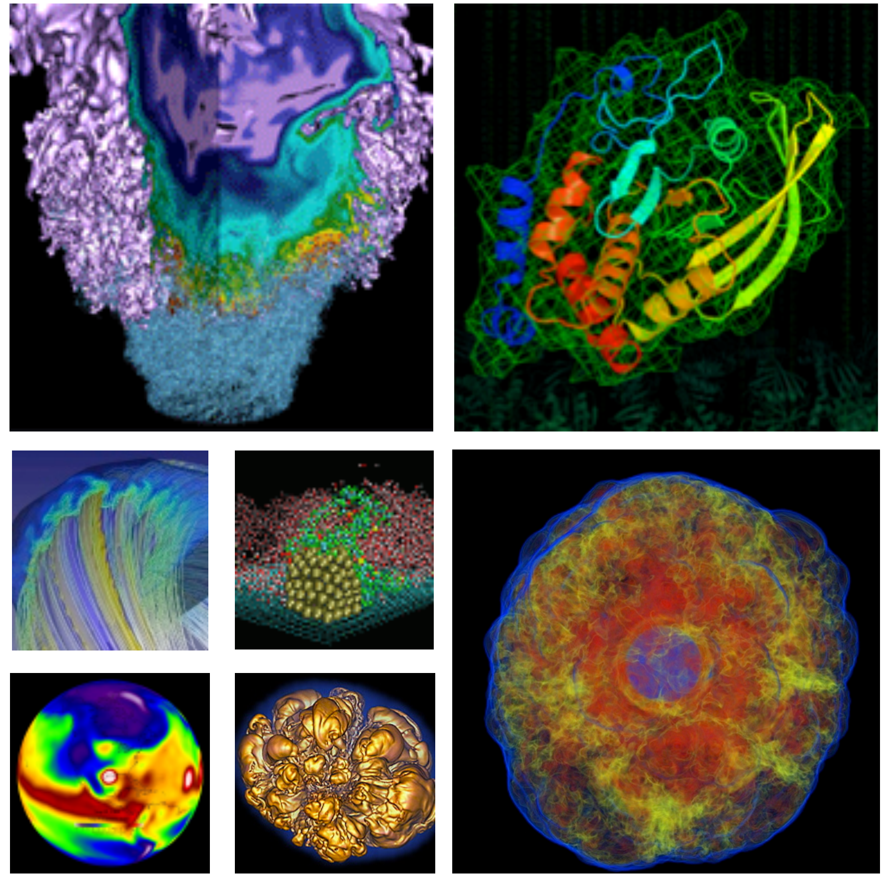
NERSC Role in HEP and Research and Emerging Technologies



NERSC

Sudip Dosanjh
Director

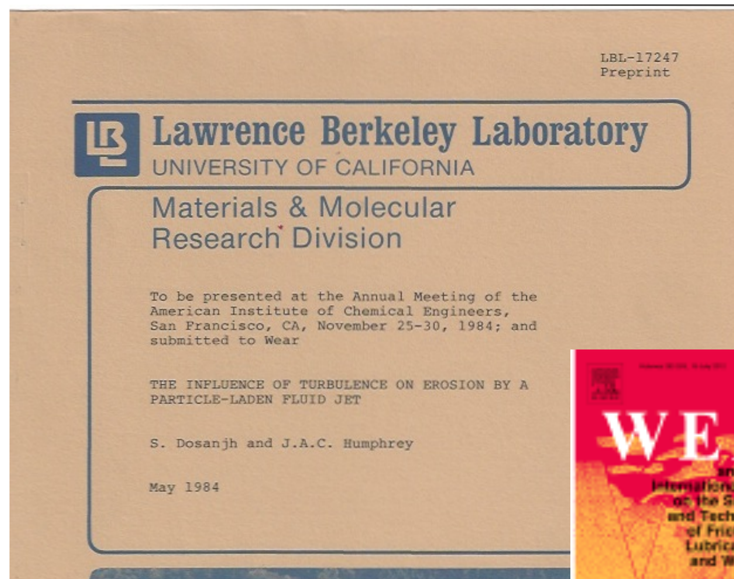
November 27, 2012

U.S. DEPARTMENT OF ENERGY | Office of Science

BERKELEY LAB
Lawrence Berkeley National Laboratory

Career History

- **1980: Summer Intern at LBL**
- **1977-1986: U.C. Berkeley student**
- **1986-2012: Sandia National Labs**
  - Modeled Three Mile Island on Cray YMPs
  - Massively parallel computing (chemically reacting flows, material science, computational science, algorithms)
  - Computational Science and Applications
  - Extreme-scale Computing
    - **Exascale**
    - **Co-design**
    - **Computer architectures**
    - **Algorithms**



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Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

Materials & Molecular
Research Division

To be presented at the Annual Meeting of the American Institute of Chemical Engineers, San Francisco, CA, November 25-30, 1984; and submitted to Wear

THE INFLUENCE OF TURBULENCE ON EROSION BY A PARTICLE-LADEN FLUID JET

S. Dosanjh and J.A.C. Humphrey

May 1984

Wear, *102* (1985) 309 - 330

THE INFLUENCE OF TURBULENCE ON EROSION BY A PARTICLE-LADEN FLUID JET

SUDIP DOSANJH and JOSEPH A. C. HUMPHREY

Materials and Molecular Research Division, Lawrence Berkeley Laboratory, University of California, Berkeley, CA 94720 (U.S.A.)

(Received July 2, 1984; accepted February 7, 1985)

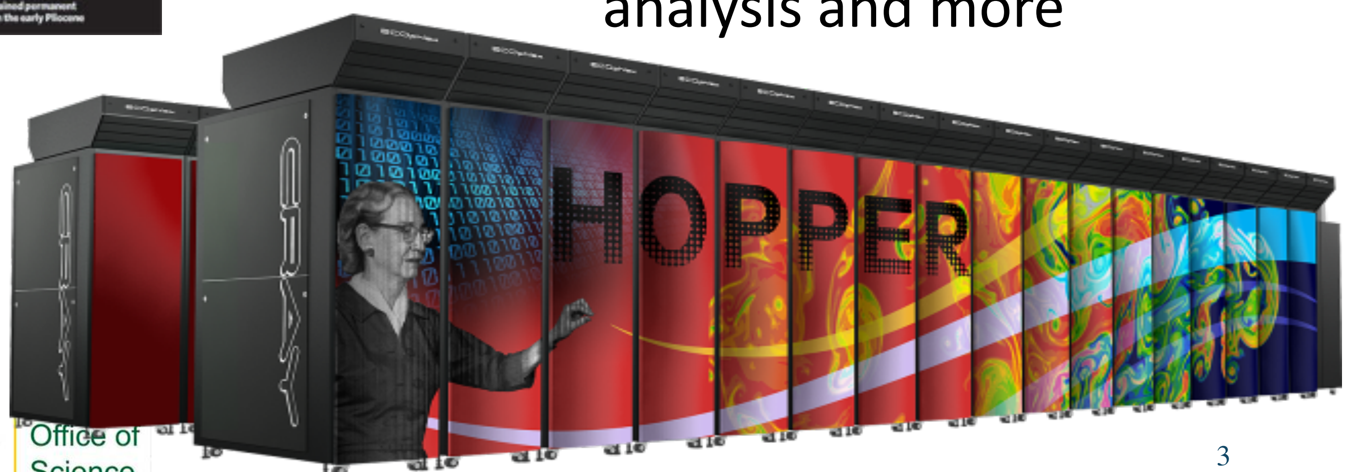
NERSC Provides Computing for Science

Broad user community

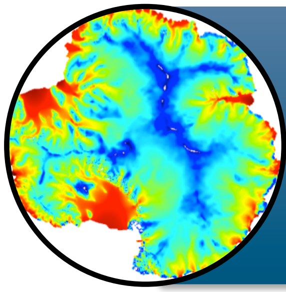
- 4844 users, 663 projects
- 48 states; 65% from universities
- Hundreds of users each day
- ~1500 publications per year

Systems for science

- 1.3PF Hopper + .5 PF clusters
- Services for consulting, data analysis and more

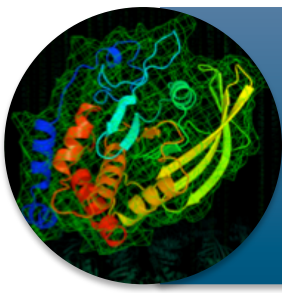


NERSC Has a Broad Range of Computational Problems



Science at Scale

Petaflops to Exaflops



Science through Volume

Thousands to Millions of Simulations

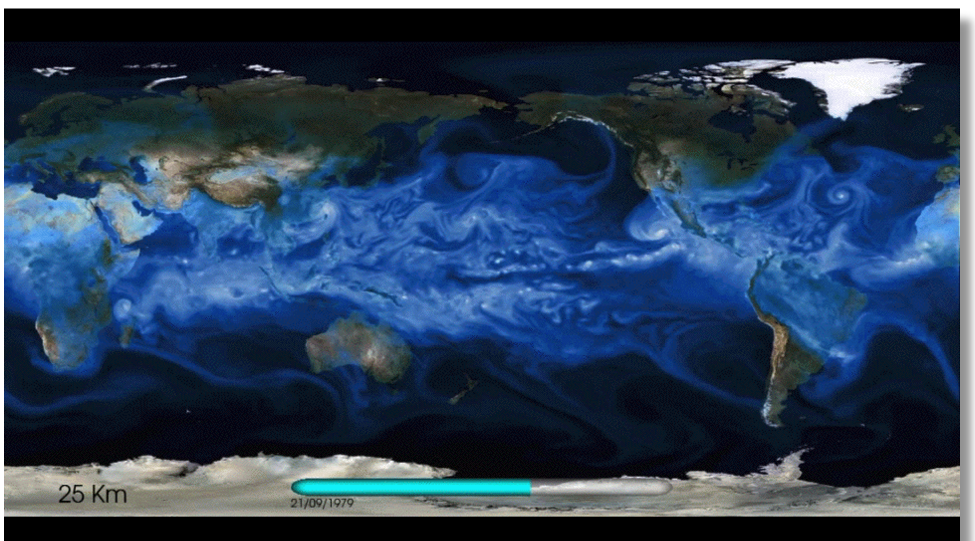
Science in Data

Petabytes to Exabytes of Data

Computational Modeling and Big Data

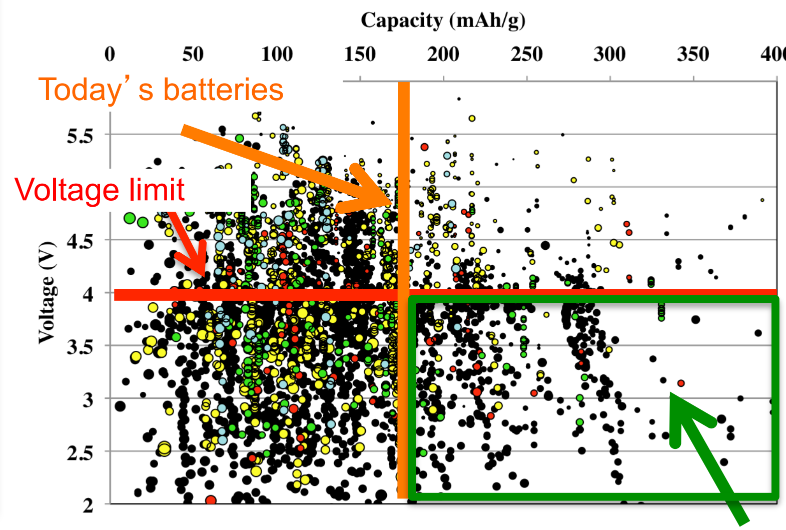
Large-Scale discovery of Events

- Petascale simulations produce data too large for manual analysis
- Data analysis using new algorithms (FastBit, Machine Learning) discover events

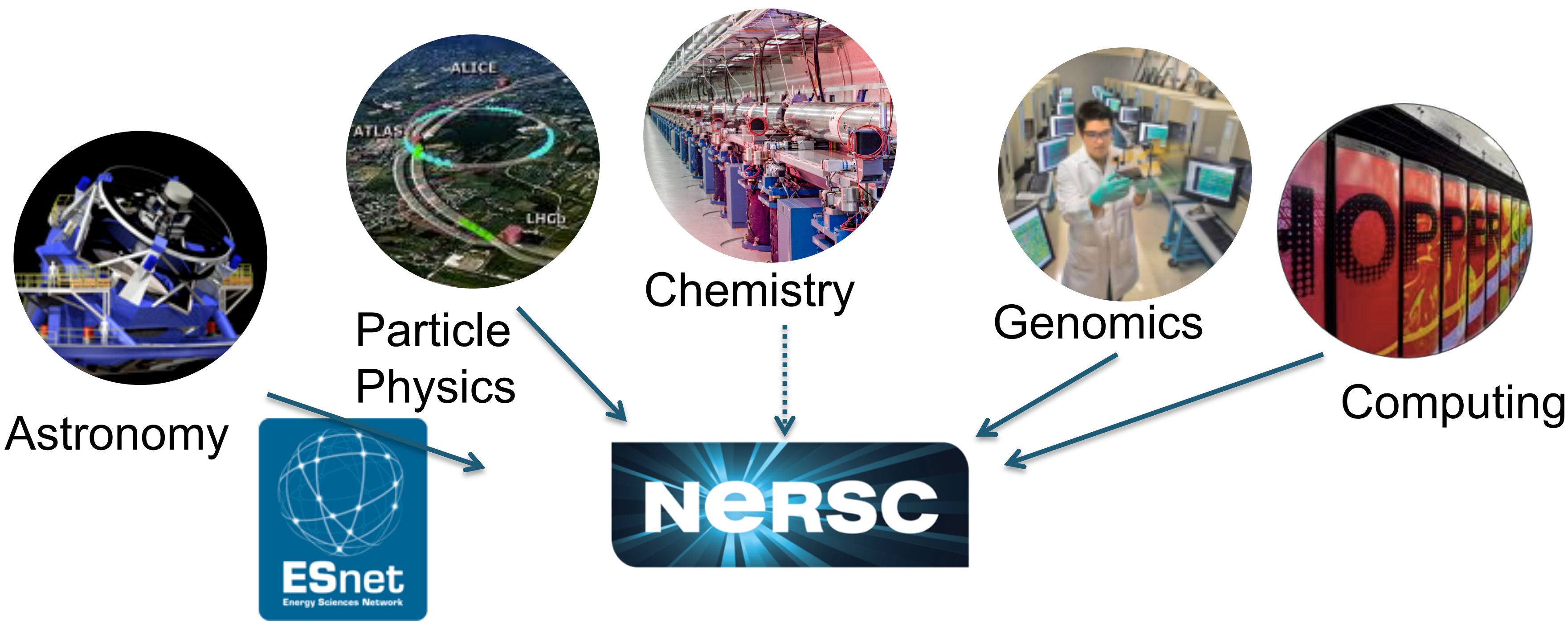


Materials Project

- Tens of thousands of simulations screen materials
- Goal: cut in half the 18 year from design to manufacturing
- Advance machine learning and data systems



DOE has Unique Data Challenges

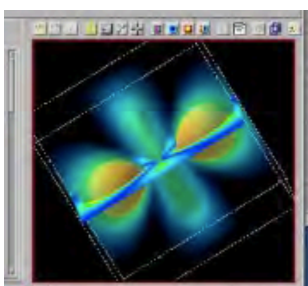


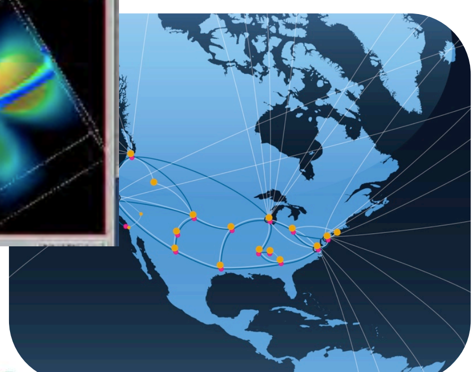
- **DOE provides many of the large scale user facilities**
- **Some are producing Petabytes of data today**
- **NERSC has about 4 Petabytes of disk and 40 of tape**

Petaflops to the People

Vision: Accelerate scientific discovery across a broad community through advanced computing

- **Energy efficient computing:** Improve application performance per Watt by 100x necessary for exascale
- **High throughput computing:** Provide tools and infrastructure for ensemble runs and deliver database of results to science community
- **Data driven computing:** Improve insight through access to and analysis of data from experimental facilities

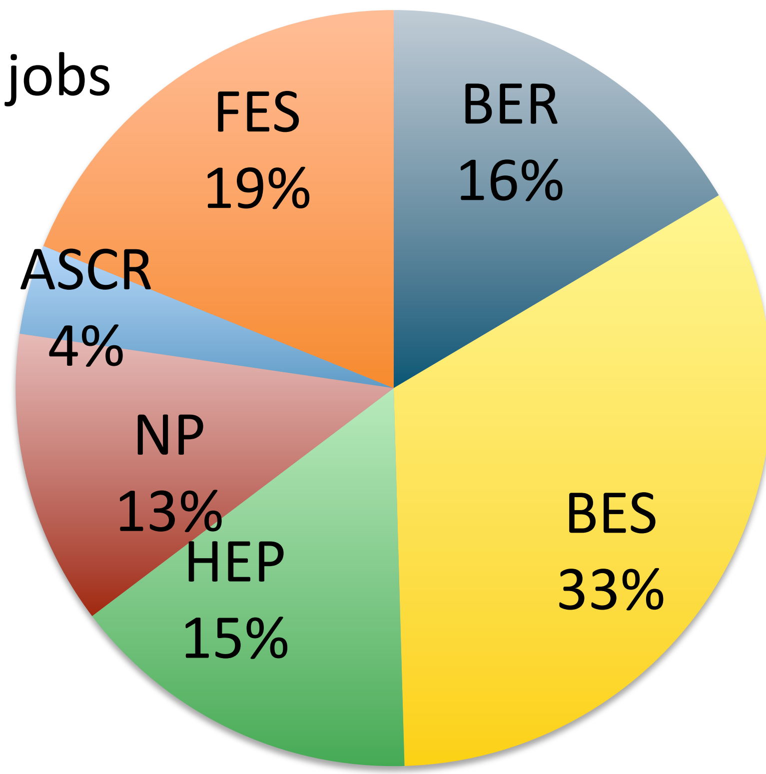




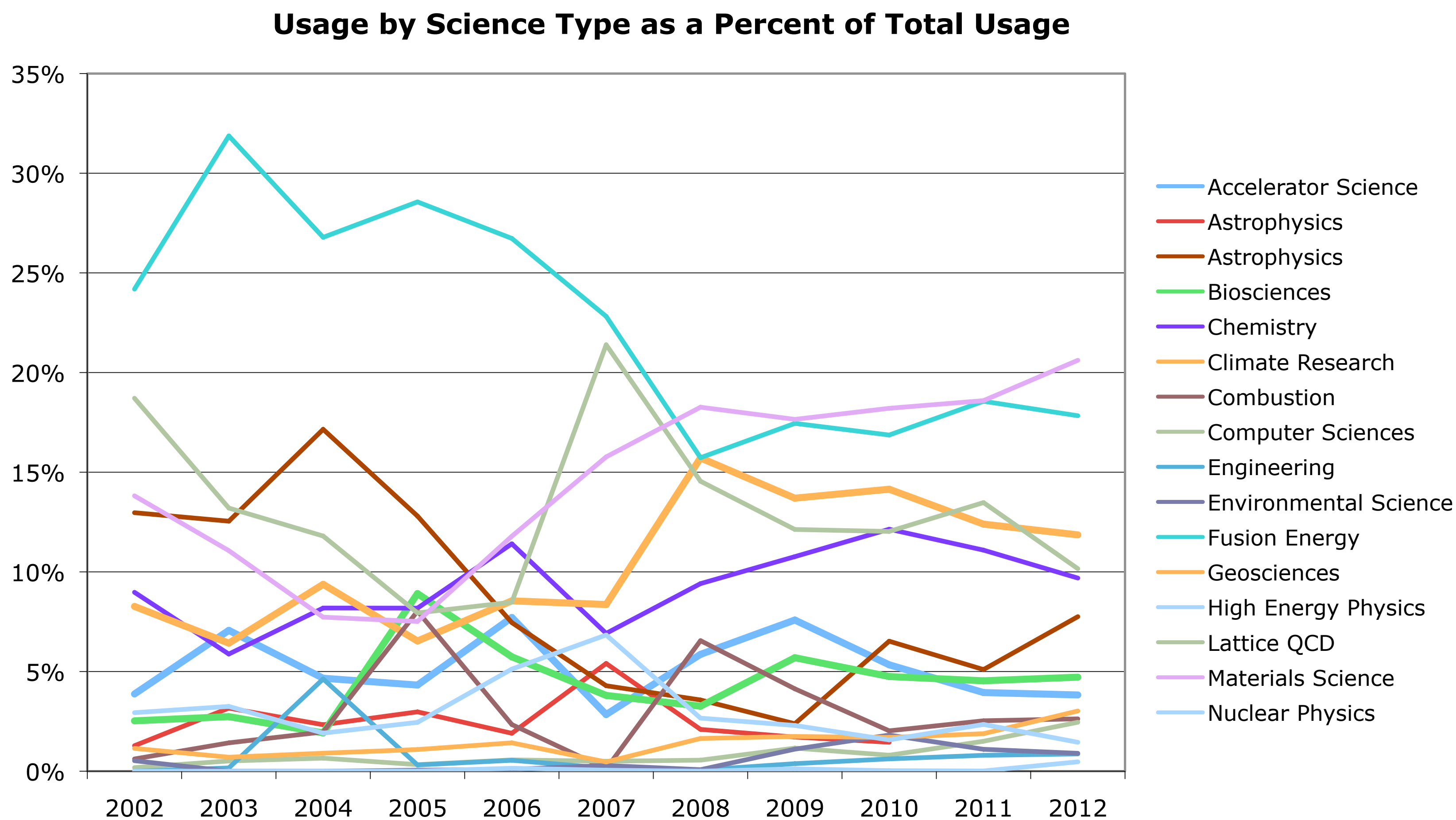
The Production Facility for DOE SC

- **NERSC Focus on unique resources**
  - –High end computing systems
    - Configured for both large-scale jobs and large numbers of jobs
  - –High end storage systems
    - Large shared file system
    - Tape archive
  - –Interface to high speed network
    - ESnet 100 Gb/s
- **Allocate time / storage**
  - –Current processor hours and tape storage

% Use in 2011



DOE's Changing Computing Priorities



ASCR's Computing Facilities

Production Computing at NERSC / LBNL	Leadership Computing at ANL and ORNL
• **100s of Projects** • **Allocations** – 80% divided and allocated by each Science Office – 10% ASCR Leadership Computing Challenge – 10% Directors' reserve • **Limited to DOE-relevant science** • **Includes storage and computing allocations**	• **10s of projects** • **Allocations** – 60% by INCITE program managed by ANL/ORNL – 30% ASCR Leadership Computing Challenge – 10% Director's reserve • **Includes industry and non-DOE applications** • **Focused on applications at scale**

NERSC is Very Cost Effective Relative to Clouds

Component	Annual Cost
Compute Systems (1.38B hours)	$181M
HPSS (17 PB)	$12M
File Systems (2 PB)	$3M
Total (Annual Cost)	**~$200M**

NERSC cost/core hours dropped 10x (1000%) from 2007 to 2011
Amazon pricing dropped 15% in the same period

These are "list" prices, which overestimate cloud costs, but several factors underestimate the cost:

- Doesn't include the measured performance slowdown 2x-50x.
- Only accounts for about 65% of NERSC's $57M annual budget.
  No consulting staff, no account management, no software support.

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Current NERSC Systems

Large-Scale Computing Systems

Hopper (NERSC-6): Cray XE6
- 6,384 compute nodes, 153,216 cores
- 144 Tflop/s on applications; 1.3 Pflop/s peak

Edison (NERSC-7): Cray Cascade
- To be delivered in 2013
- Over 200 Tflop/s on applications, 2 Pflop/s peak

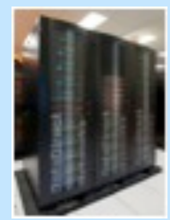

Midrange
140 Tflops total

Carver
- IBM iDataplex cluster
- 9884 cores; 106TF

PDSF (HEP/NP)
- ~1K core cluster

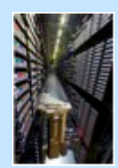
GenePool (JGI)
- ~5K core cluster
- 2.1 PB Isilon File System

NERSC Global Filesystem (NGF)



Uses IBM's GPFS
- 8.5 PB capacity
- 15GB/s of bandwidth

HPSS Archival Storage



- 240 PB capacity
- 5 Tape libraries
- 200 TB disk cache

Analytics & Testbeds

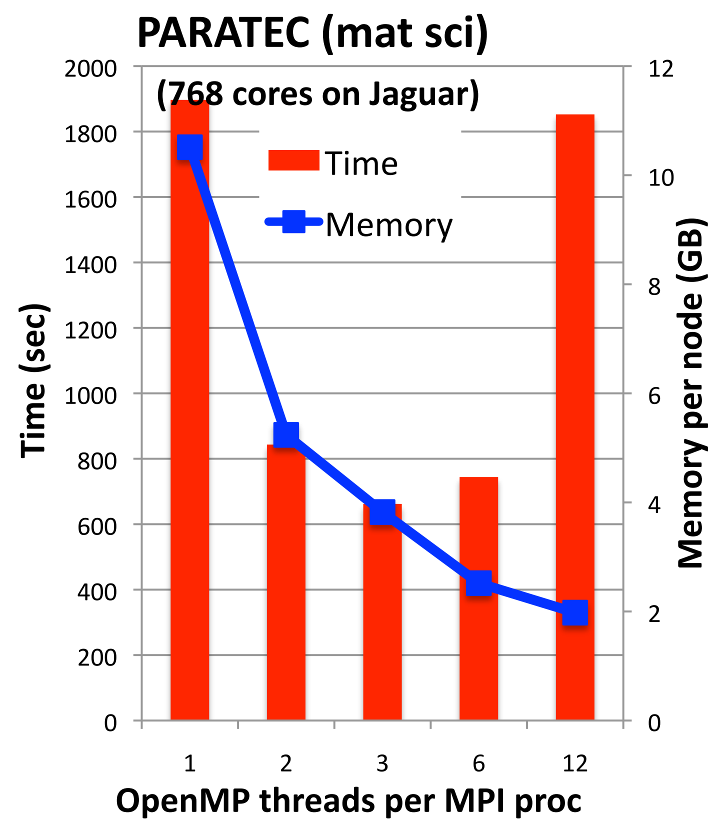
Euclid
(512 GB shared memory)

Dirac 48 Fermi GPU nodes

Magellan Hadoop

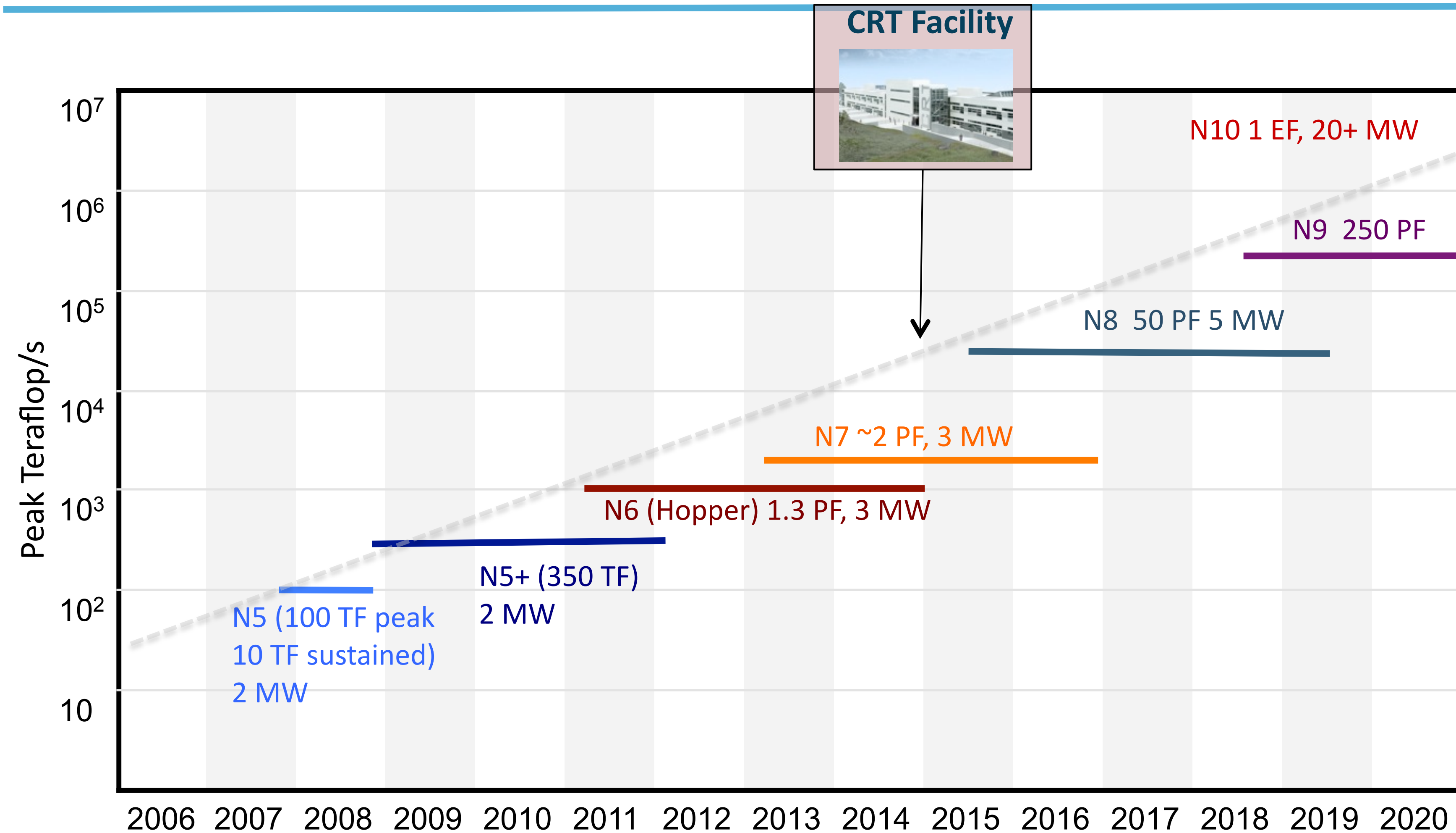
Limitations of Existing Programming Models

- **We can run 1 MPI process per core, but there are problems with 6-12+ cores/socket:**
  - Insufficient memory: user level data and internal buffers
  - Runtime overheads: copying and synchronization
- **OpenMP, Pthreads, or other shared memory models**
  - No control over locality, e.g., Non-Uniform Memory Access
  - No explicit memory movement, e.g., accelerators or NVRAM
- **Even on petascale systems, tuning is non-obvious**



Nick Wright, John Shalf et al, NERSC/Cray Center of Excellence

NERSC Roadmap



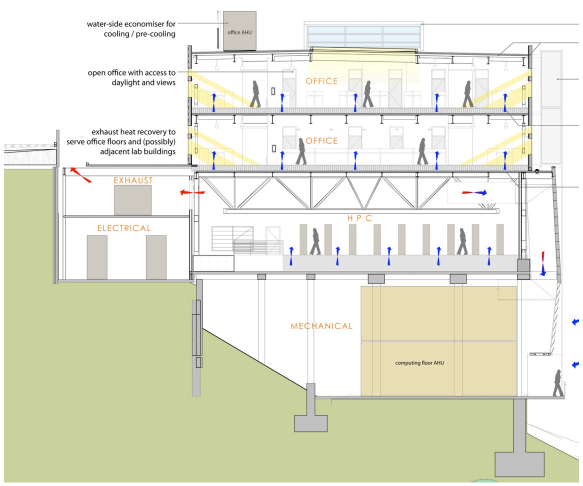
- NERSC performance has traditionally grown at 10x every 3-4 years

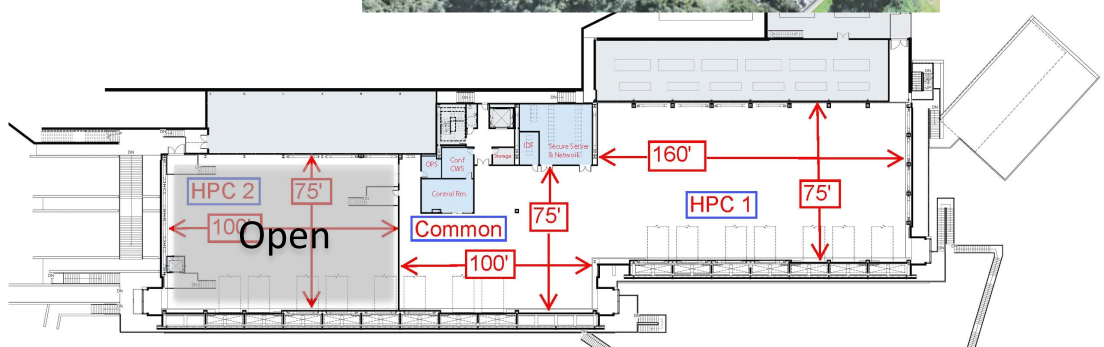
NERSC-7 Coming Soon

- **NERSC will install a Cray "Cascade" system in 2013**
  - First all new Cray design since Red Storm; developed for the DARPA HPCS program (including >$70M from DOE)
  - Intel Processors with >2PF peak performance
  - New "Aries" interconnect using a "dragonfly" topology
  - 6.5PB storage using Cray Sonexion Lustre appliances
- **Good match for diverse NERSC user needs**
  - Both High-throughput and high-concurrency workloads.
- **Excellent energy efficiency**
  - Allows chiller-less "free cooling" with only 10% "overhead"
- **Will deliver ~1B Hopper-equivalent core hours**
  - 18

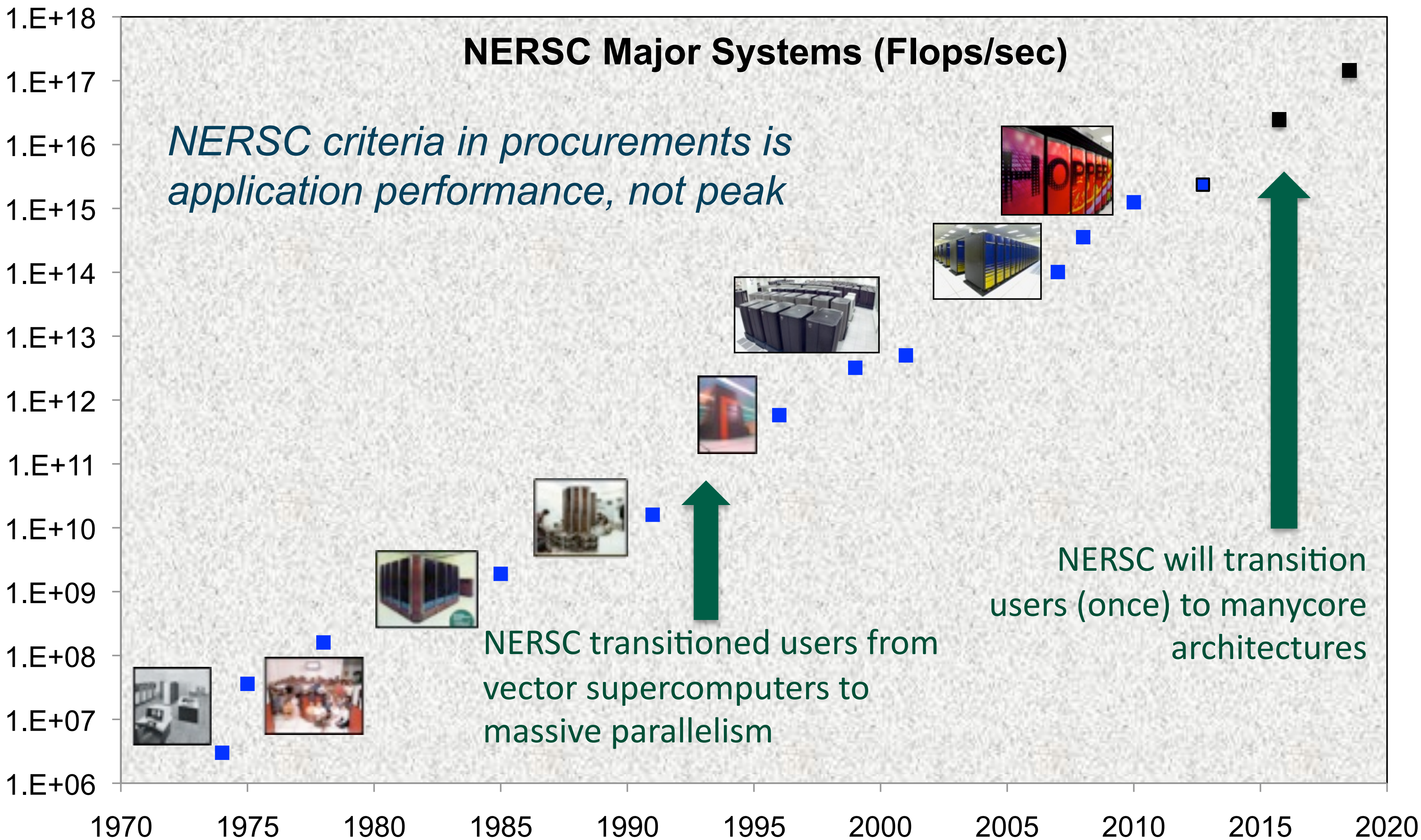
UC's Computational Research and Theory (CRT) Facility

- **Unique energy efficient design from weather / hillside**
- **Collaborative space for 300**
- **$124M UC Project (up $12M)**
- **$20M DOE Project**
- **100 MW at Berkeley Lab and space for 2 exascale systems**





NERSC Plan Will Help Take Science through Technology Transition



NERSC-8 Plans

NERSC

Trinity/NERSC-8 Collaboration

Sandia National Laboratories

Los Alamos NATIONAL LABORATORY EST. 1943

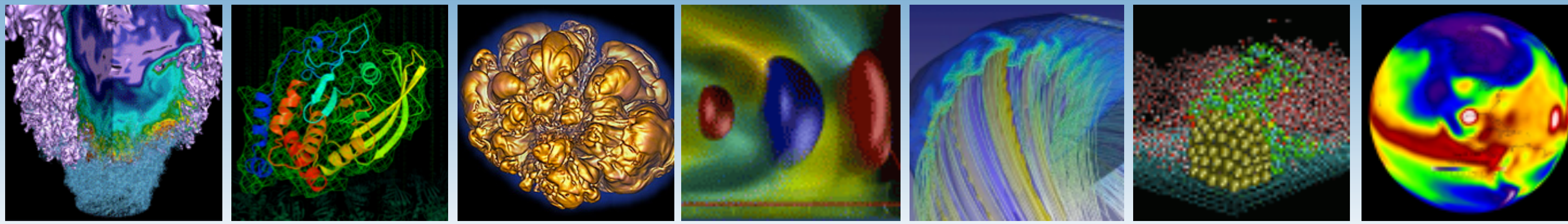
NERSC

Goals:

- 10x-50x increase in application performance over Hopper
- Transition to energy-efficient architectures
- High applications performance per watt
- Most energy efficient machine in most energy efficient facility

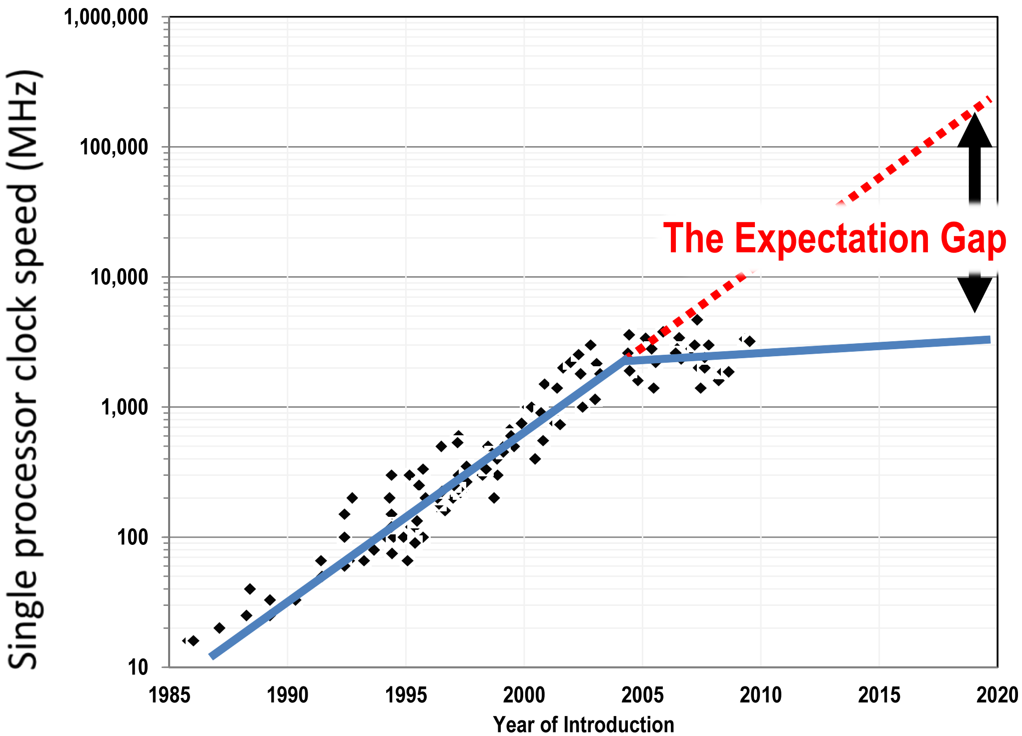
Plans:

- Production HPC resources for 2015/2016.
- Transition to new energy-efficient architectures on road to exascale
- Collaborate with Trinity/ACES to share expertise, reduce risk, and strengthen SC/NNSA alliance on road to exascale



Technology Challenges and Strategies

Power Limits Computing Performance Growth



Processor industry running at "maneuvering speed"

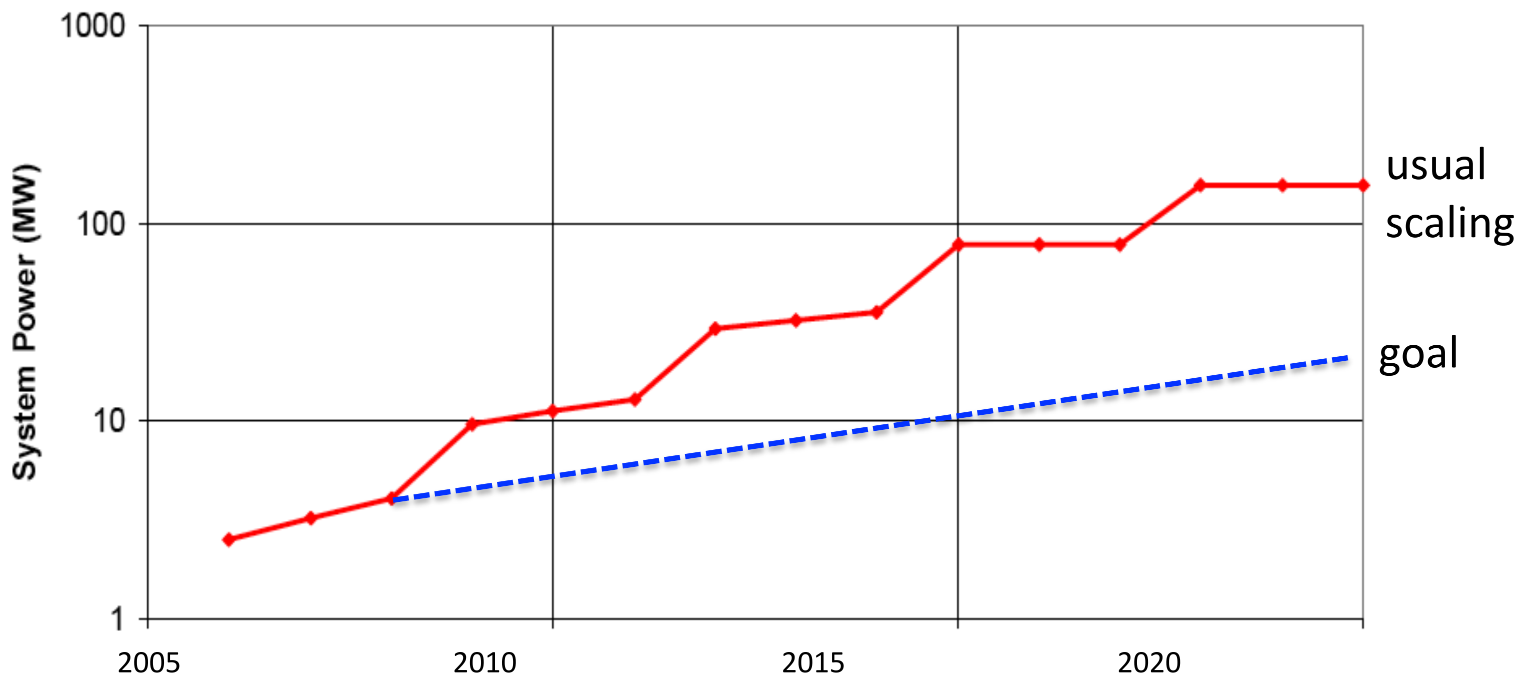
- David Liddle

- Power density limits single processor performance
- Strategy: Redesign architecture, memory, software, algorithms for low power and (implied need) resilience

Energy Efficient Computing is Key to Performance Growth

At $1M per MW, energy costs are substantial

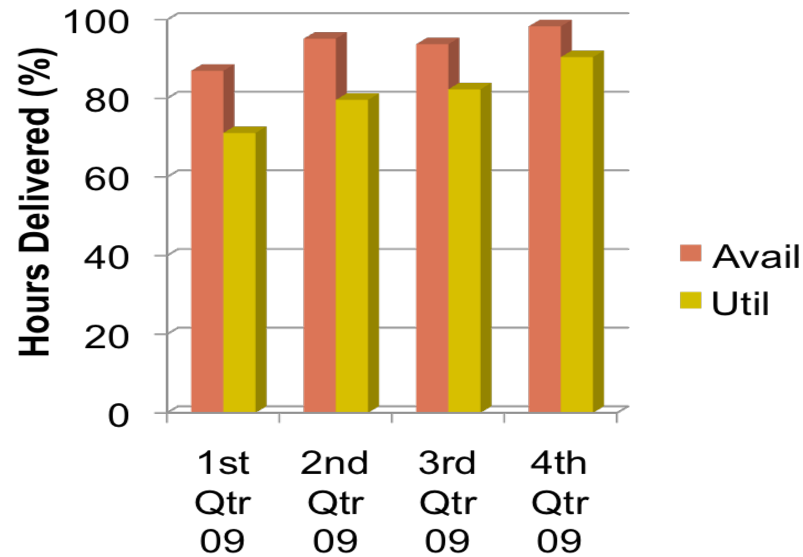
- **1 petaflop in 2010 used 3 MW**
- **1 exaflop in 2018 would use 130 MW with “Moore’s Law” scaling**



This problem doesn’t change if we were to build 1000 1-Petaflop machines instead of 1 Exasflop machine. It affects every university department cluster and cloud data center.

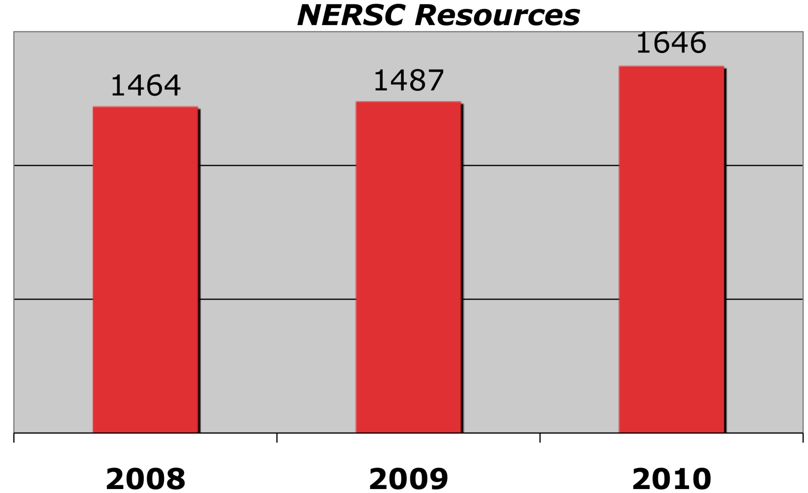
Measuring Efficiency

- **One important factor in computing efficiency is utilization**



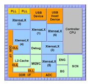
- **If we measure productivity by publications…**
  - *NERSC in 2010 ran at 450 publications per MW-year*

Number of Refereed Publications Using NERSC Resources



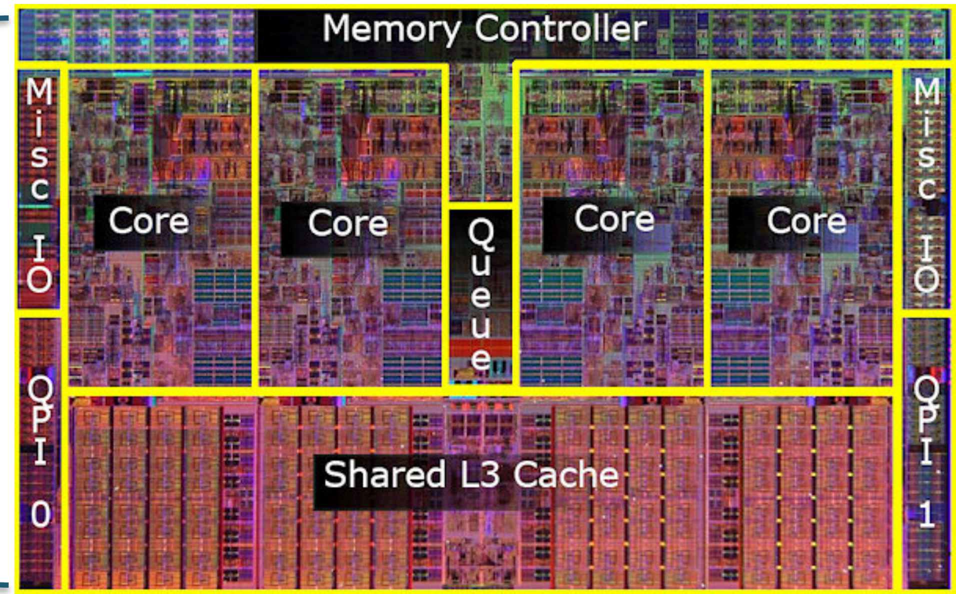
- **Application performance per Watt**

New Processor Designs are Needed to Save Energy



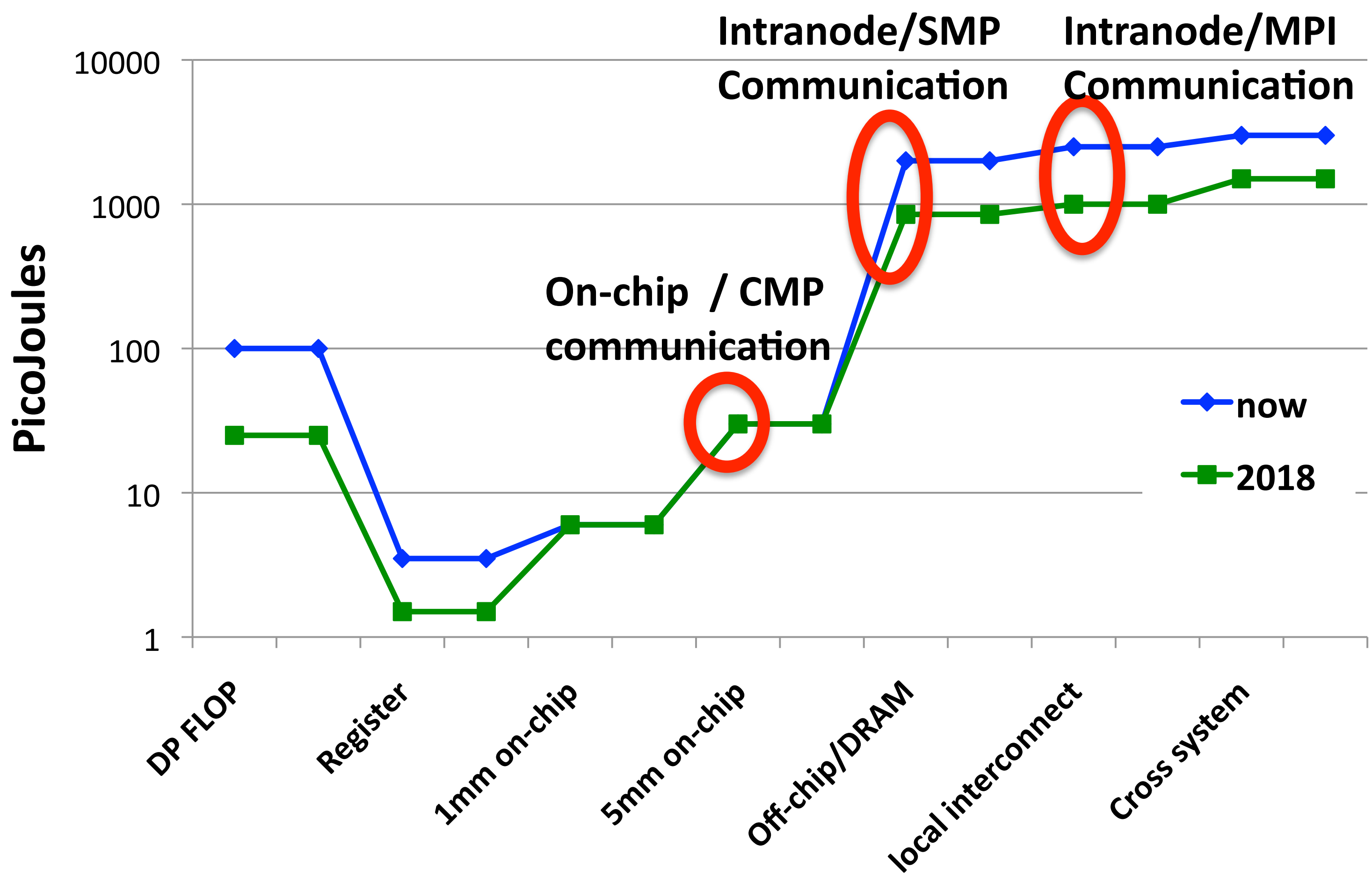
Cell phone processor (0.1 Watt, 4 Gflop/s)

Server processor (100 Watts, 50 Gflop/s)

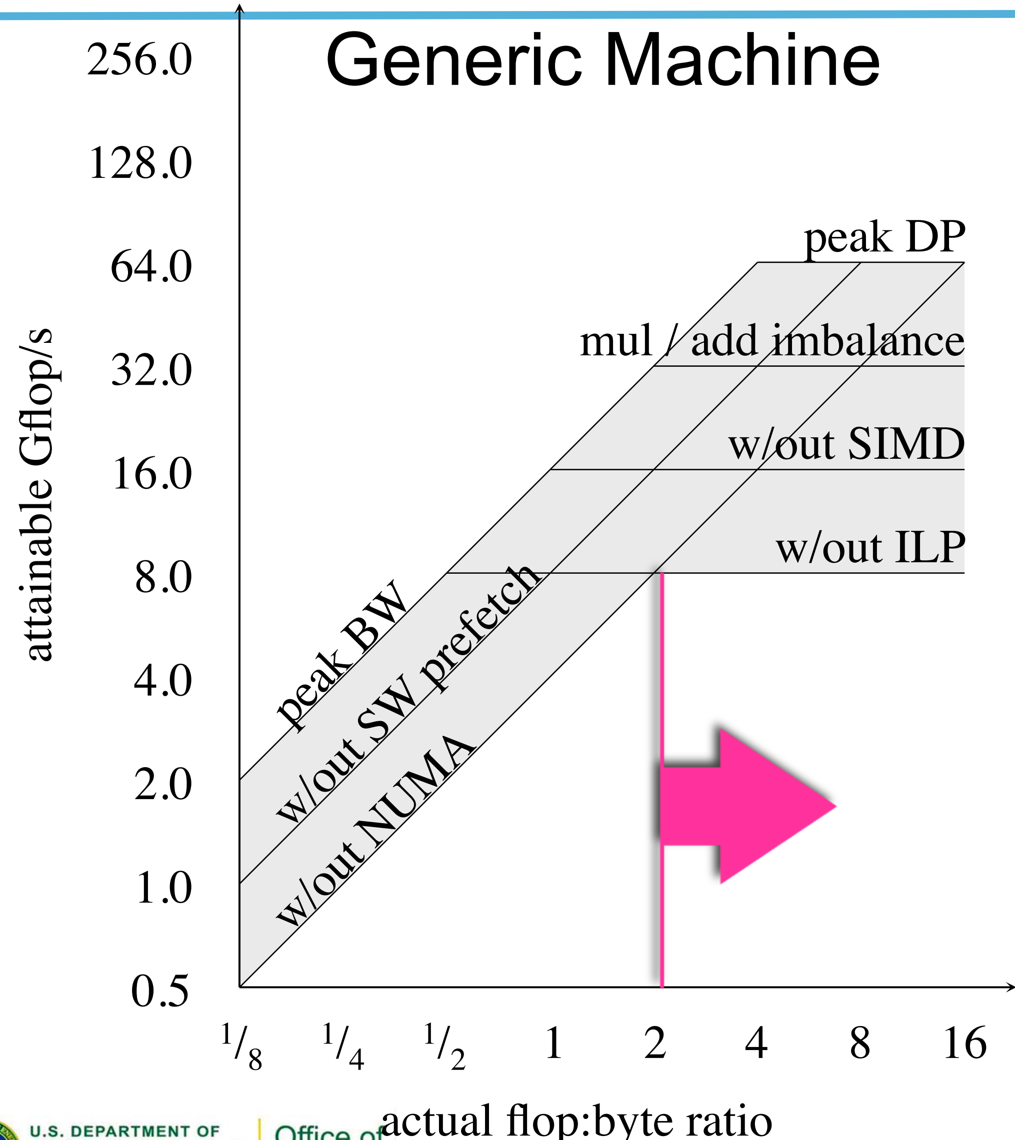


- **Server processors have been designed for performance, not energy**
  – Graphics processors are 10-100x more efficient
  – Embedded processors are 100-1000x
  – Need manycore chips with thousands of cores

Where does the Power Go?

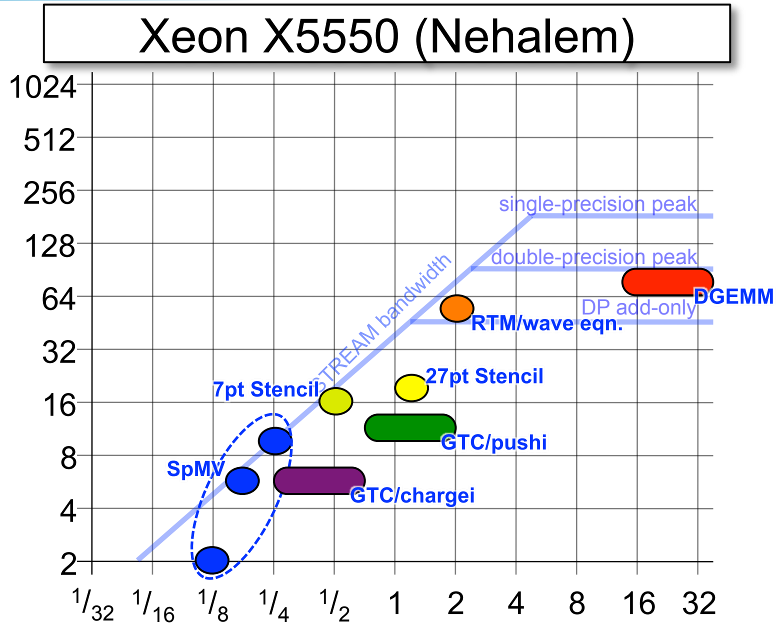


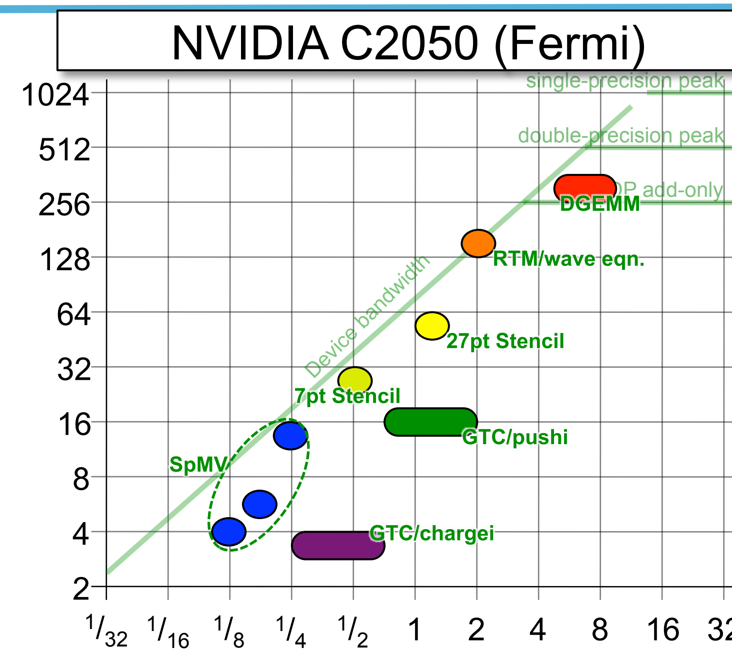
The Roofline Performance Model: Understanding Communication Limits



- The flat room is determined by arithmetic peak and instruction mix
- The sloped part of the roof is determined by peak DRAM bandwidth (STREAM)
- X-axis is the computational intensity of your computation

Exascale Programming: Memory System Structure





Known: Communication wall will get worse;

- Optimizing for memory/network more important than ever
- Automatic data movement (caches, VM) can be wasteful
- Autotuning (search) helps reach bandwidth limits

Unknown:

- How much explicit memory be management?

What is Manycore?

- **NVIDIA, AMD/ATI, Intel MIC, are all Manycore processors**
- **Case for manycore**
  - Many small cores are needed for energy efficiency and power density; could have their own PC or use a wide SIMD
  - May need at least one fat core (heterogeneity) for running the OS, etc.
- **Local store, explicitly managed memory hierarchy**
  - More efficient (get only what you need) and simpler to implement in hardware
- **Co-Processor interface and PCI between CPU and Accelerator**
  - Market: GPUs are separate chips for specific domains
  - Hoping this will go away
- **Transition at NERSC-8, not NERSC-7**

NERSC's Computing Strategy

- **Two major systems on the floor in steady state**
  - Maximize stability and usability rather than peak flops
- **Optimization for application performance not peak**
  - Procurements done using application benchmarks
- **Balance computing with growth in data services**
  - Disk, tape, network, data transfer nodes, gateways
- **Provide for large jobs and large numbers of jobs**
  - Both full OS support and lightweight OS
- **Minimize number of technology transitions**
  - Need to move to manycore is necessary
  - Transition programming model once and choose carefully

Requirements Gathering Ensures NERSC Meets DOE Needs

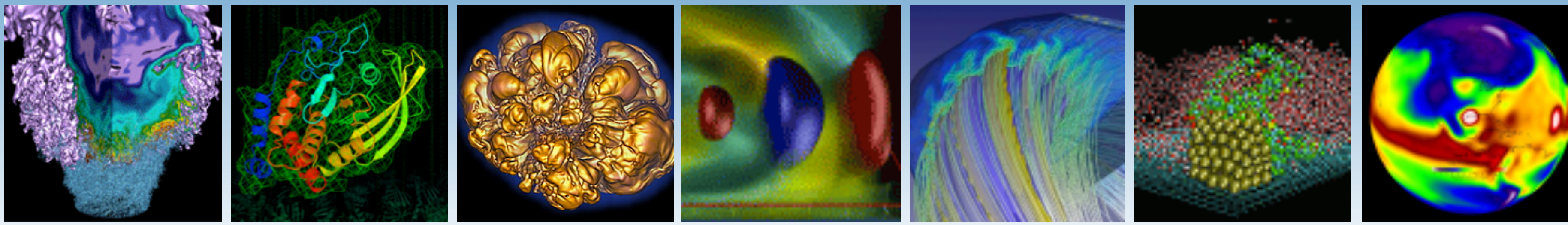
How we use your input

- Communicate science needs and impact with case studies
- Direct input into Mission Need for NERSC-9 and 10
- Inform priorities for computing, storage, infrastructure
- Inform priorities for staffing and services
- Set clear, quantitative needs

Conclusions

- **NERSC requirements**
  – Qualitative requirements shape NERSC functionality
  – Quantitative requirements set the performance
  "What gets measure gets improved"

- **Goals:**
  – Your goal is to make scientific discoveries
  – Our goal is to enable you to do science



Backup Slides

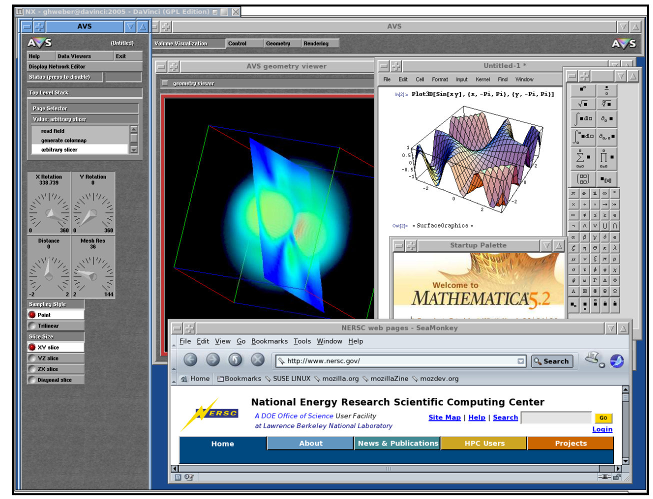
~~Challenges to Exascale~~ Performance Growth

1) **System power** is the primary constraint
2) **Concurrency** (1000x today)
3) **Memory** bandwidth and capacity are not keeping pace
4) **Processor** architecture is open, but likely heterogeneous
5) **Programming model** heroic compilers will not hide this
6) **Algorithms** need to minimize data movement, not flops
7) **I/O bandwidth** unlikely to keep pace with machine speed
8) **Resiliency** critical at large scale (in time or processors)
9) **Bisection bandwidth** limited by cost and energy

Unlike the last 20 years most of these (1-7) are equally important across scales, e.g., 1000 1-PF machines

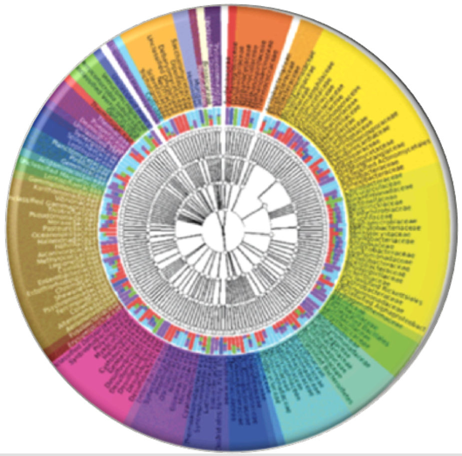
Accelerating Remote Display

- **Problem: remote display operations are very slow due to network latency.**
- **Solution: deploy new technology at NERSC that hides network latency in remote display operations to improve user productivity.**
- **Deployed Summer 2008 to entire NERSC user community.**
- **Results: improves remote display by a factor of about 10x.**

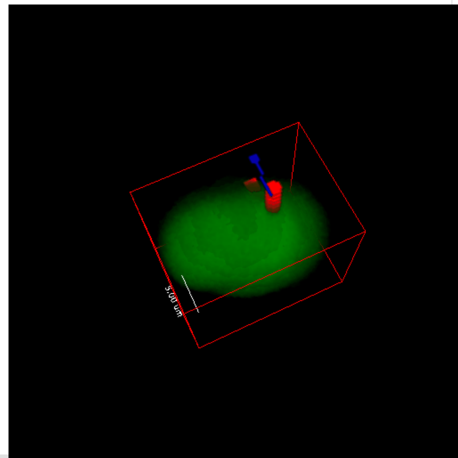


Screenshot of a remote display session running multiple 3D visual data analysis applications.

Berkeley Lab's Big-Data Activities in Biology and Environment



JGI @ NERSC, Genomics pipelines (IMG), Knowledge Base (KBase)



Bioimaging

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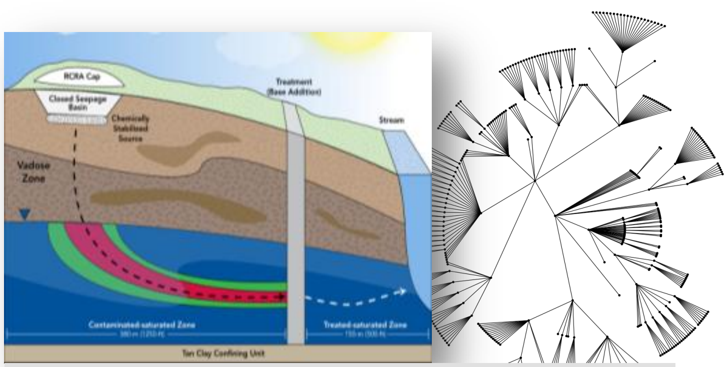
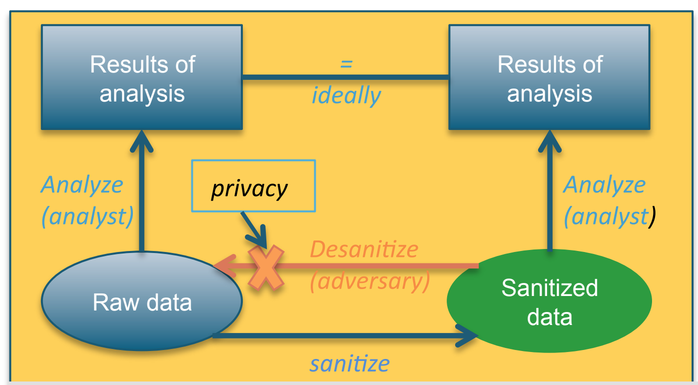
SDAV
Scalable Data Management, Analysis, and Visualization

SDAV: Scalability Data Analytics and Visualization at LBNL



End-to-end solutions for data management, curation and analysis



Medical record sanitation and analysis

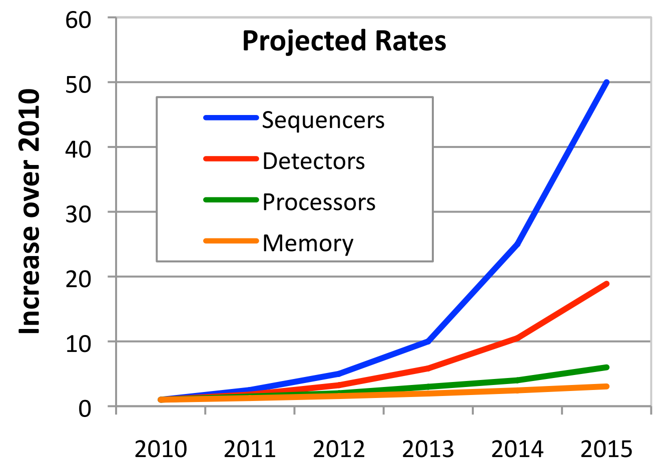
Science in Data: From Simulation to Image Analysis

LBNL Computing on Data key in 4 of 10 Breakthroughs of the decade

- 3 Genomics problems + CMB

Data rates from experimental devices will require exascale volume computing

- Cost of sequencing > Moore's Law
- Rate from CCDs > Moore's Law
- Computing needs > Data size
- Computer performan < Moore Law



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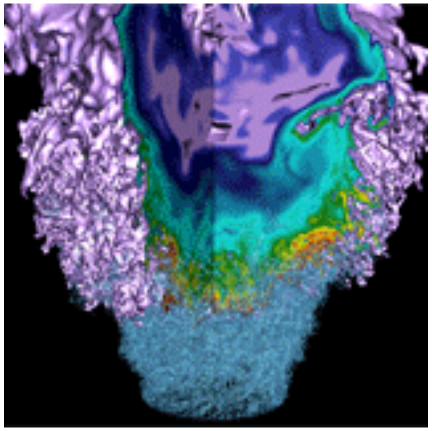
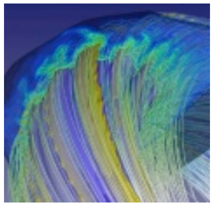
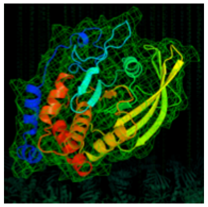
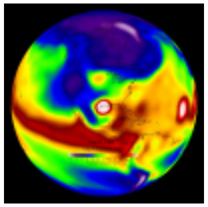
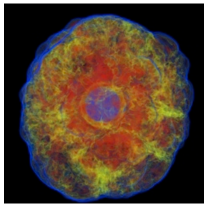
Section Title

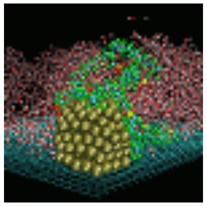












Template Info

- **Fonts**
  - Title: Helvetica Neue Bold Condensed
  - Body: Calibri; bold level 1, regular 2+
- **Title**
  - Single line at 32pt.
  - Autofit.
  - Wraps with proper second line that fits in title box

Theme Colors & Variants

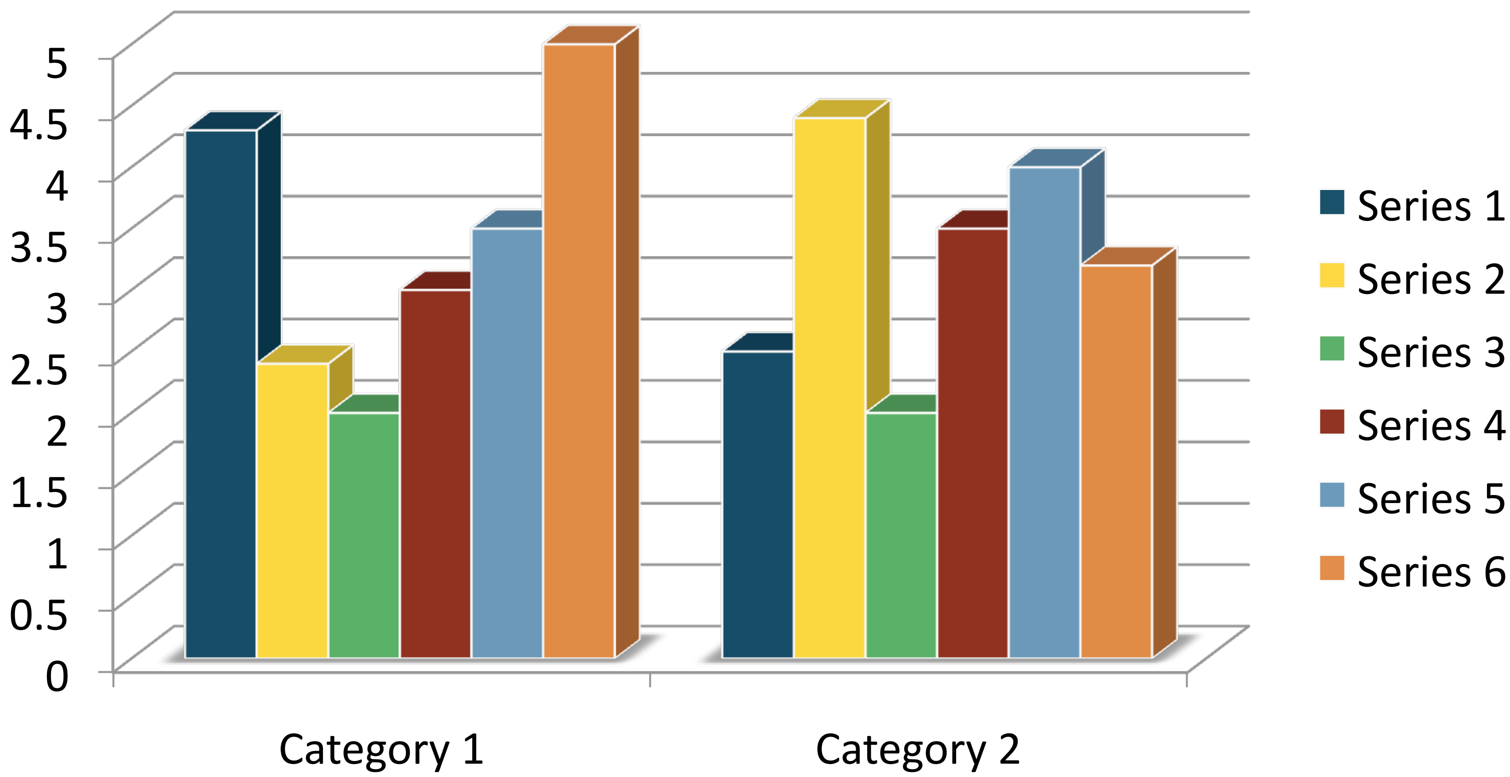
	Back-ground 1	Text 1	Back-ground 2	Text 2	Accent 1	Accent 2	Accent 3	Accent 4	Accent 5	Accent 6
Theme Color										
Lighter 80%										
Lighter 60%										
Lighter 40%										
Darker 25%										
Darker 50%										

Sample Tables

Light Style - Accent 5

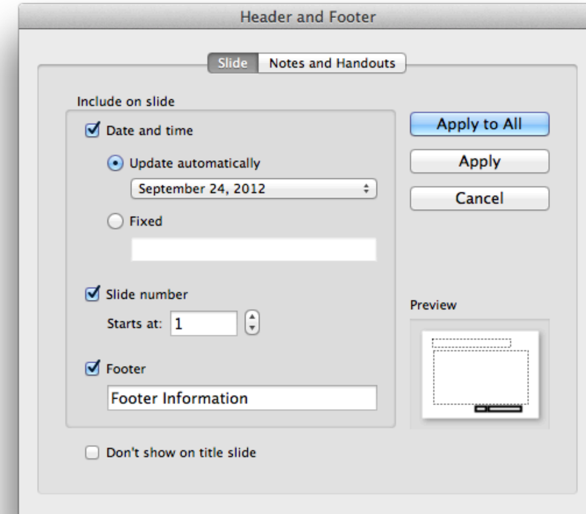
Medium Style - Accent 1	

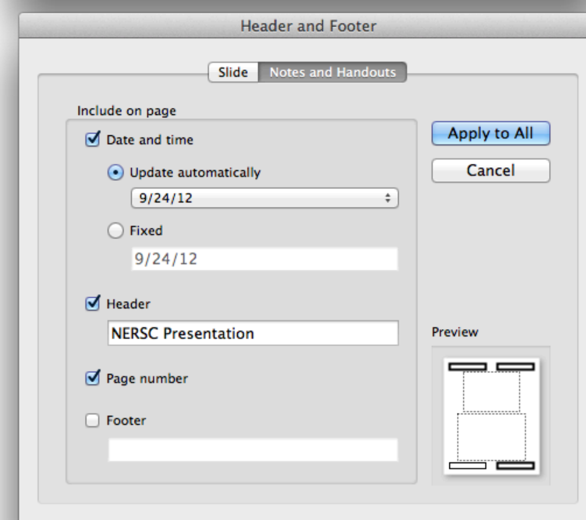
Sample Chart



Headers, Footers and Dates

- **All controlled by “View/Headers and Footers” Menu**
- **The date appears on the title and handout pages**
  - Use “fixed” for a known presentation date.
  - Use “update automatically” to track the current date.
- **Footer information appears to the right of the Lab logo**
  - Optional. Use for name of presentation, copyright info or other usage designations.
- **Notes and handout pages have separate header, footer and date information.**
  - Need to set this redundantly





Importing from Existing Presentations

- **Works OK if the source presentation used a well-formed template**
  - May need to reapply the slide template one or two times.
  - Then correct text size directly or with autofit.

- **Doesn't work well if it was manually formatted.**
  - Observe text frames after importing
  - May need to cut and paste to the text boxes generated from the master slides.

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Backup Slides Follow Big Logo

- **Never have a slide that says "Backup"**
  - Especially if the backup slides address issues that you would rather not cover.
  - It will only invite discussion.

Web Color Palette

Primary Color Palette

Slate R11 G33 B57	Mute Turquoise R0 G143 B184	Turquoise R35 G171 B227	Light Grey Blue R210 G227 B235

Secondary Color Palette

Dark Teal R25 G73 B99	Teal R35 G108 B144	Orange R248 G150 B29	Green R34 G146 707

Earlier Web Color Palette

NERSC

Primary Color Palette

Slate	Mute Turquoise	Turquoise
R 12 G 21 B 39	R 0 G 144 B 189	R 0 G 175 B 229
HEX 0c1527	HEX 0090bd	HEX 00afe5

Secondary Color Palette

Gold	Dark Teal	Bright Cyan	Orange
R 255 G 185 B 0	R 17 G 71 B 102	R 107 G 212 B 251	R 255 G 101 B 0
HEX ffb900	HEX 114766	HEX 6bd4fb	HEX ff6500

Neutral Color Palette

Cream	Light Warm Gray	Medium Warm Grey	Dark Teal
R 255 G 247 B 220	R 218 G 218 B 218	R 137 G 148 B 150	R 17 G 71 B 102
HEX fff7dc	HEX dadbda	HEX 899496	HEX 114766