NERSC Overview

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NERSC User Services

EETD Seminar
June 22, 2011

U.S. DEPARTMENT OF ENERGY | Office of Science

NERSC National Energy Research Scientific Computing Center

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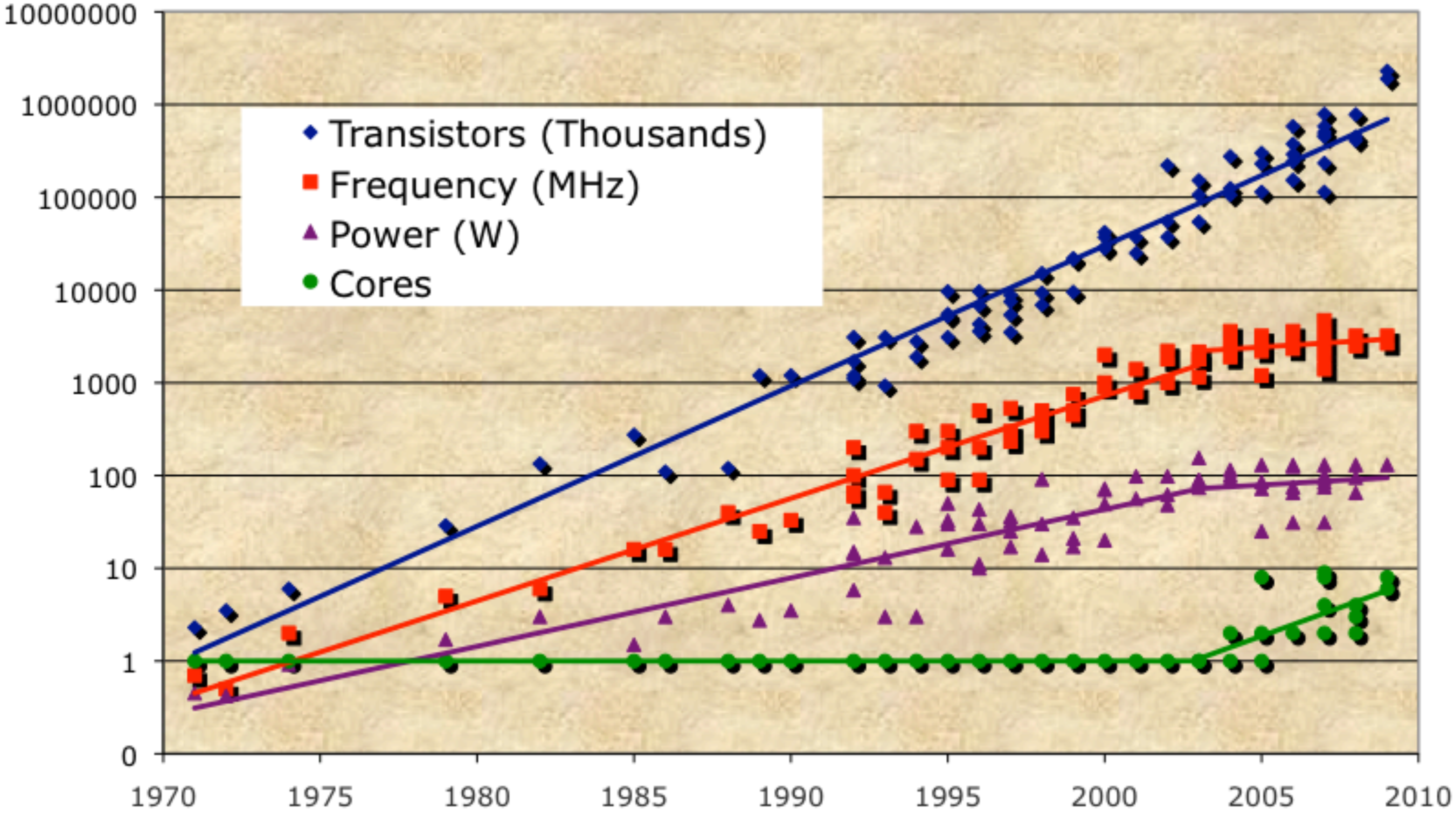
EETD and NERSC

- **NERSC's mission is to provide computing and storage resources for energy-related research and engineering**
- **Broad support for fusion, materials, chemistry research**
  - Hydrogen storage, artificial photosynthesis, solar energy storage, wind farm design, efficient combustion, understanding LED droop
- **Energy efficiency research is an important part of this picture**
  - If there is a place for HPC in EETD, NERSC is capable and eager to help
- **If you remain tied to single-threaded serial computing, you are going to be quickly left behind**
  - Flops are cheap, so use them
  - Cost per Gflop: $1.1 Trillion in 1960, $15 M in 1984, $30,000 in 1997, $600 in 2003, $0.42 in 2007, $0.13 in 2009

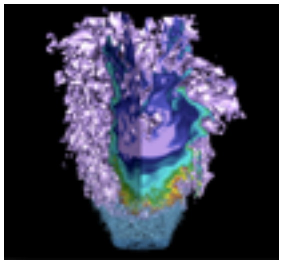
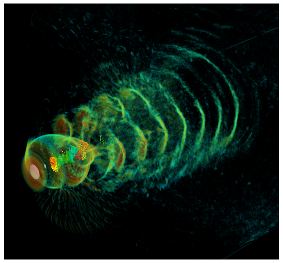
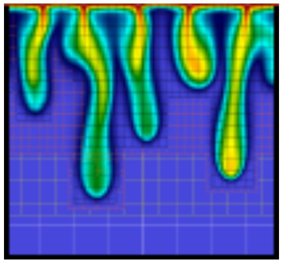
Revolution in Processors

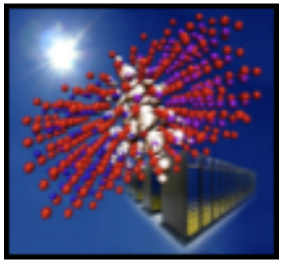
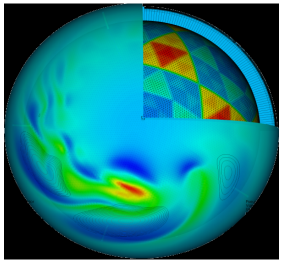


- Chip density is continuing increase ~2x every 2 years
- Clock speed is not
- Number of processor cores may double instead
- Power is under control, no longer growing

Moore's Law reinterpreted

- Number of cores per chip will double every two years
- Clock speed will not increase (possibly decrease)
- Need to deal with systems with millions of concurrent threads
- Need to deal with inter-chip parallelism as well as intra-chip parallelism
- Your take-away:
  - *Future performance increases in computing are going to come from exploiting parallelism in applications*

Why NERSC?

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Expert Services

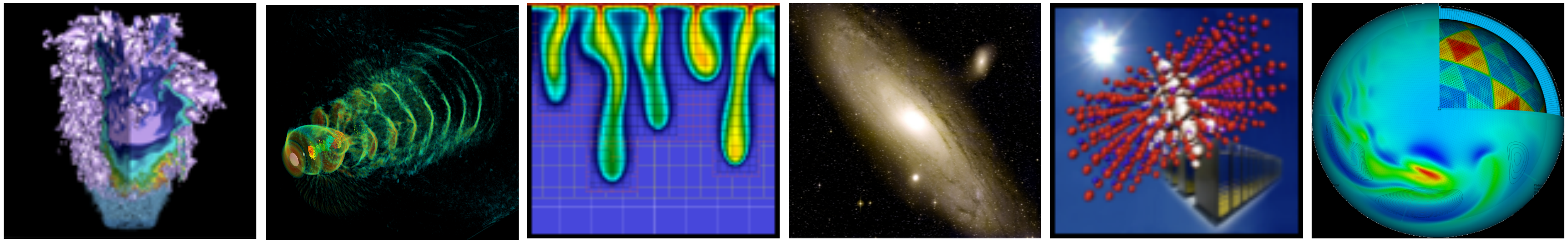
- NERSC's emphasis is on its users
  - Helping scientists and engineers be successful
- User-oriented systems and services
  - Sets NERSC apart from other centers
- Help Desk / Consulting
  - Immediate access to consultants (7 Ph.Ds)
- User group (NUG) has tremendous influence
  - Monthly teleconferences & yearly meetings
- Requirement-gathering workshops with scientists
- Agile response to special requests from users

Advantages (to you) of NERSC

- **Expert services**
  - Updated OS, software
  - NERSC does system administration, 24x7
  - Consulting and advice
  - Emphasis on helping users being successful
  - Reliable systems; auto backups for disaster recovery
- **Free access to vast amounts of computing, software, storage**
  - Play "what if" scenarios
  - Pre-compute a large library of configurations at high resolution/level of detail (or whatever)
  - Add physics and/or more parameters
  - Get compute-intensive results quickly

Disadvantages (to you)

- **NERSC computers are shared**
  - Not generally interactive
  - “Long” turnaround time: hours to days to a week
  - Per user, per system limits on # of active jobs
- **You must fill out an application for new projects**
  - Startup projects are easy to get
- **You have to learn how to use the systems**
  - You are busy already
- **You will probably have to change your code and/or your workflow to take best advantage of NERSC resources**



What is NERSC?

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NERSC Facility Leads DOE in Scientific Computing Productivity

THE JOURNAL OF CHEMICAL PHYSICS
APPLIED PHYSICS LETTERS
nature
Journal of Fluid Mechanics
nature
WINDS OF CLIMATE CHANGE
Struct
Dynamomics: Protein Folding and Dynamics Go Large-Scale!

NERSC computing for science

- •4000 users, 500 projects
- •From 48 states; 65% from universities
- •Hundreds of users each day
- ***•1500 publications per year***

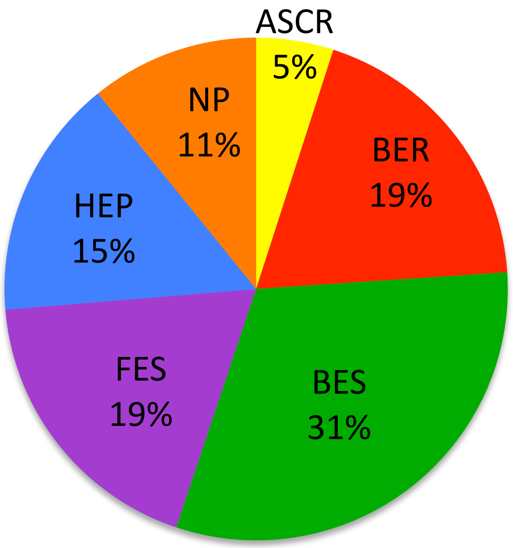
Systems designed for science

- •1.3 PF Petaflop Cray: Hopper
  - 3rd fastest computer in US
  - Fastest open Cray XE6
  - Additional .5 PF in Franklin and smaller clusters

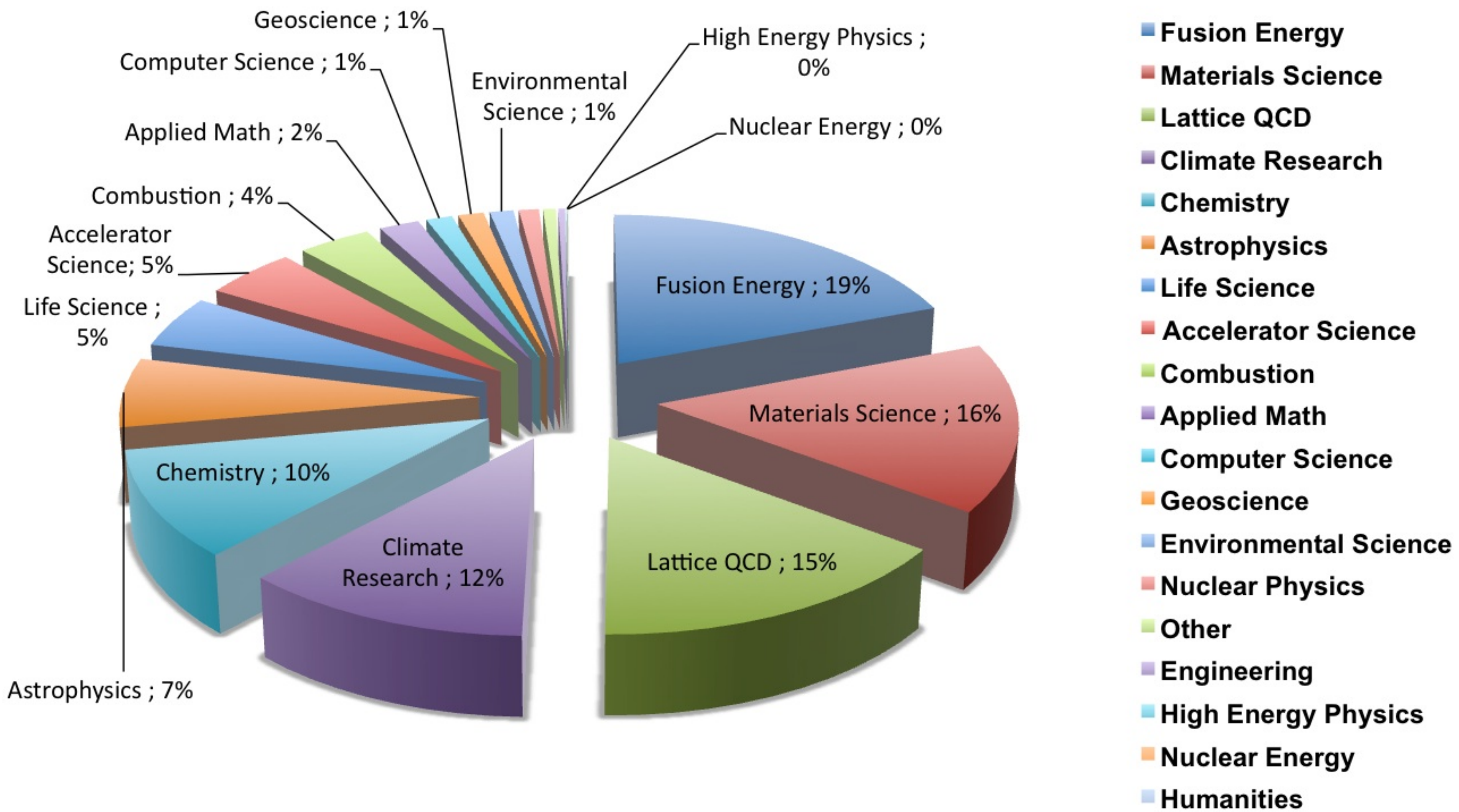
NERSC is the Production Facility for DOE Office of Science

- **NERSC serves a large population**
  - About 4,000 users
  - 400 projects
  - 500 codes
- **Unique resources**
  - Expert consulting and other services
  - High end computing systems
  - High end storage systems
  - Interface to high speed networking
- **Science-driven services**
  - Machines procured competitively using application benchmarks from DOE/SC
  - Allocations controlled by DOE/SC Program Offices to couple with funding decisions

2010 Allocations



NERSC Workload



NERSC 2011 Allocations By Science Area

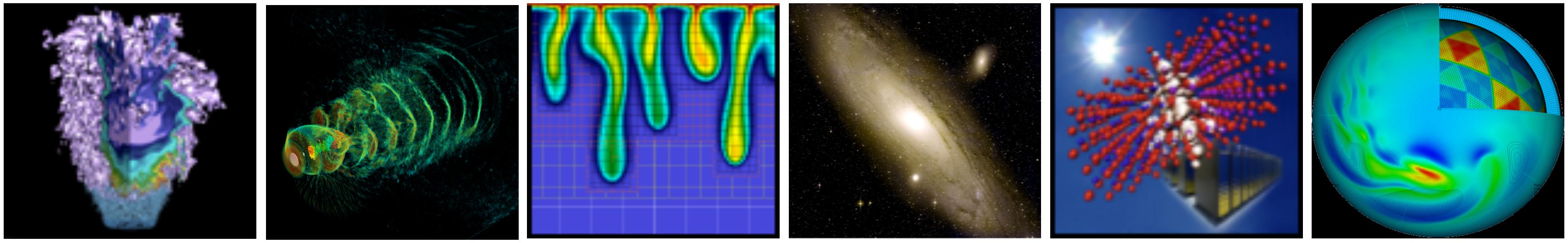
DOE Office of Advanced Scientific Computing Facilities

NERSC at LBNL

- **1000s users,100s projects**
- **Allocations:**
  - 80% DOE program managers
  - 10% ASCR Leadership Computing Challenge
  - 10% NERSC reserve
- **Science includes all of DOE Office of Science**
- **Machines procured competitively**

“Leadership Facilities” at Oak Ridge & Argonne

- **100s users 10s projects**
- **Allocations:**
  - 60% ANL/ORNL managed INCITE process
  - 30% ACSR Leadership Computing Challenge[*]
  - 10% LCF reserve
- **Science limited to largest scale; no commitment to DOE/SC offices**
- **Machines procured through partnerships**



High Performance Computing Systems

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Distributed Memory Systems

- **Most HPC systems are "distributed memory"**
  - Many nodes, each with its own local memory and distinct memory space
  - Nodes communicate over a specialized high-speed, low-latency network
  - SPMD (Single Program Multiple Data) is the most common model
    - Multiple copies of a single program (tasks) execute on different processors, but compute with different data
    - Explicit programming methods (MPI) are used to move data among different tasks

NERSC Systems

Large-Scale Computing Systems

Hopper (NERSC-6): Cray XE6

6,384 compute nodes, 153,216 cores

110 Tflop/s on applications; 1.27 Pflop/s peak

Franklin (NERSC-5): Cray XT4

9,532 compute nodes; 38,128 cores

~25 Tflop/s on applications; 356 Tflop/s peak

Clusters

140 Tflops total

Carver

IBM iDataplex cluster

PDSF (HEP/NP)

~1K core cluster

Magellan Cloud testbed

IBM iDataplex cluster

GenePool (JGI)

~5K core cluster

NERSC Global File system (NGF)

Uses IBM's GPFS

1.5 PB capacity

5.5 GB/s of bandwidth

HPSS Archival Storage

40 PB capacity

4 Tape libraries

150 TB disk cache

Analytics

Euclid

512 GB shared mem

Dirac

GPU testbed

48 nodes

Major Compute Systems

- **Hopper**
  - Hopper is NERSC's flagship computer for running high-performance parallel scientific codes.
- **Franklin**
  - Franklin, an earlier-generation Cray computer, augments the Hopper system.
- **Carver**
  - Carver provides a generic full Linux environment for codes that need operating system features that are not available on the Cray systems or don't demand massive parallelism.

Hopper - Cray XE6

- 1.2 GB memory / core (2.5 GB / core on "fat" nodes) for applications
- /scratch disk quota of 5 TB
- 2 PB of /scratch disk
- Choice of full Linux operating system or optimized Linux OS (Cray Linux)
- PGI, Cray, Pathscale, GNU compilers

- 153,408 cores, 6,392 nodes
- "Gemini” interconnect
- 2 12-core AMD 'MagnyCours' 2.1 GHz processors per node
- 24 processor cores per node
- 32 GB of memory per node (384 "fat" nodes with 64 GB)
- 216 TB of aggregate memory

Use Hopper for your biggest, most computationally challenging problems.

Franklin - Cray XT4

38,288 compute cores

9,572 compute nodes

One quad-core AMD 2.3 GHz Opteron processors (Budapest) per node

4 processor cores per node

8 GB of memory per node

78 TB of aggregate memory

1.8 GB memory / core for applications

/scratch disk default quota of 750 GB

Light-weight Cray Linux operating system

No runtime dynamic, shared-object libs

PGI, Cray, Pathscale, GNU compilers

Use Franklin for all your computing jobs, except those that need a full Linux operating system.

Carver - IBM iDataPlex

3,200 compute cores

400 compute nodes

2 quad-core Intel Nehalem 2.67 GHz processors per node

8 processor cores per node

24 GB of memory per node (48 GB on 80 "fat" nodes)

2.5 GB / core for applications (5.5 GB / core on "fat" nodes)

InfiniBand 4X QDR

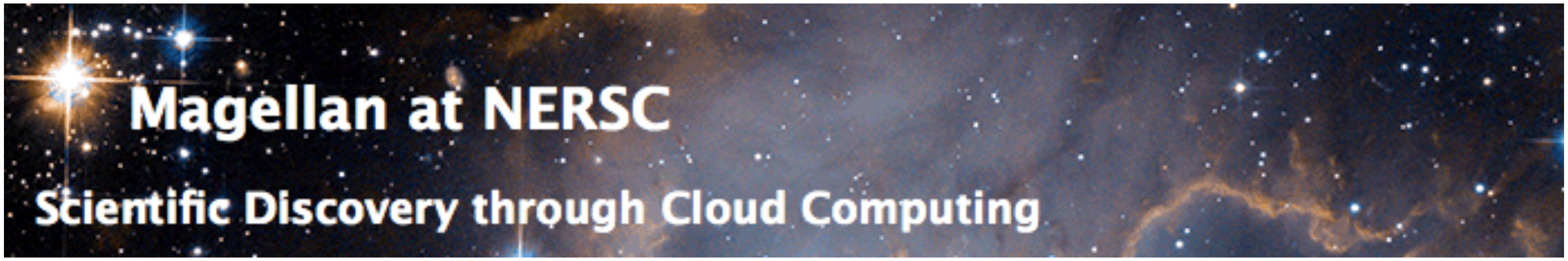
NERSC global /scratch directory quota of 20 TB

Full Linux operating system

PGI, GNU, Intel compilers

Use Carver for jobs that use up to 512 cores, need a fast CPU, need a standard Linux configuration, or need up to 48 GB of memory on a node.

Magellan - IBM IDataPlex



Dedicated to HPC Cloud Computing research

4,480 compute cores

560 compute nodes

Two quad-core Intel Nehalem 2.67 GHz processors per node

8 processor cores per node

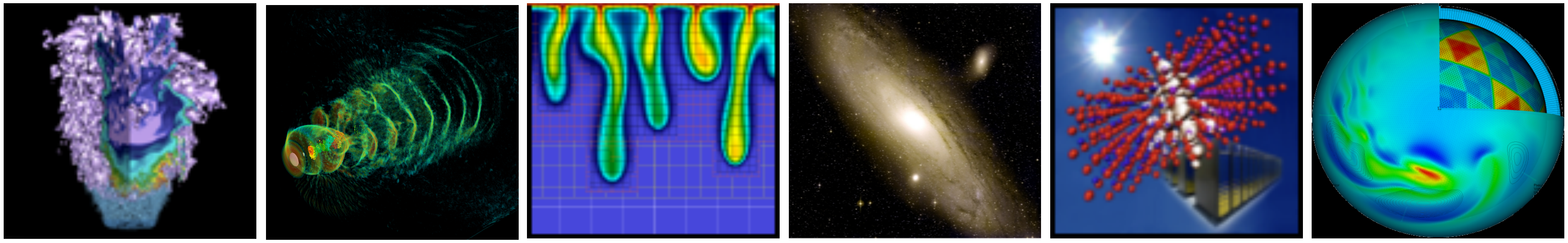
24 GB of memory per node (48 GB on 160 "fat" nodes)

2.5 GB / core for applications (5.5 GB / core on "fat" nodes)

NERSC global /scratch directory quota of 20 TB

Full Linux operating system

PGI, GNU, Intel compilers



Using NERSC

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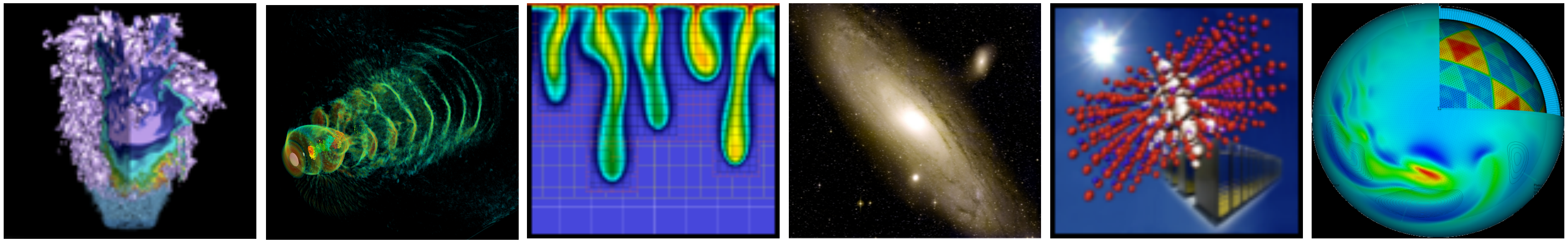
Allocations

- You must have an allocation of time to run jobs at NERSC (be a member of a "repo")
- Project PIs apply through the ERCAP process
- Computer time and storage allocations are awarded by DOE Program Offices
- Most allocations are awarded in the fall
  - Allocation year starts in January
  - 2011: Additional awards made for May 1 start of Hopper production service
  - Small startup allocations are awarded throughout the year
  - Additional time available through NISE and ALCC

Jobs at NERSC

- Most jobs are parallel, using 10s to 100,000+ cores.
- Mostly run as batch scripts; limited interactive access
- Many use custom codes; others use pre-installed applications
- Typically run a few hours, up to 48. Longer runs can be accommodated if needed and logistically possible.
- Many jobs “package” lower concurrency runs into one job
  - Even many “serial jobs”
  - Load balance may be an issue



System Architecture

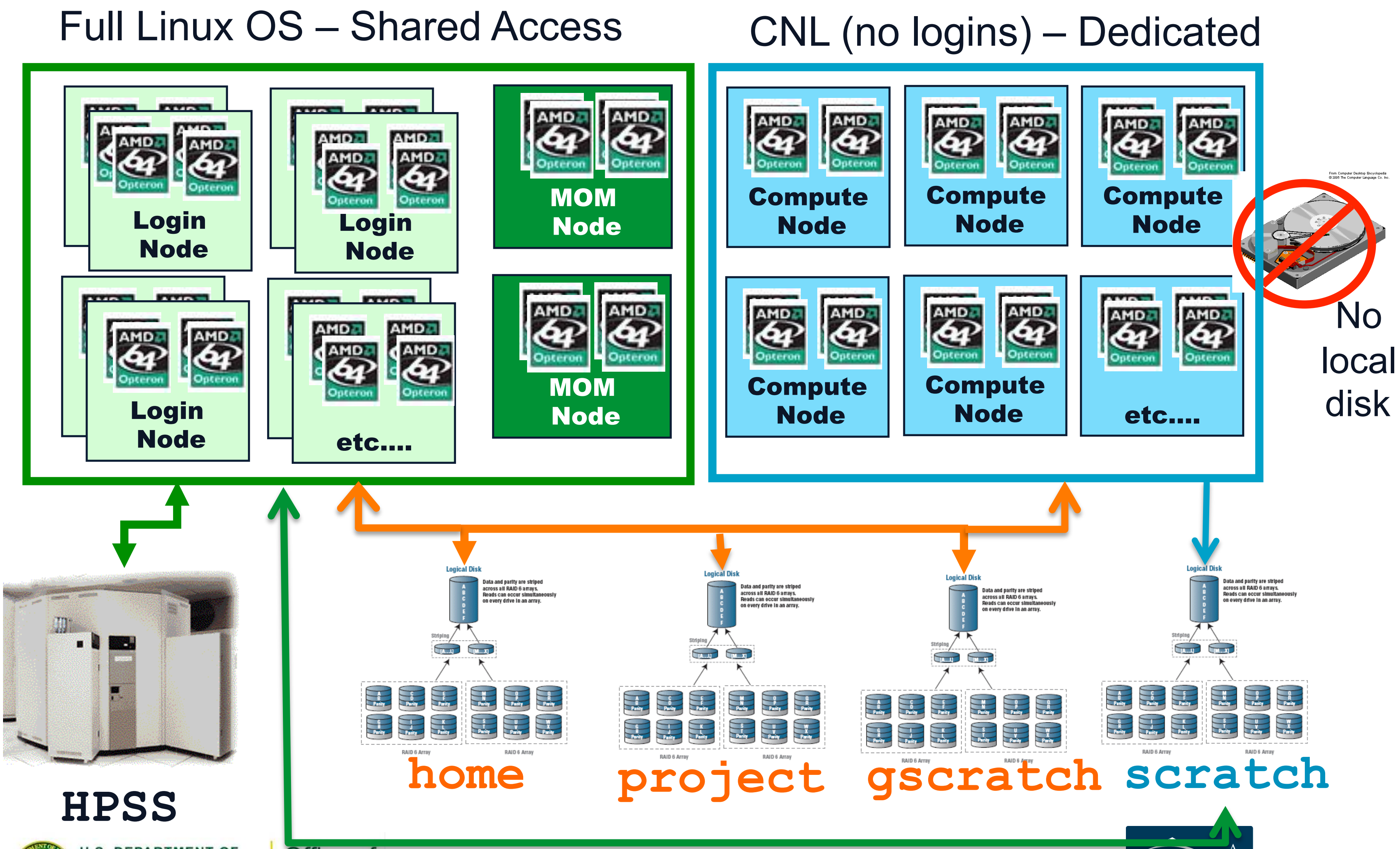
HPC Node

- **A “node” is a (physical) collection of CPUs, memory, and interfaces to other nodes and devices.**
  - Single memory address space
  - Memory access “on-node” is significantly faster than “off-node” memory access
  - Often called an “SMP node” for “Shared Memory Processing”
    - Not necessarily “symmetric” memory access as in “Symmetric Multi-Processing”

Login Nodes and Compute Nodes

- Each supercomputer has 3 types of nodes that you will use directly
  - Login nodes
  - Compute nodes
  - “MOM” nodes
- Login nodes
  - Edit files, compile codes, run UNIX commands
  - Submit batch jobs
  - Run short, small utilities and applications
- Compute nodes
  - Execute your application; dedicated to your job
  - No direct login access
- “MOM” nodes
  - Execute your batch script commands
  - Carver: “head” compute node; Cray: shared “service” node

Cray Systems



Full Linux OS – Shared Access

CNL (no logins) – Dedicated

No local disk

HPSS

home

project

gscratch

scratch

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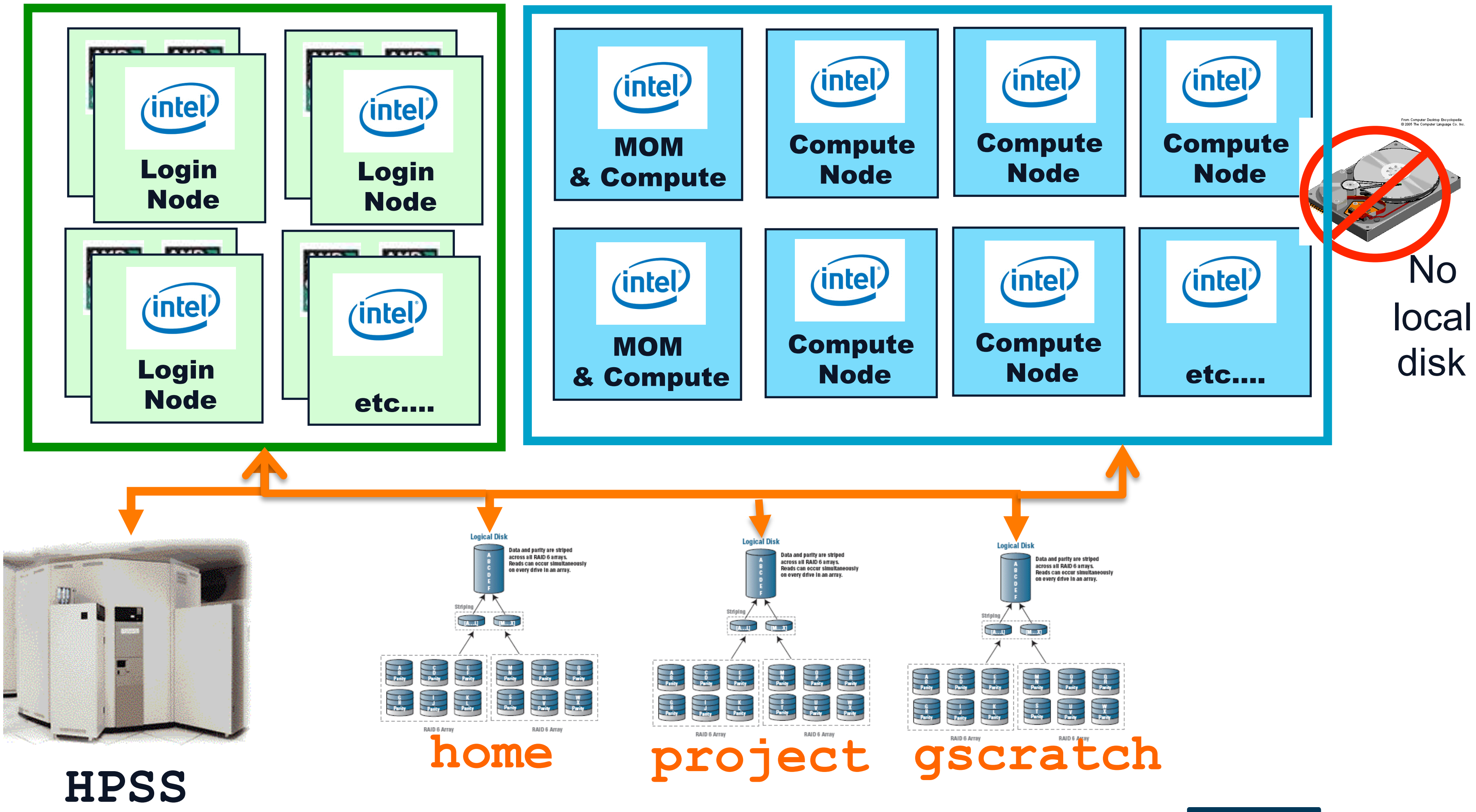
Carver / Magellan / Dirac

Full Linux OS – Shared

Full Linux (no logins) – Dedicated



Login Node

Login Node

Login Node

etc....

MOM & Compute

Compute Node

Compute Node

Compute Node

MOM & Compute

Compute Node

Compute Node

etc....

No local disk

HPSS

home

project

gscratch

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Parallel Models

- **SPMD**
  - Single Program, Multiple Data
  - Most common way to run codes at NERSC
  - *N* copies of your program/application/ code execute at the same time
  - Each instance does calculations involving a portion of a large data set
  - Temperature in a house grid example

SPMD Execution Model

- Each code instance executes on one compute “core”
- Each instance holds its data in local private memory
- If other instances need data or the results of calculations owned by another instance, the two must “pass the data (message)” to where it is needed
- Library of functions (MPI)

Shared-Memory Threaded Parallelism

- A single executable creates multiple process threads of execution that all have access to a shared pool of memory
- Typically one thread per compute core
- Number of threads limited to the number of cores on a node
- Computational work distributed to threads by programmer or maybe compiler

Hybrid Model

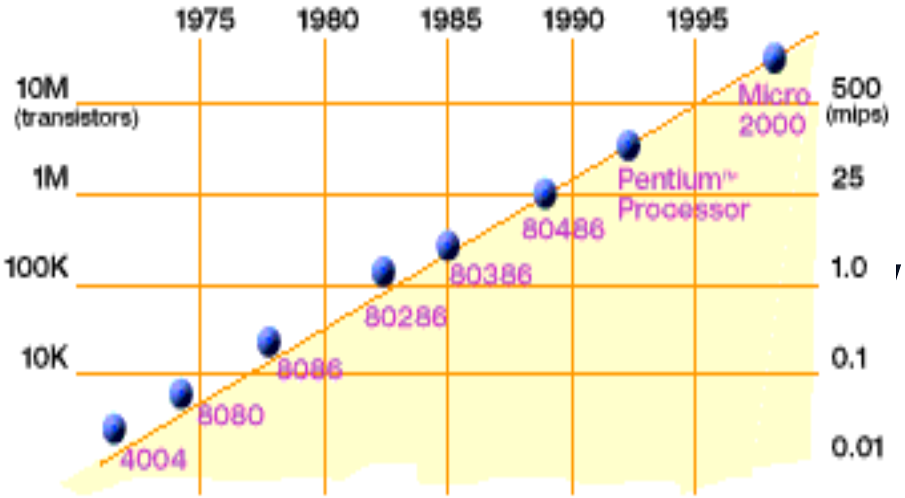
- **Run multiple instances**
  - Communicate via MPI function calls
- **Multiple threads per instance**
  - Often 1 MPI task and cores_per_node threads per task
  - Architecture may dictate best ratio of threads/ MPI task
- **Now two layers of parallelism**

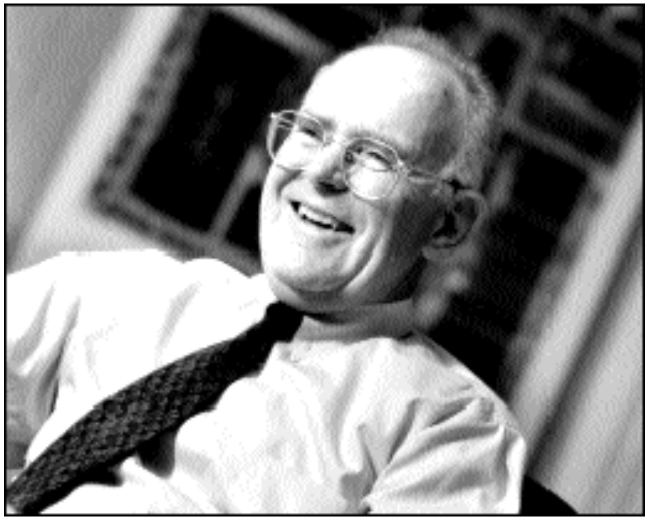
GPUs

- **NVIDIA Tesla “gaming chip”**
  - 515 Flops
  - vs. ~ 50 Gflops on AMD hex-core on Hopper
  - 448 lightweight cores w/ private memory
  - Currently implemented as a “coprocessor” on a PCI card
- **Program with CUDA**
- **“Disaster” from a programming perspective**
  - Third layer of parallelism: MPI+Threads+CUDA
  - You do the memory management between GPU and CPU
  - A new API to learn
  - Few and immature programming tools
  - Future of CUDA and “coprocessor” paradigm uncertain at best
- **Not all codes will benefit from GPU acceleration**
- **There is hope for tighter integration of CPU and GPU and better programming models**

Why Do You Care About Parallelism?

Moore's Law





2X transistors/Chip Every 1.5 years

Called "Moore's Law"

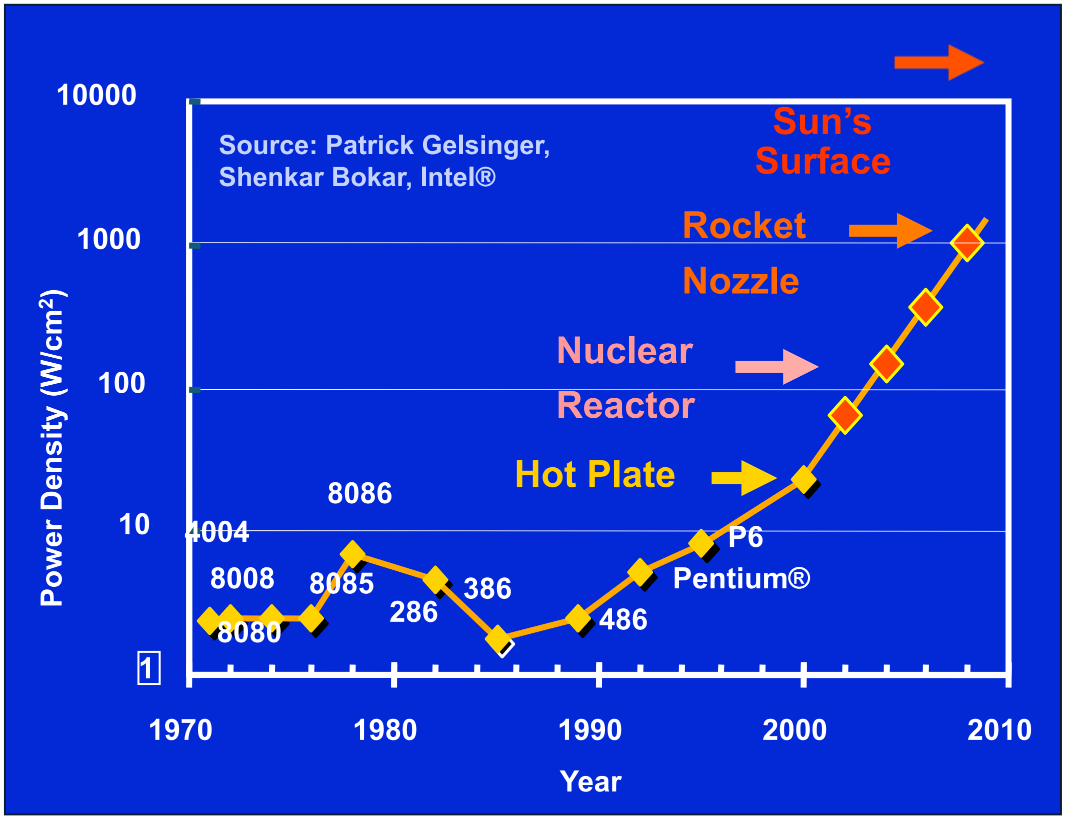
Microprocessors have become smaller, denser, and more powerful.

Gordon Moore (co-founder of Intel) predicted in 1965 that the transistor density of semiconductor chips would double roughly every 18 months.

Slide source: Jack Dongarra

Power Density Limits Serial Performance

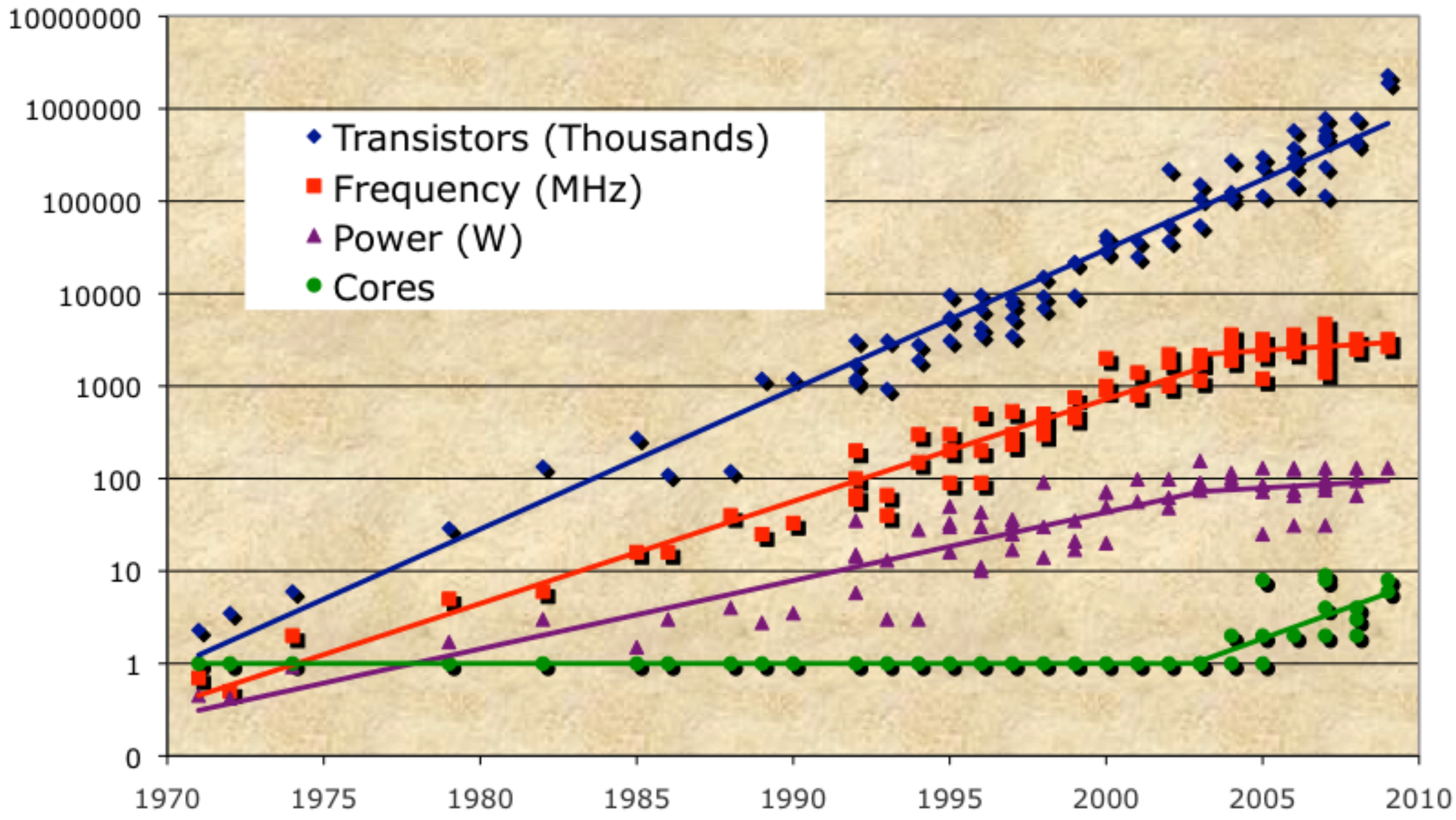
- Concurrent systems are more power efficient
  - Dynamic power is proportional to V^2fC
  - Increasing frequency (f) also increases supply voltage (V) → cubic effect
  - Increasing cores increases capacitance (C) but only linearly
  - Save power by lowering clock speed



Source: Patrick Gelsinger, Shenkar Bokar, Intel®

- High performance serial processors waste power
  - Speculation, dynamic dependence checking, etc. burn power
  - Implicit parallelism discovery
- More transistors, but not faster serial processors

Revolution in Processors



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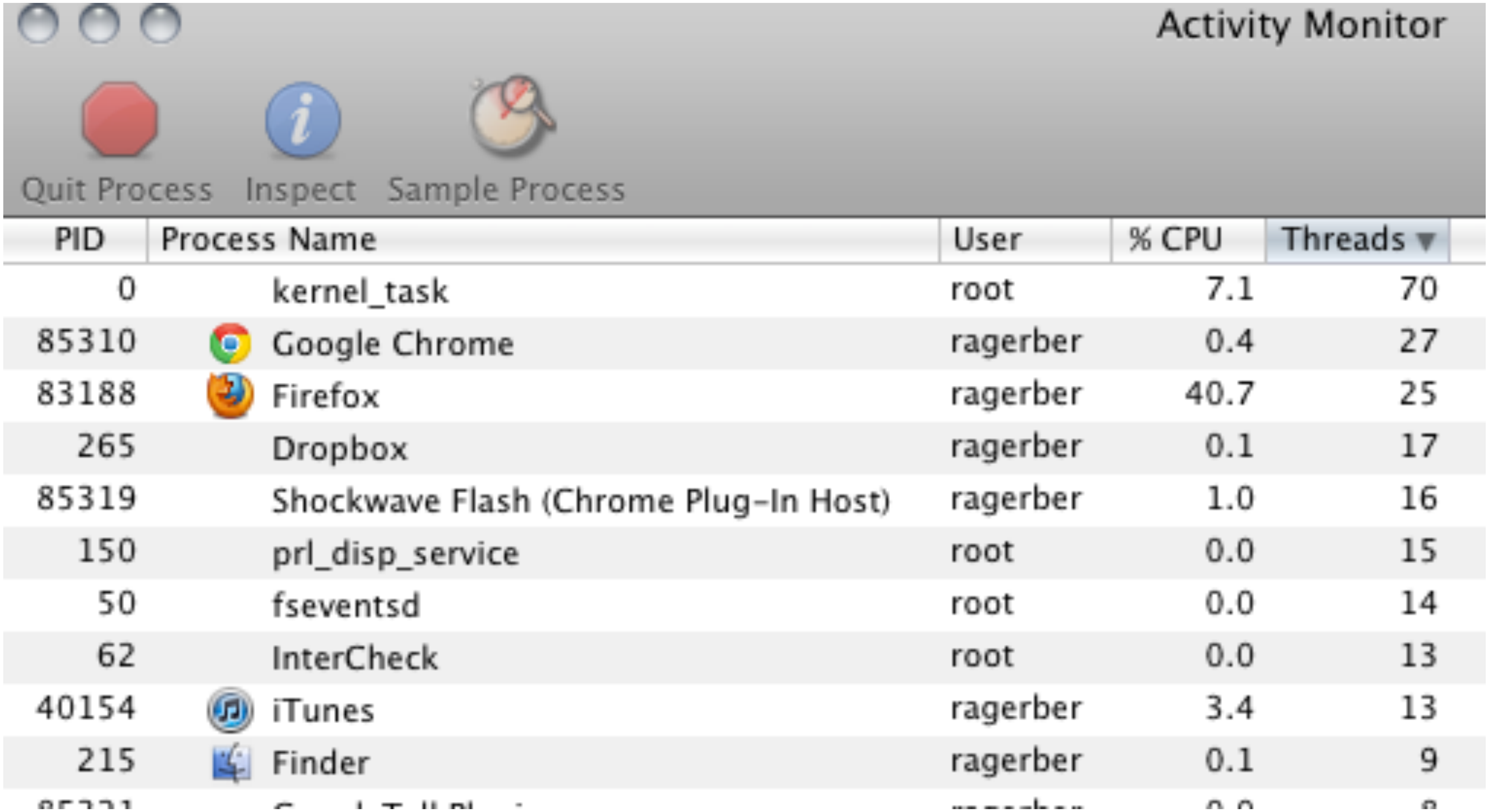
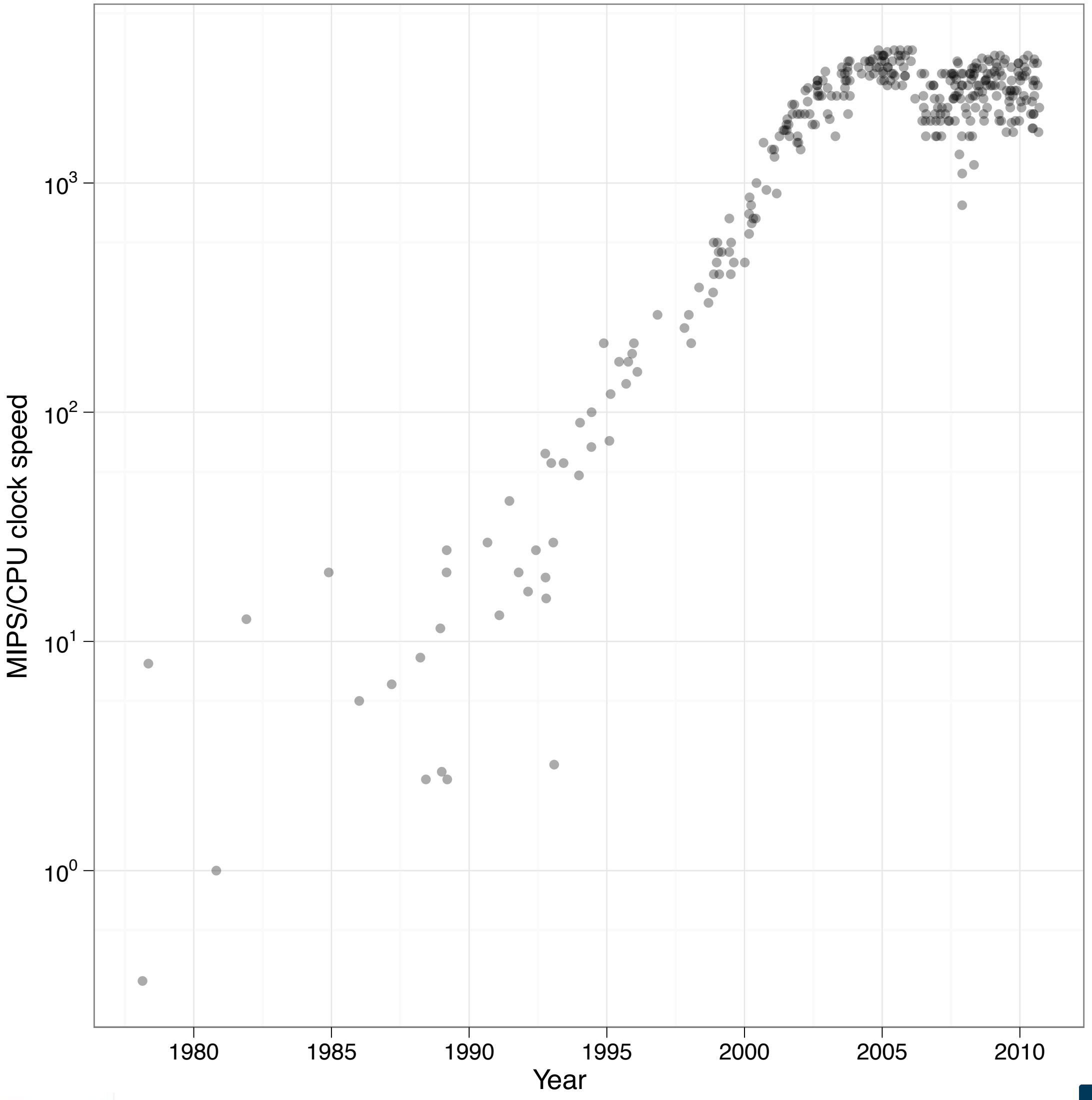


PID	Process Name	User	% CPU	Threads ▼
0	kernel_task	root	7.1	70
85310	Google Chrome	ragerber	0.4	27
83188	Firefox	ragerber	40.7	25
265	Dropbox	ragerber	0.1	17
85319	Shockwave Flash (Chrome Plug-In Host)	ragerber	1.0	16
150	prl_disp_service	root	0.0	15
50	fseventsd	root	0.0	14
62	InterCheck	root	0.0	13
40154	iTunes	ragerber	3.4	13
215	Finder	ragerber	0.1	9

CPU Clock Frequency



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