

## **Getting Started at NERSC**

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#### Purpose

# • This presentation will help you use NERSC and its facilities

- Practical information
- Introduction to terms and acronyms
- Help you get things done efficiently
- This is not a programming tutorial
  - But you will learn how to get help and what kind of help is available

 We can give presentations on programming languages and parallel libraries – just ask







### Outline

- What is NERSC?
- Computing Resources
- Storage Resources
- How to Get Help
- Accounts and Allocations
- Connecting to NERSC
- Computing Environment
- Compiling Code
- Running Jobs









## What is NERSC?

#### National Energy Research Scientific Computing Center





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#### NERSC Facility Leads DOE in Scientific Computing Productivity



#### 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

- •1.3PF Petaflop Cray system, Hopper
  - 2<sup>nd</sup> Fastest computer in US
  - Fastest open Cray XE6 system
  - Additional .5 PF in Franklin system and smaller clusters



#### Location



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Science



**NERSC** is a **DOE** Office of Science National Center located at **Berkley Lab** 





#### Location





...... BERKELEY LAB



#### 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







### **NERSC Workload**



#### NERSC 2011 Allocations By Science Area



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- Fusion Energy
- Materials Science
- Lattice QCD
- Climate Research
- Chemistry
- Astrophysics
- Life Science
- Accelerator Science
- Combustion
- Applied Math
- Computer Science
- Geoscience
- Environmental Science
- Nuclear Physics
- Other
- Engineering
- High Energy Physics
- Nuclear Energy
- Humanities





## **Computing Resources**





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#### **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

Office of

Science

GenePool (JGI)

~5K core cluster

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NERG



1.5 PB capacity

5.5 GB/s of bandwidth

#### 40 PB capacity 4 Tape libraries

150 TB disk cache







Euclid 512 GB shared mem Dirac GPU testbed 48 nodes



#### 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, sharedobject 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)



NERSC global /scratch directory quota of 20 TB Full Linux operating system PGI, GNU, Intel compilers

InfiniBand 4X QDR

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

#### **Magellan at NERSC**

Scientific Discovery through Cloud Computing

- 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







## **Data Storage Resources**





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## **Data Storage Types**

## "Spinning Disk"

- Interactive access
- I/O from compute jobs
- "Home", "Project", "Scratch"
- Note: No on-node direct-attach disk at NERSC

## Archival Storage

- Permanent, Long-Term Storage
- Tapes, fronted by disk cache
- "HPSS" (High Performance Storage System)







## **Home Directory**

- When you log in you are in your "Home" directory.
- Permanent storage
  - No automatic backups
- The full UNIX pathname is stored in the environment variable \$HOME

hopper04% echo \$HOME /global/homes/r/ragerber

- \$HOME is a global file system
  - You see all the same directories and files when you log in to any NERSC computer.
- Your quota in \$HOME is 40 GB and 1M inodes (files and directories).
  - Use "myquota" command to check your usage and quota







### **Scratch Directories**

- Each system has a large, high-performance "scratch" file system.
- Significant I/O from your compute jobs should be directed to \$SCRATCH
- Each user has a personal directory referenced by \$SCRATCH (and maybe \$SCRATCH2).
- Data in \$SCRATCH is purged (12 weeks from last access)
- Always save data you want to keep to HPSS (see below)
- \$SCRATCH is local on Franklin and Hopper, but Carver and future systems use a global scratch file system.
- Data in \$SCRATCH is not backed up and could be lost if a file system fails.







- All NERSC systems mount the NERSC global "Project" file system.
- "Project directories" are created upon request for projects (groups of researchers) to store and share data.
- The default quota in /project is 4 TB.
- While data can be written and read from a parallel job on all system, performance will may not be as good as on \$SCRATCH.
- Data in /project is not purged, but there are no automatic user backups either.







### **IO** Tips

• Use \$SCRATCH for good IO performance from a production compute job

- Write large chunks of data (MBs or more) at a time from your code
- Use a parallel IO library (e.g. HDF5)
- Read/write to as few files as practical from your code (try to avoid 1 file per MPI task)
- Use \$HOME to compile unless you have too many source files or intermediate (\*.o) files
- Do not put more than a few 1,000s of files in a single directory
- Save any and everything important to HPSS







## **Navigating NERSC File Systems**

#### A NERSC Training Event NERSC Oakland Facility & Web Broadcast

http://www.nersc.gov/users/training/events/nersc-file-systems/





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#### **Archival Storage (HPSS)**

For permanent, archival storage

- You transfer files to and from HPSS using one of ftp, pftp, or the HPSS hsi client.
- For more info see the NERSC web site: type "hpss getting started" in the search box



Hostname: archive.nersc.gov Over 15 Petabyes of data stored Data increasing by 1.7X per year 120 M files stored 150 TB disk cache 8 STK robots 44,000 tape slots 44 PB maximum capacity today Average data xfer rate: 100 MB/sec





## **Data Transfer and Archiving**

#### A NERSC Training Event NERSC Oakland Facility & Web Broadcast

http://www.nersc.gov/users/training/events/data-transfer-and-archiving/





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## How to Get Help





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### **NERSC Services**

- NERSC's emphasis is on enabling scientific discovery
- User-oriented systems and services
  - This is what sets NERSC apart from other centers
- Help Desk / Consulting
  - Immediate direct access to consulting staff that includes 7 Ph.Ds
- User group (NUG) has tremendous influence
  - Monthly teleconferences & Yearly meetings
- Requirement-gathering workshops with top scientists
  - Completed five, including BER

 Microbial Genome and Metagenome Data Processing and Analysis with the IMG Family of Systems; Victor M. Markowitz, LBNL; Natalia N. Ivanova and Nikos C. Kyrpides, Genome Biology Program, JGI

• Ask, and we'll do whatever we can to fulfill your request







#### How to Get Help

#### http://www.nersc.gov/

#### 1-800-666-3772 (or 1-510-486-8600)

Computer Operations\* = menu option 1 (24/7)

Account Support (passwords) = menu option 2, accounts@nersc.gov

HPC Consulting = menu option 3, or <u>consult@nersc.gov</u> (8-5, M-F Pacific time)

Online Help Desk = https://help.nersc.gov/

\* Passwords during non-business hours







## **Accounts & Allocations**





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#### Accounts

There are two types of "accounts" at NERSC. It is important to differentiate between them.

- 1. Your personal, private account
  - Associated with your "login" or "user name"
  - Identifies you to our systems and is used when logging into NERSC systems and web services.
  - Your PI requests an account for you.
- 2. An allocation account, or "repository" (aka "repo")
  - Like a bank account you use to "pay" for computer time.
  - PIs request allocations of time and/or storage
  - An individual user may belong to one or many repositories.

To apply for either type of account, see the NERSC web site at http://www.nersc.gov/.







#### 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
- 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

• If your repo runs out of time, you can request more through your project's DOE program manager who handles NERSC allocations (list available on NERSC web site)







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### Accounting Web Interface (NIM)

• Log into the NERSC NIM web site at https:// nim.nersc.gov/ to manage your NERSC accounts.

 In NIM you can check your daily allocation balances, change your password, run reports, update your contact information, change your login shell, etc.







## **Connecting to NERSC**





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## **Computing Environment**





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- NERSC installs dot-files in your home directory (e.g. .login, .profile)
  - Commands in dot-files are executed when you log in (or start a new shell)
  - Do not modify these or your jobs and compiles will not work correctly.
- Each dot-file sources an additional file with the same name, but with an .ext extension.
  - Put your local modifications in these .ext files
  - (e.g. .login.ext, .profile.ext)







#### Modules

- Easy access to NERSC's extensive software collection is controlled by the modules utility.
- With modules, you manipulate your computing environment to use applications and programming libraries.
- In many cases, you can ignore modules because NERSC has already loaded a rich set of modules for you when you first log in.
- If you want to change that environment you "load," "unload," and "swap" modules.
- A small set of module commands can do most of what you'll want to do







### module list

- Shows you your currently loaded modules.
- When you first log in, you have a number of modules loaded for you. Here is an example from Hopper.

```
hopper03% module list
Currently Loaded Modulefiles:
                                           11) xpmem/0.1-2.0301.25333.20.2.gem
  1) modules/3.2.6.6
                                           12) xe-sysroot/3.1.61
  2) xtpe-network-gemini
  3) pqi/10.9.0
                                           13) xt-asyncpe/4.9
  4) xt-libsci/10.5.01
                                           14) atp/1.1.2
  5) xt-mpich2/5.2.1
                                           15) PrgEnv-pgi/3.1.61
  6) udreg/2.2-1.0301.2966.16.2.gem
                                           16) eswrap/1.0.8
  7) ugni/2.1-1.0301.2967.10.23.gem
                                           17) xtpe-mc12
  8) pmi/2.1.1-1.0000.8296.10.8.gem
                                           18) xt-shmem/5.2.1
  9) dmapp/3.0-1.0301.2968.22.24.gem
                                           19) torque/2.4.8-snap.201004261413
 10) gni-headers/2.1-1.0301.2931.19.1.gem
                                           20) moab/5.3.6-s14846
```

• The most important module is called "PrgEnv-pgi", which lets you know that the environment is set up to use the Portland Group compiler suite.







#### module avail

- The "module avail" command will list all the available modules. It's a very long list, so I won't list it here
- You can use the module's name stem to do a useful search

```
nid00163% module avail PrgEnv
PrgEnv-cray/1.0.1(default) PrgEnv-pathscale/2.2.48B(default)
PrgEnv-gnu/2.2.48B(default) PrgEnv-pgi/2.2.48B(default)
```

• Here you see that four programming environments are available using the Cray, GNU, Pathscale, and PGI compilers.

• The word "default" is confusing here; it does not refer to the default computing environment, but rather the default version of each specific PrgEnv module. (It just happens that in this case, there is only one version available of each.)







#### module swap

Let's say you want to use the Cray compiler instead of PGI.

%module swap PrgEnv-pgi PrgEnv-cray

Now you are using the Cray compiler suite. That's all you have to do.

You don't have to change your makefiles, or anything else in your build script unless they contain PGI or Cray-specific options or features.





### module load

- There is plenty of software that is not loaded by default.
- You can consult the NERSC web pages to see a list, or you can use the "module avail" command to see what modules are available
- For example, if you want to use the NAMD molecular dynamics application. Try "module avail namd".

nid00163% module avail namd namd/2.6(default) namd/2.7b1\_plumed namd/cvs namd/2.7b1 namd/2.7b2

 The default version is 2.6, but say you'd rather use some features available only in version 2.7b2. In that case, just load that module.

nid00163% module load namd/2.7b2

• The "namd2" binary for version 2.7b2 is now in your UNIX search path.







## **Compiling Code**





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- Let's assume that you're compiling
  - a parallel application
  - using MPI and the code is
  - written in Fortran, C, or C++
- Then compiling is easy
  - You will use standard compiler wrapper
  - All the include file and library paths are set
  - Linker options are set







### **Parallel Compilers**

	Platform	Fortran	С	C++
	Cray	ftn	СС	CC
	Others	mpif90	mpicc	mpiCC
!Filenam program imp inc	ne hello.f90 hello plicit none lude "mpif.h"			% ftn –o hello.x hello.f90 That's it!
inte inte call	eger:: myRank eger:: ierror I mpi_init(ierror) I mpi_comm_rank(N	/IPI_COMM_WORI	LD,myRank)	<b>No</b> -I/path/to/ mpi/include <b>or</b> - L/path/to/mpi/ lib
prir cal u.s. departmen ENER	nt *, "MPI Rank ",my I mpi_finalize(ierror) I Office of Science	/Rank," checking ir	ו!" 50	It's all taken care of for you.



- You can use serial compilers as you would on a typical Linux cluster
  - gcc, gfortran, pgf90, etc.
  - Won't run on compute nodes on Crays
  - You need to supply all the compiler and linker options

May have to load a module to access a given compiler (e.g. module load pgi/11.2.0)







### Using Programming Libraries (Cray)

All you have to do is load the appropriate module and compile.

Let's compile an example code that uses the HDF5 I/O library. First let's try it in the default environment.

```
nid00195% cc -o hd_copy.x hd_copy.c
INFO: linux target is being used
Can't find include file hdf5.h (hd_copy.c: 39)
```

The compiler doesn't know where to find the include file. Now let's load the hdf5 module and try again.

```
nid00195% module load hdf5
nid00195% cc -o hd_copy.x hd_copy.c
```

We're all done and ready to run the program! No need to manually add the path to HDF5; it's all taken care of by the scripts.







### Using Programming Libraries (non-Cray)

% mpicc -o hd\_copy.x hd\_copy.c Can't find file hdf5.h (hd\_copy.c: 39) PGC/x86-64 10.8-0: compilation aborted % module load hdf5 % mpicc -o hd\_copy.x hd\_copy.c Can't find file hdf5.h (hd\_copy.c: 39) PGC/x86-64 10.8-0: compilation aborted

# Even with the module loaded, the compiler doesn't know where to find the HDF5 files.







### Using Programming Libraries (non-Cray)

We have to use environment variables defined in the module (use "module show" to see them).

- % mpicc -o hd\_copy.x hd\_copy.c \$HDF5
- % module show hdf5

/usr/common/usg/Modules/modulefiles/hdf5/1.8.3:

conflict hdf5-parallel module load szip module load zlib HDF5 DIR /usr/common/usg/hdf5/1.8.3/serial setenv HDF5\_-L/usr/common/usg/hdf5/1.8.3/serial/lib setenv lhdf5 cpp -lhdf5 fortran -lhdf5 hl -lhdf5 -L/usr/common/usg/zlib/ default/lib -lz -L/usr/common/usg/szip/default/lib -lsz -I/usr/ common/usg/hdf5/1.8.3/serial/include -I/usr/common/usg/ hdf5/1.8.3/serial/lib -I/usr/common/usg/zlib/default/include -I/ usr/common/usg/szip/default/include HDF5 INCLUDE -I/usr/common/usg/hdf5/1.8.3/ setenv serial/include prepend-path PATH /usr/common/usg/hdf5/1.8.3/serial/bin LD LIBRARY PATH /usr/common/usg/hdf5/1.8.3/ prepend-path serial/lib





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#### You can try some example compiles and run some jobs by following

https://www.nersc.gov/users/training/events/getting-started/ hands-on/







## **Running Jobs**





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- Most jobs are parallel, using 10s to 100,000+ cores.
- Many use custom codes; others use preinstalled 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





## **NERSC** 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**





#### **Carver / Magellan / Dirac**





- A "job launcher" distributes your code to all the nodes in your parallel job, starts them, and manages their execution.
- On Cray the job launcher is called "aprun" and on other systems it is "mpirun".
- Only the job launcher can start your job on compute nodes
- You can't run the job launcher from login nodes







- To run a job on the compute nodes you must write a "batch script," which contains
  - Batch directives to allow the system to schedule your job
  - An aprun or mpirun command that launches your parallel executable
- Submit the job to the queuing system with the qsub command
  - %qsub my\_batch\_script







### **Sample Hopper Batch Script**

```
#PBS -q debug
#PBS -1 mppwidth=96
#PBS -1 walltime=00:10:00
#PBS -N my_job
#PBS -e my_job.$PBS_JOBID.err
#PBS -o my_job.$PBS_JOBID.out
#PBS -V
cd $PBS_O_WORKDIR
aprun -n 96./my executable
```

The PBS directives required for each system are different, so consult the NERSC web site for details.







#### **Job Limits**

There are per user, per machine job limits. See the NERSC web site for details. Here are the limits on Hopper as of June 22, 2011.

Submit Queue	Execution Queue <sup>1</sup>	Nodes	Processors	Max Waliclock	Relative Priority	Run Limit <sup>2</sup>	Queued Limit <sup>3</sup>	Queue Charge Factor
interactive	interactive	1-256	1-6.144	30 mins	2	1	1	1
debug	debug	1-512	1-12,288	30 mins	3	1	1	1
regular	reg_1hour	1-256	1-6,144	1 hr	5	8	8	1
	reg_short	1-683	1-16,392	6 hrs	5	8	8	1
	reg_small	1-683	1-16,392	24 hrs	5	8	8	1
	reg_med	684- 2,048	16,393- 49,152	24 hrs	5	3	3	0.75
	reg_big	2,049- 4,096	49,153- 98,304	24 hrs	4	1	1	0.75
	reg_xbig <sup>4</sup>	4,097- 6,100	98,305- 146,400	12 hrs	1	1	1	0.75
low	low	1-683	1-16,392	12 hrs	6	6	6	0.5
premium	premium	1-2,048	1-49,152	12 hrs	3	1	1	2







## **Monitoring Your Job**

- Once your job is submitted, it will start when resources are available
- Monitor it with
  - qstat –a
  - qstat –u username
  - showq
  - qs
  - NERSC web site "Queue Look"







- You can run small parallel jobs interactively for up to 30 minutes
  - % qsub -I -V -lmppwidth=32
    [wait for job to start]
    % cd \$PBS\_O\_WORKDIR
    % aprun -n 32 ./mycode.x







#### **How Your Jobs Are Charged**

- Your repository account is charged for each core your job was allocated for the entire length of your job.
  - The minimum allocatable unit is a node. Hopper has 24 cores/node, so your minimum charge on Hopper is 24\*walltime.
  - e.g., mppwidth=96 for 1 hour of run time is
    charged 96\*1 = 96 MPP Hours (assuming the default
    setting of mppnppn=24)
  - You are charged for your actual run time, not the value of walltime in your batch script.
- If you have access to multiple repos, pick which one to charge in your batch script
  - #PBS -A repo\_name







### **Charge Factors & Discounts**

• Each machine has a "machine charge factor" (mcf) that multiplies the "raw hours" used

- Hopper and Franklin have mcf=1.0
- Carver has mcf=1.5
- Queues have "priority charge factors" (pcf) and corresponding relative scheduling priorities
  - Premium pcf=2.0
  - Low pcf=0.5
  - Everything else pcf=1.0
- On Hopper only:
  - reg\_med, reg\_big, reg\_xbig jobs get a 25% discount

## Storage and bandwidth are allocated and charged for HPSS

- Exhausting an HPSS allocation is rare
- See the NERSC web site for details

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## Aside: Why Do You Care About Parallelism?





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#### **Moore's Law**



2X transistors/Chip Every 1.5 years Called "<u>Moore's Law</u>" 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<sup>2</sup>fC
  - Increasing frequency (f) also increases supply voltage (V)  $\rightarrow$  cubic effect
  - Increasing cores increases capacitance (C) but only linearly
  - Save power by lowering clock speed
  - Year High performance serial processors waste power
    - Speculation, dynamic dependence checking, etc. burn power
    - Implicit parallelism discovery
  - More transistors, but not faster serial 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



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- 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



