Intro to Parallel Computing

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PHY1610 Winter 2025

Motivation for Parallel Computing

Why is Parallel Computing necessary?

- **Big Data:**
  Modern experiments and observations yield vastly more data to be processed than in the past.
- **Big Science:**
  As more computing resources become available, the bar for cutting edge simulations is raised.
- **New Science:**
  which before could not even be done, now becomes reachable.

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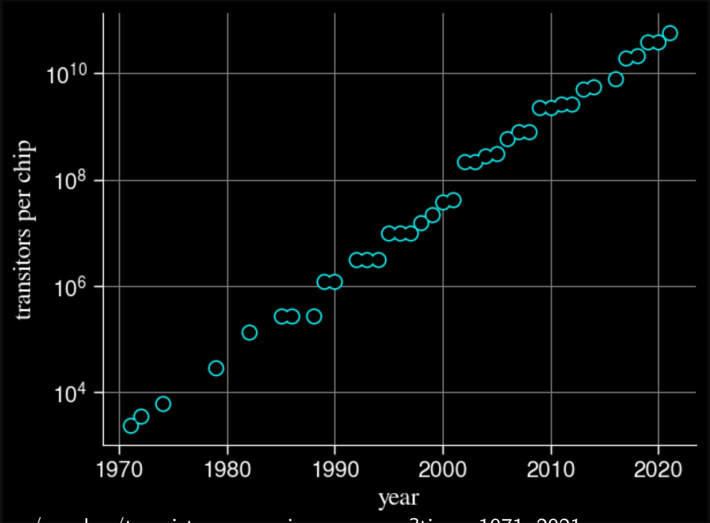
- So parallel computing is necessary.

Wait, what about Moore's Law?



https://ourworldindata.org/grapher/transistors-per-microprocessor?time=1971..2021

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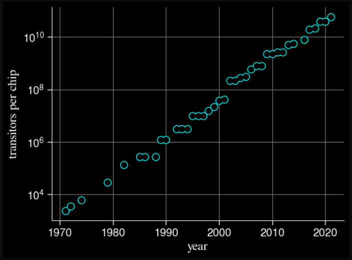
(source: Moore's law, wikipedia)



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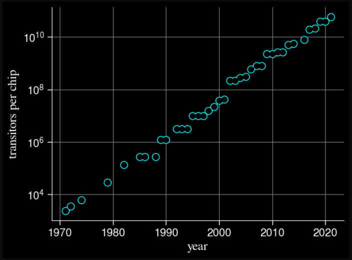

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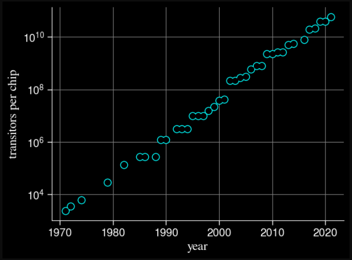

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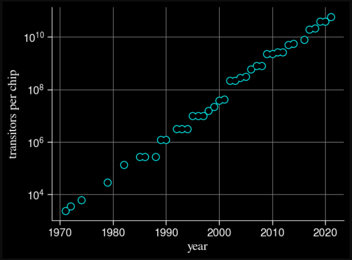

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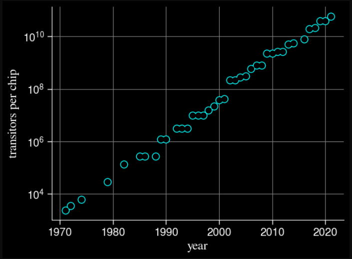

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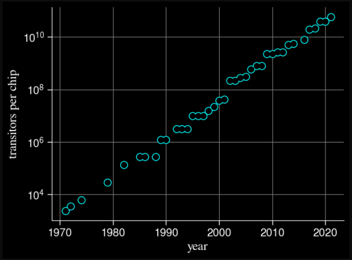

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- We've gotten more transistors but it's getting hard to push clock-speed up. Power density is the limiting factor.
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- (Also, it is physically reaching its limits)

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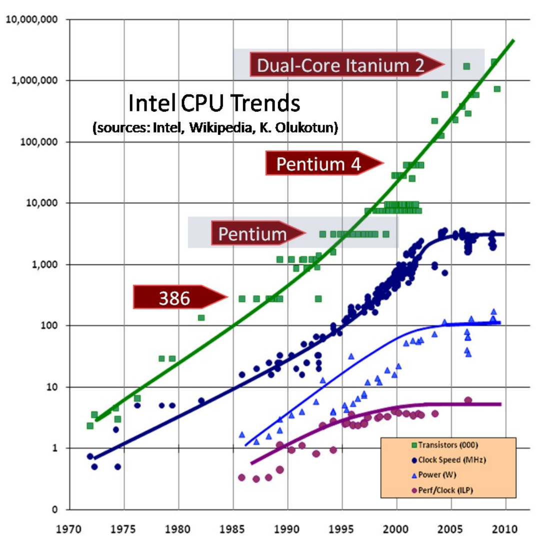

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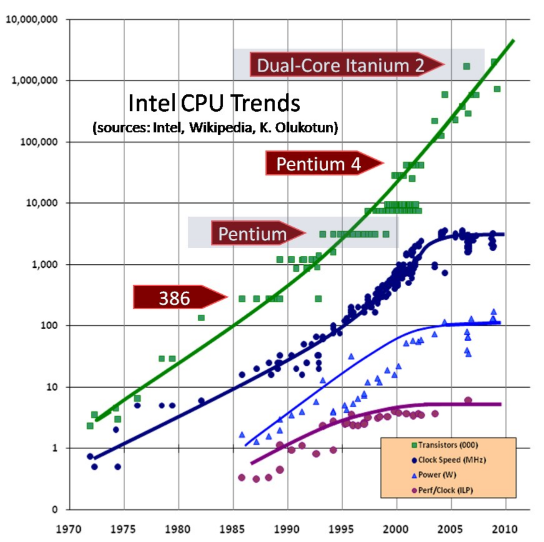

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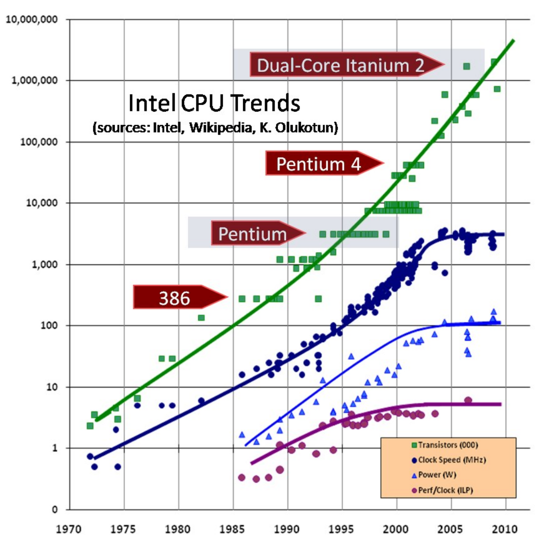

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All curves flatten except the transitor count.

This shows that the continuation of Moore's law is due to the presence of multiple cores, which require parallel programming.

(source: www.extremetech.com)

Concurrency

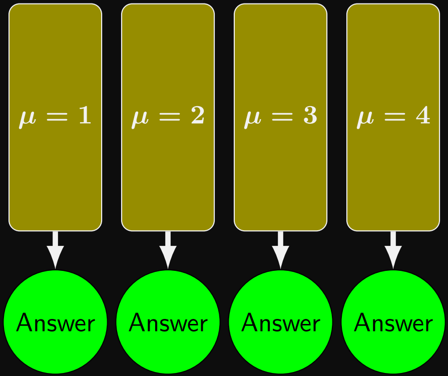
- All these cores need something to do.
- We need to find parts of the program that can done independently, and therefore on different cores concurrently.
- We would like there to be many such parts.
- Ideally, the order of execution should not matter either.
- However, data dependencies limit concurrency.

(source: http://flickr.com/photos/splorp)

Parallel computing

Parameter study: best case scenario

- Suppose the aim is to get results from a model as a parameter varies.
- We can run the serial program on each processor at the same time.
- Thus we get ‘more’ done.



Throughput

- How many tasks can you do per unit time? **throughput** $= H = \frac{N}{T}$

  N is the number of tasks, T is the total time.
- Maximizing H means that you can do as much as possible.
- Independent tasks: using P processors increases H by a factor of P.

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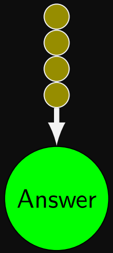

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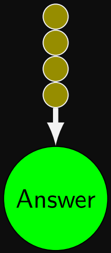

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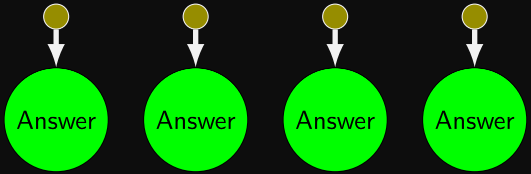


$$T = NT_1/P$$

$$H = P/T_1$$

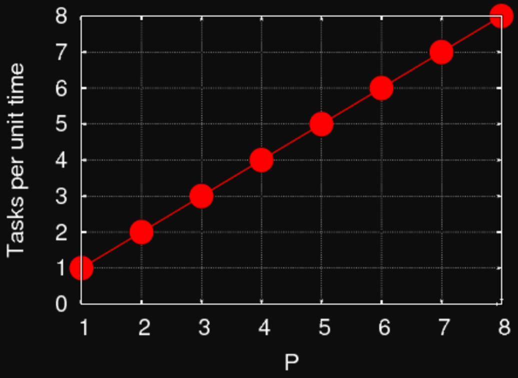
Scaling

Scaling: Throughput

- How a given problem's throughput scales as processor number increases is called strong scaling
- In the previous case, linear scaling:

$$H \propto P$$

- This is perfect scaling. These are called "embarrassingly parallel" calculations.

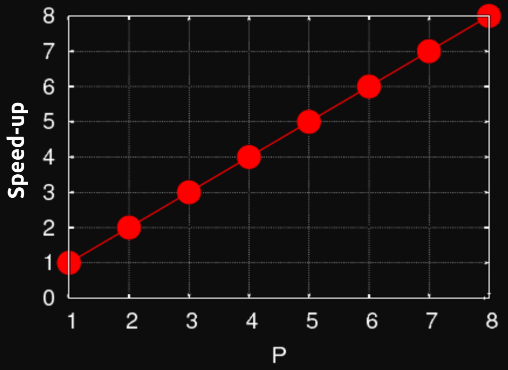


Scaling: Speedup

- Speedup: how much faster the problem is solved as processor number increases.
- This is measured by the serial time divided by the parallel time

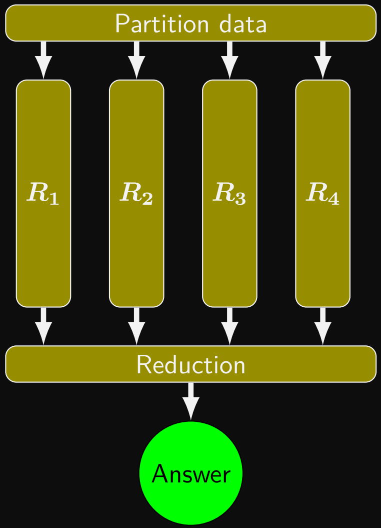
$$S = \frac{T_{\text{serial}}}{T(P)}$$

- For embarrassingly parallel applications, $S \propto P$: linear speed up.



Non-ideal cases

- Say we want to integrate some tabulated experimental data.
- Integration can be split up, so different regions are summed by each processor.
- Non-ideal:
  - We first need to get data to each processor.
  - At the end we need to bring together all the sums: *reduction*.



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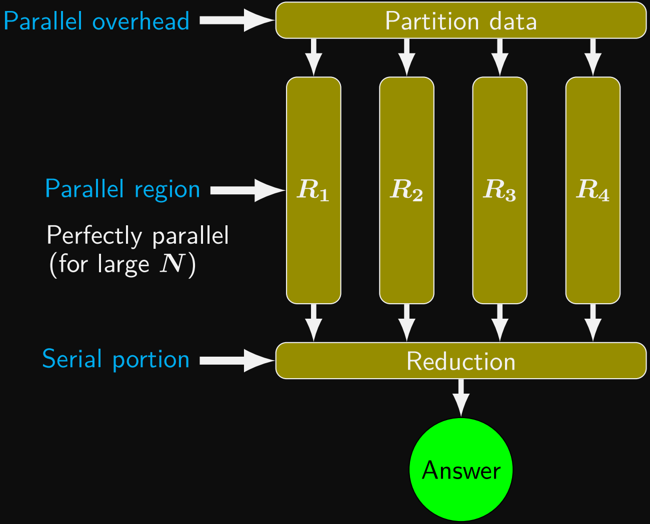

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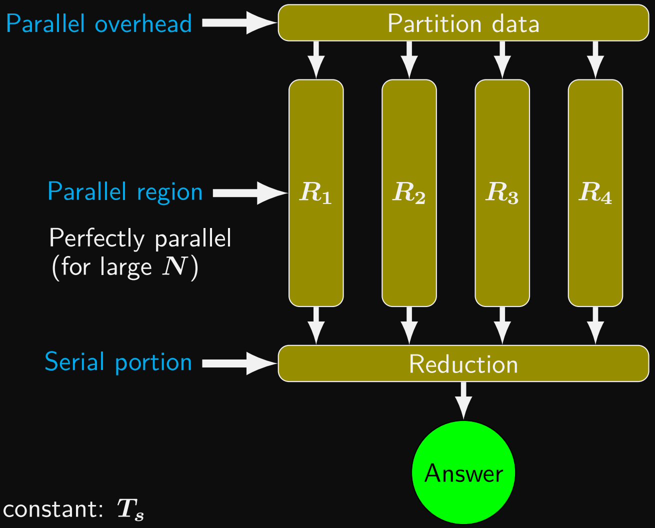

Suppose non-parallel part is constant: T_s

Amdahl's law

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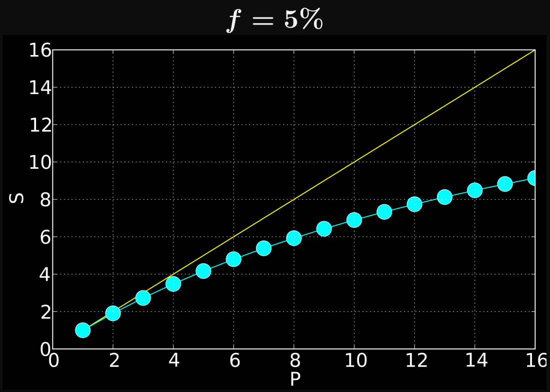
Speed-up (without parallel overhead):

$$S = \frac{T_{\text{serial}}}{T(P)} = \frac{NT_1 + T_s}{\frac{NT_1}{P} + T_s}$$

or, calling $f = T_s/(T_s + NT_1)$ the serial fraction,

$$S = \frac{1}{f + (1-f)/P} \quad \xrightarrow{P\to\infty} \quad \frac{1}{f}$$



The serial part dominates asymptotically.
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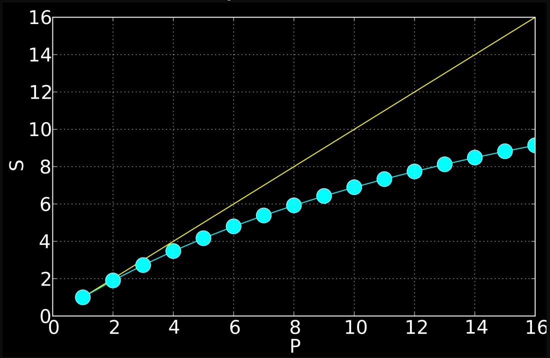
$f = 5\%$



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Aim to structure your program to minimize the serial portions of the code!

Scaling efficiency

Speed-up compared to ideal factor P:

$$\text{Efficiency} = \frac{S}{P}$$

This will invariably fall off for larger P, except for embarrassingly parallel problems.

$$\text{Efficiency} \sim \frac{1}{fP} \xrightarrow{P\to\infty} 0$$

You cannot get 100% efficiency in any non-trivial problem.\[0.3cm]

All you can aim for here is to make the efficiency as high as possible.

Hardware Architectures

Supercomputer architectures

Supercomputer architectures comes in a number of different types:

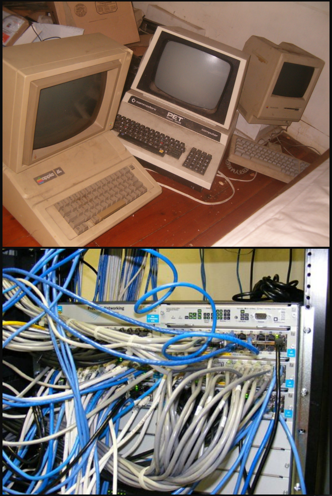
- Clusters, or distributed-memory machines, are in essence a bunch of desktops linked together by a network ("interconnect"). Easy and cheap.
- Multi-core machines, or shared-memory machines, are a collection of processors that can see and use the same memory. Limited number of cores, and much more expensive when the machine is large.
- Accelerator machines, are machines which contain an "off-host" accelerator, such as a GPGPU or Xeon Phi, that is used for computation. Quite fast, but complicated to program.
- Vector machines were the early supercomputers. Very expensive, especially at scale. These days most chips have some low-level vectorization, but you rarely need to worry about it.

Most supercomputers are a hybrid combo of these different architectures.

Distributed Memory: Clusters

Clusters are the simplest type of parallel computer to build:

- Take existing powerful standalone computers,
- and network them.
- Easy to build and easy to expand.
- SciNet's Niagara supercomputer and the teach cluster are examples.



(source: http://flickr.com/photos/eurleif)

Compute Resources at SciNet

Teach Cluster

Number of nodes: 8
Interconnect: Infiniband
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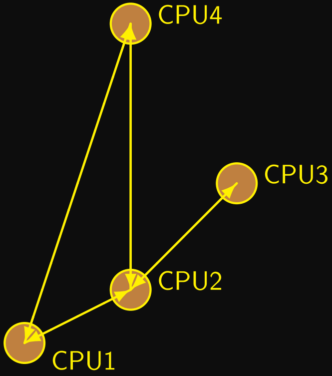
Niagara, Must and Rouge to be retired and replaced by Trillium

Distributed Memory: Clusters

- Each processor is independent! Programs run on separate processors, communicating with each other when necessary. Each processor has its own memory! Whenever it needs data from another processor, that processor needs to send it.
- All communication must be hand-coded: ~harder to program.
- MPI programming is used in this scenario.



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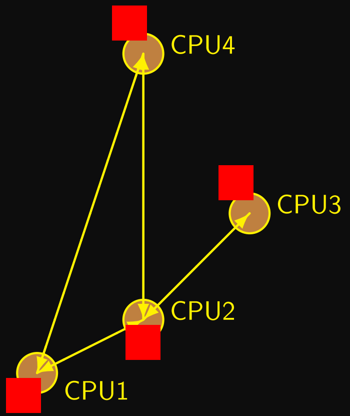
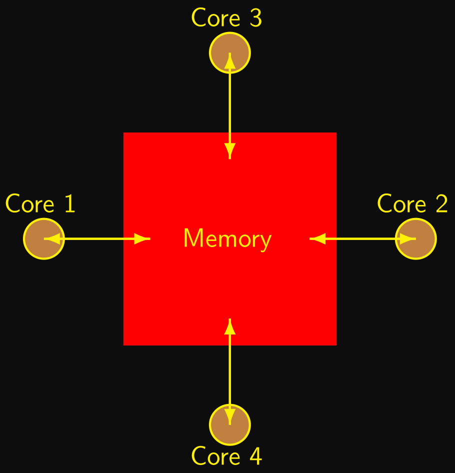


Shared memory

Shared Memory

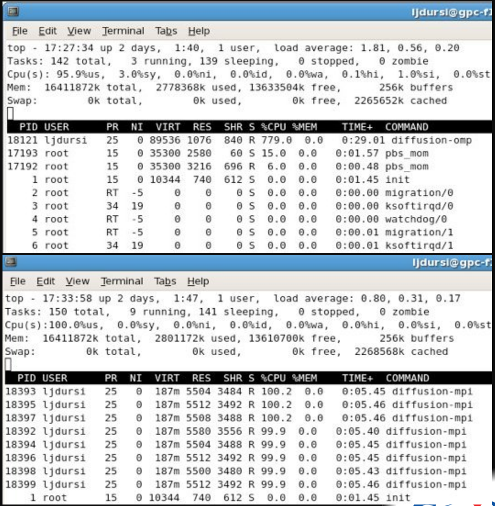
- Different processors acting on one large bank of memory. All processors “see” the same data.
- All coordination/communication is done through memory.
- Each core is assigned a thread of execution of a single program that acts on the data.
- Your desktop uses this architecture, if it’s multi-core.
- Can also use hyper-threading: assigning more than one thread to a given core.
- OpenMP is used in this scenario.



Threads versus Processes

Threads Threads of execution within one process, with access to the same memory etc.

Processes Independent tasks with their own memory and resources



Share memory communication cost

Interconnect	Latency	Bandwidth
Gigabit Ethernet	10μs (10,000 ns)	1 Gb/s (60 ns/double)
Infiniband	2μs (2,000 ns)	2-10 Gb/s (10 ns/double)
NUMA (shared memory)	0.1μs (100 ns)	10-20 Gb/s (4 ns/double)

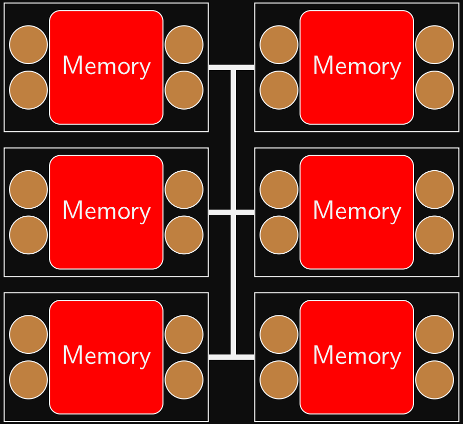
Processor speed: $\mathcal{O}$(GFlop) $\sim$ a few ns or less.

Communication is always the slowest part of your calculation!

Hybrid systems

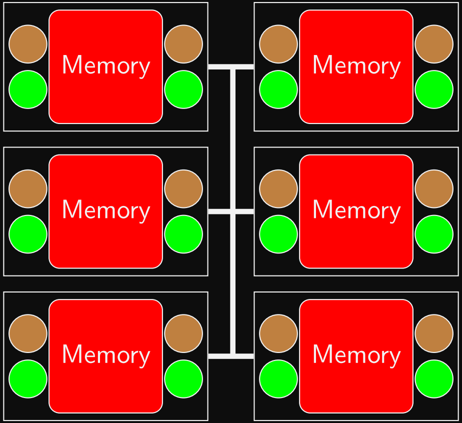
Hybrid architectures

- Multicore nodes linked together with an (high-speed interconnect.
- Many cores have modest vector capabilities.
- Teach cluster has sixteen cores, and 64 GB of memory, per node.
- Niagara has forty cores, and 202 GB of memory, per node.
- OpenMP + MPI can be used in this scenario.



Hybrid architectures: accelerators

- Multicore nodes linked together with an (high-speed) interconnect.
- Nodes also contain one or more accelerators, e.g. GPUs.
- These are specialized, super-threaded (500-2000+) processors.
- Specialized programming languages, CUDA and OpenCL, are used to program these devices.
- Can be combined with MPI and OpenMP.



Using Supercomputers

Choosing your programming approach

The programming approach you use depends on the type of problem you have, and the type of machine that you will be using:

- Embarrassingly parallel applications: scripting, GNU Parallel[1].
- Shared memory machine: OpenMP, p-threads.
- Distributed memory machine: MPI, PGAS (UPC, Coarray Fortran).
- Graphics computing: CUDA, OpenACC, OpenCL.
- Hybrid combinations.

[1] O. Tange (2011): GNU Parallel - The Command-Line Power Tool, ;login; The USENIX Magazine, February 2011:42-47.

Using a scheduler

- When you log in, you are on a login nodes.
- These are shared.
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- The scheduler will run your jobs will run on some of Teach 8 compute nodes.
- When and where your job runs is determined by the scheduler.
- Teach uses SLURM as its job scheduler.

Example

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=4
#SBATCH --time=3:00:00
#SBATCH --job-name serialjobs
#SBATCH --output=serial_output_%j.txt
#SBATCH --mail-type=FAIL

module load gcc

parallel -j $SLURM_NPROCS ./myapp ::: {0..99}
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- First line indicates that this is a bash script.

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parallel -j $SLURM_NPROCS ./myapp ::: {0..99}
```

```
teach-login01:~$ sbatch serialjobs.sh
```

- First line indicates that this is a bash script.
- Lines starting with #SBATCH go to SLURM.

Example

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#!/bin/bash
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=4
#SBATCH --time=3:00:00
#SBATCH --job-name serialjobs
#SBATCH --output=serial_output_%j.txt
#SBATCH --mail-type=FAIL

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- sbatch reads these lines as a job request
- In this case, SLURM looks for 4 cores to be put on the same one node to be run for 3 hours.
- Once it found such a node, script is run:
  - Loads modules
  - Has gnu-parallel load-balance 99 tasks over 4 cores.

Using the Scheduler

Some of the most common sbatch parameters are:

`-t`	`--time`	amount of time
`-N`	`--nodes`	number of nodes
`-n`	`--ntasks`	number of tasks
	`--ntasks-per-node`	number of tasks per node
`-c`	`--cpus-per-task`	number of threads per task
`-G`	`--gpus-per-node`	number of gpus per node
	`--mem`	amount of memory
`-A`	`--account`	scheduler account to use
	`--reservation`	use reserved nodes

Using the Scheduler

Commands to interact with the scheduler

`sbatch`	submit job
`squeue`	see queued jobs and their status
`scancel`	cancel a job
`salloc`	get short interactive job on a compute node
`debugjob -n P`	get short interactive job on a compute node