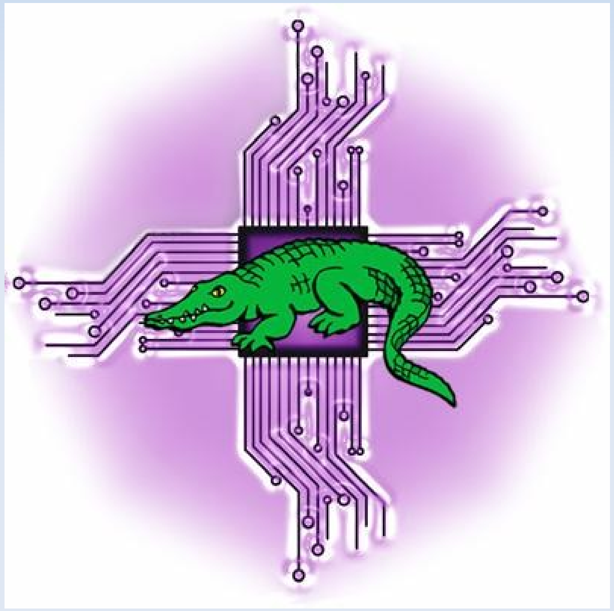
The Spartan HPC System at the University of Melbourne

COMP90024 Cluster and Cloud Computing



University of Melbourne, March 22, 2018

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Outline of Lecture

"*This is an advanced course but we get mixed bag: students that have 5+ years of MPI programming on supercomputers, to students that have only done Java on Windows.*"

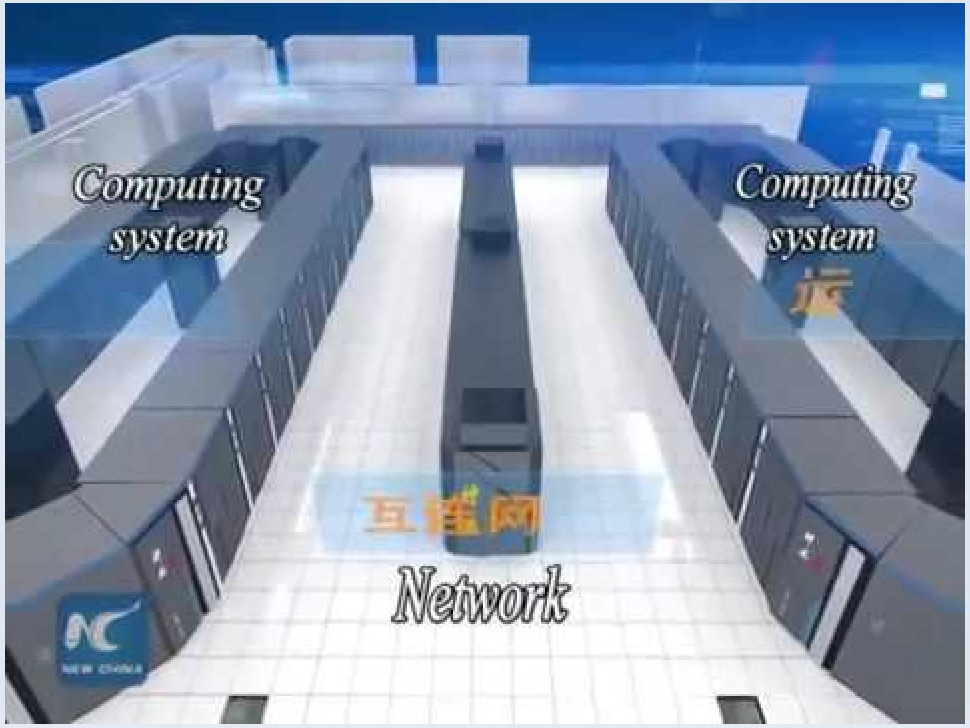
- Some background on supercomputing, high performance computing, parallel computing, scientific computing (there is overlap, but they're not the same thing).
- An introduction to Spartan, University of Melbourne's HPC/Cloud hybrid system
- Logging in, help, and environment modules.
- Job submission with Slurm workload manager; simple submissions, multicore, job arrays, job dependencies, interactive jobs.
- Parallel programming with shared memory and threads (OpenMP) and distributed memory and message passing (OpenMPI)
- Tantalising hints about more advanced material on message passing routines.

Supercomputers

'Supercomputer” arbitrary term with no specific definition. In general use it means any single computer system (itself a contested term) that has exceptional processing power for its time. A well-adopted metric is the number of floating-point operations per second (FLOPS) such a system can carry out.

Supercomputers, like any other computing system, have improved significantly over time. The Top500 list is based on FLOPS using LINPACK - HPC Challenge is a broader, more interesting metric. The current number #1 system is Sunway TaihuLight, a supercomputer operated by China’s National Super Computer Center.

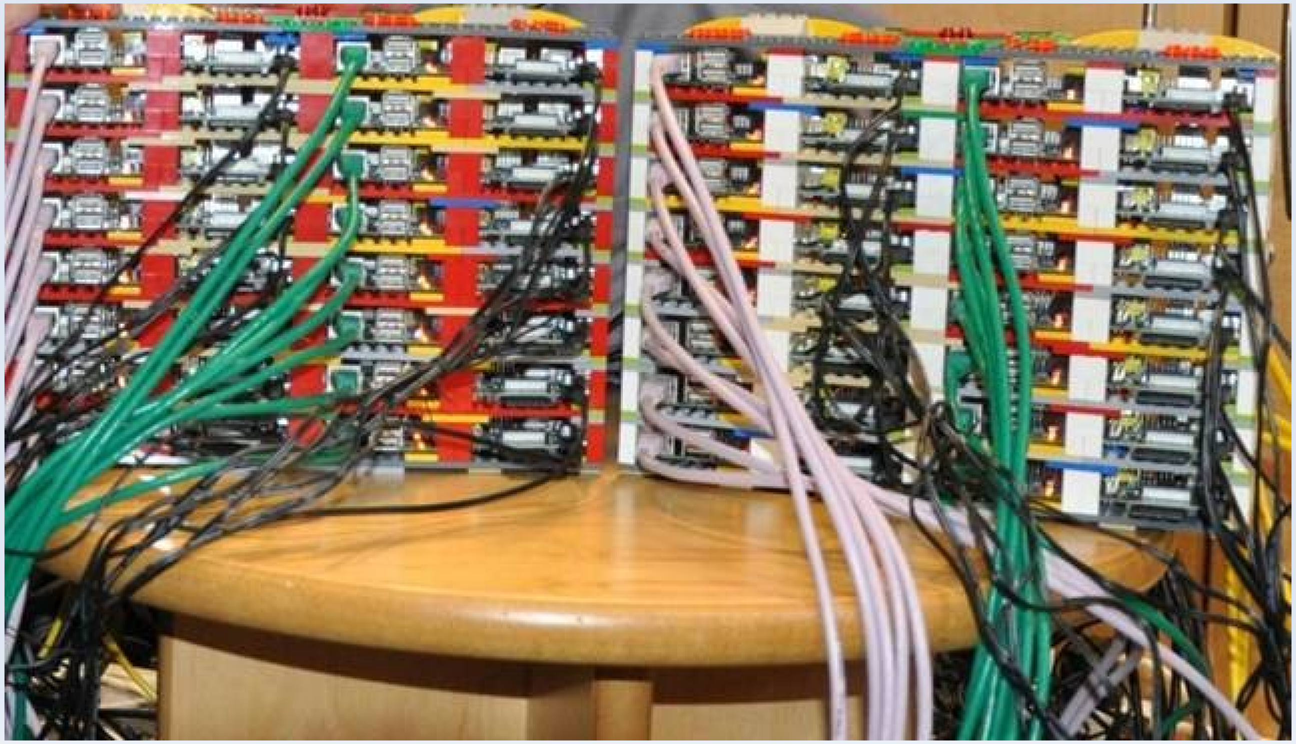
1994: 170.40 GFLOPS
1996: 368.20 GFLOPS
1997: 1.338 TFLOPS
1999: 2.3796 TFLOPS
2000: 7.226 TFLOPS
2004; 70.72 TFLOPS
2005: 280.6 TFLOPS
2007: 478.2 TFLOPS
2008: 1.105 PFLOPS
2009: 1.759 PFLOPS
2010: 2.566 PFLOPS
2011: 10.51 PFLOPS
2012: 17.59 PFLOPS
2013: 33.86 PFLOPS
2014: 33.86 PFLOPS
2015: 33.86 PFLOPS
2016: 93.01 PFLOPS
2017: 93.01 PFLOPS (125.46 PFLOPS peak)



High Performance Computing

High-performance computing (HPC) is any computer system whose architecture allows for above average performance. A system that is one of the most powerful in the world, but is poorly designed, could be a "supercomputer".

Clustered computing is when two or more computers serve a single resource. This improves performance and provides redundancy in case of failure system. To describe simply, there are a collection of smaller computers strapped together with a high-speed local network (e.g., Myrinet, InfiniBand, 10 Gigabit Ethernet), although a low-speed network system could certainly be used. Even a cluster of Raspberry Pi with Lego chassis (University of Southampton, 2012)!



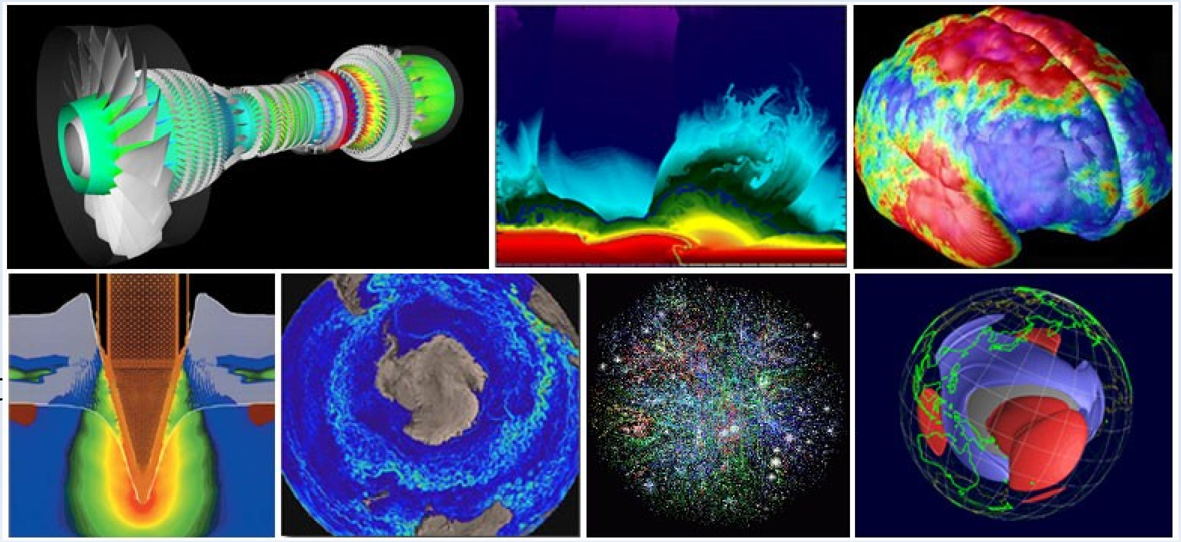
Horse and cart as a computer system and the load as the computing tasks. Efficient arrangement, bigger horse and cart, or a teamster? The clustered HPC is the most efficient, economical, and scalable method, and for that reason it dominates supercomputing today.

Parallel and Research Programming

With a cluster architecture, applications can be more easily parallelised across them. Parallel computing refers to the submission of jobs or processes over multiple processors and by splitting up the data or tasks between them (random number generation as data parallel, driving a vehicle as task parallel).

Research computing is the software applications used by a research community to aid research. Does not necessarily equate with high performance computing, or the use of clusters. This skills gap is a major problem and must be addressed because as the volume, velocity, and variety of datasets increases then researchers will need to be able to process this data.

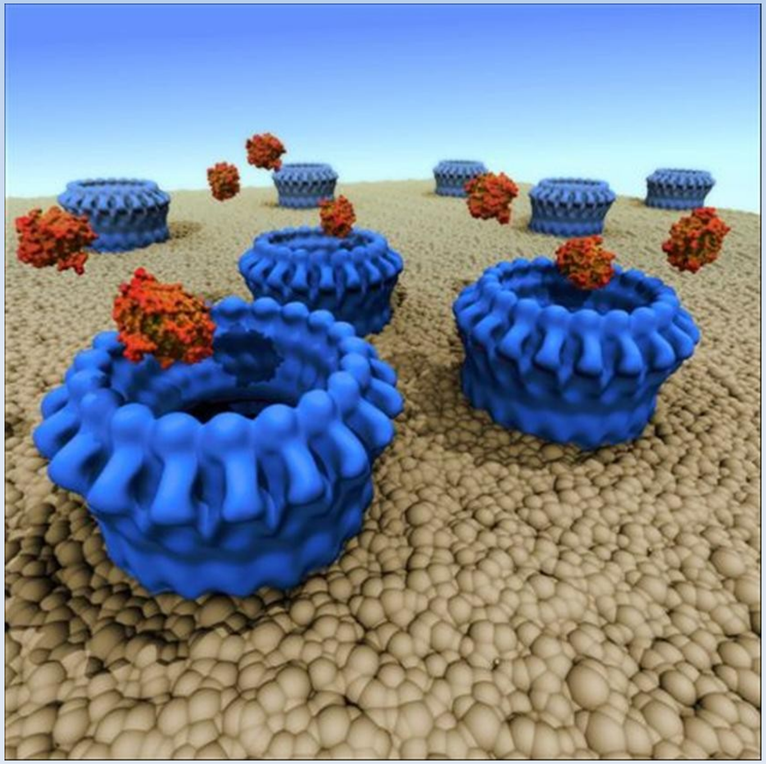
Computational capacity does have a priority (the system must exist prior to use), in order for that capacity to realised in terms of usage a skill-set competence must also exist. The the core issue is that high performance compute clusters is just speed and power but also usage, productivity, correctness, and reproducibility.
(image from Lawrence Livermore National Laboratory)



There is nascent research that shows a strong correlation between research out and availability of HPC facilities.
(Apon et al 2010)

Some Local Examples

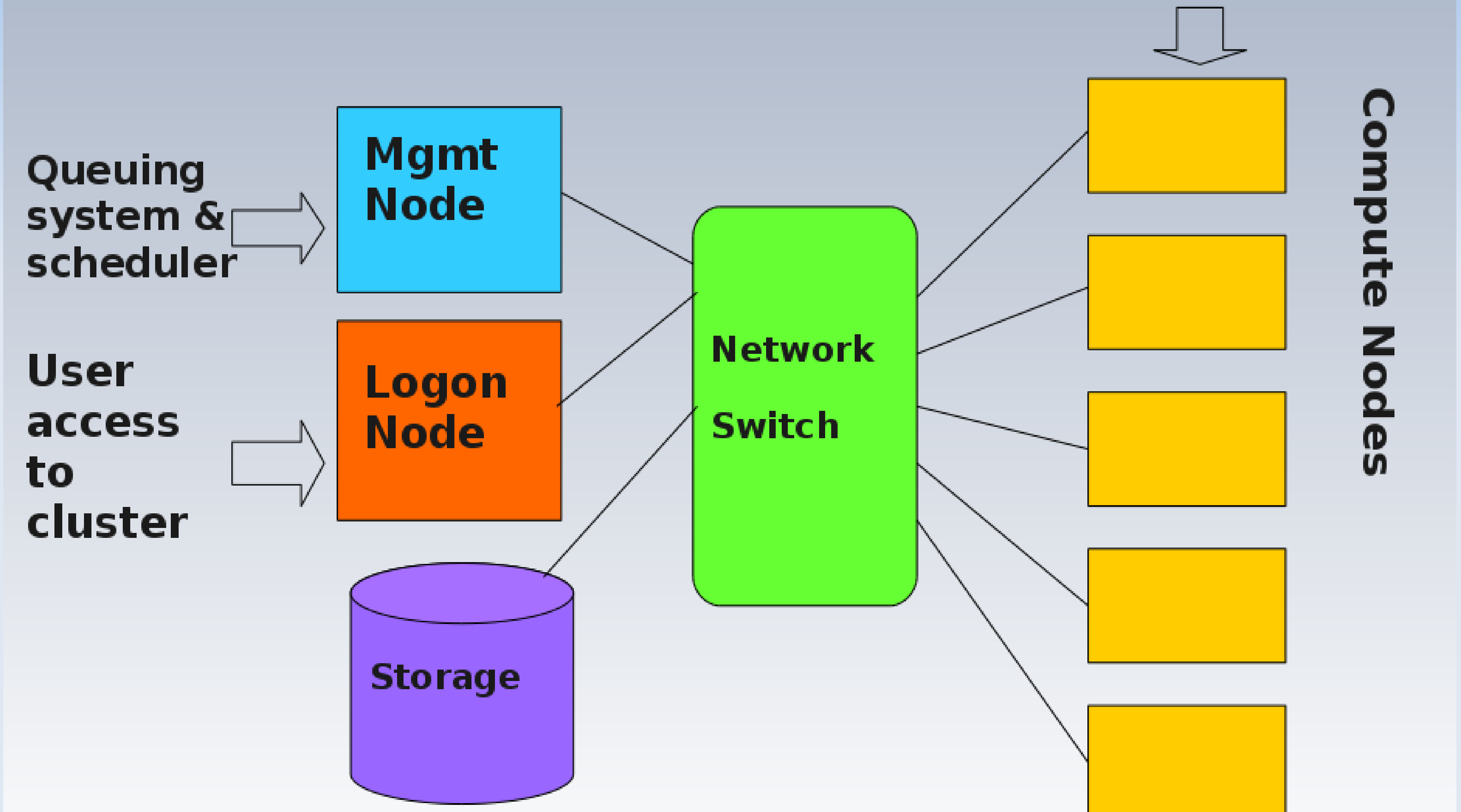
Researchers from Monash University, the Peter MacCallum Cancer Institute in Melbourne, the Birkbeck College in London, and VPAC in 2010 unravelled the structure the protein perforin to determine how pathogenic cells are attacked by white
blood cells.



In 2015 researchers from VLSCI announced how natural antifreeze proteins bind to ice to prevent it growing which has important implications for extending donated organs and protecting crops from frost damage.

In 2016 CSIRO researchers successfully manipulated the behaviour of Metallic Organic Frameworks to control their structure and alignment which provides opportunities for real-time and implantable medical electric devices.

HPC Cluster Design



It's A GNU/Linux World

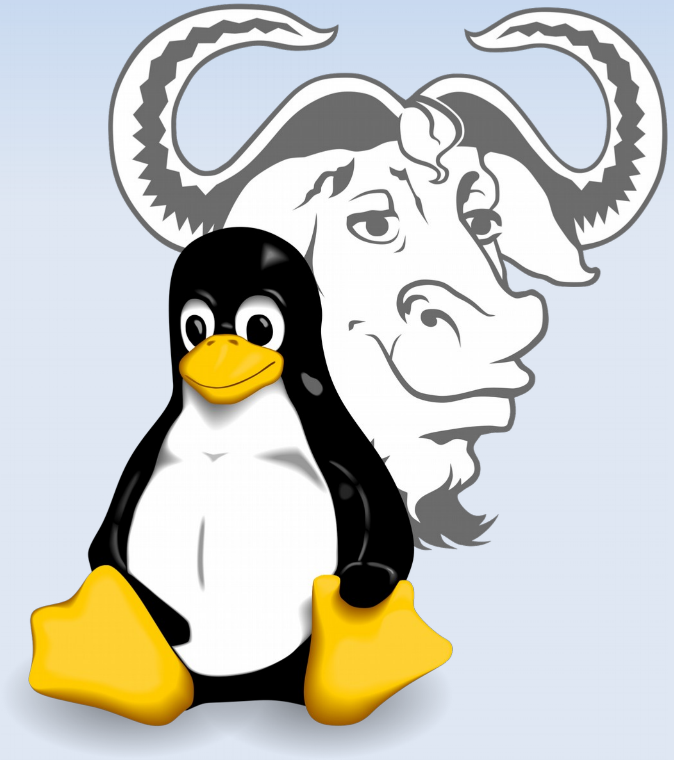
In November 2017 of the Top 500 Supercomputers worldwide, *every single machine* used Linux.
`http://www.zdnet.com/article/linux-totally-dominates-supercomputers/`

The command-line interface provides a great deal more power and is very resource efficient.

GNU/Linux scales and does so with stability and efficiency. Critical software such as the Message Passing Interface (MPI) and nearly all scientific programs are designed to work with GNU/Linux.

The operating system and many applications are provided as "free and open source", which means that not only are there are some financial savings, were also much better placed to improve, optimize and maintain specific programs.

Free or open source software (not always the same thing) can be can be compiled from source for the specific hardware and operating system configuration, and can be optimised according to compiler flags. There is necessary where every clock cycle is important.



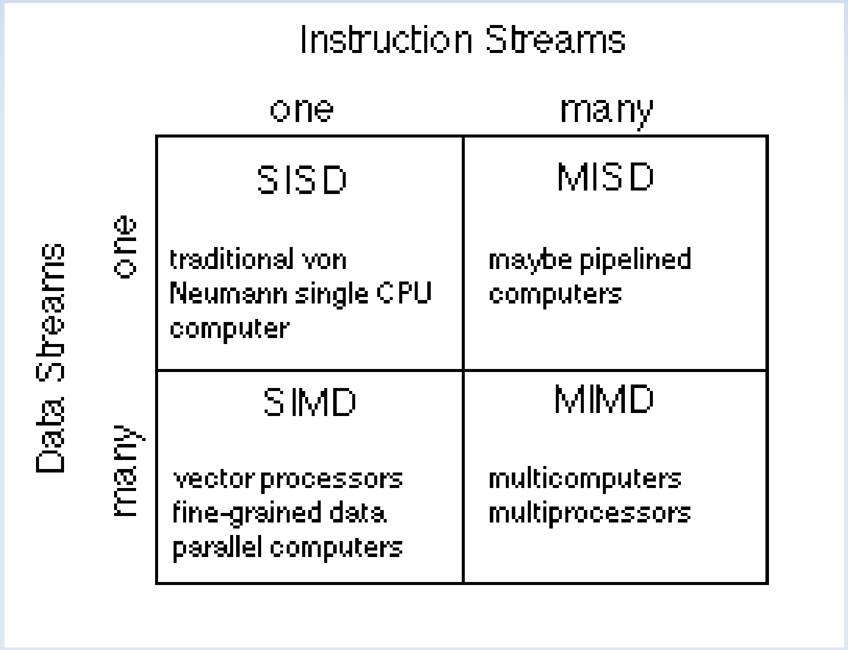
Flynn's Taxonomy and Multicore Systems

It is possible to illustrate the degree of parallelisation by using Flynn's Taxonomy of Computer Systems (1966), where each process is considered as the execution of a pool of instructions (instruction stream) on a pool of data (data stream).

Over time computing systems have moved towards multi-processor, multi-core, and often multi-threaded and multi-node systems.

The engineering imperative to these systems comes down to heat. From the mid-2000s clock speed on CPUs have largely stalled.

Some trends include GPGPU development, massive multicore systems (e.g., The Angstrom Project, the Tile CPU with 1000 cores) and massive network connectivity and shared resources (e.g., Plan9 Operating System).



		Instruction Streams	
		one	many
Data Streams	one	SISD traditional von Neumann single CPU computer	MISD maybe pipelined computers
	many	SIMD vector processors fine-grained data parallel computers	MIMD multicomputers multiprocessors

(Image from Dr. Mark Meyer, Canisius College)

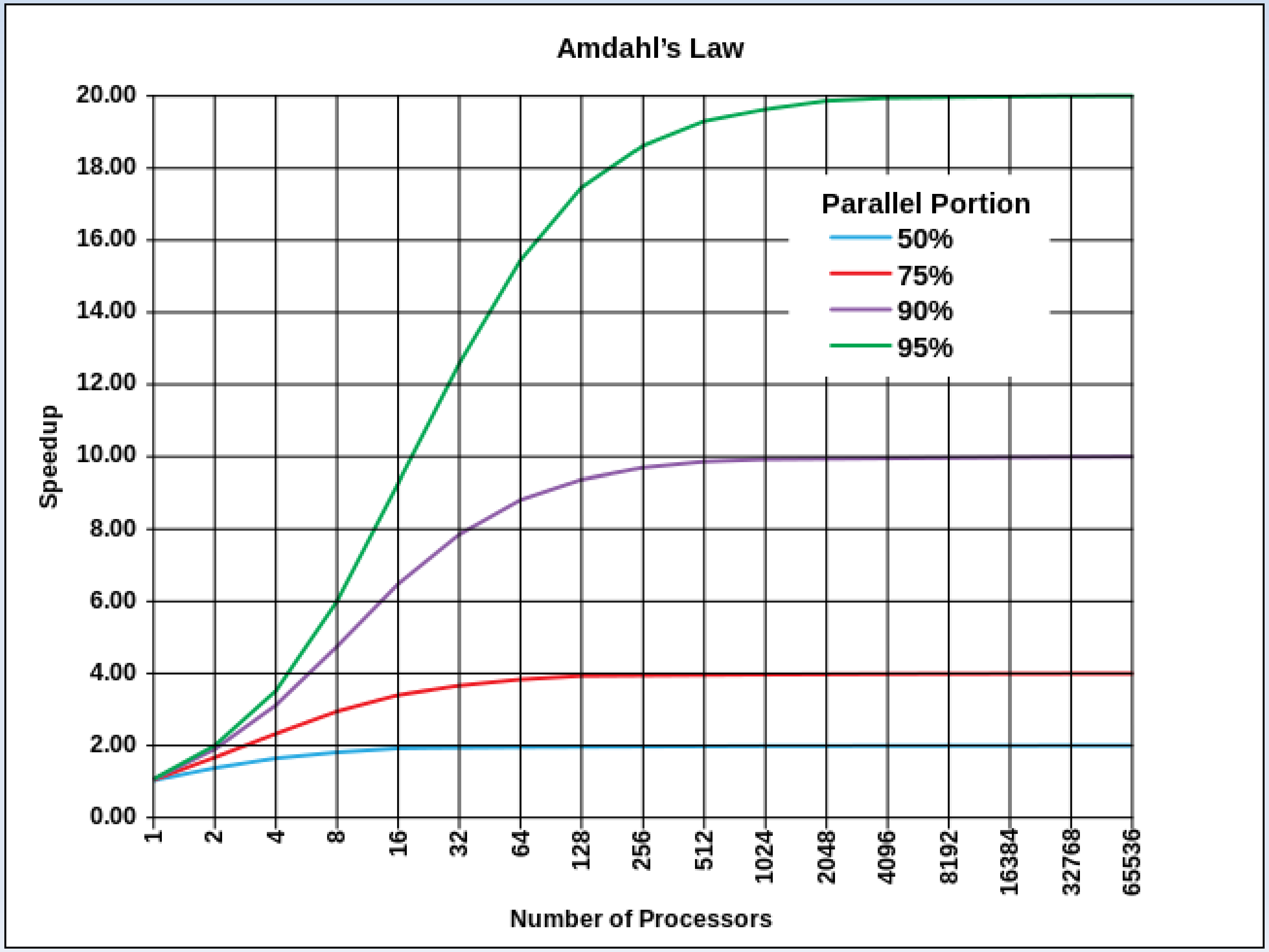
Limitations of Parallel Computation

Parallel programming and multicore systems should mean better performance. This can be expressed a ratio called speedup

Speedup (p) = Time (serial)/ Time (parallel)

Correctness in parallelisation requires synchronisation (locking). Synchronisation and atomic operations causes loss of performance, communication latency.

Amdahl's law, establishes the maximum improvement to a system when only part of the system has been improved. Gustafson and Barsis noted that Amadahl's Law assumed a computation problem of fixed data set size.



New UniMelb System: Spartan

A detailed review was conducted in 2016 looking at the infrastructure of the Melbourne Research Cloud, High Performance Computing, and Research Data Storage Services. University desired a 'more unified experience to access compute services'

Recommended solution, based on technology and usage, is to make use of existing NeCTAR Research cloud with an expansion of general cloud compute provisioning and use of a smaller "true HPC" system on bare metal nodes.

The 'bare metal' HPC component really will be laconic. "Real" HPC is a mere c276 cores, 21 GB per core. 2 socket Intel E5-2643 v3 CPU with 6-core per socket, 192GB memory, 2x 1.2TB SAS drives, 2x 40GbE network. “Cloud” partitions is almost 400 virtual machines with over 3,000 cores. There is also a GPU partition (big expansion this year), and departmental partitions (water and ashley).

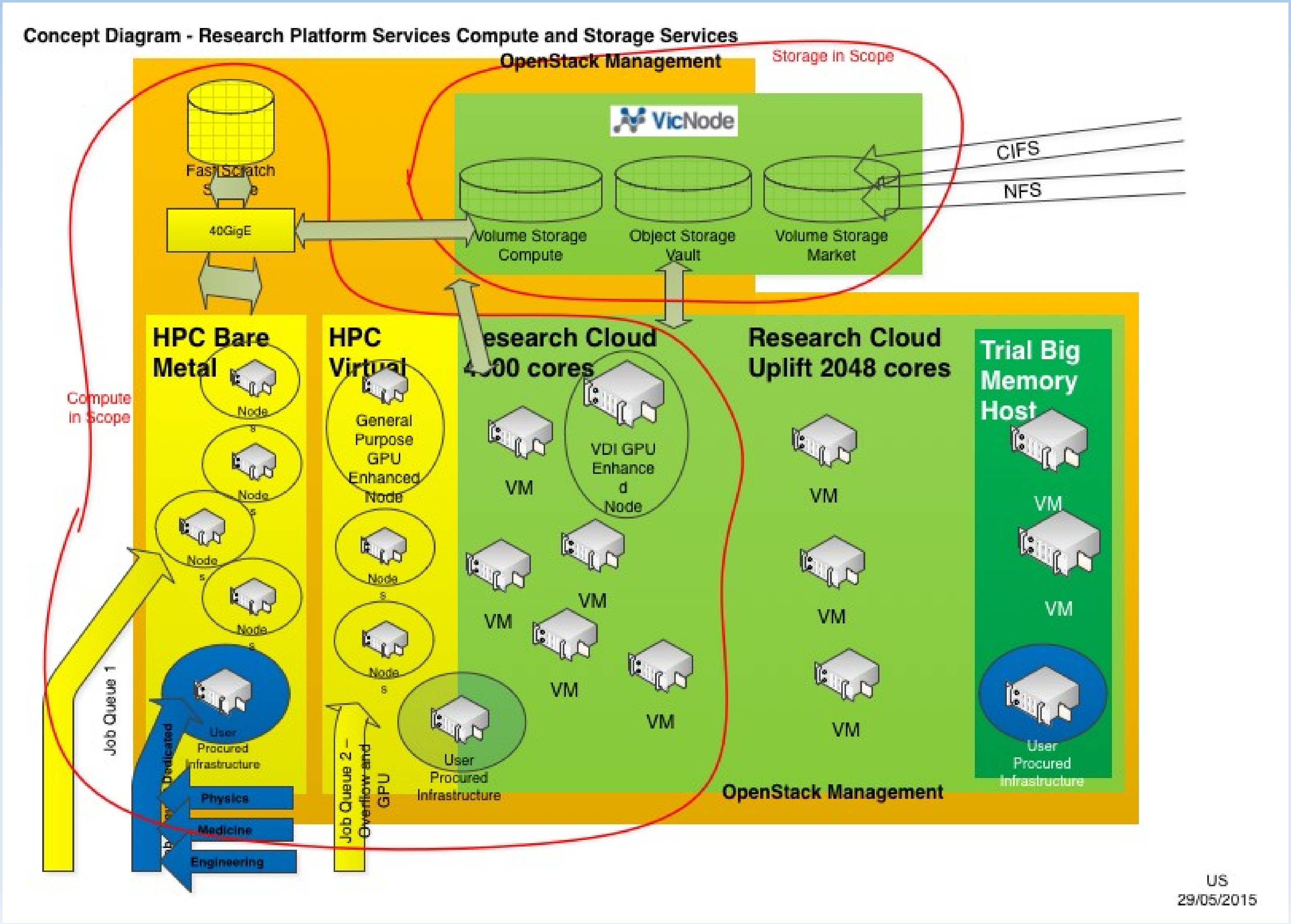
Spartan is Small but Important

This is not a big cluster by international standards! c.f., *The Provision of HPC Resources to Top Universities http://levlafayette.com/node/528*

But it is important! Spartan and the model of an HPC-Cloud Hybrid has been featured at Multicore World, Wellington, 2016, 2017; eResearchAustralasia 2016, Center for Scientific Computing (CSC) Goethe University Frankfurt, 2016, High Performance Computing Center (HLRS) University of Stuttgart, 2016, High Performance Computing Centre Albert-Ludwigs-University Freiburg, 2016; European Organization for Nuclear Research (CERN), 2016, Centre Informatique National de l'Enseignement Supérieur, Montpellier, 2016; Centro Nacional de Supercomputación, Barcelona, 2016, and the OpenStack Summit, Barcelona 2016.
https://www.youtube.com/watch?v=6D1lobuCZqE

Also featured in OpenStack and HPC Workload Management in Stig Telfer (ed), The Crossroads of Cloud and HPC: OpenStack for Scientific Research, Open Stack, 2016
http://openstack.org/assets/science/OpenStack-CloudandHPC6x9Booklet-v4-online.pdf

Moving Towards A New System



Spartan's Performance

Service	Network Device	Network	Protocol	Latency (usecs)
UoM HPC Traditional	Mellanox	56Gb	Infiniband FDR	1.17
Legacy Edward HPC	Cisco Nexus	10Gbe	TCP/IP	19
Spartan Cloud nodes	Cisco Nexus	10Gbe	TCP/IP	60
Spartan Bare Metal	Mellanox	40Gbe	TCP/IP	6.85
Spartan Bare Metal	Mellanox	25Gbe	RDMA Ethernet	1.84
Spartan Bare Metal	Mellanox	40Gbe	RDMA Ethernet	1.15
Spartan Bare Metal	Mellanox	56Gbe	RDMA Ethernet	1.68
Spartan Bare Metal	Mellanox	100Gbe	RDMA Ethernet	1.3

Job	Task	Resources	Control	HPC	Spartan Cloud
BWA	Disk	8 core Single Node	1:18:49	1:02:56	1:40:21
GROMACS	Compute	128 core Multinode	0:30:02	0:30:10	0:30:32
NAMD	Compute, I/O	128 core Multinode	1:11:41	1:00:46	1:55:54

Setting Up An Account and Training

Spartan (like Edward) uses its own authentication that is tied to the university Security Assertion Markup Language (SAML). The login URL is `https://dashboard.hpc.unimelb.edu.au/karaage`

Users on Spartan must belong to a project. Projects must be led by a University of Melbourne researcher (the "Principal Investigator") and are subject to approval by the Head of Research Compute Services.

Participants in a project can be researchers or research support staff from anywhere.

The University, through Research Platforms, has an extensive training programme for researchers who wish to use Spartan. This includes day-long courses in “Introduction to Linux and HPC Using Spartan”, “Edward to Spartan Transition Workshop”, “Linux Shell Scripting for High Performance Computing”, and “Parallel Programming On Spartan”.

Logging In and Help

To log on to a HPC system, you will need a user account and password and a Secure Shell (ssh) client. Most HPC cluster administrators do not allow connections with protocols such as Telnet, FTP or RSH as they insecurely send passwords in plain-text over the network, which is easily captured by packet analyser tools (e.g., Wireshark). Linux distributions almost always include SSH as part of the default installation as does Mac OS 10.x, although you may also wish to use the Fugu SSH client. For MS-Windows users, the free PuTTY client is recommended. To transfer files use scp, WinSCP, Filezilla, and especially rsync.

Logins to Spartan are based on POSIX identity for the system

`ssh your-username@spartan2.hpc.unimelb.edu.au` or

Note `spartan2`. This is a second login node that was created specifically for this class.

For help go to http://dashboard.hpc.unimelb.edu.au or check `man spartan`. Lots of example scripts at `/usr/local/common`

Need more help? Problems with submitting a job, need a new application or extension to an existing application installed, if job generated unexpected errors etc., an email can be sent to: `hpc-support@unimelb.edu.au`

The Linux Environment and Modules

Assumption here is that everyone has had exposure to the Linux command line. If not, you'd better get some! At least learn the twenty or so basic environment commands to navigate the environment, manipulate files, manage processes. Plenty of good online material available (e.g., my book "Supercomputing with Linux", https://github.com/VPAC/superlinux)

Environment modules provide for the dynamic modification of the user's environment (e.g., paths) via module files. Each module contains the necessary configuration information for the user's session to operate according according to the modules loaded, such as the location of the application's executables, its manual path, the library path, and so forth.

Modulefiles also have the advantages of being shared with many users on a system and easily allowing multiple installations of the same application but with different versions and compilation options. Sometimes users want the latest and greatest of a particular version of an application for the feature-set they offer. In other cases, such as someone who is participating in a research project, a consistent version of an application is desired. Having multiple version of applications available on a system is essential in research computing.

Modules Commands

Some basic module commands include the following:

`module help`
The command module help , by itself, provides a list of the switches, subcommands, and subcommand arguments that are available through the environment modules package.

`module avail`
This option lists all the modules which are available to be loaded.

`module whatis <modulefile>`
This option provides a description of the module listed.

`module display <modulefile>`
Use this command to see exactly what a given modulefile will do to your environment, such as what will be added to the PATH, MANPATH, etc. environment variables.

More Modules Commands

`module load <modulefile>`
This adds one or more modulefiles to the user's current environment (some modulefiles load other modulefiles.

module unload <modulefile>
This removes any listed modules from the user's current environment.

module switch <modulefile1> <modulefile2>
This unloads one modulefile (modulefile1) and loads another (modulefile2).

module purge
This removes all modules from the user's environment.

In the lmod system as used on Spartan there is also “module spider” which will search for all possible modules and not just those in the existing module path.

(Image from NASA, Apollo 9 “spider module”)

Batch Systems and Workload Managers

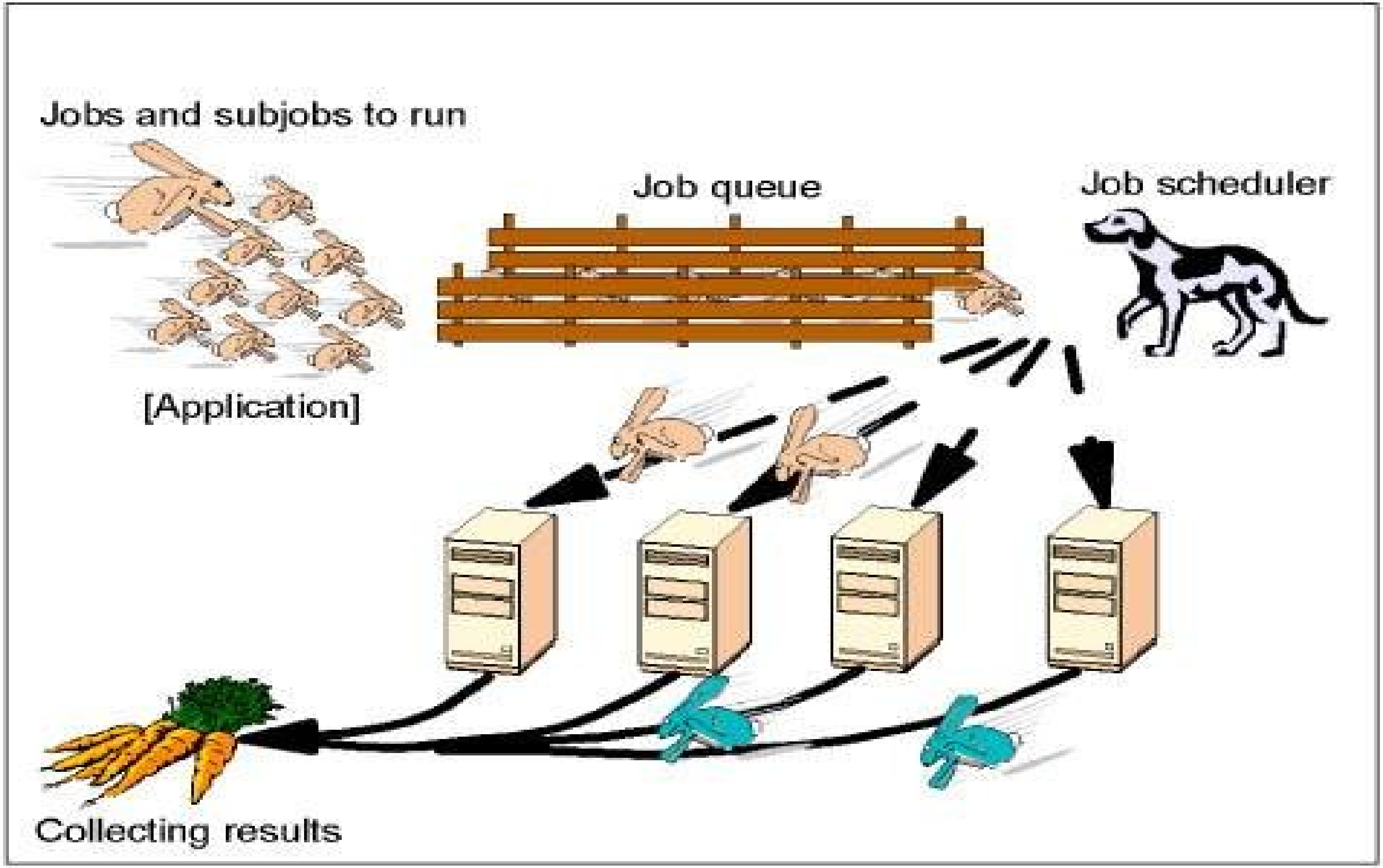
The Portable Batch System (or simply PBS) is a utility software that performs job scheduling by assigning unattended background tasks expressed as batch jobs among the available resources. The scheduler provides for paramterisation of computer resources, an automatic submission of execution tasks, and a notification system for incidents.

The original Portable Batch System was developed by MRJ Technology Solutions under contract to NASA in the early 1990s. In 1998 the original version of PBS was released as an open-source product as OpenPBS. This was forked by Adaptive Computing (formally, Cluster Resources) who developed TORQUE (Terascale Open-source Resource and QUEue Manager). Many of the original engineering team and what commercial property of exists from the original product is now part of Altair Engineering who have their own version, PBSPro. In addition to this the popular job scheduler Slurm (originally “Simple Linux Utility for Resource Management”), now simply called Slurm Workload Manager, also uses batch script where are very similar in intent and style to PBS scripts.

Spartan uses the Slurm Workload Manager. A job script written on one needs to be translated to another (handy script available pbs2slurm https://github.com/bjpop/pbs2slurm)

In addition to this variety of implementations of PBS different institutions may also make further elaborations and specifications to their submission filters (e.g., site-specific queues, user projects for accounting). (Image from the otherwise dry IBM 'Red Book' on Queue Management)

Submitting and Running Jobs



Submitting and Running Jobs

Submitting and running jobs is a relatively straight-forward process consisting of:

1) Setup and launch
2) Job Control, Monitor results
3) Retrieve results and analyse.

Don't run jobs on the login node! Use the queuing system to submit jobs.

1. Setup and launch consists of writing a short script that initially makes resource requests and then commands, and optionally checking queueing system.

Core command for checking queue:	squeue | less
Alternative command for checking queue:	showq -p cloud | less
Core command for job submission:	sbatch [jobscript]

2. Check job status (by ID or user), cancel job.

Core command for checking job in Slurm:	squeue -j [jobid]
Detailed command in Slurm:	scontrol show job [jobid]
Core command for deleting job in Slurm:	scancel [jobid]

3.Slurm provides an error and output files They may also have files for post-job processing. Graphic visualisation is best done on the desktop.

Simple Script Example

```
#!/bin/bash
#SBATCH -p cloud
#SBATCH --time=01:00:00
#SBATCH --nodes=1
#SBATCH –ntasks-per-node=1
module load my-app-compiler/version
my-app data
```

The script first invokes a shell environment, followed by the partition the job will run on (the default is 'cloud' for Spartan). The next four lines are resource requests, specifically for one compute node, one task.

After these requests are allocated, the script loads a module and then runs the executable against the dataset specified. Slurm also automatically exports your environment variables when you launch your job, including the directory where you launched the job from. If your data is a different location this has to be specified in the path!

After the script is written it can be submitted to the scheduler.

```
[lev@spartan]$ sbatch myfirstjob.slurm
```

Multithreaded, Multicore, and Multinode Examples

Modifying resource allocation requests can improve job efficiency.

For example shared-memory multithreaded jobs on Spartan (e.g., OpenMP), modify the --cpus-per-task to a maximum of 8, which is the maximum number of cores on a single instance.

```
#SBATCH --cpus-per-task=8
```

For distributed-memory multicore job using message passing, the multinode partition has to be invoked and the resource requests altered e.g.,

```
#!/bin/bash
#SBATCH -p physical
#SBATCH --nodes=2
#SBATCH –ntasks-per-node=4
module load my-app-compiler/version
srun my-mpi-app
```

Note that multithreaded jobs *cannot* be used in a distributed memory model across nodes. They can however exist be conducted on distributed memory jobs which include a shared memory component (hybrid OpenMP-MPI jobs).

Arrays and Dependencies

Alternative job submissions include specifying batch arrays, and batch dependencies.

In the first case, the same batch script, and therefore the same resource requests, is used multiple times. A typical example is to apply the same task across multiple datasets. The following example submits 10 batch jobs with myapp running against datasets dataset1.csv, dataset2.csv, ... dataset10.csv

```
#SBATCH --array=1-10
myapp ${SLURM_ARRAY_TASK_ID}.csv
```

In the second case a dependency condition is established on which the launching of a batch script depends, creating a conditional pipeline. The dependency directives consist of `after`, `afterok`, `afternotok`, `before`, `beforeok`, `beforenotok`. A typical use case is where the output of one job is required as the input of the next job.

```
#SBATCH --dependency=afterok:myfirstjobid mysecondjob
```

Interactive Jobs

For real-time interaction, with resource requests made on the command line, an interactive job is called. This puts the user on to a compute node.

This is typically done if they user wants to run a large script (and shouldn't do it on the login node), or wants to test or debug a job. The following command would launch one node with two processors for ten minutes.

```
[lev@spartan interact]$ sinteractive --nodes=1 --ntasks-per-node=2
srun: job 164 queued and waiting for resources
srun: job 164 has been allocated resources
[lev@spartan-rc002 interact]$
```

X-Windows Forwarding

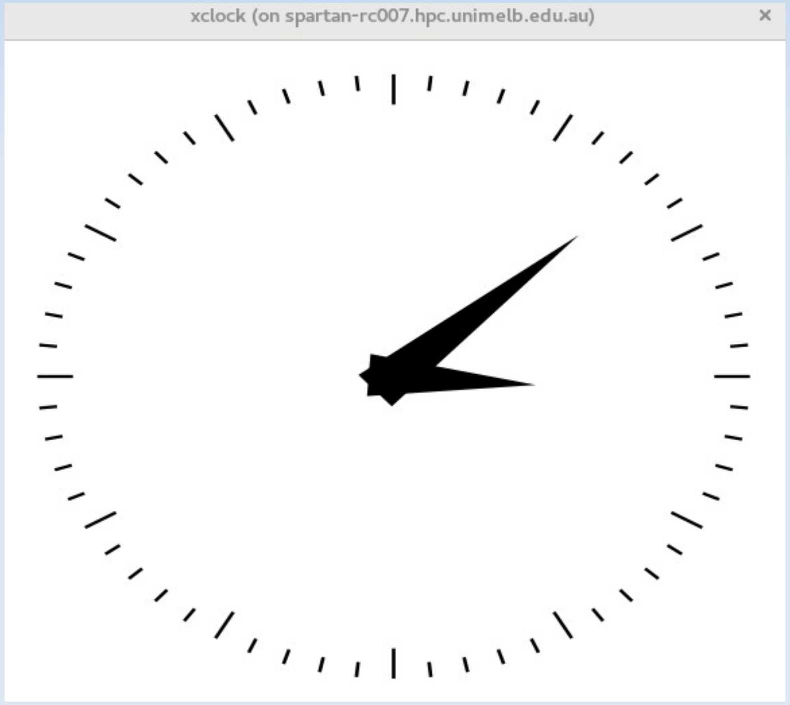
In almost all cases it is much better to do computation on the cluster and visualisation on a local system. In some cases however it is unavoidable to require x-windows forwarding.

It is best to login with the -Y option for security and then to login with -X to the login node. The compute node with then pass through the graphics via the login node to the desktop system.

Please note that you will need an x-windows client on your desktop for the visualisation.

```
[lev@cricetomys ~]$ ssh
lev@spartan.hpc.unimelb.edu.au -Y

[lev@spartan]$ sinteractive --nodes=1 --ntasks-per-
node=2 --x11=first
srun: job 602795 queued and waiting for resources
srun: job 602795 has been allocated resources
[lev@spartan-rc002 ~]$ xclock
```



PBS, SLURM Comparison

User Commands	**PBS/Torque**	**SLURM**
Job submission	qsub [script_file]	sbatch [script_file]
Job submission	qdel [job_id]	scancel [job_id]
Job status (by job)	qstat [job_id]	squeue [job_id]
Job status (by user)	qstat -u [user_name]	squeue -u [user_name]
Node list	pbsnodes -a	sinfo -N
Queue list	qstat -Q	squeue
Cluster status	showq, qstatus -a	squeue -p [partition]
Environment		
Job ID	$PBS_JOBID	$SLURM_JOBID
Submit Directory	$PBS_O_WORKDIR	$SLURM_SUBMIT_DIR
Submit Host	$PBS_O_HOST	$SLURM_SUBMIT_HOST
Node List	$PBS_NODEFILE	$SLURM_JOB_NODELIST
Job Array Index	$PBS_ARRAYID	$SLURM_ARRAY_TASK_ID

PBS and SLURM Comparison

Job Specification	**PBS**	**SLURM**
Script directive	#PBS	#SBATCH
Queue	-q [queue]	-p [queue]
Job Name	-N [name]	--job-name=[name]
Nodes	-l nodes=[count]	-N [min[-max]]
CPU Count	-l ppn=[count]	-n [count]
Wall Clock Limit	-l walltime=[hh:mm:ss]	-t [days-hh:mm:ss]
Event Address	-M [address]	--mail-user=[address]
Event Notification	-m abe	--mail-type=[events]
Memory Size	-l mem=[MB]	--mem=[mem][M|G|T]
Proc Memory Size	-l pmem=[MB]	--mem-per-cpu=[mem][M|G|T]

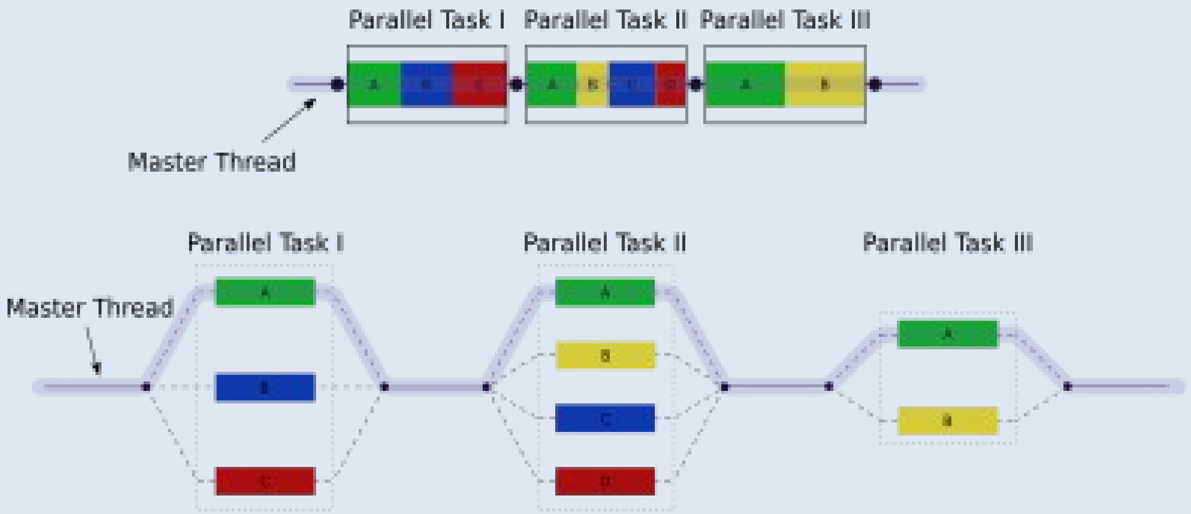
Shared Memory Parallel Programming

One form of parallel programming is multithreading, whereby a master thread forks a number of sub-threads and divides tasks between them. The threads will then run concurrently and are then joined at a subsequent point to resume normal serial application.

One implementation of multithreading is OpenMP (Open Multi-Processing). It is an Application Program Interface that includes directives for multi-threaded, shared memory parallel programming. The directives are included in the C or Fortran source code and in a system where OpenMP is not implemented, they would be interpreted as comments.

There is no doubt that OpenMP is an easier form of parallel programming, however it is limited to a single system unit (no distributed memory) and is thread-based rather than using message passing. Many examples in `` `/usr/local/common/OpenMP` ``.

(image from: User A1, Wikipedia)



Shared Memory Parallel Programming

```
#include <stdio.h>
#include  "omp.h"
int main(void)
{
    int id;
    #pragma omp parallel num_threads(8) private(id)
    {
    int id = omp_get_thread_num();
    printf("Hello world %d\n", id);
    }
return 0;
}
```

```
program hello2omp
    include "omp_lib.h"
    integer :: id
    !$omp parallel num_threads(8) private(id)
      id = omp_get_thread_num()
           print *, "Hello world", id
    !$omp end parallel
end program hello2omp
```

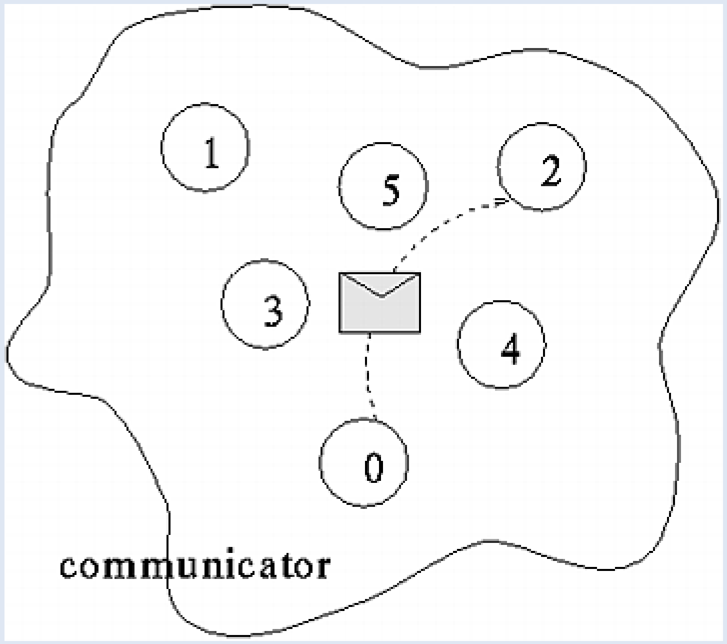
Distributed Memory Parallel Programming

Moving from shared memory to parallel programming involves a conceptual change from multi-threaded programming to a message passing paradigm. In this case, MPI (Message Passing Interface) is one of the most well popular standards and is used here, along with a popular implementation as OpenMPI.

The core principle is that many processors should be able cooperate to solve a problem by passing messages to each through a common communications network.

The flexible architecture does overcome serial bottlenecks, but it also does require explicit programmer effort (the "questing beast" of automatic parallelisation remains somewhat elusive).

The programmer is responsible for identifying opportunities for parallelism and implementing algorithms for parallelisation using MPI.

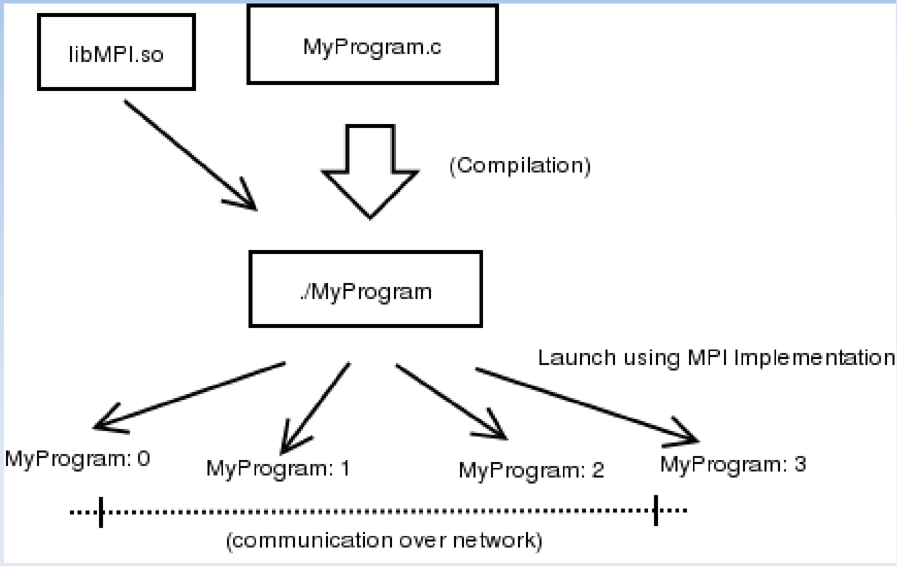


Distributed Memory Parallel Programming

```
#include <stdio.h>
#include "mpi.h"
int main( argc, argv )
int  argc;
char **argv;
{
    int rank, size;
    MPI_Init( &argc, &argv );
    MPI_Comm_size( MPI_COMM_WORLD, &size );
    MPI_Comm_rank( MPI_COMM_WORLD, &rank );
    printf( "Hello world from process %d of %d\n", rank, size );
    MPI_Finalize();
    return 0;
}

!       Fortran MPI Hello World
        program hello
        include 'mpif.h'
        integer rank, size, ierror, tag, status(MPI_STATUS_SIZE)

        call MPI_INIT(ierror)
        call MPI_COMM_SIZE(MPI_COMM_WORLD, size, ierror)
        call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierror)
        print*, 'node', rank, ': Hello world'
        call MPI_FINALIZE(ierror)
        end
```



MPI Compilation and Job Scripts

The OpenMP example needs to be compiled with OpenMP directives. The OpenMP example cannot run across compute nodes; therefore it is best run on the “cloud” partition. The OpenMPI compilation needs to call the MPI wrappers.

```
module load OpenMPI/1.10.0-GCC-4.9.2
gcc -fopenmp helloomp.c -o helloompc
mpigcc mpihelloworld.c -o mpihelloworld
```

```
#!/bin/bash
#SBATCH -p cloud
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH --cpus-per-task=16
export OMP_NUM_THREADS=16
module load GCC/4.9.2
mpiexecu helloompc
```

```
#!/bin/bash
#SBATCH -p physical
#SBATCH --nodes=2
#SBATCH --ntasks=16
module load OpenMPI/1.10.2-GCC-4.9.2
mpiexec mpi-helloworld
```

MPJ Express for Java

Java can be compiled with MPI bindings; we have done this with OpenMPI/3.0.0 only. A more common option is to use MPJ-Express. The following “HellowWorld.java” program is compiled and executed.

```
import mpi.*;
public class HelloWorld {
public static void main(String args[]) throws Exception {
        MPI.Init(args);
        int me = MPI.COMM_WORLD.Rank();
        int size = MPI.COMM_WORLD.Size();
        System.out.println("Hi from <"+me+">");
        MPI.Finalize();
        }
}
```

```
sinteractive --time=1:00:00 --nodes=1 --ntasks=2
module load MPJ-Express
javac -cp .:/usr/local/easybuild/software/MPJ-Express/0.44-goolf-
2015a-Java-9.0.4/lib/mpj.jar HelloWorld.java
mpjrun.sh -np 2 HelloWorld
```

MPI4Py Express for Python

Python too has various MPI bindings available. The most common used is MPI4Py. Sample assignment data is provided from the 2016 and 2015 in the Spartan directory, `/usr/local/common`. As a package it can be simply imported (e.g., `from mpi4py import MPI`).

But remember! With environment modules with extensions you do not necessarily get all the packages/libraries/extensions that you might expect. See the README file for an explanation of how to review the extensions already installed.

Examples provided in the directory of various Python jobs with MPI bindings with Slurm submissions scripts for single-core, dual core, eight-core, sixteen-core (different partition), and two-nodes with four cores each.

The actual Python script for the above is `twitter_search_541635.py`

MPI Communication: A Game of Ping-Pong

A very popular and basic use of MPI Send and Recv routines is a ping-ping program. Why? Because it can be used to test latency within and between nodes and partitions if they have different interconnect (like on Spartan).

An example is given in `/usr/local/common/MPI` as `mpi-pingpong.c` with a job submission script that can be modified accord to the test case `mpi-pingpong.slurm`. There are some routines here which manage the communication in the ping-pong activity.

`MPI_Status()` MPI_Status is not a routine, but rather a data structure and is typically attached to an MPI_Recv() routine.

`MPI_Request()` A wrapper for MPI Requests such as wait, waitany, waitall, waitsome, start, cancel, startall.

`MPI_Barrier()` Enforces synchronisation between MPI processes in a group by placing a barrier on communication between groups. An MPI barrier completes after all group members have entered the barrier.

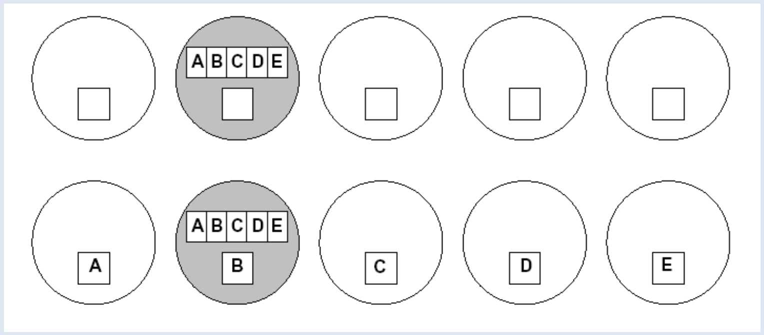
`MPI_Wtime()` - Returns an elapsed time as a floating-point number of seconds on the calling processor from an arbitrary time in the past.

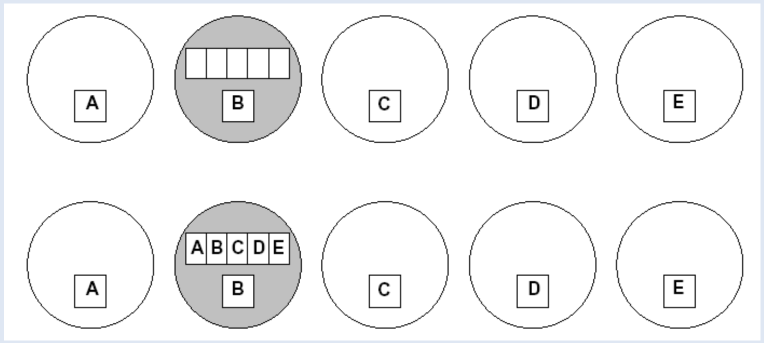
MPI Collective Communications

There are *many* other MPI routines which are *not* going to explored here! However just as a little taste one of the most popular is MPI collective communications and reduction operations. Collective communications include `MPI_Broadcast`, `MPI_Scatter`, `MPI_Gather`, `MPI_Reduce`, and `MPI_Allreduce`.

`MPI_Bcast` Broadcasts a message from the process with rank "root" to all other processes of the communicator, including itself. It is significantly more preferable than using a loop.

`MPI_Scatter` sends data from one task to all tasks in a group; the inverse operation of `MPI_Gather.` The outcome is as if the root executed n send operations and each process executed a receive. `MPI_Scatterv` scatters a buffer in parts to all tasks in a group.

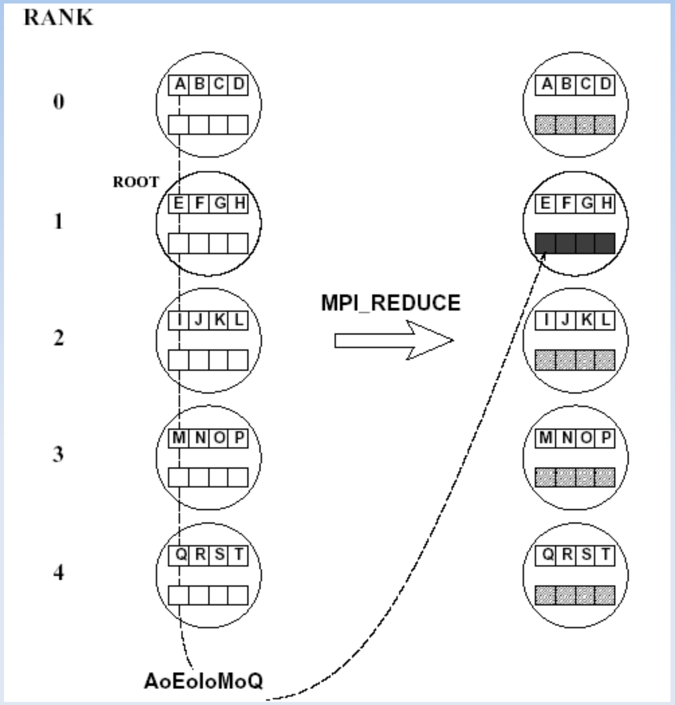


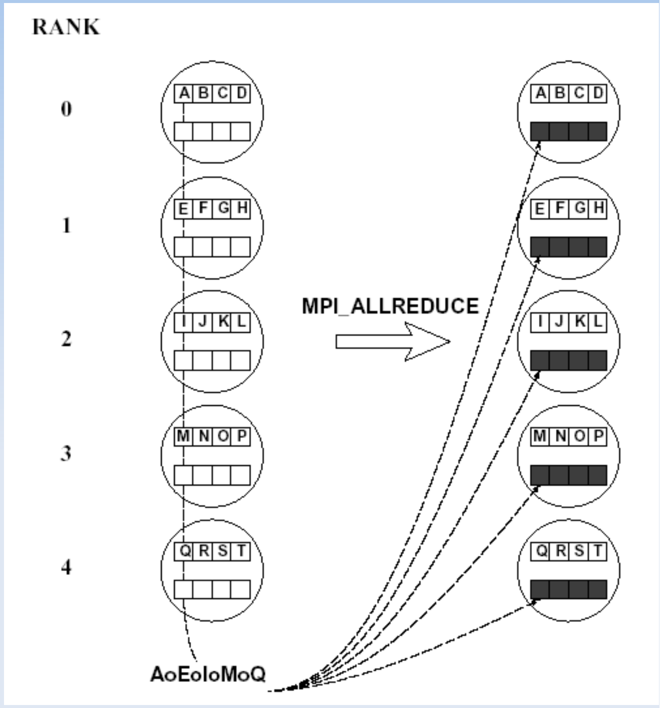


MPI Reduction Communications

`MPI_Reduce` performs a reduce operation (such as sum, max, logical AND, etc.) across all the members of a communication group.

`MPI_Allreduce` conducts the same operation but returns the reduced result to all processors.





The general principle in Reduce and All Reduce is the idea of reducing a set of numbers to a small set via a function. If you have a set of numbers (e.g., [1,2,3,4,5]) a reduce function (e.g., sum) can convert that set to a reduced set (e.g., 15). MPI_Reduce takes in an array of values as that set and outputs the result to the root process. MPI_AllReduce outputs the result to all processes.

THANKS FOR WATCHING
& LISTENING PATIENTLY
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