Kavli IPMU High-Performance Computing Tutorial

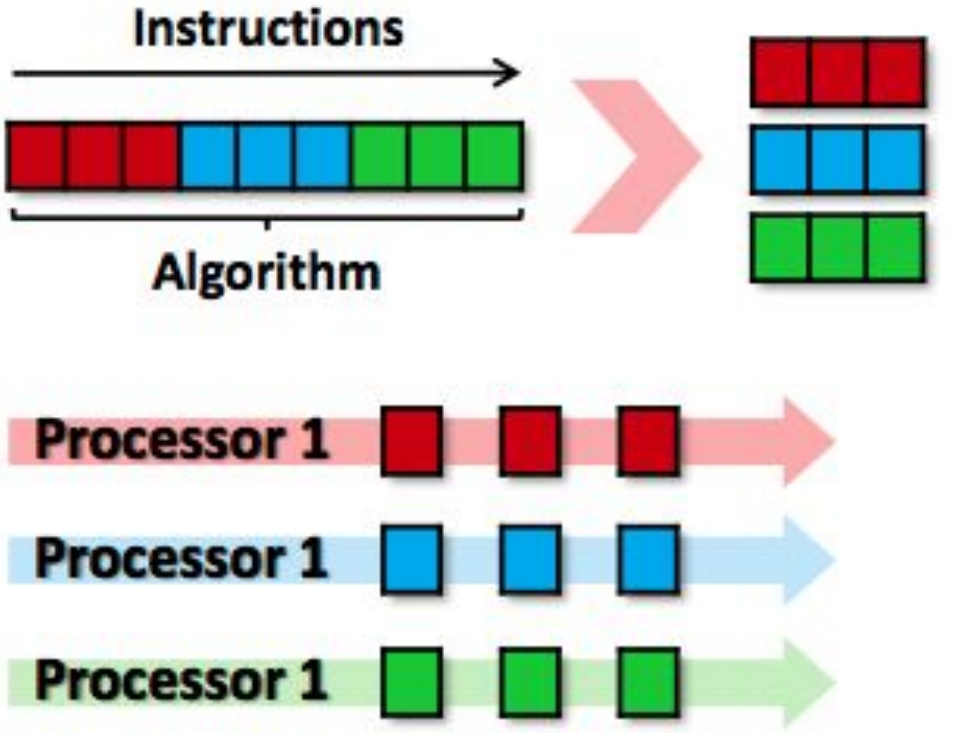
Connor Bottrell and Youngsoo Park
6/24/2021

Serial and parallel computing

Serial and Parallel Computing

Serial tasks

- A list of commands performed sequentially.
- All commands are carried out on a single CPU (core/processor).
- Multiple tasks (job) using the same commands are also carried out sequentially.
- Generally difficult to break up an individual serial task (colour in the right plot).
- Very efficient for small operations.



https://skirt.ugent.be/skirt8/_parallel_computing.html

Example of a set (**seri**es) of tasks (colours) carried out in **seri**al. Each task comprises a set of instructions which are performed sequentially (blocks).

Serial and Parallel Computing

Example of a serial task

Write a file whose whose contents are determined by some (set of) input argument(s).

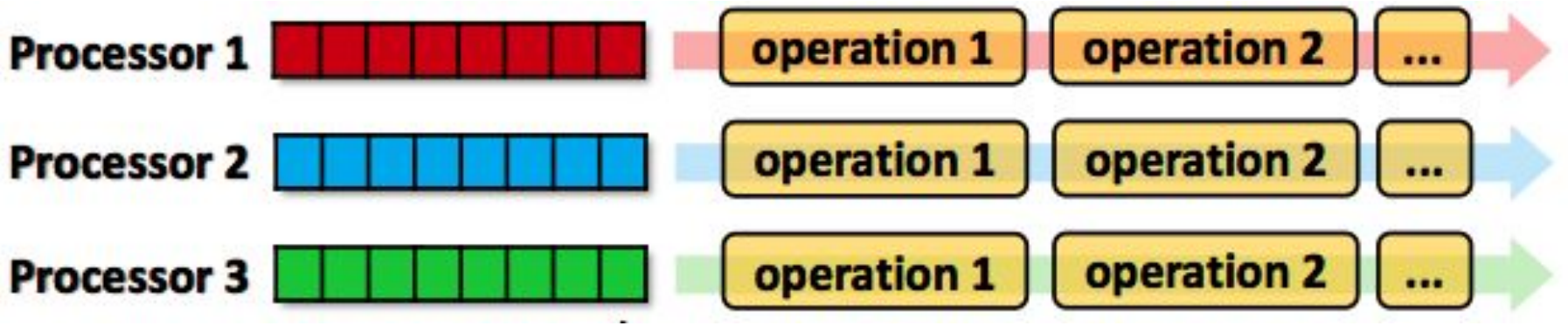
In the example to the right, **the serial task is the code inside the function** `serial_task`.

The function uses `idx` to determine the name of the output file and its contents.

In this example, each serial task takes ~0.5 s. But what if each took 1 min? 1 hour? 1 day?

```
1  # Example Serial Job
2  import time
3
4  # Serial task
5  def serial_task(idx):
6      time.sleep(0.5)
7      filename = f'Serial.{idx}.txt'
8      with open(filename,'w') as f:
9          for i in range(idx+1):
10             f.write(f'{i**2}\n')
11     return
12
13 def main():
14     # Main code
15     start = time.time()
16     for i in range(16):
17         serial_task(i)
18     runtime = time.time()-start
19     print(f'Time: {runtime}s')
20
21 if __name__=='__main__':
22     main()
```

Serial and Parallel Computing



https://skirt.ugent.be/skirt8/_parallel_computing.html

Example of a series of tasks (colours) carried out in parallel. Each task is independent and assigned to a different processor. Alternatively, each block may represent a chunk of a large dataset.

Parallel job

- Parallelization maps a set of tasks (colours) to multiple processors.
- Three different types of parallelization: *multithreading* (OpenMP), *message-passing* (MPI) and *hybrid parallelization* -- which combines message-passing and multi-threading.

Serial and Parallel Computing

Example of a parallel job

Here we see the same serial task as in the serial job example. But what is different about the main() function?

In this case, instead of a *for loop*, the tasks are being mapped to different threads (CPUs) using *multi-threading* parallelism (multiprocessing package in Python).

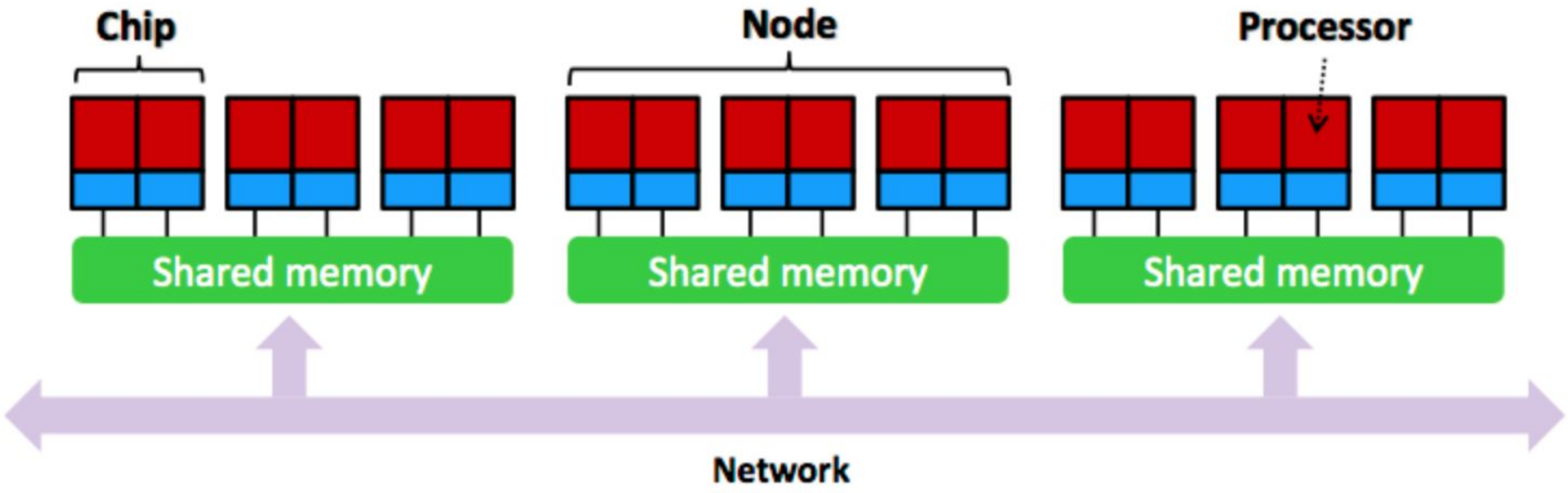
The job executes ~nthreads times faster than the serial job -- since each task is assigned to a separate CPU.

Once a CPU is done with a task, it accepts the arguments for the next unassigned task.

```
1  # Example Parellel OpenMP Job
2  import time
3  from multiprocessing import Pool
4
5  # Serial task
6  def serial_task(idx):
7      time.sleep(0.5)
8      filename = f'OpenMP.{idx}.txt'
9      with open(filename,'w') as f:
10         for i in range(idx+1):
11             f.write(f'{i**2}\n')
12     return
13
14 def main():
15     # Main code
16     start = time.time()
17     args = range(16)
18     nthreads = 8
19     with Pool(nthreads) as pool:
20         pool.map(serial_task,args)
21     runtime = time.time()-start
22     print(f'Time: {runtime}s')
23
24 if __name__=='__main__':
25     main()
```

Computing and the Queue System on IPMU's iDark Cluster

Cluster Computing



A cluster is made up of a large number of CPUs organized onto ***nodes*** -- on which the CPUs share a block of memory. Each CPU on a node share the total memory on that node. Each node is also connected via a ***network*** -- which enables rapid distribution of tasks, passing of information, and even memory sharing across multiple nodes.

iDark Cluster at IPMU

When you login to iDark, you will be connected to a ***head node*** shared by all users. All heavy-lifting should be done via the ***compute nodes*** which are accessed via a queue system:

Node Name	CPU count	Memory
ansys[01-40]	52	376.4 GB
ansys[1-2]	56	1.510 TB

Queue System: PBS Professional (next slides)

User Manual:
https://github.com/cbottrell/HPC_IPMU/blob/main/Docs/idark_users_manual_en.pdf

Check node status with:

```
pbsnodes -a
```

Queue system on idark

Many large computing clusters are shared between many users. This means competition for resources. Some clusters use a ***priority-based queue*** system where a ***fair share*** is enforced by reducing priority when resources are being overused. This ***forces*** users to take care about the jobs they submit.

IPMU clusters use an ***honour-based queue*** system -- which is to say that there is no regulation of resource usage. Therefore, in consideration of other users, it is important to consider the efficiency of your jobs (e.g. CPUs/memory used vs requested), and the duration of jobs.

At the end of this tutorial, we will explain how to monitor/check the efficiencies of current jobs.

Queue system on idark

queue	Maximum number of jobs to be executed /user	Maximum number of cores in use /job	Maximum number of nodes in use /job
tiny	256	1	1
mini	6	52	1
small	3	208	4
large	1	1040	20
mini2	1	56	1

There are currently 5 queues on idark -- each with different restrictions on (1) number of active jobs (2) maximum number of CPUs/job and (3) maximum number of active nodes/job.

One thing to consider, however, is the role of memory. Each CPU on a node uses shared memory. If I request a single CPU in the tiny queue with 376 GB of memory, I am effectively blocking off the whole node for myself and other users. So be careful, and considerate, about memory requests.

Running jobs

Running an *interactive* job

An ***interactive job*** is a resource allocation which will connect the user to (a) compute node(s) via ssh. Interactive jobs are useful for:

1) Testing and debugging programs on the compute nodes before deployment in the main queue.
2) Regular work to relieve congestion on the login node (e.g. jupyter lab sessions).

```
qsub -l select=1:ncpus=1:mem=4gb -l walltime=3:0:0 -q tiny -I
```

This interactive job request asks for 1 chunk of resources (discussed later) with 1 CPU/chunk and 4GB of memory per chunk for 3 hours 0 minutes 0 seconds on the `tiny` queue.

Running an *interactive* job

Let's run the serial job script in interactive mode using the resources we have requested. First, ssh onto iDark and request the interactive job:

```
qsub -l select=1:ncpus=1:mem=4gb -l walltime=3:0:0 -q tiny -I
```

Then, from the compute node, clone the tutorial repository to a directory of your choice (current directory) with git:

```
git clone https://github.com/cbottrell/HPC_IPMU.git
cd HPC_IPMU/Code/Serial
```

The scripts are written in Python 3, which needs to be activated from conda or by activating your own virtual Python 3 environment.

```
source /home/anaconda3/bin/activate
python Serial_Example.py
```

Running a job

Interactive jobs are for testing with limited resources (less than 3 hours with only the CPUs needed to test the code).

All long/resource-intensive jobs should be submitted to the queue via a job script:

```
#!/bin/bash
#PBS -N Serial_Example
#PBS -o /home/connor.bottrell/Scratch/pbs
#PBS -e /home/connor.bottrell/Scratch/pbs
#PBS -l select=1:ncpus=1:mem=4gb
#PBS -l walltime=00:30:00
#PBS -u bottrell
#PBS -M connor.bottrell@ipmu.jp
#PBS -m ae
#PBS -V
#PBS -q tiny

# activate Python 3
source /home/anaconda3/bin/activate
# you can set environment variables in the job script
export HPC_DIR=$HOME/Demos/HPC_IPMU
cd $HPC_DIR/Code/Serial
# run program
python Serial_Example.py
```

Options:

-N: Job name in queue
-o: Output file full path (non-dynamic)
-e: Error file full path (non-dynamic)
-l: Resources requested
(1 CPU with 4GB mem for 30 minutes)
-u: Username
-M: Mail address for job updates
-m: Options for when to receive mail
-V: Import environment
-q: The queue in which to run the job

Please personalize! I don't want your job mail.

Running a job and checking job status

```
cd HPC_IPMU/Code/PBS
# edit file for your mail address and path
qsub Serial_Example.pbs
```

qsub is the job submission command. We already used it for the interactive session.

The job should complete very quickly. Too fast to look at it in the queue. Check your output/error file path for the output/error files.

Active/queued jobs can be checked using **qstat** :

```
qstat -ntr -u user_name # running jobs/subjobs
qstat -ntr # running jobs/subjobs by all users
qstat -nt  # all queued/running jobs/subjobs
```

Other job/queue management tools

Suppose you've made an error in your job script or program. Jobs can be cancelled using **qdel** and the **Job ID** from **qstat**:

```
qstat -ntr -u bottrell
```

```
idark:
                                                                  Req'd  Req'd   Elap
Job ID          Username Queue    Jobname    SessID NDS TSK Memory Time  S Time
--------------- -------- -------- ---------- ------ --- --- ------ ----- - -----
8220.idark      sunao.su small    run_mn     216318   4 208   40gb   --  R 291:3
   ansys02/0*52+ansys25/0*52+ansys03/0*52+ansys28/0*52
8221.idark      sunao.su small    run_mn     248886   4 208   40gb   --  R 291:3
   ansys29/0*52+ansys30/0*52+ansys31/0*52+ansys32/0*52
9080.idark      toshiki. small    run_mn     268982   4 208   40gb   --  R 242:3
   ansys17/0*52+ansys21/0*52+ansys22/0*52+ansys34/0*52
13356[1492].ida bottrell mini     Run_SKIRT  177020   1  50  150gb 24:00 R 01:24
   ansys06/0*50
15231.idark     bottrell tiny     TNG_Downlo 179412   1   1  512mb 36:00 R 00:00
   ansys06/1
```

```
qdel 15231
```

Checking status of a job

You may ssh onto any node on which you are running jobs. Indeed, you can ssh onto any node on iDark, but it is bad practice as you may disrupt the workflow of other users.

If I have a job running on the ansys06 compute node, I can do:

```
ssh ansys06
```

on the login node and then check the efficiency of my job with the **top** command:

```
top -u user_name
```

```
top - 11:16:48 up 79 days, 22:59,  1 user,  load average: 49.09, 46.24, 46.33
Tasks: 736 total,   7 running, 729 sleeping,   0 stopped,   0 zombie
%Cpu(s): 96.2 us,  0.0 sy,  0.0 ni,  3.8 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
GiB Mem :    376.4 total,    340.3 free,     14.5 used,     21.6 buff/cache
GiB Swap:      8.0 total,      8.0 free,      0.0 used.    360.7 avail Mem

  PID USER      PR  NI    VIRT    RES    SHR S  %CPU %MEM     TIME+ COMMAND
 2724 bottrell  20   0 1692736 785440   6000 R 999.0  0.2  32:22.67 skirt
 2725 bottrell  20   0 1697260 787996   6012 R 999.0  0.2  32:23.90 skirt
 2726 bottrell  20   0 1697260 789848   5992 R 998.7  0.2  32:23.15 skirt
 2727 bottrell  20   0 1697260 787952   5992 R 998.7  0.2  32:23.34 skirt
 2723 bottrell  20   0 1697268 790040   6020 R 998.3  0.2  32:22.98 skirt
 2905 bottrell  20   0  166924   3072   1692 R   0.3  0.0   0:00.79 top
```

Use **SHIFT+e** to toggle between KiB, MiB, and GiB and **q** to quit top.

Running multi-core and multi-node jobs

Running a parallelized job

A parallelized job script is submitted in the same way as a serial job script. The difference is the resources requested and the program (which is now parellelized).

Below, 1 chunk of 8 CPUs and 4GB total memory is requested.

```
#!/bin/bash
#PBS -N Serial_Example
#PBS -o /home/connor.bottrell/Scratch/pbs
#PBS -e /home/connor.bottrell/Scratch/pbs
#PBS -l select=1:ncpus=8:mem=4gb
#PBS -l walltime=00:30:00
#PBS -u bottrell
#PBS -M connor.bottrell@ipmu.jp
#PBS -m ae
#PBS -V
#PBS -q mini

# activate Python 3
source /home/anaconda3/bin/activate
# you can set environment variables in the job script
export HPC_DIR=$HOME/Demos/HPC_IPMU
cd $HPC_DIR/Code/OpenMP
# run program
python OpenMP_Example.py
```

You can be clever about how the numbers of CPUs/nodes are communicated to a program by setting these as environment variables in the job script that can then be grabbed by the program.

```
cd HPC_IPMU/Code/PBS
# edit file for your info
qsub OpenMP_Example.pbs
```

Running a parallelized job

Resource Specifications:

```
#PBS -l select=4:ncpus=6:mem=8gb
```

select: how many chunks of [ncpus, mem] do you want
ncpus: number of CPUs per chunk
mem: memory requested per chunk

The request above is for 4 x 6 = 24 CPUs and 4 x 8 = 32 GB of total memory. The **select** request ***does not restrict CPUs to the same node*** and ***allocates to empty space wherever it exists*** (starting with nodes that are already busy). ***This maximizes cluster usage efficiency -- leaving as many empty nodes as possible***. If you wish all 24 CPUs to be on the same node:

```
#PBS -l select=1:ncpus=24:mem=32gb
```

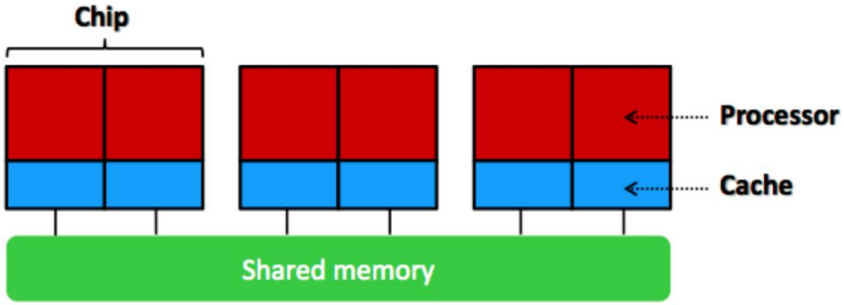
is the resource-equivalent request.

Types of parallelization: Which is right for you?

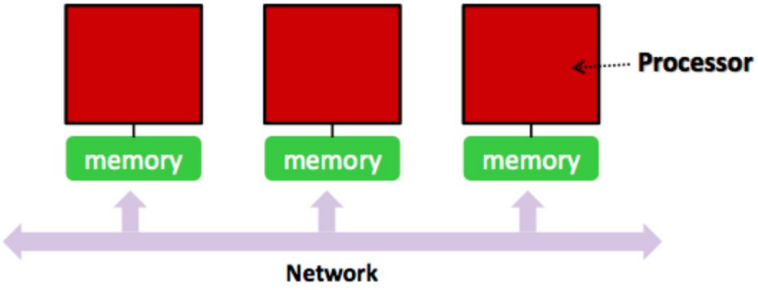
The multi-threading parallel job used in these examples is called an ***embarrassingly parallel job*** because no communication is required between CPUs. These are very useful.

When communication is required, the options are:

Multi-threading, Shared Memory



Message-passing, Distributed memory

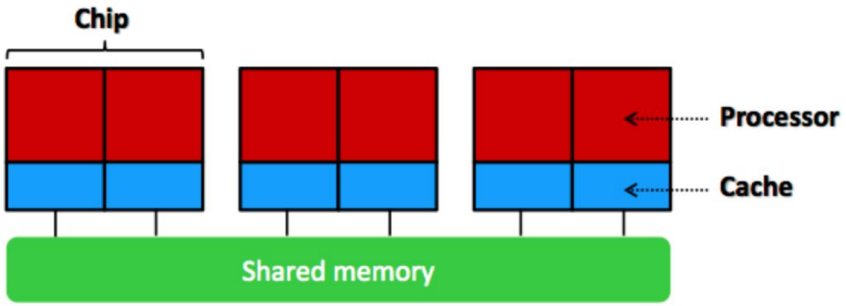


And hybrid parellelization, which combines both by creating multiple instances of the data in memory which can be accessed by all threads connected to each instance.

Types of parallelization: Which is right for you?

The advantage of multi-threaded parallelism is that all CPUs can access and update the same information in memory, and these changes are immediately seen by all other CPUs.

The disadvantage is that it is not scalable to large numbers of threads because of the competition for access to memory between threads.



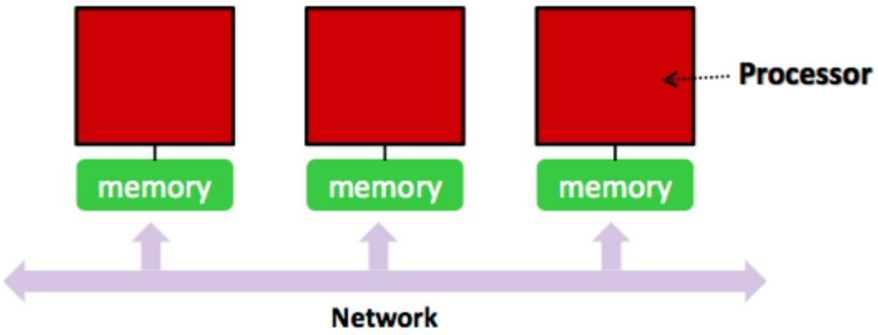
Multi-threading, Shared Memory

All processors share have access to the same memory chunk. Multi-threading is efficient on memory -- but can become CPU inefficient when too many CPUs are competing for read/write access to a large dataset stored in memory.

Types of parallelization: Which is right for you?

The advantage of distributed memory parallelization is that each chunk of CPUs has access to a unique instance of the data -- so little competition and high efficiency.

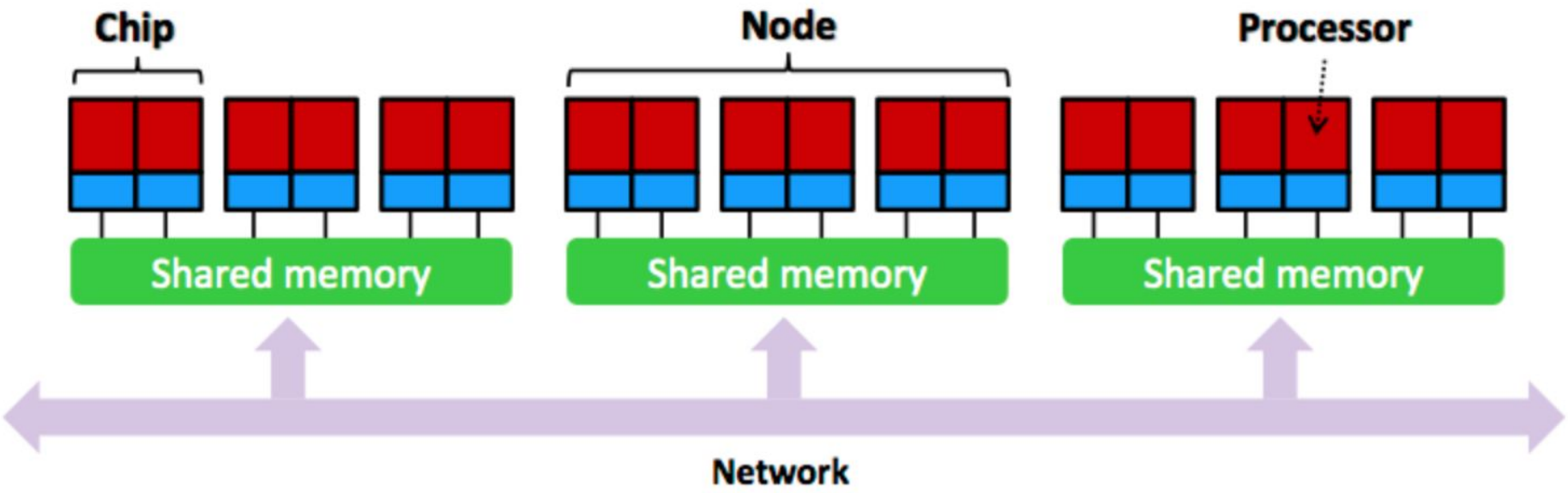
The disadvantage is that the memory requirements scale with the number of chunks and communication between chunks is not as fast as communication from processors to their own shared memory.



Message Passing, Distributed memory

Each processor has access to its own copy of the data in a separate memory chunk. Changes to the data are communicated via the network.

Types of parallelization: Which is right for you?



In *hybrid* parallelization, shared memory parallelism (threading) is used together with distributed memory parallelism (multiple chunks/tasks).

E.g. NxN gravity solver with a huge data set. ***Each chunk*** (process/task) needs the whole data set -- but only updates the output (force table) for only Nparticles/Ntasks particles. In each task, the force calculations on each particle use thread-based parallelism.

Message Passing Interface (MPI)

Array Jobs:
Gold Standard of HPC Computing

The array job

Job Script

```
#!/bin/bash
#PBS -N Serial_Example
#PBS -o /home/connor.bottrell/Scratch/pbs
#PBS -e /home/connor.bottrell/Scratch/pbs
#PBS -l select=1:ncpus=1:mem=32mb
#PBS -l walltime=00:30:00
#PBS -J 0-256:1
#PBS -u bottrell
#PBS -M connor.bottrell@ipmu.jp
#PBS -m ae
#PBS -V
#PBS -q tiny

# activate Python 3
source /home/anaconda3/bin/activate
# you can set environment variables in the job script
export HPC_DIR=$HOME/Demos/HPC_IPMU
cd $HPC_DIR/Code/Array
# run program
python Array_Example.py $PBS_ARRAY_INDEX
```

Use job arrays whenever you have several independent tasks.

Program

```
# Example Array Job Program
import time
# To access $PBS_ARRAY_INDEX
import sys

# subjob task
def serial_task(idx):
    time.sleep(0.5)
    filename = f'Array.{idx}.txt'
    with open(filename,'w') as f:
        for i in range(idx+1):
            f.write(f'{i**2}\n')
    return

def main():
    # Get subjob idx from python arg vars
    program_name, pbs_array_idx = sys.argv
    pbs_array_idx = int(pbs_array_idx)
    # Code performed for each subjob
    start = time.time()
    serial_task(pbs_array_idx)
    runtime = time.time()-start
    print(f'Time: {runtime}s')

if __name__=='__main__':
    main()
```

Rationale for the array job

Array jobs generate an array of indices which become unique environment variables ($PBS_ARRAY_INDEX) in each ***subjob*** of the array. Advantages:

- Array jobs can parallelize programs across the *entire cluster* wherever there are empty resources (within queue limits). ***Accelerates your work***!
- Array subjobs can be made short (~minutes) which ***creates availability for other users*** in the queue.
- Two scripts: job script and program. ***No need for generator scripts*** for submitting jobs to the queue.
- Each subjob gets unique output/error files. Good for debugging, ***other subjobs unaffected by errors***.

Thank you for attending the Kavli IPMU HPC Tutorial

We hope you use the information, tips, and tricks in this tutorial to accelerate your computing!

Connor & Youngsoo