HIGH PERFORMANCE COMPUTING

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COMPUTER CLUSTERS OR SUPERCOMPUTER

- So far we have been performing all of our numerical calculations on laptops.
- We also have been limiting our calculations to tasks that can finish in a reasonable time on our laptops.
- But what if we want to do calculations that would involve thousands or millions more operations.
- We could wait a month or longer for them to finish.
- Or we could instead run our code on a computer cluster or supercomputer.
- A supercomputer is just really big cluster.

WORLD ECONOMIC FORUM

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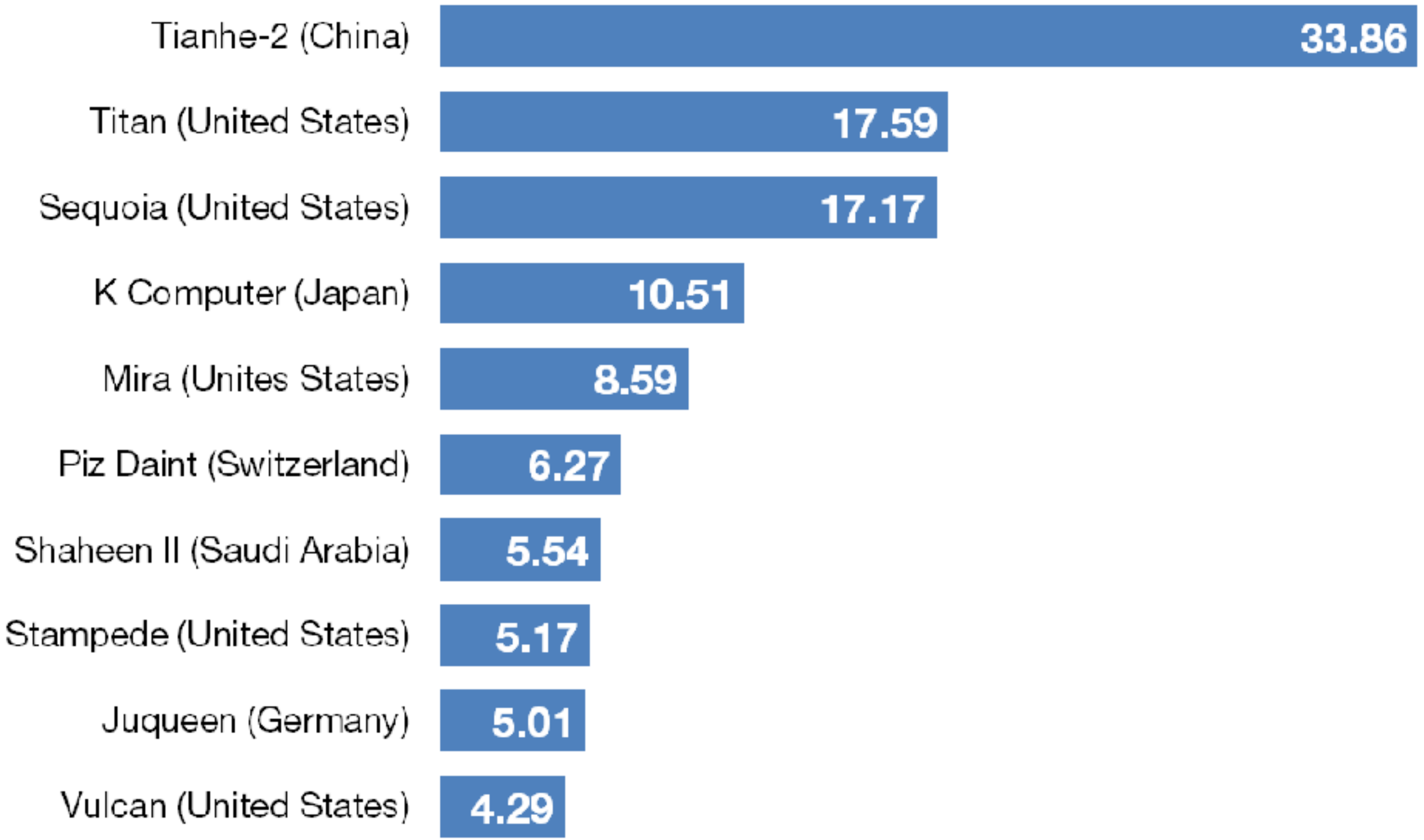
Top 10 supercomputers

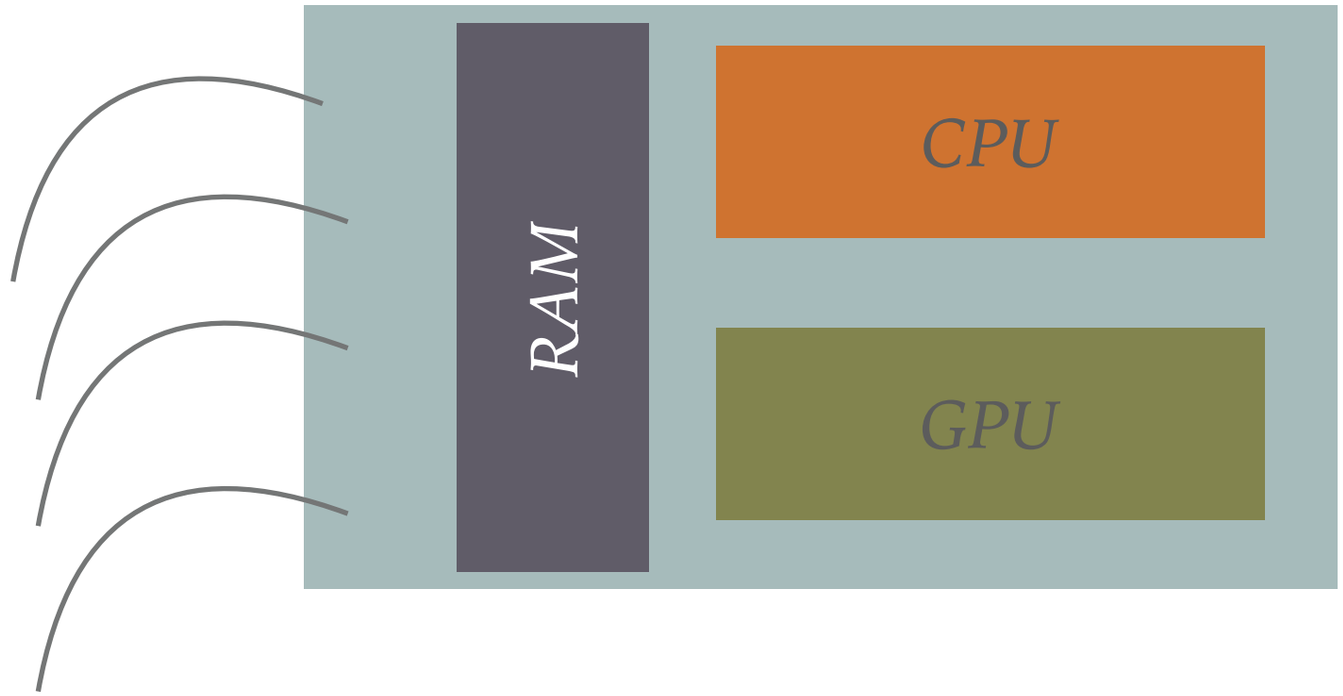
Petaflop/s on the Linpack benchmark



Source: top500.org

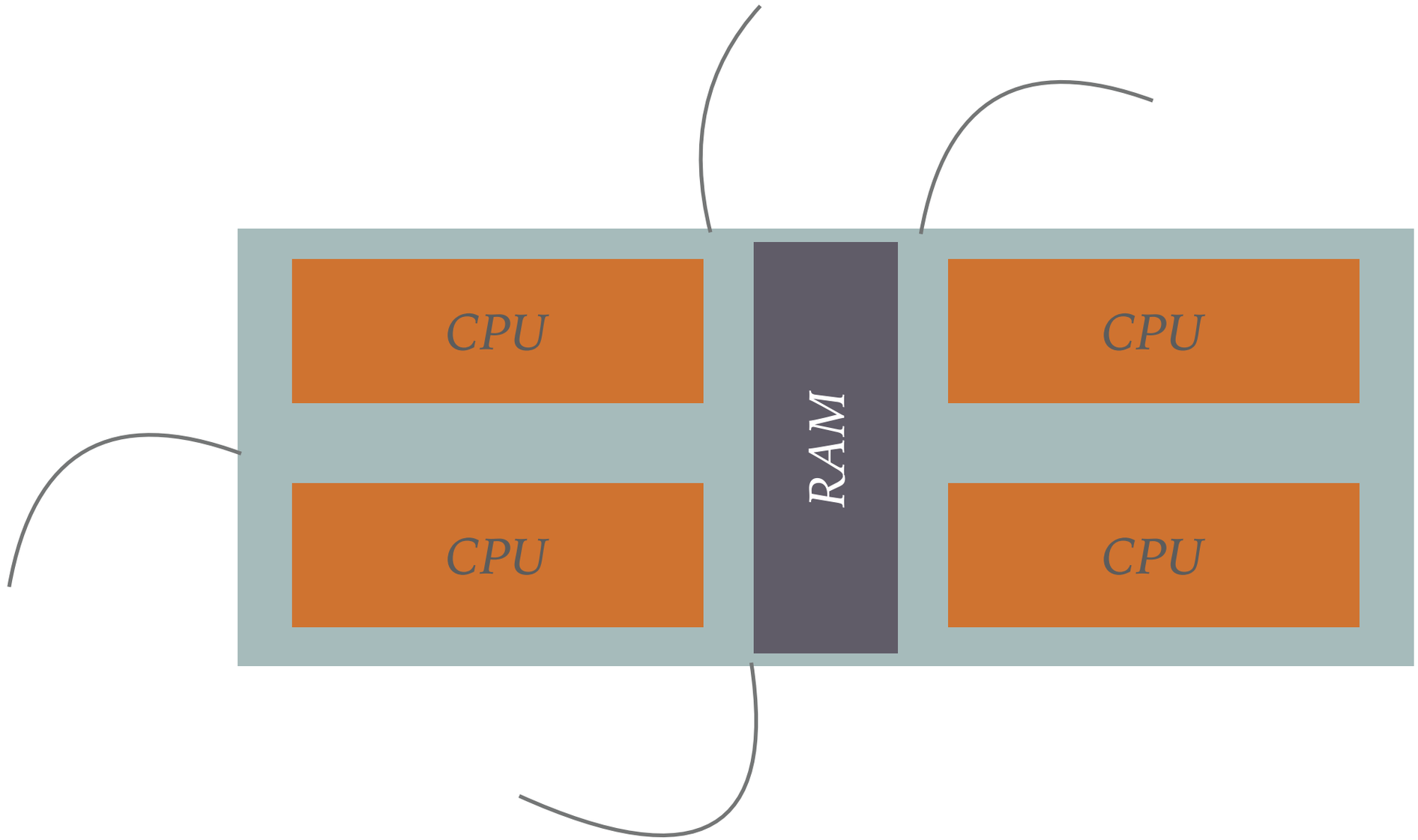
COMPUTE NODE

- Before we start discussing what a supercomputer is let us discuss what is a computer.
- A computer combines a number of hardware pieces into a single device. Most importantly these include
  - CPU - central processing unit
  - GPU - graphical processing unit
  - RAM - random access memory
  - Hard Drive - memory storage
  - Input devices - keyboard, mouse, screen
  - Output devices - screen, speakers


RAM
CPU
GPU

COMPUTER NODES

- However, thing aren't that simple anymore. Now days chips are designed to act as if they contain more than one CPU.
- Language can get a bit confusing here. Let's think of the CPU as a single chip. But the ability to process instructions let us call a core.
- A multi-core processor (dual-core, quad-core, etc.) means that one one chip you can run multiple instructions at the same time.
- In addition, a chip can have multi-threading. This is additional way to get multiple thing done, but it isn't a separate a having a different core. That is it can't take different instructions, but can branch out part of an instruction.
- Finally on a single motherboard you can place more than one CPU. The different CPU's will share the same RAM. This gives us the modern basic unit of a computer, the *computer node*.
- In summary a single computer node can have multiple CPUs. Each CPU can have multiple cores and each core can have multiple threads.



Compute Node

COMPUTER CLUSTER

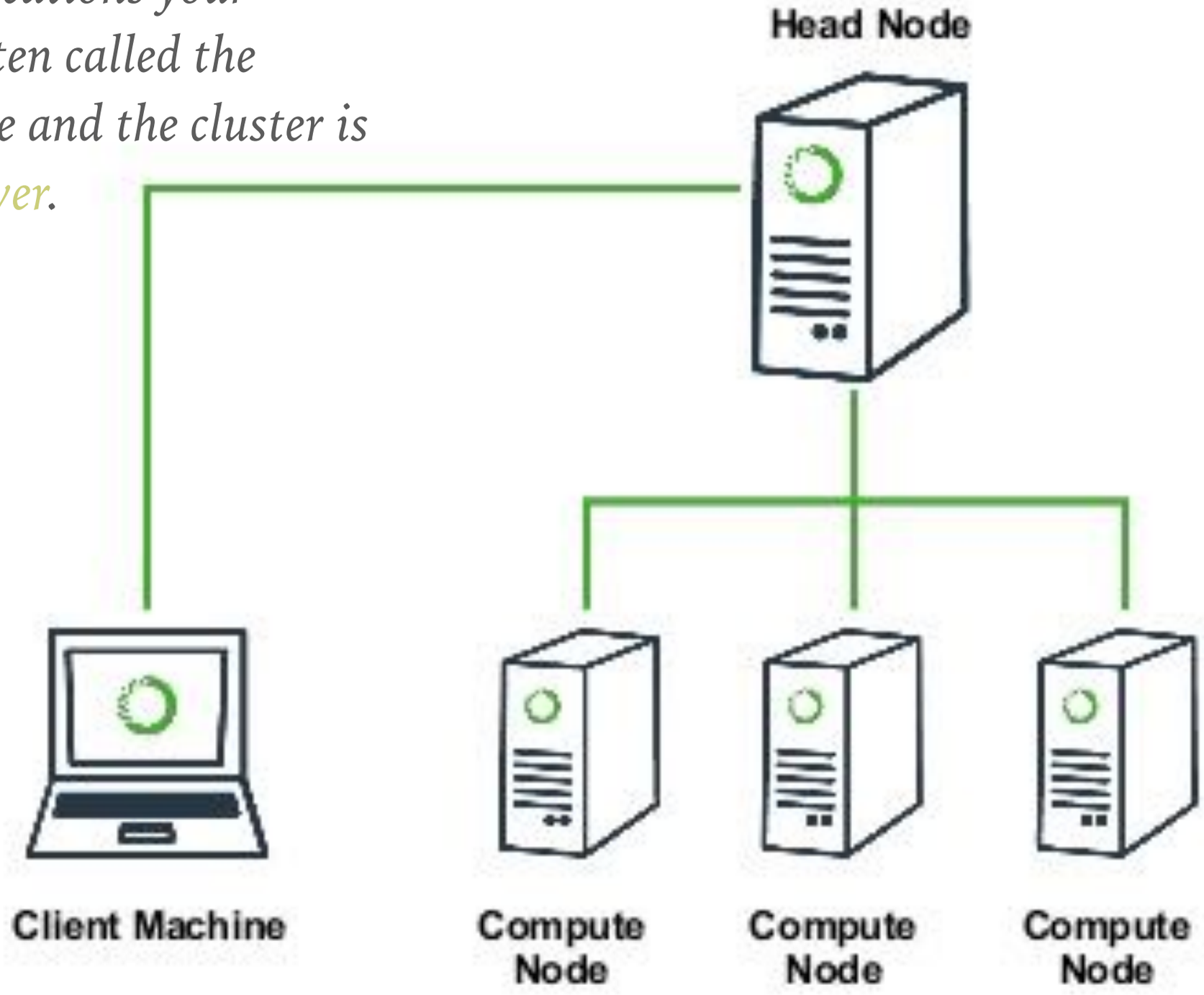
- A computer cluster is made of many compute nodes. This can be as few as 4 or 8 and a many as 40,960 (Sunway TaihuLight current world champ).
- A cluster with thousands of node is called a supercomputer.
- Each of the nodes can contain multiple cores, the Sunway TaihuLight has 256 cores per node so this supercomputer has a total of 10,649,600 CPU cores which basically can act like 10 million computers running at once.
- However, this does not mean this supercomputer is 10 million times faster than your laptop. A lot depends on what you are using it to do.

CLUSTER ARCHITECTURE

- The most common way the nodes are set up in a cluster is to have one head node that tells all the other nodes what to do.
- This way normal users only interact with this head node and tell it what they want it to do. The head node then takes those instructions (a job) and makes decisions as to which compute nodes should run different pieces of code.
- In order to be more efficient, jobs are usually placed in a queue. The job will wait there until the resources it needs are freed up. Unlike on your laptop the process doesn't start running as soon as you hit enter. Instead your job may wait in the queue for a long time before it starts running.
- This has the huge advantage that you don't have to sit around waiting until resources are freed up. Instead you simply submit your job and the head node will run it as soon as it possibly can.

Cluster Architecture Diagram

For web applications your machine is often called the client machine and the cluster is called the server.



REMOTE LOGIN

- As a user, it is likely you will never have physical access to the cluster. Instead you will log in to the head node remotely.
- This is almost always done with the ssh (secure shell) protocol. On Linux and Mac you will have this program installed. On Windows you will need to install a program that runs ssh, Putty is one choice (and it is free).
- On the command line ssh works like this:

```
ssh username@remotehost
```

- alternatively you can leave out the username and it will ask
- you will need to give a password after this step.

SSH CONFIG

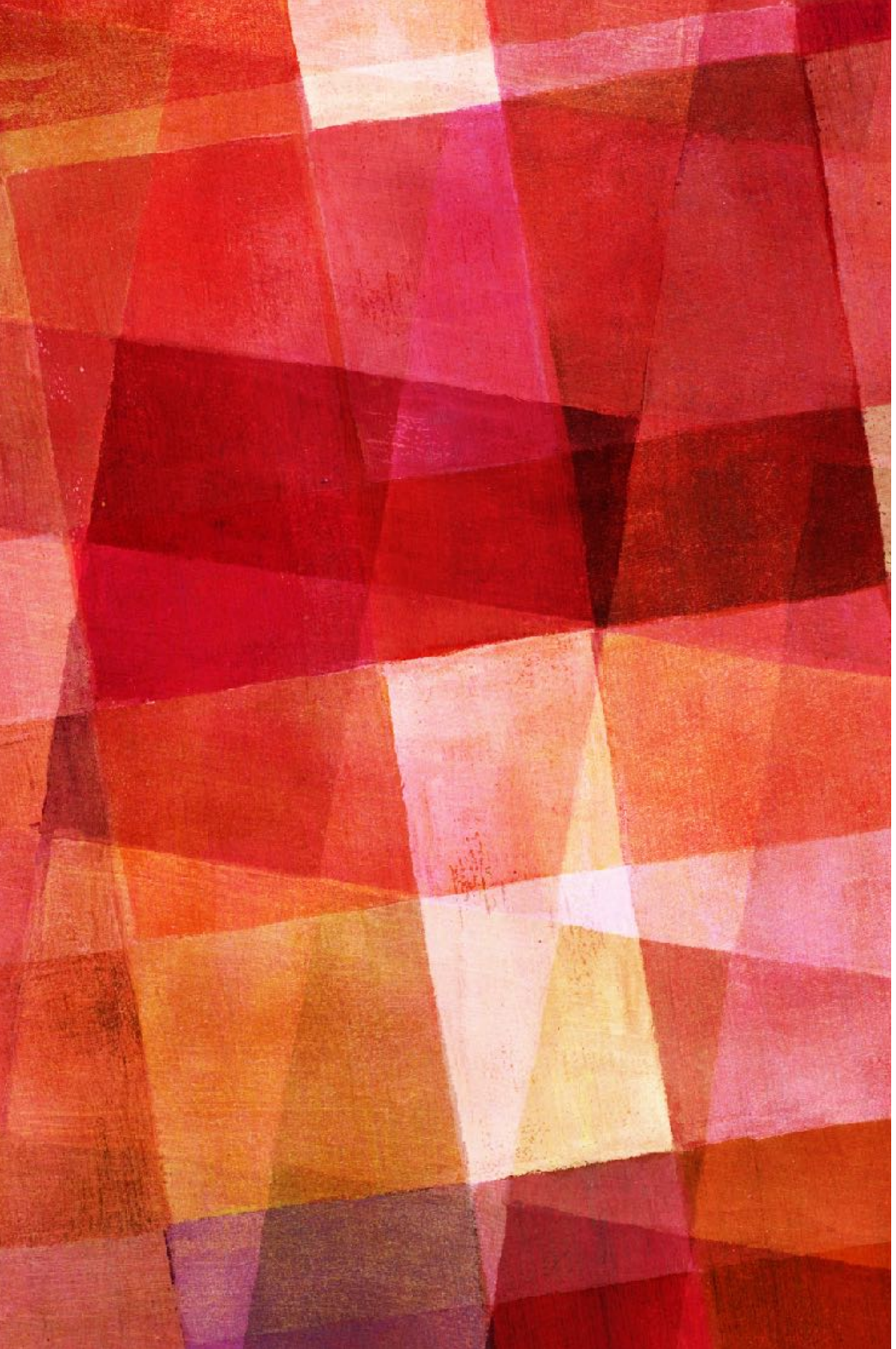
- There is a useful config file for ssh that lives in the director .ssh under your home directory.
- Like all unix programs there are dozens of things you can set in the file but the most useful are your username and an alias for the host. For example:

```
Host ursa

    Hostname ursa.major.edu

    User JohnDoe

    HostKeyAlias ursa
```

- This allows one to just type ssh ursa and it knows the host name and username.

PUBLIC KEYS

- public/private key sharing is a more secure way to access remote machines than using a password.
- The idea is you create a key that can be sent to other machines and then it recognizes you when you log in. The public key recognizes your private key, but can't be used to recover it.
- To create a key in a terminal you can use ssh-keygen. There are tons of options but just ssh-keygen should get you started.
- This will ask for a passphrase and a location for the keys, using the default should create public and private keys in .ssh/ as the files id_rsa.pub and id_rsa. The .pub one is your public key which you need to copy to any machine you wish to use it for.



EX 13.1

- Let's create a set of keys and share them with your GitHub account. If for some reason you need to use ssh to connect to GitHub this will be useful.
- First generate a key with ssh-keygen if you don't already have one.
- Then copy your key. You can use pbcopy < .ssh/id_rsa.pub or open it in a text editor and copy it.
- Go to GitHub settings SSH and GPG keys and add the key. Test it in the terminal with ssh -T git@github.com

PBS SUBMISSION SCRIPT

- In order to run a job on a cluster you have to write what is called a submission script. This is a file that contains the instructions for what you would like head node to do.
- You submit with something like

qsub my_submision_script.pbs

- You can check on your submission with the command qstat.
- There are many other commands and options that are dependent on the program being used to control the submission que.
- Your script might look something like:

PBS SUBMISSION SCRIPT

```
#!/bin/sh


#PBS -N job-name
#How many nodes and processors per node (ppn) you request:
#PBS -l nodes=4:ppn=32
#PBS -j oe
#PBS -o outputfile

echo "Starting  job"
cd $PBS_O_WORKDIR
python mycode.py
python more_code.py
echo "Job finished"
```

PARALLELIZATION

- To make use of multiple nodes or cores you need to send different instructions to each core. For this to be helpful the key question is how parallel is the task you want to perform.
- For example if your code was the following:

```
for i in range(N):
    k=k+i
```

- then a different core can do nothing helpful in this calculation, because every addition needs to know what was done previously. That is the code is 100% serial.

PARALLELIZATION

- On the other hand if your code was this:

```
for i in range(N):
    array[i]=array[i]+i
```

- then each of these additions could be done on a different core. This operation is 100% parallel.

- In general coding contain both parts that can run in parallel and parts that can not. The degree to which a problem can be made to run in parallel is the degree to which using more cores will make it run faster.
- Some tasks are 100% parallel, like solving an ODE for 100 different boundary conditions. This is essentially just running the same code 100 times so it can very easily be run on 100 different cores.
- 100% parallel tasks can actually be run on 100 different computers, but you may want to combine the results are start the process based on some common conditions so that is the advantage to running on the same machine.

NODES AND CORES

- A parallel operation runs the same on a core on the same node or on a different node, but there is an important difference.
- Cores on the same node share memory. But cores on different nodes do not. So if different processes need access to the same variables, then they must be copied to the RAM of the other node.
- This can also be an advantage, one of the uses of clusters is to break up memory needs across many nodes. So if you had a 100,000×100,000 matrix, that would exceed the RAM on any machine. But you could break that matrix up into many smaller matrices and distribute them onto many nodes.

NODES AND CORES

- In either case, communication between nodes becomes a key aspect of parallel programming. Communication between nodes is much slower than operations on a chip, so a program can get stuck waiting for information from another node and not computing anything.
- Thus both the operations and the memory must be parallelized to use a cluster effectively. The degree to which this is possible will determine how a program will scale on a cluster.
- Even if not running on a cluster it can useful to think about such things because your single CPU is probably multi-cored and multi-threaded so the more parallel your code it will probably still run faster.

HOW TO PARALLELIZE

- Writing parallel code can be done a number of ways.
- At the lowest level you can write the different parts of code to be run on each processor and then write the code to start them, run them and control how they communicate.
- Most scientific users do not do this. Instead they use libraries that will handle much of the parallelization details for you. These libraries include MPICH and OpenMPI.
- MPI stands for Message Passing Interface and it takes care of some of the hardest parts of parallel programming, getting the information back and forth between nodes.

RUNNING PARALLELIZED CODE

- When you run parallelized code you don't just type a command on the command line, but instead you run a program from MPI (if using MPI) that will then deal with sending the different processes to different cores.
- Your command would look something like

mpiexec -n 16 python mycode.py

- the -n says you want to use 16 cores. You then pass python as the program you want to run. And then to python you pass your code that you want to run.
- So mpiexec is running python and python is running your code.

GPUS

- Using GPUs is in many ways similar to using a cluster. GPUs have many threads and can perform many operations in parallel.
- However, the GPU has its own memory and to perform operations you must transfer data to the GPU memory cache. Thus performance speedup will often depend on how much and how often you need to move memory around.
- To access the GPU requires using special libraries. NVIDIA has released a code library CUDA but it can only be used with their chips. The package NUMBA can call CUDA, but you may have to install the cudatoolkit.

conda install cudatoolkit
conda install numba

GPUS

- With numba using the GPU is very simple, but whether you get increased speed will depend on what you are trying to do.
- To use the GPU just do the following:

```
from numba import jit,cuda

# normal function to run on cpu

def func(a):

    for i in range(10000000):

        a[i]+= 1


# function optimized to run on gpu

@jit(target ="cuda")

def func2(a):

    for i in range(10000000):

        a[i]+= 1
```

this is called a decorator

- The @jit part tells the parser that the following function should be compiled to run on the GPU.

NUMBA

- numba can also be used to optimize your code on the cpu.
- languages like c++ use a compiler that translates the code to machine language before it is run. With optimization this can make your c++ code run very fast.
- languages like java have a *just in time* (jit) compiling that compile some code functions that are used multiple times.
- numba adds this functionality to python so that some code aspects can be optimized for your cpu.
- speed improvement will mostly depend on how many times a function is called and what it does.
- To learn about your system type numba -s on the command line

NUMBA

```
from numba import jit
import numpy as np

x = np.arange(100).reshape(10, 10)

@jit(nopython=True) # Set "nopython" mode for best performance, equivalent to @njit
def go_fast(a): # Function is compiled to machine code when called the first time
    trace = 0.0
    for i in range(a.shape[0]):   # Numba likes loops
        trace += np.tanh(a[i, i]) # Numba likes NumPy functions
    return a + trace              # Numba likes NumPy broadcasting

print(go_fast(x))
```

```
Elapsed (with compilation) = 0.33030009269714355
Elapsed (after compilation) = 6.675720214843750e-06
```

MULTIPROCESSING

- As mentioned earlier modern cpus have multiple processors on a single chip. While the python interpreter will try to make use of this you can explicitly run different parts of your code on different processors.
- The multiprocessing package can be used to send functions in your code to different processors. This is just like MPI, but because the processors are on the same chip you don't need MPI to pass information between nodes.
- This enables you to parallelize aspects of your code for running on a single compute node.
- One can use the package thread to control to send code to separate threads in a similar way.

```
import multiprocessing

def print_cube(num):
    “”" function to print cube of given num"""
    print("Cube: {}".format(num * num * num))

def print_square(num):
    """function to print square of given num"""
    print("Square: {}".format(num * num))

if __name__ == "__main__":
    # creating processes
    p1 = multiprocessing.Process(target=print_square, args=(10, ))
    p2 = multiprocessing.Process(target=print_cube, args=(10, ))

   p1.start()     # starting process 1
   p2.start()    # starting process 2
   p1.join()   # wait until process 1 is finished
   p2.join()  # wait until process 2 is finished
   print("Done!")  #both processes finished
```