

Introduction to HPC Resources and Linux

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CSC

UNIVERSITY OF CALIFORNIA SANTA BARBARA
CENTER FOR SCIENTIFIC COMPUTING

Overview

- What is High Performance Computing (HPC)?

High Performance Computing (HPC) allows scientists and engineers to solve complex science, engineering, and business problems using applications that require **high bandwidth, enhanced networking,** and very **high compute** capabilities.

From: <https://aws.amazon.com/hpc/>

- Multiple computer nodes connected by a very fast interconnect
- Each node contains many CPU cores (around 12-32)
- Allows many users to run calculations simultaneously on nodes
- Allows a single user to use many CPU cores incorporating multiple nodes
- UCSB provide access and support for multiple HPC resources and educational/training/research support.

Which resources do we have?

- UCSB Center for Scientific Computing (CSC) clusters
 - Access to all UCSB staff, free and condo clusters
- Extreme Science and Engineering Discovery Environment (XSEDE)
 - Project funded by NSF. Access to national resources. Free*
- Triton Shared Computing Cluster (TSCC) at San Diego Supercomputing Center (SDSC)
 - Mostly used for education/training and class support

<http://csc.cnsi.ucsb.edu/resources>

HPC systems at CSC

Campus available cluster Knot:

- 110 node, ~1400 core system
- 4 ‘fat nodes’ (256/512 GB RAM)
- GPU nodes (12)
- Published papers should acknowledge CNSI and MRL

Request access: <http://csc.cnsi.ucsb.edu/acct>

Condo clusters:

- Lattice (62 nodes)
- Guild (60 nodes)
- Braid (60 nodes, also has GPUs)

PIs buy nodes in the clusters, CSC handles infrastructure

XSEDE

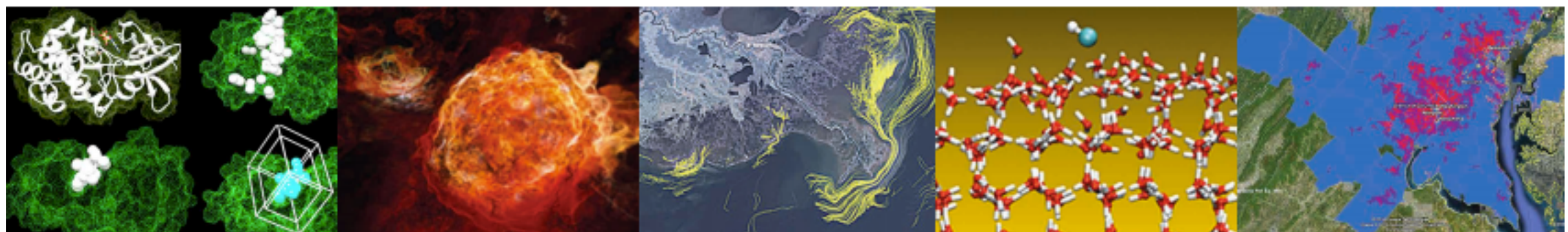
Extreme Science and Engineering
Discovery Environment

XSEDE is an NSF sponsored service organization that provides access to computing resources.

<https://portal.xsede.org>

www.xsede.org








Currently XSEDE supports more than a dozen supercomputers and high-end visualization and data analysis resources.



Summary of XSEDE systems

XSEDE Compute Resources

[Detail View](#)

Name	Status	Load	Jobs
Stampede UT Austin 	Healthy	 97%	R: 677 Q: 624 O: 186
Comet SDSC 	Healthy	 87%	R: 2327 Q: 217 O: 297
XStream Stanford U 	Healthy	 71%	R: 50 Q: 286 O: 947
SuperMIC LSU CCT 	Healthy		
Bridges Regular Memory PSC 	Healthy		
Bridges Large Memory PSC 	Healthy		
Jetstream UT Austin 	Healthy		
Gordon Compute Cluster SDSC 	Healthy	 58%	R: 179 Q: 0 O: 6
Wrangler UT Austin 	Healthy		

Top 500

General purpose
Big data

GPU

Small,
general purpose

General purpose
Big Data

Cloud (on demand)

General purpose
Big data

High I/O
data intensive

XSEDE Campus Champions Program

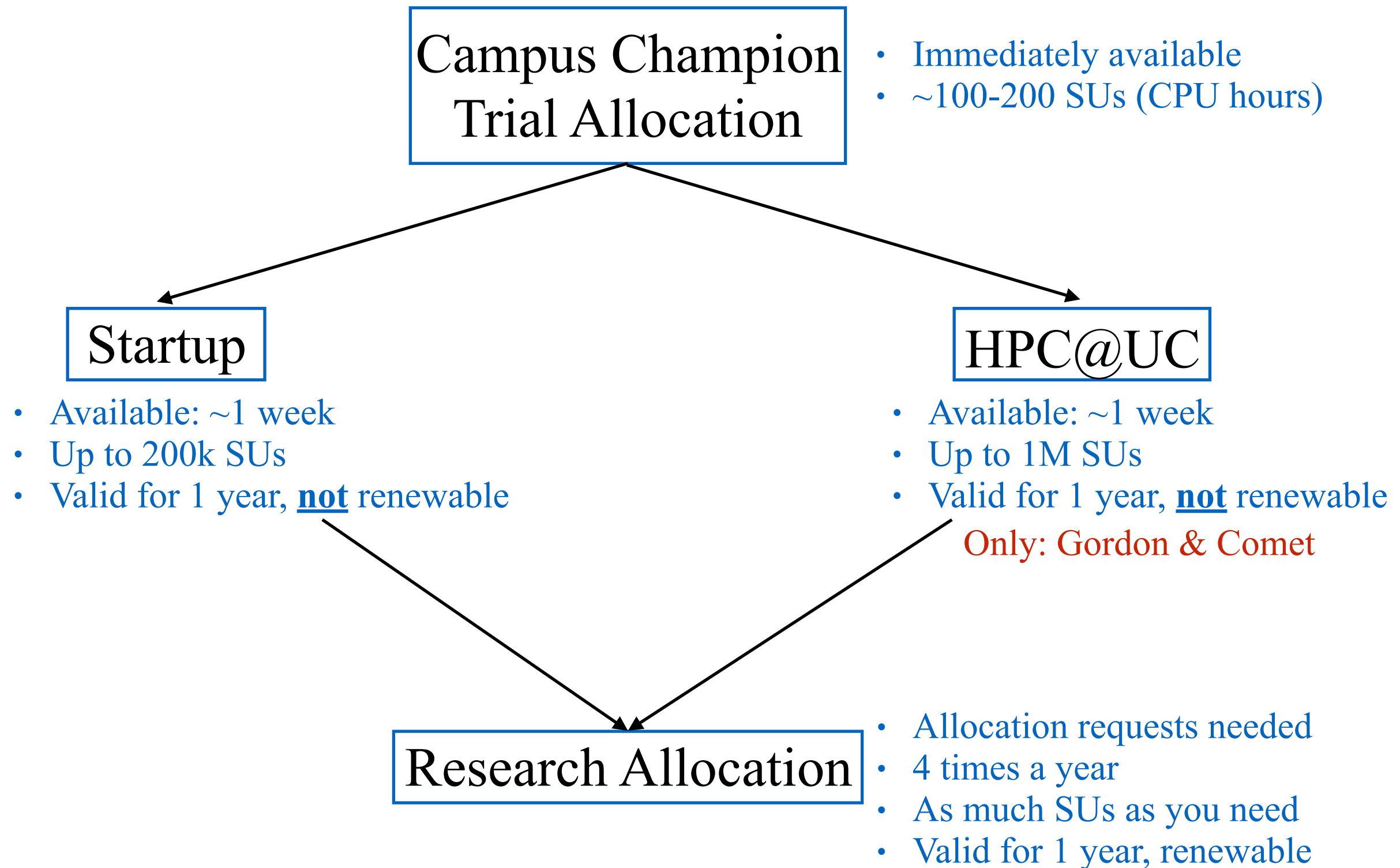
Campus Champion: Represents XSEDE on the campus

As a campus champion, I (Burak) will help you:

- Understand the capabilities of HPC and get to include it as a part of your research and educational work.
- Get access to local, regional and national resources.
- Maintenance of accounts, allocations of computing time and technical expertise.
- Connect with the broader community of HPC users in your field

How to get access?

<https://portal.xsede.org/allocations-overview>



XSEDE Portal

Get access:

- Get a username from the portal
- Send me your username
- You will get limited trial time from any resource!

On the portal you will find:

- Documentation
- Help desk
- Training sessions broadcasted from the web
- Forums

The screenshot shows the XSEDE User Portal interface. At the top, there's a header with the XSEDE logo and 'USER PORTAL' text. Below the header is a navigation bar with links: MY XSEDE, RESOURCES, DOCUMENTATION, ALLOCATIONS, TRAINING, USER FORUMS, HELP, and ECSS. Under 'MY XSEDE', there's a sub-menu with links: Summary, Allocations/Usage, Accounts, Jobs, Profile, Publications, Tickets, Change Password, and Add User. A search bar is located in the top right corner. Below the navigation bar, there's a banner for 'XSEDE USER PORTAL ON THE GO' with images of the app on a smartphone and tablet. To the left of the banner, there's a user profile section with a photo of a man and the text 'Welcome, Burak!', 'Last login: Mon 10/26/15 at 09:52:16 AM CST', and links for Profile, Allocations, Accounts, and Training. Below the profile section, there's a 'Publications' section with a 'Full List' link and a button to 'Add a Publication'. The main content area features a 'In The Past 7 Days' section with a large pie chart titled 'XD SUS Charged: Total: by Field of Science' and a smaller bar chart titled 'Number of Jobs by Field of Science'. The pie chart shows various fields of science and their corresponding charged amounts. The bar chart shows the number of jobs for different fields. At the bottom, there's a 'My XSEDE Resources' section with a table showing resource status, load, username, and my jobs. A 'System Monitor' link is also present.

XSEDE USER PORTAL
Extreme Science and Engineering Discovery Environment

Search XSEDE...

MY XSEDE | RESOURCES | DOCUMENTATION | ALLOCATIONS | TRAINING | USER FORUMS | HELP | ECSS

Summary | Allocations/Usage | Accounts | Jobs | Profile | Publications | Tickets | Change Password | Add User

Share your feedback on XSEDE Extended Collaborative Support Services with a quick 5 question survey!

Welcome, Burak!
Last login: Mon 10/26/15 at 09:52:16 AM CST

Profile | Allocations | Accounts | Training

NEW! Share your XSEDE Science Achievements

Publications: [Full List]
You have entered 3 publication(s).
Add a Publication

In The Past 7 Days

XD SUS Charged: Total: by Field of Science

Biophysics 15,496,525.0
Materials Research 12,851,897.0
Astronomical Sciences 7,212,089.0
Fluid, Particulate, and Hydraulic Systems 6,234,052.0
Molecular Biosciences 5,091,439.0
Earth Sciences 4,802,351.0
Gravitational Physics 3,786,288.0
Extragalactic Astronomy and Cosmology 4,378,987.0
Elementary Particle Physics 4,378,987.0
All 75 others 12,048,399.0

Number of Jobs by Field of Science

View Gallery

My XSEDE Resources | System Monitor

Resource	Status	Load	Username	My Jobs
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Using HPC Clusters and Basic Linux (examples on Knot)

<http://csc.cnsi.ucsb.edu/docs/getting-started>

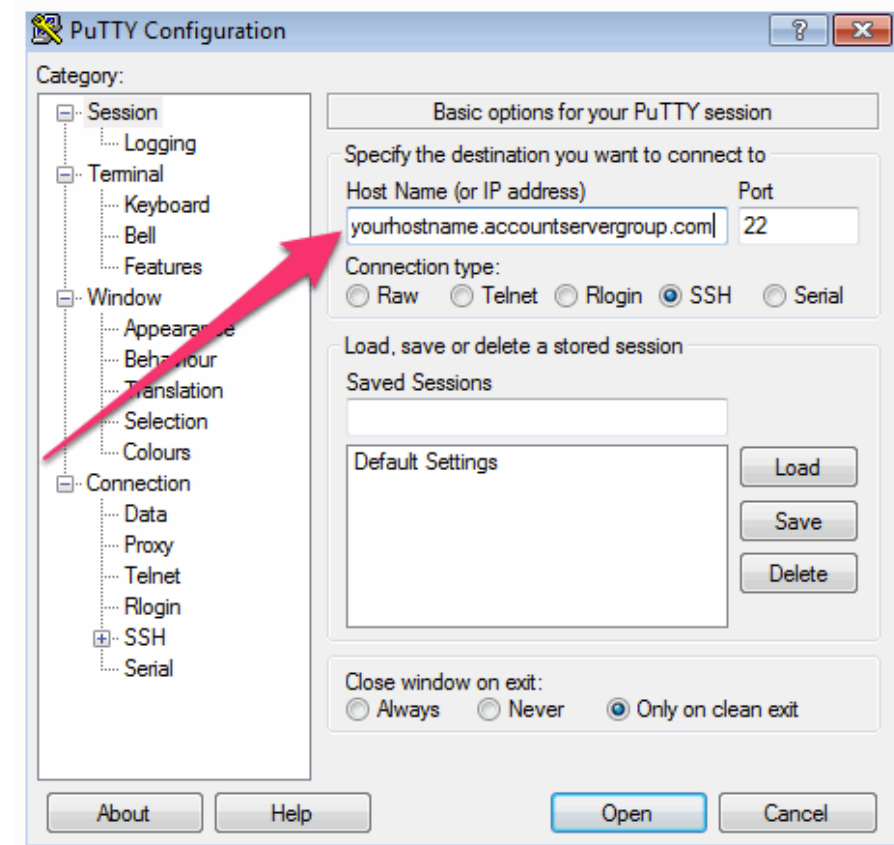
Access

For Linux and Mac, open a terminal:

```
$ ssh username@knot.cnsi.ucsb.edu
```

For Windows, you will need a client (e.g. Putty, www.putty.org)

knot.cnsi.ucsb.edu



X2go is another option (good for graphics):

<http://csc.cnsi.ucsb.edu/docs/using-x2go-windows-knot>

Remote (non UCSB) login via VPN client:

<http://www.ets.ucsb.edu/services/campus-vpn/get-connected>

File Transfer

For Linux and Mac, open a terminal, use `scp` or `rsync` commands:

E.g. Copy file.txt from your computer to your home directory on Knot

```
scp file.txt user@knot.cnsi.ucsb.edu:file_copy.txt
```

Windows users: Need a client to copy files. Usage is similar to Putty.

<https://filezilla-project.org/>

<https://winscp.net/eng/download.php>

Globus is another option (all operating systems). Preferred for large files transfers.

<http://csc.cnsi.ucsb.edu/docs/globus-online>

Running Jobs

- When you login to Knot (or any other cluster), you are on the login node
- This node is NOT for running calculations!
- All jobs must be submitted to the queue
- Submission to the queue requires a script to be written

Example job submission script (submit.job):

```
#!/bin/bash
#PBS -l nodes=2:ppn=12
#PBS -l walltime=2:00:00
#PBS -N test

cd $PBS_O_WORKDIR

mpirun -machinefile $PBS_NODEFILE -np 24 ./run.x
```

\$ qsub submit.job

<http://csc.cnsi.ucsb.edu/docs/example-scripts-running-jobs>

Running Jobs

Check status of the running jobs: `$ showq -u $USER`
 `$ qstat -u $USER`

Delete a running job: `$ qdel job_id`

More options for PBS:

https://www.olcf.ornl.gov/kb_articles/common-batch-options-to-pbs/

Available queues:

- Short queue: `$ qsub -q short submit.job`
- Large memory queues : `$ qsub -q (x)largemem submit.job`
- GPU queue: `$ qsub -q gpuq submit.job`

Extracting Information

For this example, we investigate the OUTCAR file generated from the software VASP (<http://csc.cnsi.ucsb.edu/docs/vasp-compilation>)

```
## Print direct and reciprocal lattice vectors
grep -A 3 "direct lattice vectors" OUTCAR | tail -4 > cell.info

## Print information about Forces in the unit cell
grep -A 15 "FORCE on cell" OUTCAR > force.info

## Print the calculated energy at each iteration
nIter=`grep TOTEN OUTCAR | wc -l`

for index in `seq 1 $nIter` # Grab value of energy at each iteration
do

    En=`grep TOTEN OUTCAR | head -$index | tail -1 | awk '{print $5}'`
    echo $index $En >> E_vs_iter.dat # Note the use of >> here instead of >

done
```


Example usage of Linux Commands

For this example, we investigate example.sh.

A simple shell script can be used to combine Linux commands.

The following commands are demonstrated in this script:

mkdir : <ake directory

head/tail : Display beginning/end of file

cd : Change directory

cat [file] : view file

grep [pattern] [file] : Find matching patterns in a file

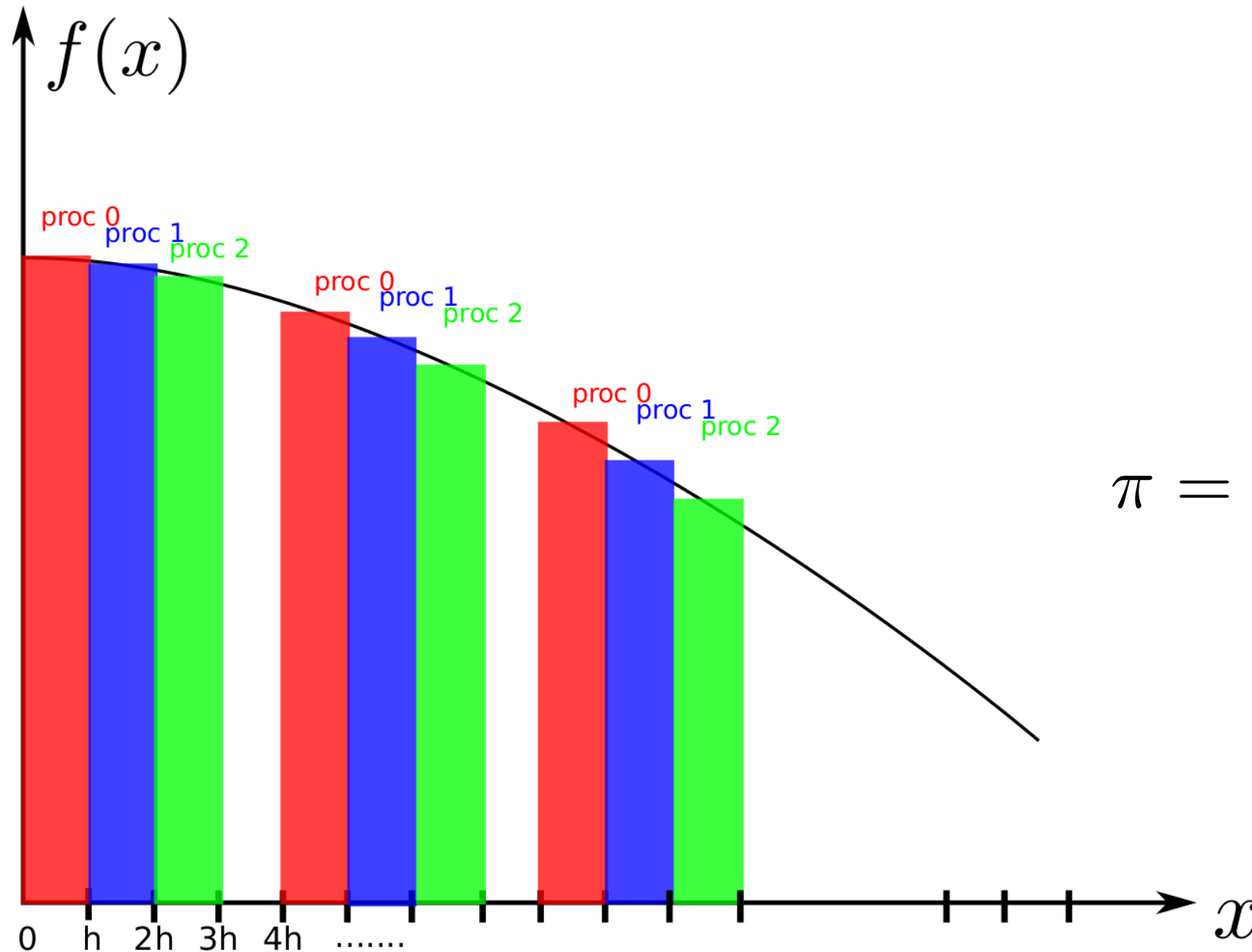
cut : Get a piece of string

| : Pipe, connecting commands

> and >> : Redirect and append

Computing Pi in parallel

For this example, look at mpi_pi.c.



$$\pi = \int_0^1 \frac{4}{1+x^2} dx$$

```
for (i=iProc+1; i <= nDivisions; i+=nProcs){  
    x = h * (i-0.5)  
    sum += f(x)  
}
```

Some Linux Commands

Some useful commands

ls [-option] : list files

mkdir : make directory

cd : change directory

man : display manual for a command

mv : mv file/folder

rm [-r] : remove file. -r to remove folders

pwd : present working directory

cat [file] : view file

less /more : view file, one screen at a time

grep [pattern] [file] : Find matching patterns in a file

Pipes and redirection

command > file : Redirect output of command to file

command >> file : Append output of command to file

command < file1 > file2 : Get input from file1, write output to file2

command1 | command2 : Join command1 & command2

Common shortcuts

* : Wildcard

~ : Home directory

. : Current directory

.. : One directory up

TAB key: Finish commands, good for typing fast

Creating/Extracting Archives

Suppose you have an archive: `package.tar.gz`

Extract: `$ tar -xzvf package.tar.gz`

Suppose you have files you want to collect together: file1, ..., file10

`$ tar czf file1 file2 .. file10 package.tar.gz`