PACE - Linux 101

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Partnership for an Advanced Computing Environment at GT September 14, 2022

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Outline

- High performance computing at Georgia Tech
- What is Linux and why use it?
- What is bash?
- Using the command line basic commands, help, and editing files
- Environment variables
- Scripting and command automation
- Session customization
- Useful material
- Movement/Screen break after ~1h



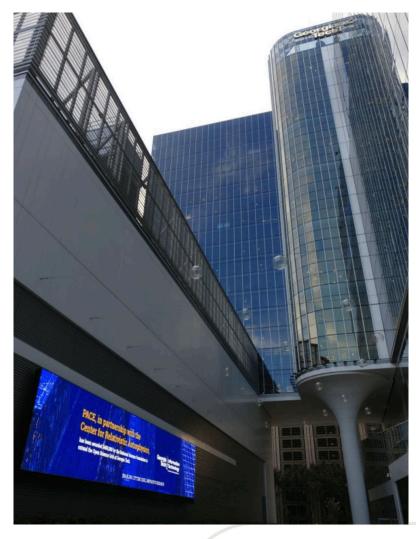
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- PACE provides faculty participants sustainable leading-edge advanced research computing resources with technical support services, infrastructure, software, and more.
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- PACE is a service which operates as a Cost Center.
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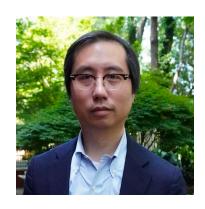
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PACE-RCF

Meet the Research Computing Facilitation team! We interact with the advanced computing research community at Georgia Tech, respond to a wide range of requests submitted by faculty & student researchers.











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"HPC brings you to an amazing parallel universe!" Michael D. Weiner, PhD Research Computing Facilitator

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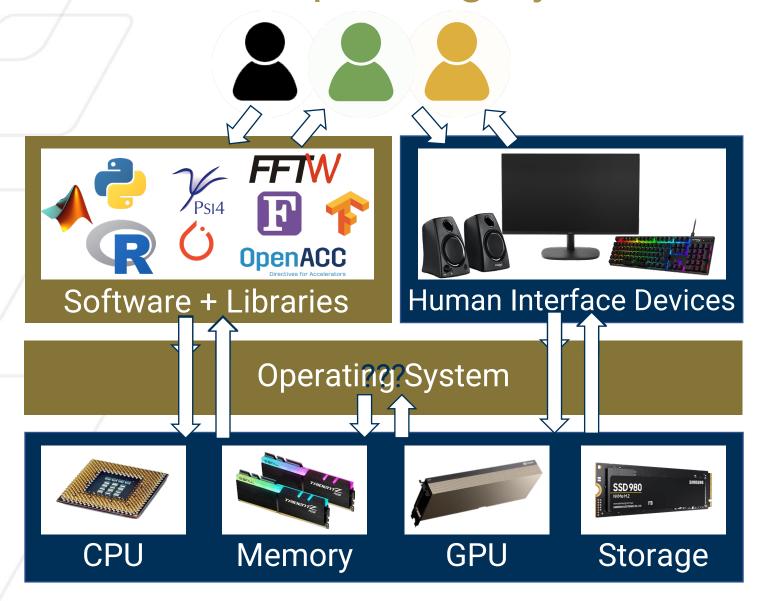
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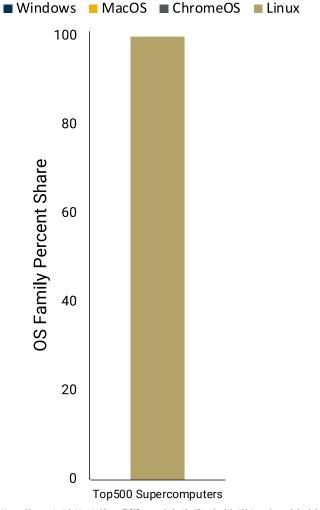
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"I like to refine business and enhance PACE customer experience.
Always ready to play chess, too!"



What is an Operating System?



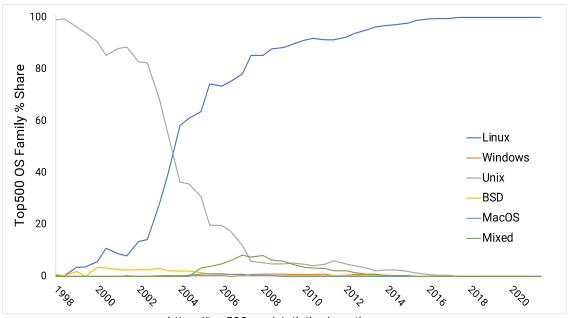


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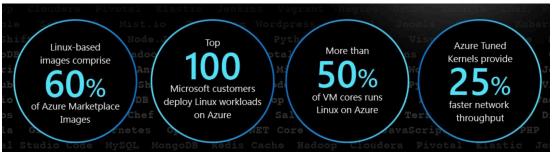


Why use Linux?

- It is free and open source
 - Exceptions for enterprise systems, but that's a choice
 - With a little know-how, you can customize everything!
- It is efficient
 - Better background process management
 - · Less "nannying"
 - Faster filesystem (although you probably won't notice)
- It is reliable
 - Reboots not required!
 - Easy access to system services



https://top500.org/statistics/overtime



https://www.linkedin.com/posts/adirron_linuxonazure-progress-activity-6665502370795003905-DY1G



How do I "use Linux"?

- Install it!
 - Distros like Ubuntu, Fedora, and openSUSE are free
 - On Windows, try out the Windows Subsystem for Linux (WSL)
- Try a browser-based emulator!
 - https://bellard.org/jslinux/
 - https://cocalc.com/features/terminal
 - https://distrotest.net/index.php
- Access a remote cluster (like those managed by PACE)!
 - OpenSSH available by default on most OSs (including Windows 10 > 18.03)
 - 3rd Party apps like PuTTY, MobaXterm, XSHELL, etc.



Using OpenSSH

- OpenSSH is a suite of secure networking tools built on the SSH protocol, and includes:
 - ssh: the remote login client
 - scp: a utility to securely copy files between a local and a remote host, or between two remote hosts
 - sftp: another secure file transfer utility based on FTP, so it can also do things like list files
 - ssh-keygen: a utility to inspect/generate keys for user and host authentication
 - On clusters like those managed by PACE, keys are generated that allow your jobs to run across multiple servers with tools like MPI
 - ssh-copy-id: gathers available keys and uses ssh to make them available for authentication on the remote host



Using SSH to Access PACE-ICE

- To login to a remote cluster like PACE-ICE, use ssh
 - Command looks like ssh <username>@<remote_host>
 - For PACE systems, use your GT username
 - PACE-ICE login hostname is 'pace-ice.pace.gatech.edu'
 - When prompted, enter your GT password (you won't see anything as you type)
 - Congratulations! You're logged in to the cluster
 - You will need to be on VPN
- If you plan on using graphical applications, you'll want to enable X11 forwarding
 - You'll need an X11 client (Xming or VcXsrv on Windows, Xquartz on MacOS)
 - Modify the above by including '-X': ssh -X <username>@<remote_host>



Using Open OnDemand to Access PACE -ICE

- You need to be connected to Georgia Tech's VPN to access the resources
 - Browser-based VPN, see https://vpn.gatech.edu/global-protect/login.esp
 - GlobalProtect client (newer option, recommended) For information about VPN access, see http://docs.pace.gatech.edu/gettingStarted/vpn/
- Navigate to: <u>https://ondemand-pace-ice.pace.gatech.edu</u> and login with your GT credentials



Using Open OnDemand to Access PACE -ICE

 Start an interactive shell session by clicking 'Clusters' and selecting '>_PACE-ICE Shell Access'



Terms of Use

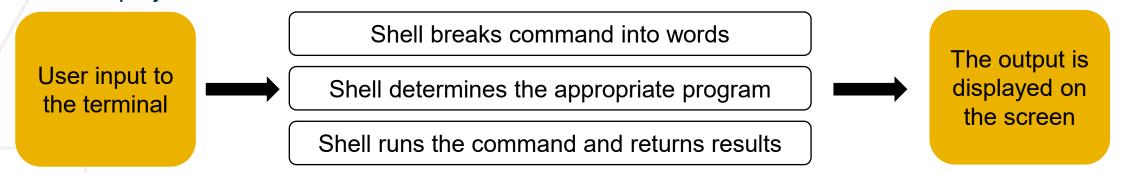
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By using this system, I acknowledge and consent to these terms.



What is a Shell...and What is Bash?

- The Bourne-Again SHell is the command language interpreter for most Linux distributions
 - Reads input from the user
 - Interprets the input into instructions, separating words according to the internal field separator, \$IFS (defaults to <space><tab><newline>)
 - Executes commands, interactively or non-interactively and synchronously or asynchronously
 - Displays the results for the user in a readable format



- Contains a large number of built-in commands
 - These would be impossible or inconvenient to obtain separately
 - Generally these should not (or cannot!) be implemented in other applications
- Can be customized with functions and aliases for ease of use



Command Line Keyboard Shortcuts

- Tab: Attempts to complete a command
- Ctrl+A: move cursor to the beginning of the command line
- Ctrl+E: move cursor to the end of the command line
- Ctrl+K: delete all characters after the cursor
- Ctrl+U: delete all characters before the cursor
- Ctrl+W: delete the word before the cursor
- Ctrl+L: clear this terminal (equivalent to typing clear)
- Ctrl+C: end a running program and return to the prompt
- Ctrl+D: log out of the current shell session (equivalent to typing exit or logout)
- Ctrl+Z: suspend a program



Bash Commands for Exploring Directories

pwd shows you the path of the current working directory

```
[gburdell3@login-pace ~]$ pwd
/storage/home/hpace1/gburdell3
```

1s shows the contents of the current directory

```
[gburdell3@login-pace ~]$ ls
dir1 file1 file2 p-gburdell3-0 scratch
```

- The color option is enabled with --color=auto (automatic on PACE):
 - White = file, blue = directory, green = executable, red* = archive file, cyan = symbolic link (references another file/directory)
 - Red with black background is broken link (black terminal = background always black!)
- Use the option −a to show all files (including hidden)



Bash Commands for Navigation

cd changes the working directory to the target directory

```
[gburdell3@login-pace ~] $ pwd
/storage/home/hpace1/gburdell3

[gburdell3@login-pace ~] $ cd p-gburdell3-0/

[gburdell3@login-pace p-gburdell3-0] $ pwd
/storage/home/hpace1/gburdell3/p-gburdell3-0
```

- If no target directory is provided to cd, it will return you to your home (~/)
- Each directory contains two special paths, . and . .
 - points to the current directory
 - . . points to the current directory's parent (one level up)

```
[gburdell3@login-pace p-gburdell3-0]$ cd ..
[gburdell3@login-pace ~]$ pwd
/storage/home/hpace1/gburdell3
```



Bash Commands for Exploring Directories (cont'd)

• Use the -1 option to show the long listing format

- Use chmod to change the permissions for files and directories
 - User, Group, Other: the order in which permissions are applied
 - 644 = user can read+write, group+other can read = -rw-r-r--
 - 755 = user can read+write+execute, group+other can read+execute = -rwxr-xr-x
 - 4 (read), 2 (write), 1 (execute); multiple permissions granted by summing
 - 6 = read+write, 5 = read+execute, 7 = read+write+execute

Bash Commands for Files

- touch can be used to create new, empty files
- mkdir can be used to create new, empty directories

```
[gburdell3@login-pace ~]$ ls
dir1 file1 file2 p-gburdell3-0 scratch
[gburdell3@login-pace ~]$ touch new_file && mkdir new_dir
[gburdell3@login-pace ~]$ ls
dir1 file1 file2 new_dir new_file p-gburdell3-0 scratch
```

file can be used to see what a file "is"

```
[gburdell3@login-pace ~]$ file p-gburdell3-0
p-gburdell3-0: symbolic link to `/storage/coda1/project/0/gburdell3/'
[gburdell3@login-pace ~]$ file file1
file1: ASCII text
Geo
```

How Do I Edit Files from the Terminal?

- Nano's ANOther editor, "An enhanced free Pico clone"
 - Small, free, and friendly editor
 - Simple in features = easier to use
 - Commands are displayed on screen for easy reference
- Vi IMproved, "A Programmer's Text Editor"
 - Operates in two modes "insert" and "command line"
 - In "insert" mode, -- INSERT -- is displayed at the bottom of the terminal
 - A thorough tutorial can be accessed via vimtutor
- Editor MACros, "The extensible, customizable, self-documenting real-time display editor"
 - Can write in many languages (human and programming), as well as compile, run, and test programs
 - Commands involve the <u>CONTROL</u> (Ctrl) and <u>META</u> (Esc) keys
 - A thorough tutorial can accessed by starting emacs and typing C-h t



mv is used to modify a file's path (including renaming)

```
[gburdell3@login-pace ~] $ ls
dir1 file1 file2 new_dir new_file p-gburdell3-0 scratch
[gburdell3@login-pace ~] * mv new_file renamed_file
[gburdell3@login-pace ~] $ ls
dir1 file1 file2 new_dir renamed_file p-gburdell3-0 scratch
[gburdell3@login-pace ~] * mv renamed_file new_dir/
[gburdell3@login-pace ~] $ mv file1 new_dir/moved_and_renamed
[gburdell3@login-pace ~] $ ls
dir1 file2 new_dir p-gburdell3-0 scratch
[gburdell3@login-pace ~] $ ls new_dir
moved_and_renamed renamed_file
```



• cp is used to copy files (to copy directories, you'll need to use -r)

```
[gburdell3@login-pace ~] $ ls
dir1 file2 new_dir p-gburdell3-0 scratch
[gburdell3@login-pace ~] $ cp file2 new_dir
[gburdell3@login-pace ~] $ cp new_dir/renamed_file .
[gburdell3@login-pace ~] $ cp renamed_file new_dir/copied_and_renamed
[gburdell3@login-pace ~] $ cp -r new_dir copied_dir
[gburdell3@login-pace ~] $ cp -r new_dir copied_dir/copied_again
[gburdell3@login-pace ~] $ ls
copied_dir dir1 file2 new_dir p-gburdell3-0 renamed_file scratch
[gburdell3@login-pace ~] $ ls new_dir
copied_again file2
                                      renamed file
copied_and_renamed moved_and_renamed
```

• rm is used to delete files (to copy directories, you'll need to use -r)

```
[gburdell3@login-pace ~] $ ls
copied_dir dir1 file2 new_dir p-gburdell3-0 renamed_file scratch
[gburdell3@login-pace ~] $ rm file2
[gburdell3@login-pace ~] $ rm new_dir/renamed_file
[gburdell3@login-pace ~] $ rm copied_dir
rm: copied_dir/: is a directory
[gburdell3@login-pace ~] $ rm -r copied_dir
[gburdell3@login-pace ~] $ ls
dir1 new_dir p-gburdell3-0 renamed_file scratch
[gburdell3@login-pace ~]$ ls new_dir
copied_again copied_and_renamed file2 moved_and_renamed
```

The -f option can be used to force remove (and ignore errors)



cat can be used to view unformatted file content

[gburdell3@login-pace ~]\$ cat somefile THE STORY OF THE THREE LITTLE PIGS.

Once upon a time there was an old sow with three little pigs, and as she had not enough to keep them, she sent them out to seek their fortune. The first that went off met a man with a bundle of straw, and said to him, "Please, man, give me that straw to build me a house; " which the man did, and the little pig built a house with it. Presently came along a wolf, and knocked at the door, and said, -



- For longer files, cat can be problematic as it prints out the whole file
- head shows content from the beginning of the file
 - Default is first 10 lines, but can use -n < int > to specify another number

```
[gburdell3@login-pace ~] $ head -n3 somefile THE STORY OF THE THREE LITTLE PIGS.
```

Once upon a time there was an old sow

- Similarly, tail shows lines from the end of the file
 - Default is also 10, and -n < int > is still allowed

```
[gburdell3@login-pace \sim]$ tail -n2 somefile him for supper, and lived happy ever afterwards.
```



- Another option is less, which displays one page at a time
 - You can scroll with the up/down arrows, use f/b to advance/backtrack a
 whole page, search forward/backward with //?, and exit with q
 - The: means you can scroll further until it changes to (END)

[gburdell3@login-pace ~]\$ less somefile THE STORY OF THE THREE LITTLE PIGS.

Once upon a time there was an old sow with three little pigs, and as she had not enough to keep them, she sent them out to seek their fortune. The first that went off met a man with a bundle of straw, and said:



grep is used to search for patterns (regex) within files

```
[gburdell3@login-pace ~]$ grep pigs somefile with three little pigs, and as she had not he did to the other little pigs, and said, -
```

• The -i option is used to ignore case

```
[gburdell3@login-pace ~]$ grep -i pigs somefile THE STORY OF THE THREE LITTLE PIGS. with three little pigs, and as she had not he did to the other little pigs, and said, -
```



Bash Filename Expansions (Globbing Patterns)

- Sometimes, you may want to operate on multiple files simultaneously
 - If there are many files, it can be convenient to describe the filenames using a pattern
 - ? can be used to represent any single character
 - * can be used to represent any number of character (including 0)
 - [] can be used to specify a list of allowed values or a range (in arguments)
 - [^] logical NOT to exclude characters
 - { } can be used to specify patterns using parameter expansion
 - \ escape character, used to protect a subsequent special character

```
[gburdell3@login-pace ~]$ ls * #lists all files in directory

[gburdell3@login-pace ~]$ rm file[124-6] #deletes file1, file2,

file4, file5, and file6

[gburdell3@login-pace ~]$ cat file1? #reads file10-file19
```

Learning More about Command -line Tools

- With so many commands, it can be helpful to get help on the terminal
 - Three main tools: man, info, and -h/--help options

[gburdell3@login-pace ~] \$ man rm

• Manual page: description, available options/arguments, associated shell variables, related man pages, author/copyright information)

```
Forward (backward) one line: e, 4, \( \text{(y, \( \))}\) Forward (backward) one window: f, z (b, w) Search forward (backward): /<pattern> (?<pattern>) End of manual: Shift+g Exit: q
```

[gburdell3@login-pace ~] \$ info gcc

• GNU project documentation: hypertext with links, very detailed (like a digital book with chapters; may open man page if no info manual exists)

```
Forward (backward) one line: \( (\frac{1}{1} \)) Forward (backward) one page: n, ] (p, [ ) Search: Ctrl+s Cycle through links: Tab Go to Main home: d Go to Topic Home: t Follow link: Enter Exit: q
```

[gburdell3@login-pace ~] \$ tar --help

• CLI tool help: documents some of the built-in commands and keywords of the shell (think of it as a cheat sheet – neat and succinct)



Environment Variables

- Environment variables are named objects that contain data used by one or more applications
 - Each environment variable has a name and a value
 - The name is case sensitive, and can include any character except = and NUL
 - The value can provide several key pieces of information
 - The location of all executable files in the file system
 - The default text editor or compiler that should be used
 - The system locale settings (language, country, character encoding, etc.)
- printenv lists the environment variables defined for the current session
- Some important environment variables:
 - HOME
 - HOSTNAME
 - USER
 - SHELL
 - PATH
 - LD_LIBRARY_PATH/LIBRARY_PATH

- PBS_O_WORKDIR
- PBS_NODEFILE
- PBS GPUFILE
- PBS_JOBID
- PBS_ARRAYID
- PBS_JOBNAME



Working with Environment Variables

- The shell uses \$ to de-reference environment variables, e.g. echo \$PATH
- Environment variable values can be changed a few ways:
 - Assignment (VARIABLE="NEWVALUE") good for local variables
 - Prepend (VARIABLE="NEWVALUE: \$VARIABLE") good if you need to point to a custom application instead of the default
 - Append (VARIABLE="\$VARIABLE: NEWVALUE") for when you just need to point to a new, unique location
- By default, all user defined variables are local they won't be visible to child processes (processes started by the shell)
 - Use export to make the variable available to all processes run from that shell
 - Amendments to an already global variable will already be exported
 - If you want the variable to persist from session to session, define and export it in your ~/.bash_profile file (discussed shortly)



...and How Software Modules Work

- An abundance of software is available, pre-compiled and configured for use on PACE clusters
 - Software environment, version all set no need to edit PATH, LD_LIBRARY_PATH, etc.
- Modules are used to set everything up
 - module avail
 lists all available modules
 - module list displays all currently loaded modules
 - module load <target> loads target module to the environment

TIP! ml can be used in place of module list AND module load <target>

- module rm <target> removes target module from the environment
- module purge removes all loaded
- module show displays the variables set by the module
- Default modules can be loaded per job in the PBS script or loaded manually on the command line



Automation with Shell Scripts

- A shell script is a text file containing shell commands that can be run in the shell non-interactively
 - Any command from the command line can be used in a bash script
- There are many benefits to implementing commands in a script
 - Task automation: write it once, use it many times
 - Consolidation: combine multiple steps into one command
 - Portable: the shell commands are the same in Bash, no matter the OS
 - · Repeatability: you can look back over the file to see what you did

NOTE: By default, files will be created with 644 permissions (-rw-r--r--); to execute a shell script by typing ./myscript.sh, change permissions to 755 to allow for execution (-rwxr-xr-x)



Developing Shell Scripts

- The first line of a script begins with #!, followed by the designated interpreter
 - Bash shell scripts start with #!/usr/bin/bash
- Any normal commands can be included as lines in the script
 - Commands can be separated by &&, ;, or a new line
- Conditional execution:

```
if <condition>; then <command>; else <command>; fi
```

• For loops:

```
for <variable> in <array>; do <command>; done
OR
```

```
for ((expr1;expr2;expr3)); do <command>; done
```

• While loops:

```
while <condition>; do <command>; done
```



Developing Shell Scripts (cont'd)

- Arguments can be passed to a Bash script:
 - If the number of arguments is fixed, use the positional variables \$1, \$2, \$3, ...
 echo \$1 \$2 \$3 #prints out the 1st, 2nd, and 3rd arguments passed via CLI
 - If the number of arguments is variable, use \$@ (which represents an array of all arguments passed to the script) and \$# (which represents the number of arguments passed to the script)

```
for ARGS in $0; do echo $ARGS; done
```

• Functions can be defined to minimize repetition (declaration is optional):

```
function my_function() {
    #insert code here
}

or

my_other_function() {
    #insert code here
}
```

• Variables can be defined (myvar="value") and read (echo \$myvar)



Passing Notes with I/O Redirects

- There are three standard streams in Linux:
 - stdin (0): carries data from a user to a program
 - stdout (1): writes data generated by a program, default to the terminal
 - stderr (2): writes errors generated by a program, defaults to the terminal
- Streams can be redirected to/from existing files, or to a new file
 - 1>filename: stdout data overwrites filename
 - 1>>filename: stdout data appends filename
 - 2>filename: stderr data overwrites filename
 - 2>>filename: stderr data appends filename
 - O<filename: stdin data is read from filename
- Streams can also be redirected to chain commands
 - command1 | command2: stdout data from command1 is fed to command2



Shell Customization: ~/.bash_profile

- The personal initialization file, executed for login shells
- Two main purposes:
 - Gets any aliases and functions from ~/ .bashrc, if it exists
 - Sets user specific environment and startup programs
- If you install Tier3 software and need to set your PATH, LD_LIBRARY_PATH, etc., this is the place to do it
- If your custom application needs to reference a shell script before running, this is the place to point to it
- To implement changes, log out and then log in, or type source ~/.bash_profile



Shell Customization: ~/.bashrc

- The personal initialization file, executed for non-interactive login shells
- Two main purposes:
 - Get any globally defined aliases and functions
 - Define any user specific aliases and functions
- Example 1: Define a function that creates and moves into a new directory

```
mcd () {
    mkdir -p $1
    cd $1
}
```

 Example 2: Define an alias that will run qstat to detail current jobs for only the current user

```
alias qme='qstat -tn1u $USER'
```



Shell Customization: ~/.bash_logout

- The personal initialization file, executed when login shells exit
- One main purposes:
 - Keep the Bash environment tidy for each time you login
- Clean up temporary files here:
 - You can simply tell it to rm any unwanted files
 - Or you can automate file compression for archiving with tar
 - Or you can copy them to remote storage for backup
- If you want to terminate all processes that you are currently running
- You can also add a line to give yourself a friendly message upon exit: echo Have a wonderful day!



One Last Thing...

https://b.gatech.edu/2TceuOq



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Always ready to play chess, too!"



External References

General Linux

- Wikibooks Guide to Linux: https://en.wikibooks.org/wiki/Linux_Guide
- Siever, Ellen. *Linux in a Nutshell*. O'Reilly Media, Inc. (2009)
- Welsh, Matt and Dalheimer, Matthias. Running Linux. O'Reilly Media, Inc. (2006)

Shells

- Linux Command: http://www.linuxcommand.org
- Explain shell: https://explainshell.com
- Kochan, Stephen G. and Wood, Patrick. *Unix Shell Programming*. O'Reilly Media, Inc. (2003)
- Newham, Cameron. Learning the Bash Shell. O'Reilly Media, Inc. (2005)
- Quigley, Ellie and Hawkins, Scott. The Complete Linux Shell Programming Training Course. Prentice Hall PTR (2000)

Text Editors

- Nano Cheat Sheet: https://www.nano-editor.org/dist/latest/cheatsheet.html
- Vim Cheat Sheet: https://vim.rtorr.com
- Emacs Reference Card: https://www.gnu.org/software/emacs/refcards/pdf/refcard.pdf



Command Cheatsheet

- pwd show current working direcory
- cd change directory
- 1s list contents of \$pwd
- chmod <permissions> <filename> change permissions (755 or u+x format) of filename
- mkdir <dirname> make new empty directory
- touch <filename> make new empty file
- cat <filename> print out file contents
- head -n X <filename> print first X lines
- tail -n X <filename> print last X lines
- less <filename> read file in 'less' reader
- grep <pattern> <filename> search for <pattern> inside <filename>
- Help commands:
 - man <command>
 - info <command>
 - <command> --help [or <command> -h]
- File Editors:
 - nano <filename>
 - vim <filename>
 - emacs <filename>

