

Managing Your HPC Software Environment

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Comet to Expanse Transition Tutorial
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XSEDE Code of Conduct

This external code of conduct for XSEDE-sponsored events represents XSEDE's commitment to providing an inclusive and harassment-free environment in all interactions regardless of race, age, ethnicity, national origin, language, gender, gender identity, sexual orientation, disability, physical appearance, political views, military service, health status, or religion. The code of conduct below extends to all XSEDE-sponsored events, services, and interactions.

XSEDE is committed to providing an inclusive and harassment-free environment in all interactions regardless of race, age, ethnicity, national origin, language, gender, gender identity, sexual orientation, disability, physical appearance, political views, military service, health status, or religion. This commitment extends to all XSEDE-sponsored events and services (in-person training, webinars, committee meetings, networking functions, online forums, chat rooms, and social media) and any interaction including staff-to-participant, participant-to-participant, and participant-to-staff. Participants are all individuals who are not XSEDE staff who attend and participate including but not limited to administrators, faculty, students, volunteers, and research computing professionals. As a project that aims to share ideas and freedom of thought and expression, it is essential that the interaction between participants, users of XSEDE services, and XSEDE staff take place in an environment that respects the inherent worth of everyone, including respect for all. The XSEDE project is committed to providing a harassment-free environment for all participants in all of its activities. Harassment is any form of behavior intended to exclude, intimidate, or cause discomfort. Harassment includes, but is not limited to, the use of abusive or degrading language, intimidation, stalking, harassing photography or recording, inappropriate physical contact, and unwelcome sexual attention. All XSEDE users, participants, and staff are governed by local laws and their organization's code of conduct and policies.

Anyone who experiences, observes, or has knowledge of threatening behavior are expected to immediately report the incident to a member of the event organizing committee, XSEDE staff, or one of the XSEDE Ombudspersons listed below, or by using the [online form](#). XSEDE reserves the right to take appropriate action.

XSEDE ombudspersons:

- Linda Aki, Southeastern Universities Research Association (aki@urus.org)
- Lizzanne Destefano, Georgia Tech (lizanne.destefano@oiamc.gatech.edu)
- Ken Hackworth, Pittsburgh Supercomputing Center (hackworth@psc.edu)
- Bryan Snead, Texas Advanced Computing Center (bryan@tacc.utexas.edu)

Key Points

- XSEDE provides an inclusive and harassment-free environment
- Code of conduct applies to all XSEDE-sponsored events and services

Related Links

[Anonymous Reporting Form](#)

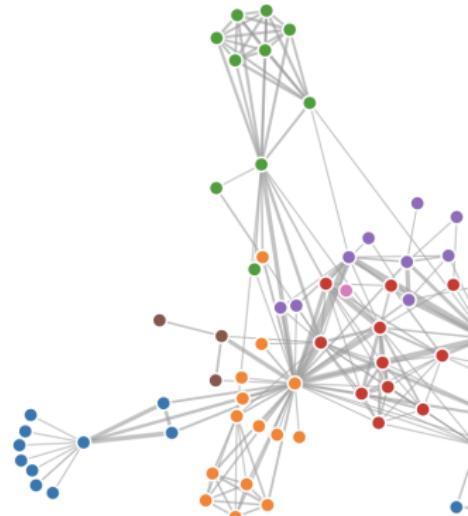
Contact Information

[Linda Aki](#)

<https://www.xsede.org/codeofconduct>

Today

- ▶ What is a software environment?
- ▶ What tools may be used to create a custom software environment?
- ▶ What are some the best practices for constructing a software environment?
- ▶ How can you configure your own software environment to get your research done?



Upcoming Events

The screenshot shows a web browser window for the SDSC (San Diego Supercomputer Center) website. The URL in the address bar is https://www.sdsc.edu/education_and_training. The page title is "Education and Training".

The main content area features several sections:

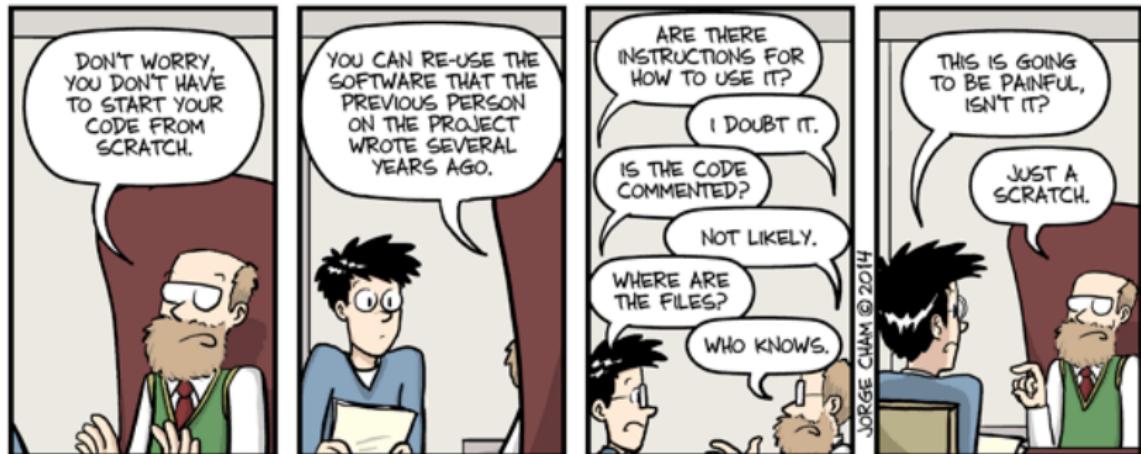
- Camps & Workshops:** An image showing people working at laptops in a classroom setting.
- Professional Development:** A list of workshops:
 - > Internet Data Analysis Workshops
 - > SDSC Annual Summer Institute
 - > XSEDE HPC Workshops
- Courses & Degree Programs:** An image showing several computer monitors displaying data visualizations.
- Text:** "Build a career in High-Performance and Data-Intensive computing through SDSC-related courses, certificates and degree programs."
 - > Big Data Specialization
 - > Data Science MicroMasters

On the right side of the page, there are sidebar sections:

- Contact Us:** Education Contact eot@sdsc.edu, Industry Partners ipp@sdsc.edu.
- Events:** [View upcoming events](#)

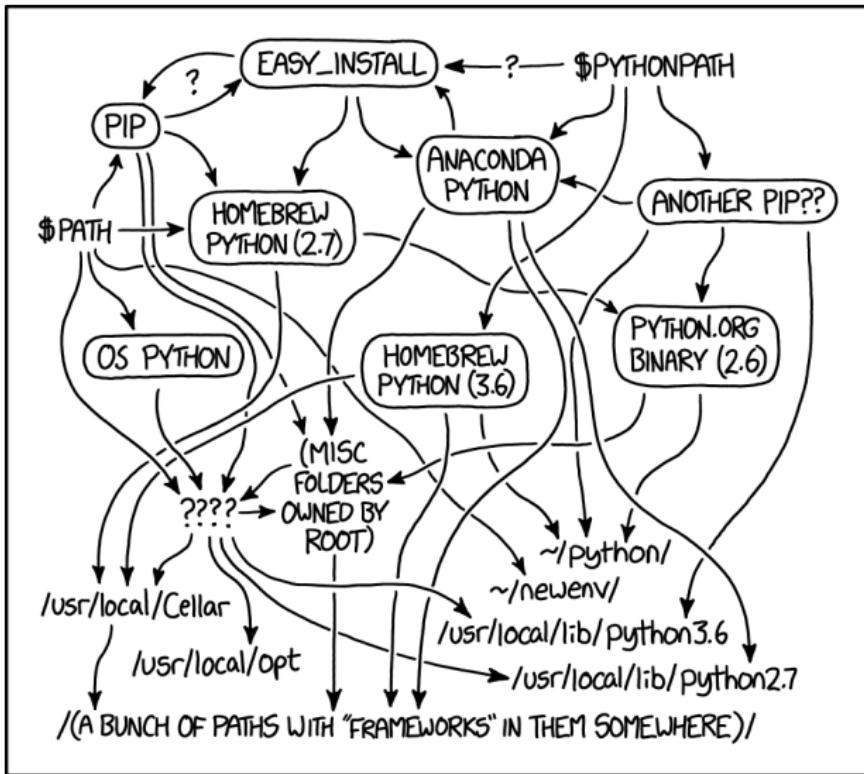
https://www.sdsc.edu/education_and_training

How It Started



WWW.PHDCOMICS.COM

How It's Going



MY PYTHON ENVIRONMENT HAS BECOME SO DEGRADED
THAT MY LAPTOP HAS BEEN DECLARED A SUPERFUND SITE.

Monty Python

What is a Software Environment?

- ▶ A software environment is the ecosystem of software packages and libraries that you depend on to run your application(s).
- ▶ The software environment for most applications usually includes software packages and libraries from the operating system, software development tools like a compiler and build system, and application- and hardware-specific software libraries.
- ▶ Software environments are (generally) unique to each system, but they can be modified to support the application(s) you want to deploy and run for your work.

Your Software Environment in a NutSHELL



A screenshot of a terminal window titled "mkandes — mkandes@login01:~ — ssh mkandes@login.expanse.sdsc.edu — 80x24". The window contains the following text:

```
[mkandes@login01 ~]$ echo "What's a ${SHELL}?"  
What's a /bin/bash?  
[mkandes@login01 ~]$
```

What is a Shell?

- ▶ A shell is a program that provides the traditional, text-only user interface for Linux and other Unix-like operating systems. Its primary function is to read in commands provided by a user, process those commands, and then executes them on the computer being run by the operating system.
- ▶ A shell is the fundamental interface between a user and a computer's operating system, which allows the user to interact with the computer and its operating system, while hiding all of the underlying details.
- ▶ A user is running a shell whenever they log into a system with their username and password.

Common Linux Shells

- ▶ sh: the original Unix shell
- ▶ bash: a Linux shell written by the GNU Project; default shell program for many of the most popular Linux distributions
- ▶ csh/tcsh: a Linux shell modeled after C programming language.

* If you would like your default shell on Expanse to be something other than bash, then please contact us via the ticketing system with a change request.

Shell Builtins

```
[mkandes@login01 ~]$ help cd
cd: cd [-L|[-P [-e]] [-@]] [dir]
      Change the shell working directory.

      Change the current directory to DIR.  The default DIR is the value of the
      HOME shell variable.

      The variable CDPATH defines the search path for the directory containing
      DIR.  Alternative directory names in CDPATH are separated by a colon (:).
      A null directory name is the same as the current directory.  If DIR begins
      with a slash (/), then CDPATH is not used.

      If the directory is not found, and the shell option `cdable_vars' is set,
      the word is assumed to be a variable name.  If that variable has a value,
      its value is used for DIR.

      Options:
      -L      force symbolic links to be followed: resolve symbolic
             links in DIR after processing instances of `..'
      -P      use the physical directory structure without following
             symbolic links: resolve symbolic links in DIR before
             processing instances of `..'
      -e      if the -P option is supplied, and the current working
             directory cannot be determined successfully, exit with
```

A shell builtin is a command or function that is executed directly in the shell itself, instead of an external executable program which the shell would load and execute.

Shell Sessions



A shell session is a running instance of a shell program.

Shell Variables

- ▶ A shell variable is a character string to which a value may be assigned a value.
- ▶ The value assigned to a shell variable could be a number, text, filename, device, or any other type of data.
- ▶ Most importantly, a shell variable is available only to the shell session in which it was defined and it is not inherited by child processes spawned by the shell.
- ▶ Shell variables are typically used to store temporary data local to a particular shell that may change frequently.

Environment Variables

- ▶ Environment variables are shell variables that have been exported to the shell's *environment* such that they may be inherited by any child processes spawned by the shell.
- ▶ Environment variables are used to define how a shell responds to user commands and how those commands are run when executed.
- ▶ Environment variables are typically used to store data that needs to be more persistent and utilized by other commands and processes run by the shell.

The PATH Environment Variable

- ▶ PATH is an environmental variable in Linux and other Unix-like operating systems that tells the shell which directories to search for executable files in response to commands issued by a user.
- ▶ PATH consists of a series of colon-separated absolute paths. Whenever a user enters a command at the command line prompt that is not a shell builtin or does not include its absolute path, the shell then searches through the PATH directories until it either finds an executable file with that name or it does not.

The LD_LIBRARY_PATH Environment Variable

- ▶ LD_LIBRARY_PATH is an environmental variable which sets the path in which the linker search while linking dynamic, shared libraries.
- ▶ LD_LIBRARY_PATH contains a colon separated list of absolute paths the linker uses to prioritize its search over the standard library paths /lib and /usr/lib. The standard paths will still be searched, but only after the list of paths in LD_LIBRARY_PATH has been exhausted.
- ▶ The best way to use LD_LIBRARY_PATH is to set it on the command line or script immediately before executing the program. This way the new LD_LIBRARY_PATH is isolated from the rest of your system.

Environment Modules



The Environment Modules system is a tool to help users manage their Unix or Linux shell environment, by allowing groups of related environment-variable settings to be made or removed dynamically.

<http://modules.sourceforge.net>

Common module commands

- ▶ module list
- ▶ module avail <package>
- ▶ module purge
- ▶ module load <package>
- ▶ module unload <package>
- ▶ module show <package>
- ▶ module spider <package>

Lmod: A New Environment Module System



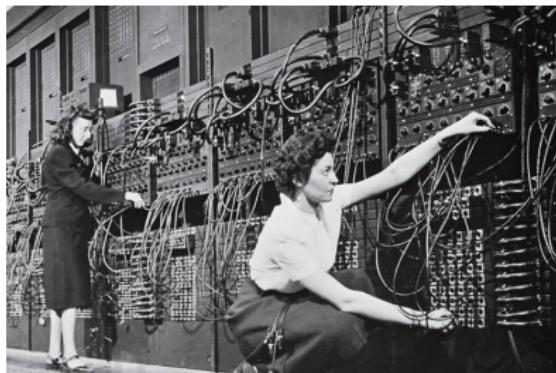
Lmod is a Lua-based environment module system that easily handles the MODULEPATH hierarchy problem. It provides a convenient way to dynamically change the users' environment through modulefiles. This includes easily adding or removing directories to the PATH and LD_LIBRARY_PATH variables.

<https://lmod.readthedocs.io>

What is Software Deployment?

- ▶ Software deployment is the process of making an application executable on a target system.
- ▶ Software is deployed into and run within a software environment.
- ▶ Do you have a reproducible software deployment process?

Evolution of Software Deployment



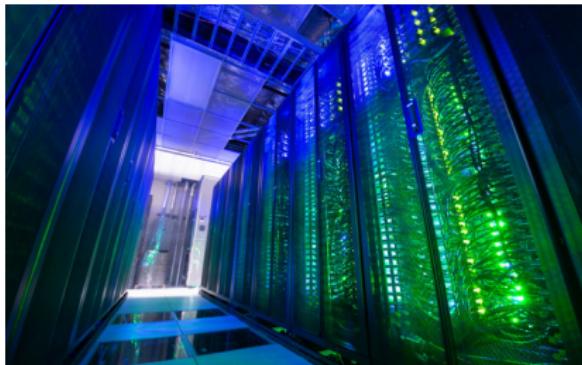
```
SONS> aws ec2 help
EC2()

NAME
    ec2 - 

DESCRIPTION
    Amazon Elastic Compute Cloud (Amazon EC2) provides resizable computing
    capacity in the Amazon Web Services (AWS) cloud. Using Amazon EC2 eliminates
    your need to invest in hardware up front, so you can develop and
    deploy applications faster.

AVAILABLE COMMANDS
    o accept-vpc-peering-connection
    o allocate-address
    o assign-private-ip-addresses
    o associate-address
    o associate-dhcp-options
    o associate-route-table
```

Software Deployment on XSEDE



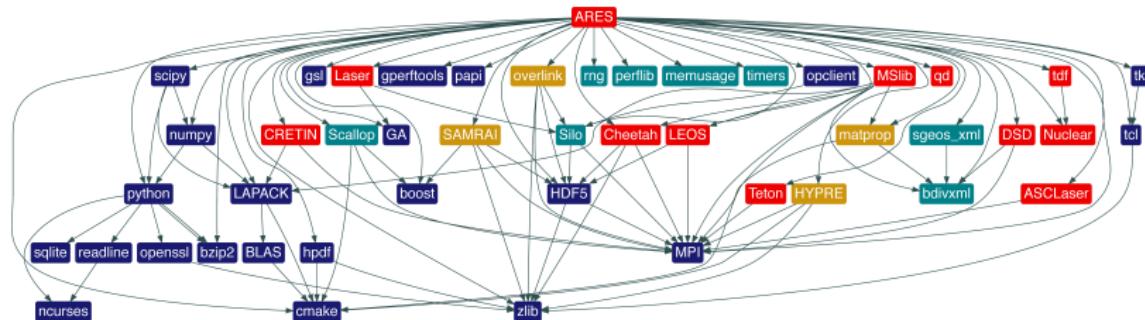
Comet vs. Stampede2

```
mkanedes@comet-ln3:~$ git clone https://github.com/mkanedes/gpse.git
Cloning into 'gpse'...
remote: Enumerating objects: 528, done.
remote: Total 528 (delta 0), reused 0 (delta 0), pack-reused 528
Receiving objects: 100% (528/528), 311.06 KiB | 1.31 MiB/s, done.
Resolving deltas: 100% (347/347), done.
Checking out files: 100% (15/15), done.
[mkanedes@comet-ln3 ~]$ cd gpse/
[mkanedes@comet-ln3 gpse]$ ls
CHANGELOG gpse.input LICENSE Makefile README source
[mkanedes@comet-ln3 gpse]$ cat /etc/os-release | grep PRETTY_NAME
PRETTY_NAME="CentOS Linux 7 (Core)"
[mkanedes@comet-ln3 gpse]$ uname -a
Linux comet-ln3.sdsu.edu 3.10.0-957.12.2.el7.x86_64 #1 SMP Tue May 14 21:24:32 U
TC 2019 x86_64 x86_64 x86_64 GNU/Linux
[mkanedes@comet-ln3 gpse]$ module list
Currently Loaded Modulefiles:
 1) intel/2018.1.163  2) mvapich2_ib/2.3.2
[mkanedes@comet-ln3 gpse]$ module purge
[mkanedes@comet-ln3 gpse]$ module load gnu/7.2.0
[mkanedes@comet-ln3 gpse]$ module load mvapich2_ib/2.3.2
[mkanedes@comet-ln3 gpse]$ module list
Currently Loaded Modulefiles:
 1) gnu/7.2.0          2) mvapich2_ib/2.3.2
[mkanedes@comet-ln3 gpse]$ make
mpiF90 -Jbuild -fimplicit-none -fmodule-private -ffree-form -ffree-line-length-n
one -std=gnu -fdefault-real-8 -O2 -mtune=native -c source/math.f90 -o build/math.o
source/math.f90:45:23:
      USE, INTRINSIC :: ISO_FORTRAN_ENV
      1
Warning: Use of the NUMERIC_STORAGE_SIZE named constant from intrinsic module IS
O_FORTRAN_ENV at (1) is incompatible with option -fdefault-real-8
mpiF90 -Jbuild -fimplicit-none -fmodule-private -ffree-form -ffree-line-length-n
one -std=gnu -fdefault-real-8 -O2 -mtune=native -c source/io.f90 -o build/io.o
source/io.f90:45:23:
      USE, INTRINSIC :: ISO_FORTRAN_ENV
      1
Warning: Use of the NUMERIC_STORAGE_SIZE named constant from intrinsic module IS
O_FORTRAN_ENV at (1) is incompatible with option -fdefault-real-8
mpiF90 -Jbuild -fimplicit-none -fmodule-private -ffree-form -ffree-line-length-n
```

```
mkanedes@stampede2:~$ git clone https://github.com/mkanedes/gpse.git
Cloning into 'gpse'...
remote: Enumerating objects: 528, done.
remote: Total 528 (delta 0), reused 0 (delta 0), pack-reused 528
Receiving objects: 100% (528/528), 311.06 KiB | 2.06 MiB/s, done.
Resolving deltas: 100% (347/347), done.
[mkanedes@stampede2:~]$ cd gpse/
[mkanedes@stampede2:~]$ ls
CHANGELOG gpse.input LICENSE Makefile README source
[mkanedes@stampede2:~]$ cat /etc/os-release | grep PRETTY_NAME
PRETTY_NAME="CentOS Linux 7 (Core)"
[mkanedes@stampede2:~]$ uname -a
Linux login2.stampede2.tacc.utexas.edu 3.10.0-957.5.1.el7.x86_64 #1 SMP Fri Feb
1 14:54:57 UTC 2019 x86_64 x86_64 x86_64 GNU/Linux
[mkanedes@stampede2:~]$ module list
Currently Loaded Modules:
 1) intel/18.0.2          4) git/2.24.1           7) cmake/3.16.1
 2) libfabric/1.7.0        5) autotools/1.1       8) xalt/2.8
 3) impi/18.0.2            6) python2/2.7.15     9) TACC

[mkanedes@stampede2:~]$ sed -i 's/ := ffortran/ := ifort/g' Makefile
[mkanedes@stampede2:~]$ make
mpiF90 -Jbuild -fimplicitnone -free -stand none -module build -real-size 64 -ipo
-O3 -no-prec-div -fp-model fast2 -xhost -c source/math.f90 -o build/math.o
ifort: command line warning #10006: ignoring unknown option '-Jbuild'
mpiF90 -Jbuild -fimplicitnone -free -stand none -module build -real-size 64 -ipo
-O3 -no-prec-div -fp-model fast2 -xhost -c source/grid.f90 -o build/grid.o
ifort: command line warning #10006: ignoring unknown option '-Jbuild'
source/grid.f90(255): warning #6178: The return value of this FUNCTION has not b
een defined. [GRID_BINARY_SEARCH]
INTEGER RECURSIVE FUNCTION grid_binary_search()
=====
mpiF90 -Jbuild -fimplicitnone -free -stand none -module build -real-size 64 -ipo
-O3 -no-prec-div -fp-model fast2 -xhost -c source/pmc.a.f90 -o build/pmc.a.o
ifort: command line warning #10006: ignoring unknown option '-Jbuild'
mpiF90 -Jbuild -fimplicitnone -free -stand none -module build -real-size 64 -ipo
-O3 -no-prec-div -fp-model fast2 -xhost -c source/vex.f90 -o build/vex.o
ifort: command line warning #10006: ignoring unknown option '-Jbuild'
mpiF90 -Jbuild -fimplicitnone -free -stand none -module build -real-size 64 -ipo
-O3 -no-prec-div -fp-model fast2 -xhost -c source/rot.f90 -o build/rot.o
```

And it gets more complicated ...



Software dependency hell is a colloquial term for the frustration of some software users who have installed software packages which have dependencies on specific versions of other software packages.

Problem by Example

Dear SDSC,

I need to install the software package libmpich-dev on Expanse.
Can you help me install it?

I tried to install the package with the following command from
the documentation I found online, but it failed to install.

```
[profX@login01 ~]$ sudo apt-get install libmpich-dev
```

We trust you have received the usual lecture from the local
System Administrator. It usually boils down to these three
things:

- #1) Respect the privacy of others.
- #2) Think before you type.
- #3) With great power comes great responsibility.

PIN+Yubi:

Sorry, try again.

Is the problem here that I'm using the wrong PIN? Or is this a
permissions issue?

Thanks for your help,

Professor X

Problem by Example

```
sudo apt-get install libmpich-dev
```

Problem #1: The use of **apt**.

- ▶ **apt** is a command-line package management tool used to handle the installation, updating, and removal of software packages on Debian-based Linux distributions.
- ▶ Comet, Expanse, Bridges2, and Stampede2 all run CentOS as their operating system, which is NOT a Debian-based Linux distribution.
- ▶ Know your operating system!

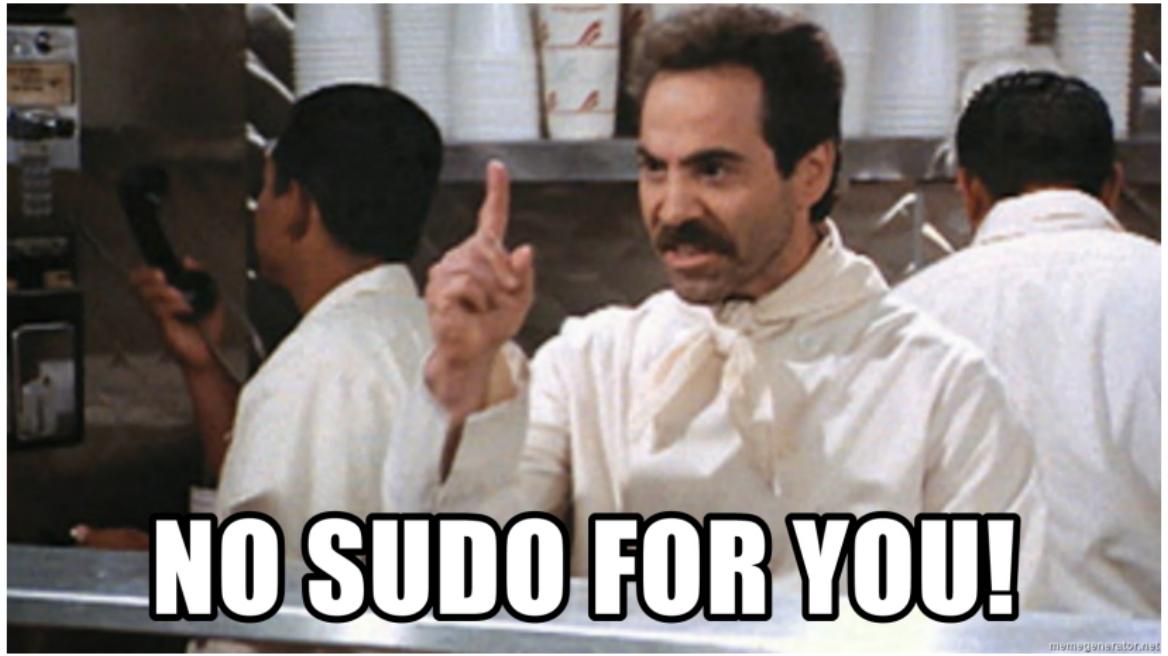
```
[prof@logino1 ~]$ cat /etc/os-release | grep PRETTY_NAME  
PRETTY_NAME="CentOS Linux 8 (Core)"
```

Problem by Example

```
sudo apt-get install libmpich-dev
```

Problem #2: The use of **sudo**.

- ▶ sudo is a command in Unix-like operating systems that allows a user to execute programs with the security privileges of another user, which, by default, is the superuser — a special user account used for system administration.
- ▶ When you install software via an operating system's package manager (e.g., using apt or yum), you are modifying the common software packages and libraries that will be available *system-wide* for ALL users to run.
- ▶ Do you really think we'd let you do that?



memegenerator.net

Problem by Example

```
sudo apt-get install libmpich-dev
```

Problem #3: The library being installed: **libmpich-dev**.

- ▶ MPICH is a freely available, portable implementation of MPI, a standard message-passing interface for distributed-memory applications used in parallel computing.
- ▶ OS-level package managers like apt or yum download and install pre-compiled binary packages. This requires the software packager to make a certain set of assumptions about the system hardware and software configuration the package rely on once installed.
- ▶ HPC is not the default assumption.

Problem by Example

```
sudo apt-get install libmpich-dev
```

Problem #3: The library being installed: **libmpich-dev**.

- ▶ Many HPC applications and software libraries need to be compiled from source against the specialized hardware and software that is unique to each system, especially if you want to obtain maximum performance when running your code.
- ▶ On Expanse, we build, install, and maintain several different MPI distributions for you. These builds include special features that would not be found in an MPI distribution installed from a standard Linux package repository. e.g., Slurm scheduler integration; Infiniband support; GPU-awareness

Types of Software in Your Environment

- ▶ System software - Built, installed, and maintained by SDSC HPC Systems Group. Includes operating system, your Shell, common command-line tools and utilities, filesystem software. Limited set of packages and versions. Managed by standard Linux package managers.
- ▶ Shared application software - Built, installed, and maintained by SDSC HPC User Services Group. Includes all common scientific and engineering application software. Available to all users. Accessed via Lmod-based Environment Modules.
- ▶ Local application software - Built, installed, and maintained by YOU in your \$HOME directory. May include software compiled from source using compilers and libraries from SDSC's shared application software, software installed using a user-level package manager (e.g., pip, conda, install.packages()).

Questions?

