Data Management in the HPC

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osf.io/ugrq6

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What you will learn

What: understand how to transfer, organize, and use data on the HPC.

Why: Nice data makes things easier: collaboration, reproducibility => better research

Assume

- Basic understanding of how to use the Unix shell
- Ability to log in to the HPC (optional but recommended)

How

- Overview of storage options on the HPC
- Methods of transferring data in and out
- Basic HPC data management /good enough practices
- Moving data around in jobs

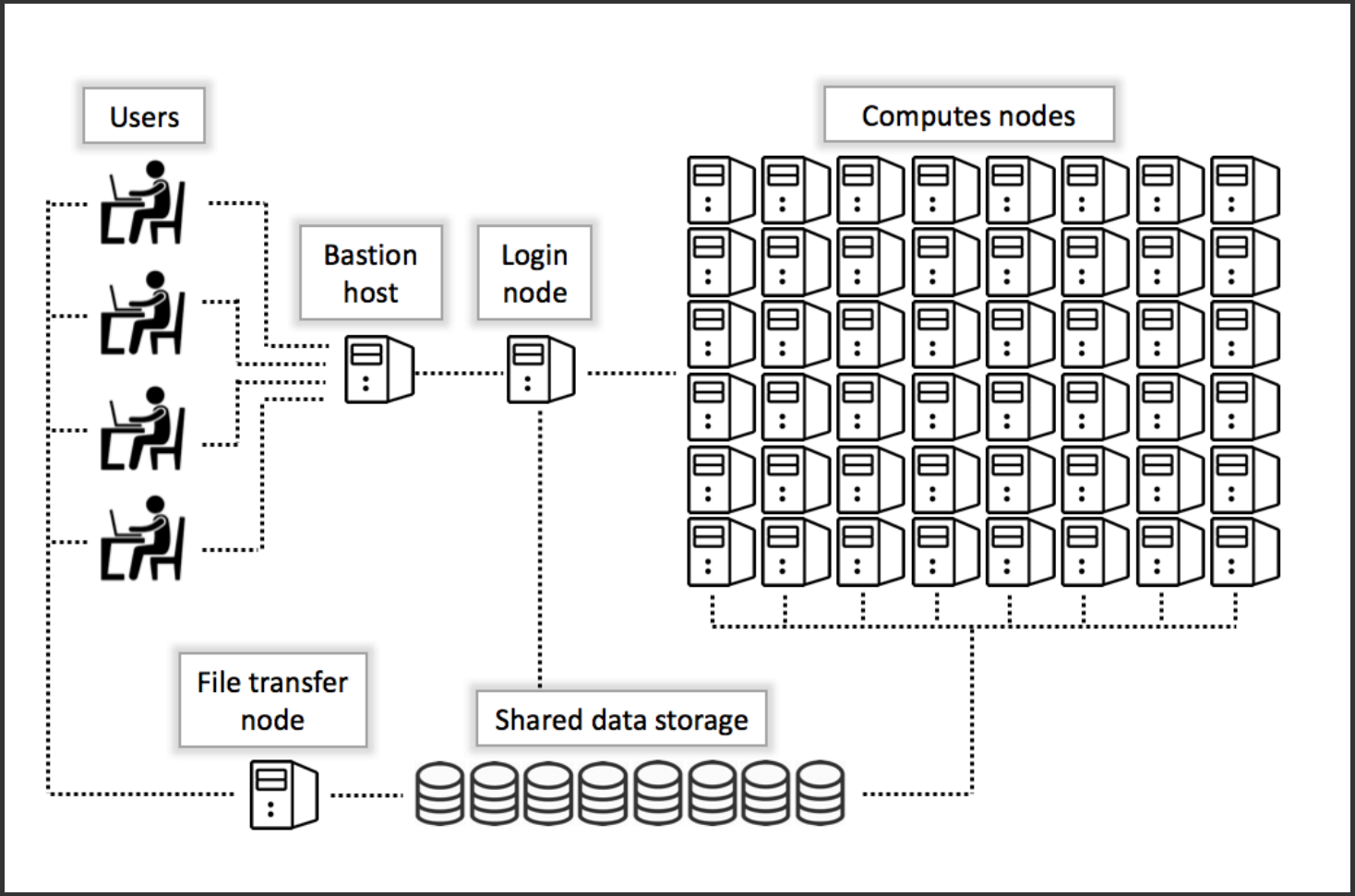
Basic Pipeline

- Data input, processing, collaboration, sharing

- Fill in details of what, where, how

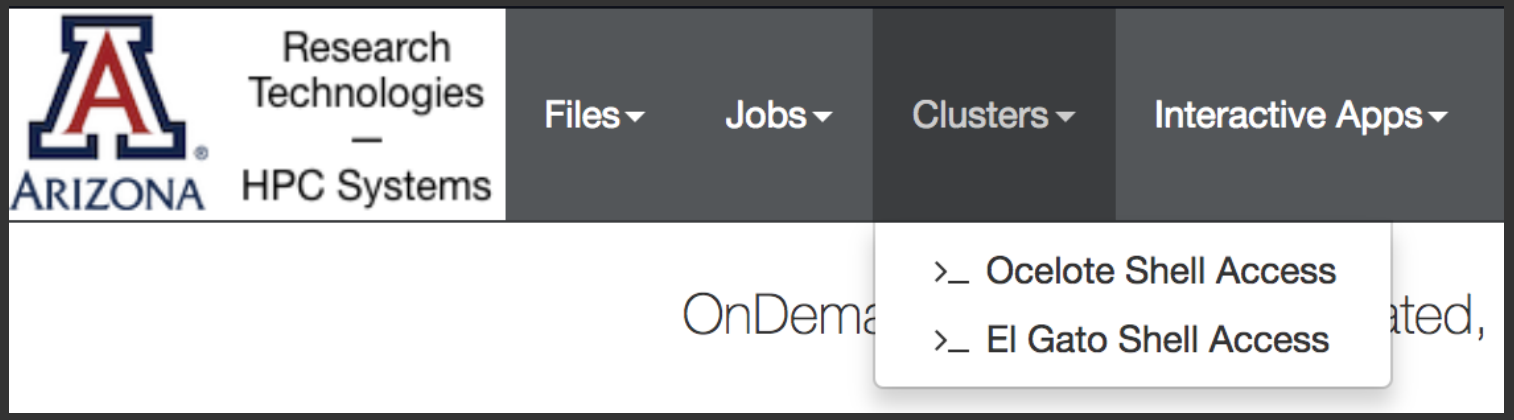
Logging in

The diagram of the UA HPC cluster



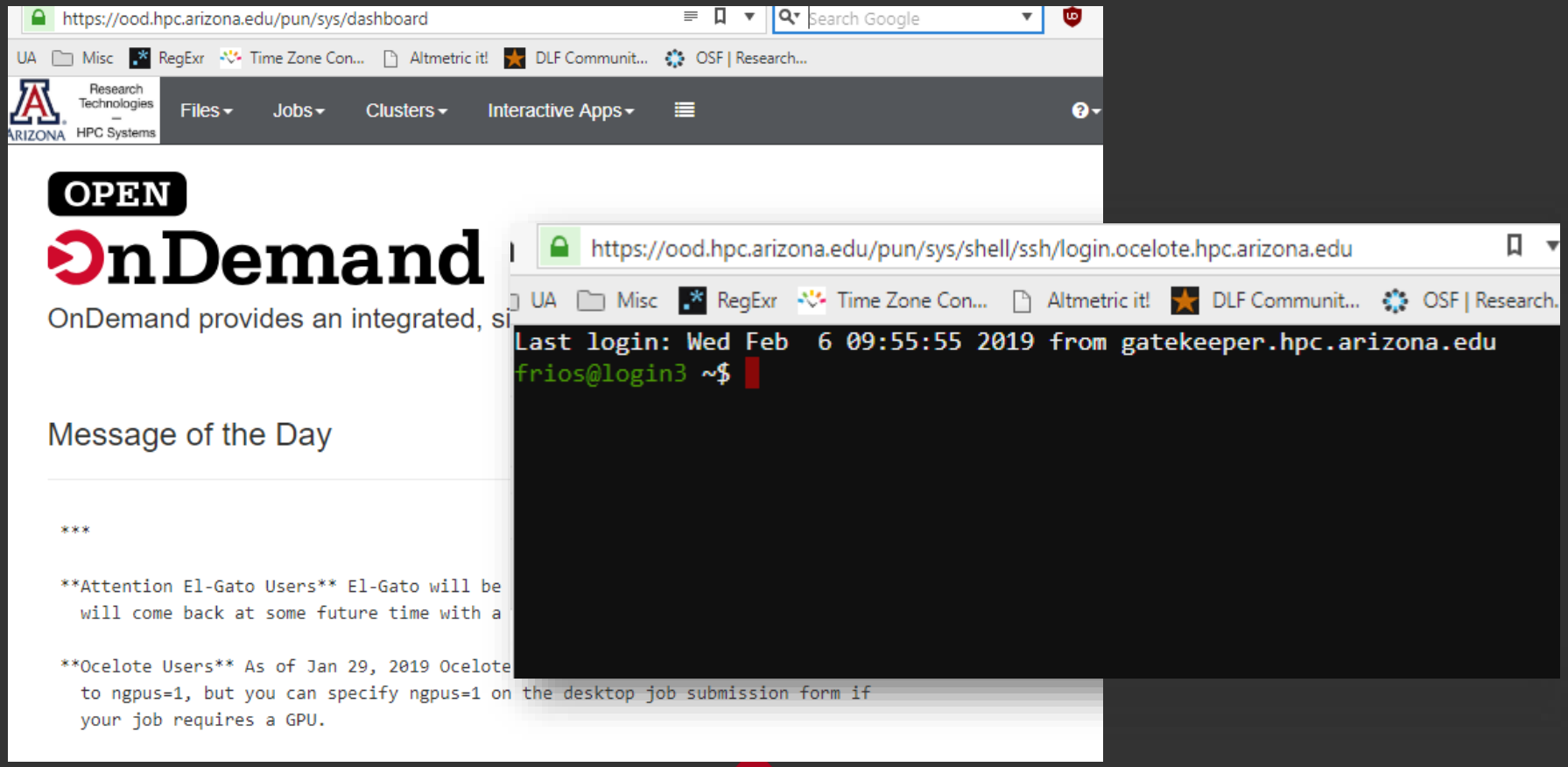
Login

- Open **ood.hpc.arizona.edu** in your web browser and login with your NetID and password.
- From the “Clusters” drop-down menu choose which HPC cluster you would like to access:



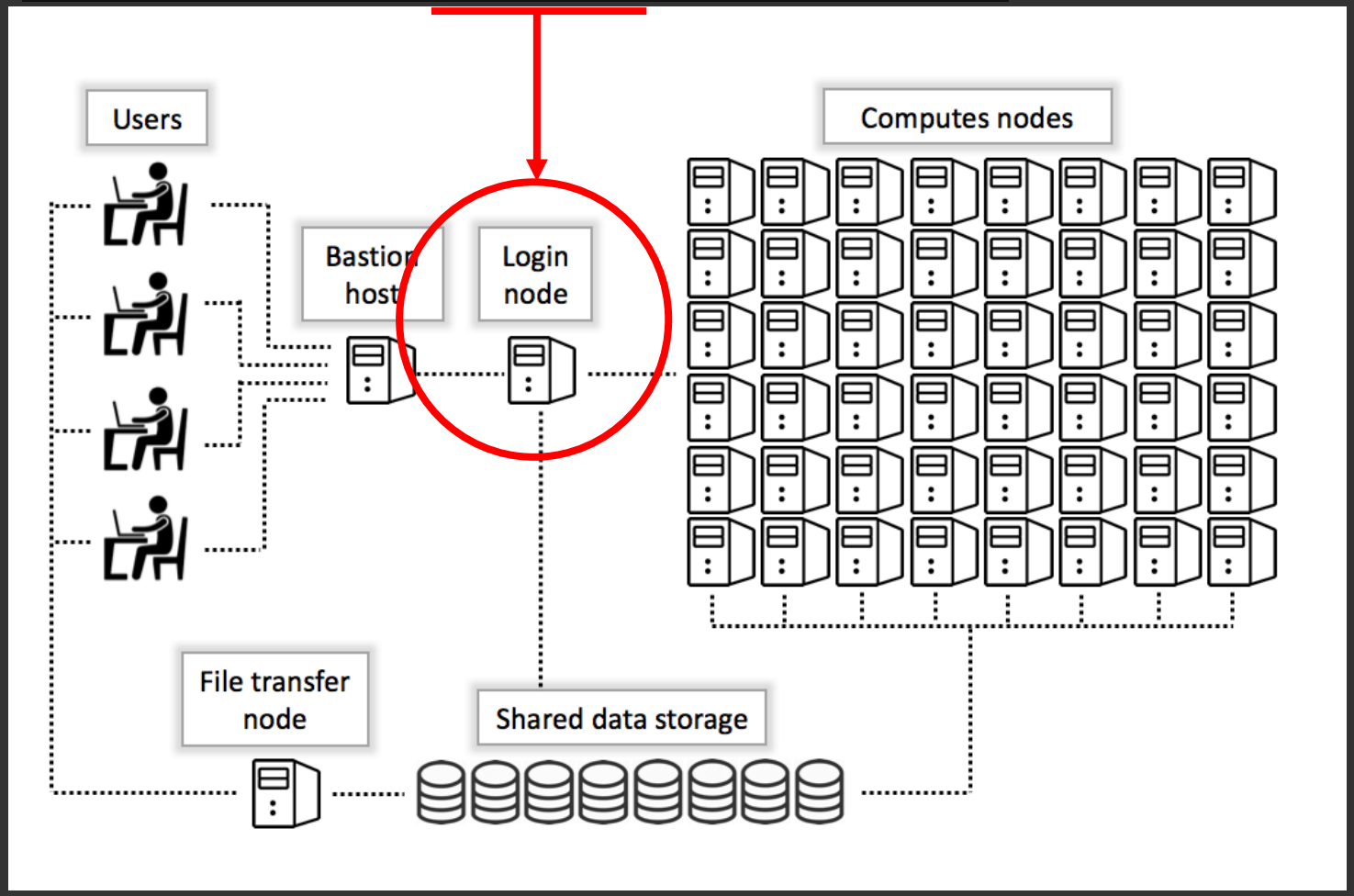
Warm-up exercise

- Log in to Ocelote
  - Ssh, PuTTY/KiTTY
  - ondemand.hpc.arizona.edu or ood.hpc.arizona.edu



Login node

```
[dshyshlov@login2 ~]$
```



Login node is like an elevator

Login node is like an elevator

Data Storage Options

HPC Storage

- Every users gets two default storage locations:
  - /home
    - the default home directory
    - 15GB
    - the only backed up storage on UA HPC/extra
  - /extra
    - full path: /extra/NetID
    - 200GB
    - not backed up
    - has file count limit 600 files/GB

```
[dshyshlov@login2 ~]$ uquota
                     used  soft limit  hard limit      files/limit
dshyshlov home & PBS      0G        14G        15G          0
/extra/dshyshlov          0G       200G       200G          0/120000
```

HPC Storage

- Other storage options:
  - /xdisk
    - temporary “scratch” storage
    - from 200GB to 1TB for up to 45 days
    - not backed up

```
$ xdisk -c help
*************************************************************
  USAGE on login2:


  xdisk -c create [-h hostname] [-m GB] [-d days]
  xdisk -c delete -h hostname
  xdisk -c expire [-h hostname] -d days
  xdisk -c resize [-h hostname] -m GB
  xdisk -c cancel -h hostname
  xdisk -c query [-h hostname]
  xdisk -c help

  NOTE: Commands given in parenthesis are optional, in which
        case you will get system defaults
```

HPC Storage

- Other storage options:
  - /rsgrps
    - rented storage for research groups
    - shared between all members of the group
    - current rate: $39/TB/year
    - not backed up
    - file count limit 600 files/GB
  - /tmp
    - local disk on compute nodes
    - not connected to the main storage
    - the best performance for calculation
    - <1TB is available on each node
    - data is removed once the job is finished, so need to script copying input/output data to the main storage

HPC Storage – Summary

	Storage	Back-up	File limits	Speed
/home	15 GB	Nightly	None	
/extra	200 GB	None	600 files / GB	
/xdisk	200 – 1000 GB (45 day limit)	None	None	
/rsgrps	Rented space	None	600 files / GB	
/tmp	Varies ~ 800 GB (Ocelote)	None	None	Fastest (on node)

COMING SOON for 2020

- Scheduler: PBS -> Slurm
  - Slurm can run PBS scripts
  - Some options in PBS scripts not supported
- New HPC System
  - 19200 AMD CPUs

New Storage!

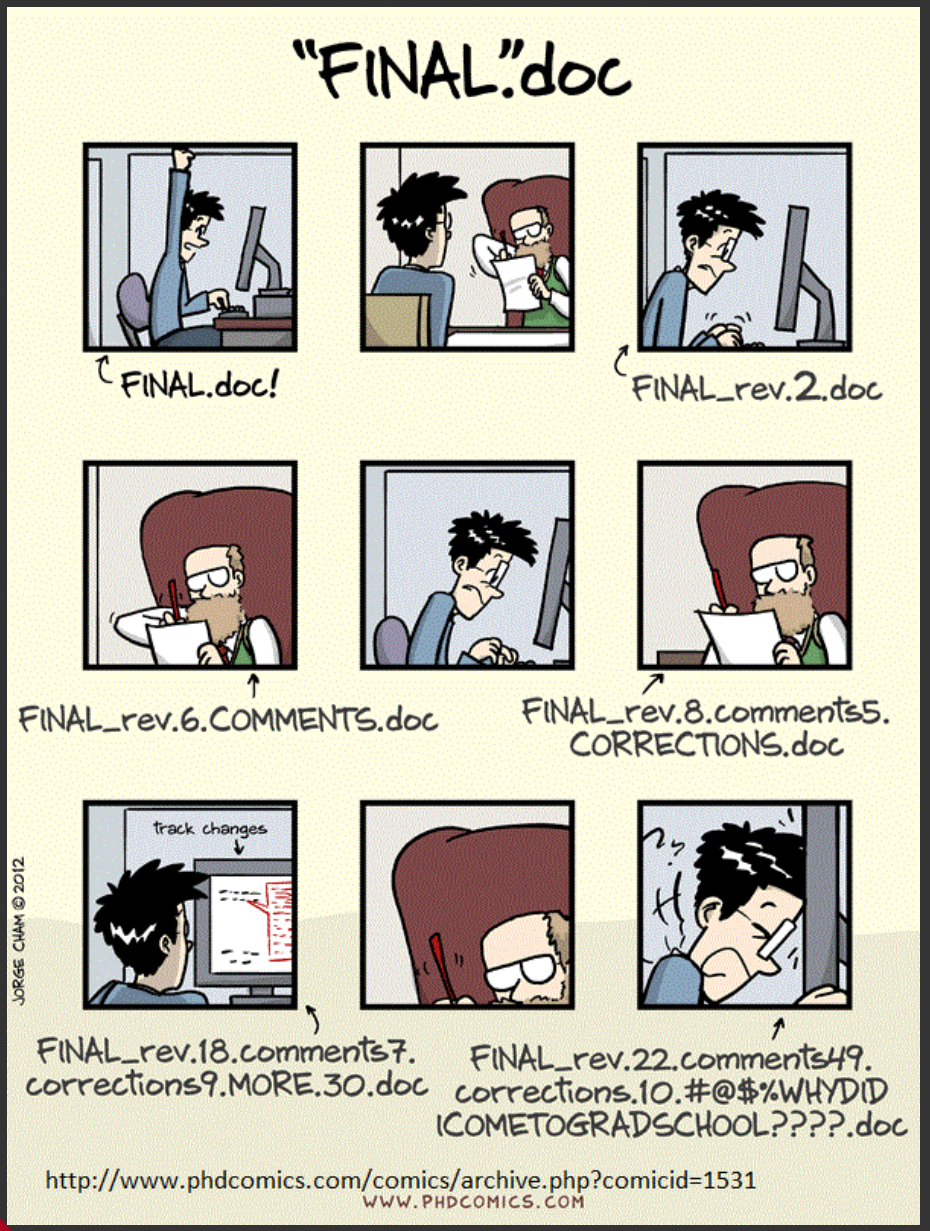
	Old	New
Storage	DDN 7200 RPM Spinning Disk	Qumulo Solid State Disk
	1.5 PB + 20 TB (astronomy purchased)	2 PB
Policy	Free Storage /home 15 GB	Merging together /home and /extra /home 50 GB (Less /wherearemyfiles/path confusion!)
	/rsgrps rental space $39 per (TB*year)	All PIs get a free 500 GB allocation in /rsgrps All members of PI group has access to space
	/xdisk 1 TB for up to 90 days	/xdisk (free) 20 TB up to 150 days (requested at PI level, not per user) renewable for another 150 days
Data Plan	Never intended or architected for long-term file storage Reality: Used for long-term file storage because it was cheap and there were not many other options	1. Data will be maintained and managed on another platform (Google Drive, S3 bucket, Box, *etc*) 2. Data that needs to be analyzed is pulled down to HPC storage for analysis 3. The results are pushed back up to other platform 4. Original data pulled down is deleted because it already exists elsewhere

File Management

Data Management Best Practice: Naming & Organization

"I don't follow a consistent approach for keeping my data organized, so it often takes time to find things."

- Use a schema to determine file names
- Avoid using confusing labels such as revision, final, final2, or definitive copy.
- Use only alphanumeric characters and . _ -
- Max name length on HPC= 255



Data Management Best Practice: Versioning

- Add dates and/or version numbers
- Convention is to use ordinal numbers such as 1, 2, and 3 for version changes
- Document changes to your data/code. Within the file or use separate log as needed

Better

Document the naming scheme

Study001_Raw
└ BiopsyData
- 20161101_Study001_Biopsy_visit1.xls
- 20161101_Study001_Biopsy_visit1_v2.xls
- 20161101_Study001_Biopsy_visit1_v3.xls

Add version and/or date (ISO 8601)

These are your friends:
sprintf (C/C++)
str.format (Python)

File	Date	Person	Changes
filename_v1.csv	3/5/2017	Arthur N.	Initial dataset
filename_v2_FR.csv	4/14/2017	Fernando R.	Cleaned up a few null values

Data Management Best Practice: Folders

- Folder names should be unique and descriptive
- Try not to nest more than 3 levels deep
- Use a consistent folder organization structure
  - Different data stages should have their own folders (i.e., raw data, processed data, analyzed data , figures and charts)

Bad

```
GW_model
├ elevation.mat
├ depth_wt.csv
├ well_loc.csv
├ flow_model.m
├ flow_model2.m
├ flow_model_final.m
├ flowlines1.png
├ flowlines2.png
├ contours.png
```

Better

```
GroundwaterModel
└ Code
        ├ 20170402_FlowModel_v1.m
        ├ 20170410_FlowModel_v2.m
        ├ 20170511_FlowModel_v3.m
└ Inputs
        ├ TerrainElevation.mat
        ├ DepthToWaterTable.csv
        ├ WellLocations.csv
└ Outputs
        ├ 20170402_Flowlines_FlowModelv1.png
        ├ 20170402_Contours_FlowModelv1.png
        ├ 20170415_Flowlines_FlowModelv2.png
```

Exercise 1: Project Setup

- Applying good folder organization automatically


```
.
├── AUTHORS.md
├── LICENSE
├── README.md
├── bin                <- Your compiled model code can be stored here (not tracked by git)
├── config             <- Conf                                  doxygen or for your model if needed
├── data
│   ├── external       <- Data from third party sources.
│   ├── interim        <- Intermediate data that has been transformed.
│   ├── processed      <- The final, canonical data sets for modeling.
│   └── raw            <- The original, immutable data dump.
├── docs               <- Documentation, e.g., doxygen or scientific papers (not tracked by git)
├── notebooks          <- Ipython or R notebooks
├── reports            <- For                                   LaTeX, Markdown, etc., or any project reports
│   └── figures        <- Figu                                  reports
└── src                <- Sour
    ├── data           <- scripts and programs to process data
    ├── external       <- Any external source code, e.g., pull other git projects, or external libraries
    ├── models         <- Source code for your own model
    ├── tools          <- Any helper scripts go here
    └── visualization  <- Scripts for visualisation of your results, e.g., matplotlib, ggplot2 related.
```

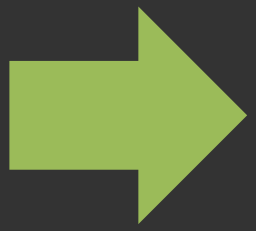
Basic Metadata

Each stage of data in it's own folder

Software in it's own folder

Getting Data

Getting External Data In



	Storage	Back-up	File limits
/home	15 GB	Nightly	None
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/xdisk	200 – 1000 GB (45 day limit)	None	None
/rsgrps	Rented space	None	600 files / GB

- 2-factor authentication may get in the way…

Exercise 2: Get Data

```
$ wget
```

- Download some ecology data from the Figshare data repository into the data/external folder

Ernest, Morgan; Brown, James; Valone, Thomas; White, Ethan P. (2018): Portal Project Teaching Database. figshare. Fileset.

https://doi.org/10.6084/m9.figshare.1314459.v9

```
.
├── AUTHORS.md
├── LICENSE
├── README.md
├── bin                <- Your compiled model code can be stored here (not tracked by git)
├── config             <- Configuration files, e.g., for doxygen or for your model if needed
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│   ├── external       <- Data from third party sources.
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├── notebooks          <- Ipython or R notebooks
├── reports            <- For a manuscript source, e.g., LaTeX, Markdown, etc., or any project reports
│   └── figures        <- Figures for the manuscript or reports
└── src                <- Source code for this project
    ├── data           <- scripts and programs to process data
    ├── external       <- Any external source code, e.g., pull other git projects, or external libraries
    ├── models         <- Source code for your own model
    ├── tools          <- Any helper scripts go here
    └── visualization  <- Scripts for visualisation of your results, e.g., matplotlib, ggplot2 related.
```

Data Mgmt Best Practice: Storage & Backup

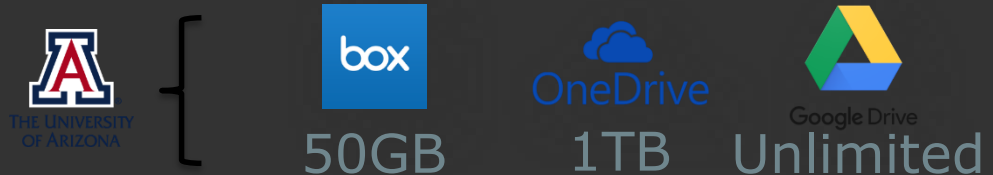
"I decide what data is important while I am working on it and typically save it in a single location"

Do

- 3-2-1: If possible, 3 copies, 2 different storage types, 1 copy offsite
- Keep offline backups if possible. Sync clients could be propagate changes unintentionally

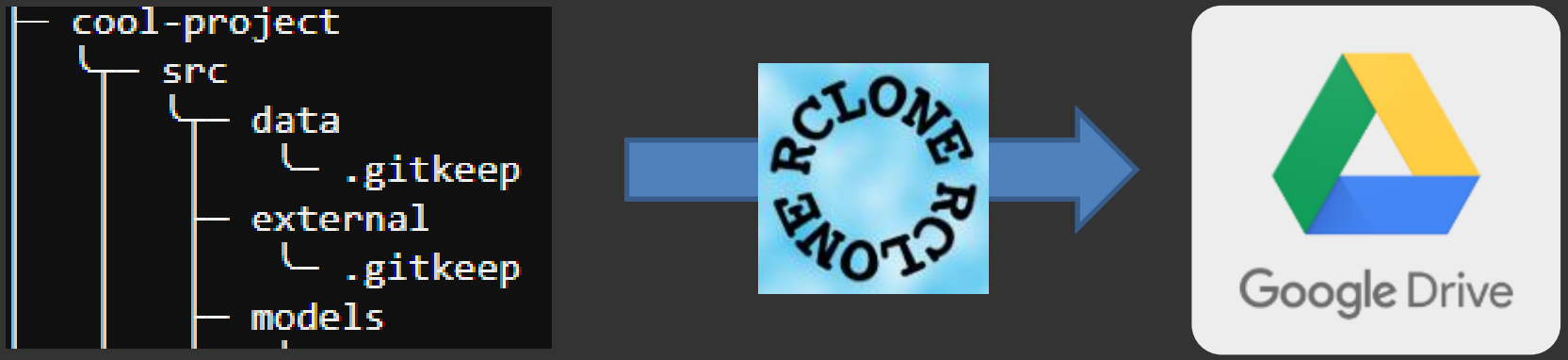
Avoid:

- Storing sensitive data on an unencrypted laptop or flash drive or insecure servers
- Relying on cloud storage for the only copy!
  http://www.cnet.com/news/dropbox-fixes-file-deletion-bug-offers-year-of-free-service/



For HIPAA compliance, use UA Box Health account.

Backup and Restore to Google Drive



- Rclone to transfer directly to/from Google Drive, Dropbox, S3, Box… many more
- Exercise 2a: set up Rclone - Do up to step 5

  rclone lsf <remote>:/
  rclone copy <remote>:/path/to/file <dest>/path/to/file

Managing Files

Sharing data between HPC users

- You can share data with another HPC user without moving the data
- Open file permissions
- Create symbolic links

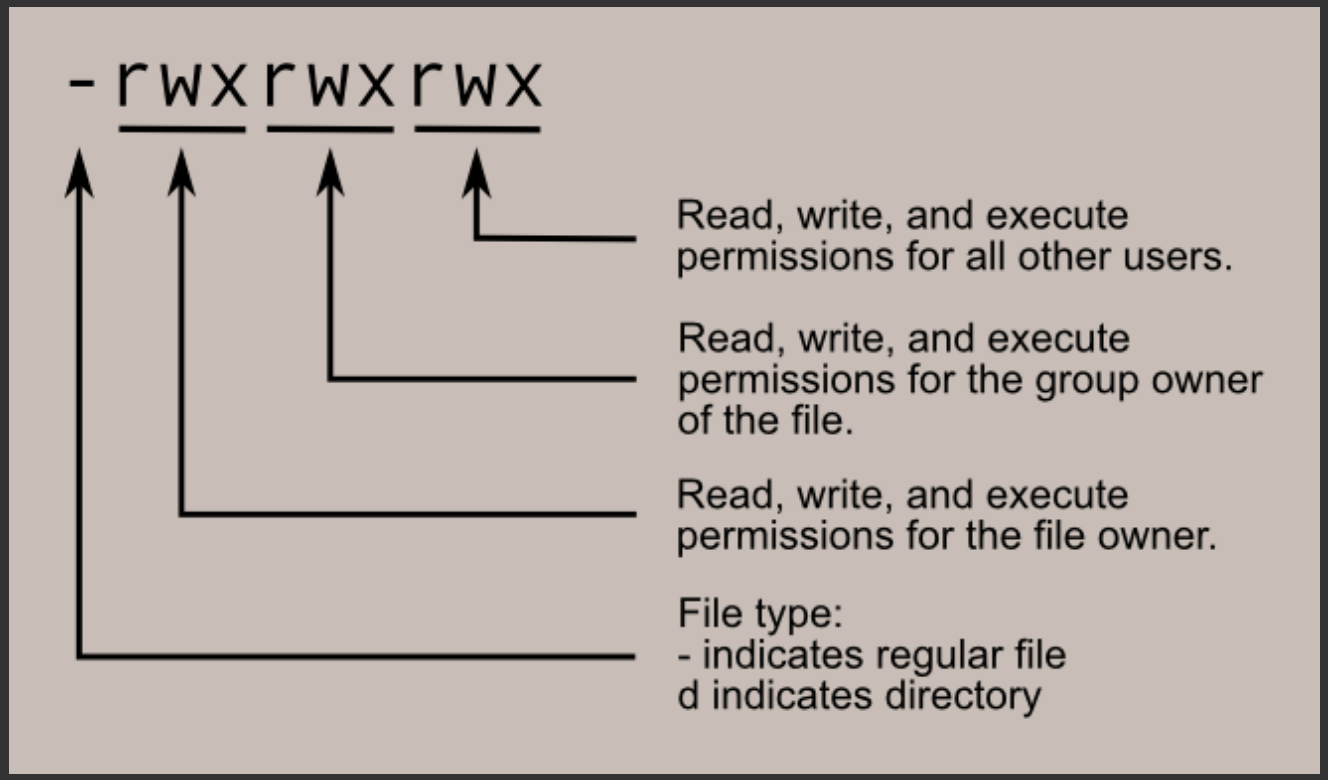
File permissions

- Check file permissions – *ls -l*

-rw-r--r-- 1 dshyshlov rc 639 Oct 10 15:58 script.pbs

Owner

Group



Change file permissions

- Command to change permissions – *chmod*
  - *chmod +x filename* - make file executable
  - *chmod g+rwx filename* - open all permissions for you group
  - *chmod 777 filename* - open all permissions for everyone
  - *chmod –R 777 filename* - same as above but recursively

Symbolic links

- Create a soft link to a file or directory
  - *ln –s path/to/the/destination link_name*
  - perfect for situations when you need to share read only data
  - requires permissions to link directory of another user
- Examples:
- Create a shortcut to your /extra in your /home
  - *ln –s /extra/NetID ~/my_extra*
- link to a directory with shared data
  - *ln –s /rsgrps/NetID/project/data ~/collaboration_data*

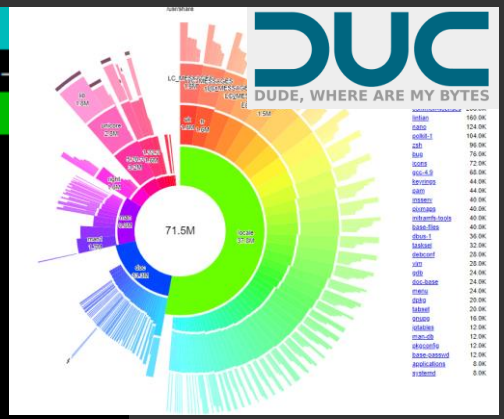
File & Space Management Tools

- Checking your space & file limit: uquota

```
frios@login2 ~$ uquota
                                          used   soft limit  hard limit        files/limit
frios home & PBS                        46.84M         14G         15G         1044
/extra/frios                            56.72G        200G        200G            2/120000
```

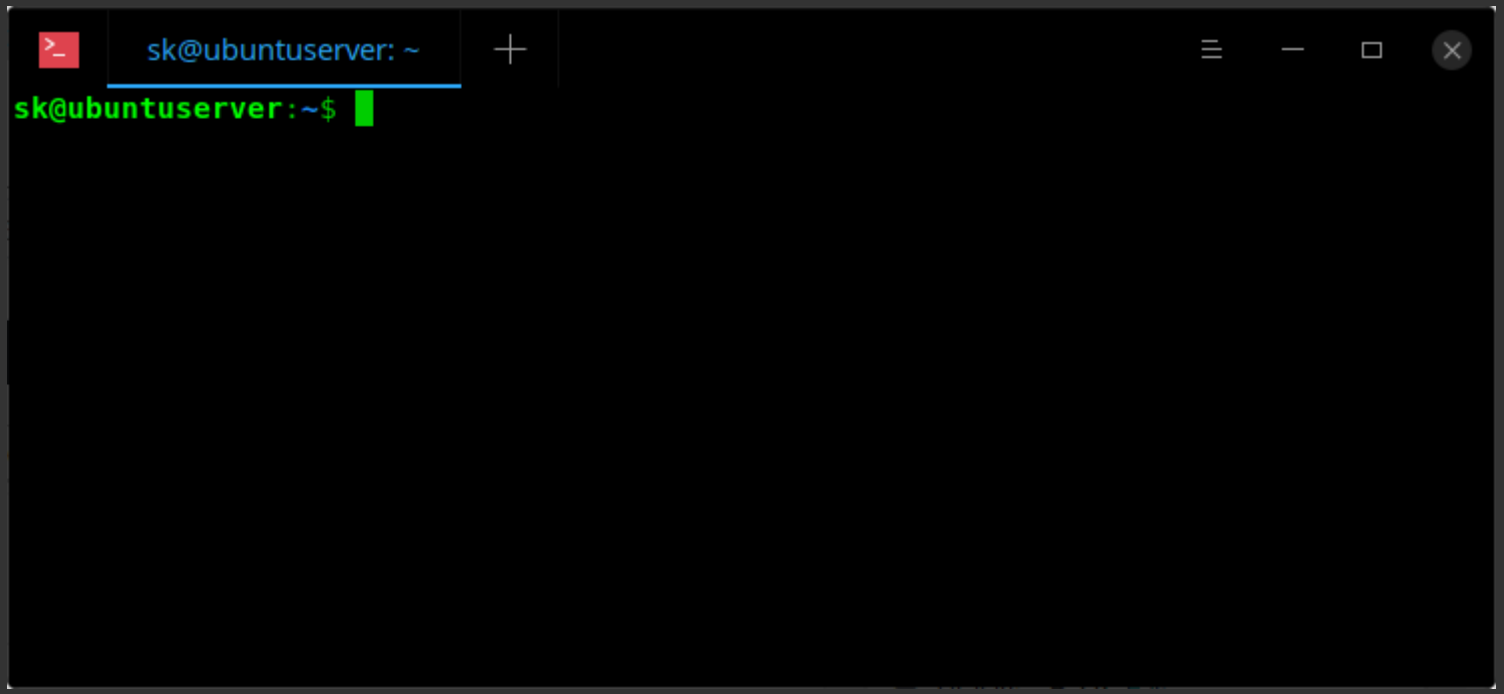
- Checking folder usage and count: NCDU

```
ncdu 1.14 ~ Use the arrow keys to navigate, press ? for help
--- /home/u17/frios ----------------------------------------------
  20.8 MiB [##########]       4 /rclone-v1.42-linux-amd64
  12.2 MiB [#####     ]     619 /renameutils-0.12.0
   9.7 MiB [####      ]      13 /tmsu-x86_64-0.7.4
   2.7 MiB [#         ]     149 /.local
   2.0 MiB [          ]      92 /ncdu-1.14
   1.0 MiB [          ]      37 /hpc-test1
 392.0 KiB [          ]         duc-1.4.3.zip
 256.0 KiB [          ]         .duc.db
 200.0 KiB [          ]      76 /.cache
 144.0 KiB [          ]         ncdu-1.14.tar.gz
  16.0 KiB [          ]       9 /ondemand
  16.0 KiB [          ]         .bash_history
   8.0 KiB [          ]     143 /.cookiecutters
```



File & Space Management Tools

- Keeping file names tidy with renameutils



Credit: ostechnix.com

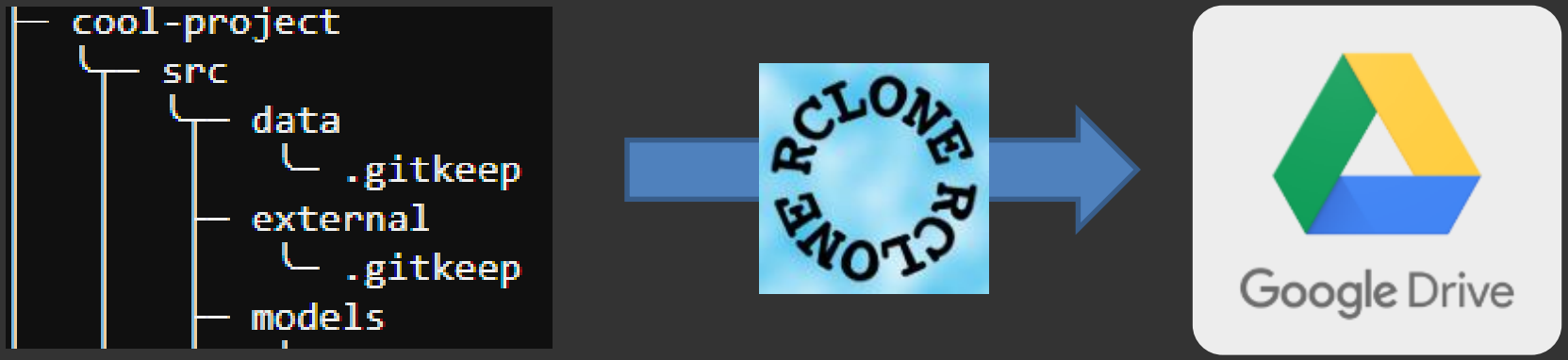
Operate on Data

- Things that can “break” the system:
  - heavy use of the login node
  - too many jobs
  - too many files
  - heavy I/O jobs
  - copying GB of data

- Exercise 3 – Using /tmp

Finish Project and Export

- Exercise 4 - Export to Google Drive



- What do you notice about the transfer speed?

Sample Transparent and Reproducible Research Pipeline

- Data input, processing, sharing/collaborating

globus

Get data

Process & Manage on UA HPC

Export

RCLONE

Google Drive

data, figures

Dropbox

box

MENDELEY

Co-author files & literature

GitHub

Get code

Connect to OSF

Share, collaborate, Publish (w/ DOI)

Connect to OSF

Open Science Framework