

Transferring Data

- After logging into the XSEDE Single Sign-On Hub, you can transfer data
 - using various commands in the terminal, including rsync, scp, and sftp
 - using specialized programs, as specified in the user manuals, but this requires installing programs, which you might not want to do
- On the terminal, I recommend rsync because you don't need to copy (and wait for) the whole directory
- A good template is: `rsync -Cuavz --port 2222 source_path destination_path`
 - Cuavz are options, which can be seen by ``man rsync``
 - port 2222 means that you go through the XSEDE SSO
 - the paths have the format `user_name@directory/file_name`
 - if `user_name@` is omitted, it assumes the same user name as on the current system
 - if `directory` is omitted, the home directory is assumed
 - if `file_name` is omitted, the whole directory is assumed

- Try copying a local directory with the ubiquitin pdb file and python script for OpenMM

```
Minh-IIT-MBP2018:[~/Documents/GitHub/Chem456/static_files/tutorials]: rsync -Cua  
vz --port 2222 ubq-md dminh@data.bridges.psc.edu:/home/dminh/  
building file list ... done  
ubq-md/  
ubq-md/1ubq.pdb  
ubq-md/MD_ubq.py  
  
sent 14309 bytes  received 70 bytes  9586.00 bytes/sec  
total size is 52573  speedup is 3.66  
Minh-IIT-MBP2018:[~/Documents/GitHub/Chem456/static_files/tutorials]:
```

If you don't have them on your local computer, you can download them from github:
https://github.com/daveminh/Chem456/tree/master/static_files/tutorials/ubq-md