DS 7347
High-Performance Computing (HPC) and Data Science

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Research and Data Sciences Services
Office of Information Technology
Center for Research Computing
Southern Methodist University

Course Overview

Accessing ManeFrame II (M2)

Assignment

Course Overview

- Ph.D. in Computational Chemistry from SMU in 2014 where I studied the strength of chemical bonds using local modes
- Post-doctoral fellowship using classical molecular dynamics to study protein allostery 2014-2015
- Currently HPC Research Scientist with Center for Research Computing and Office of Information Technology
- Current Research Projects
  - Machine Learning Model Development for *ab initio* Molecular Dynamics
  - Development of Finite Element Based *ab initio* Quantum Chemical Methods
  - Computational Materials Design for Small Molecule Sieving Applications
  - Computational Materials Design for Nano-Scale Flow Reactors

- 2U
- GitHub
  https://github.com/SouthernMethodistUniversity/msds_hpc
  (SMU Internal)

- ManeFrame II (M2)
- NVIDIA DGX SuperPOD
- GitHub
- Microsoft Teams
- 2U and Zoom

Accessing ManeFrame II (M2)

SSH
- Provides secure command line access to the login nodes.
- Graphical applications require X11-forwarding.
- Five login nodes all accessible via `m2.smu.edu`.
- M2 SSH Instructions

HPC Portal
- Provides web-based access to M2.
  - File access
  - Terminal access
  - JupyterLab (Notebooks)
  - RStudio
  - Remote Desktops

SFTP
- Transfer files to and from M2 using an SFTP client.
- M2 SFTP Instructions

- Provides an integrated single access point for HPC resources on the ManeFrame II (M2) supercomputer
- Accessing the Portal:
  - Access to the HPC portal requires an existing M2 account
  - Go to `hpc.smu.edu`
  - Sign in using your SMU ID and SMU password
- HPC Portal Documentation
- HPC Portal Walkthrough Video

Assignment

Assignment 1

- Get GitHub account and add SMU email address (GitHub Docs)
- Setup Microsoft Teams using SMU credentials (SMU Microsoft Teams)
- Message your GitHub handle to me on Teams (Robert Kalescky)
- Fork the class GitHub repository once you have access to it (GitHub Docs)
- Add me to your forked repository (`rkalescky`)
- Verify access to M2 via SSH and the Portal