

ECP8506 Course Overview

Shen Cheng

2024-09-06

Objectives

- ▶ Introduce ourselves
- ▶ Syllabus
- ▶ Introduce useful concepts/tools with hands-on setup session
 - ▶ Minnesota Supercomputing Institute (MSI)
 - ▶ Version control/Github
 - ▶ Reproducibility/`renv`

Myself

Shen Cheng, Ph.D.

- ▶ Assistant Professor at UMN ECP



- ▶ Contacts: cheng423@umn.edu
- ▶ Office: 717 Delaware St. Room 464

Your turn

- ▶ Your name
- ▶ Your role in this class (instructor/student/auditor)
- ▶ Your major/year in the program (if you are a student)
- ▶ Your job/experience (if you are working)
- ▶ Anything else that you'd like to share

Schedule

- ▶ 10 am -12 pm weekly on Fridays
- ▶ Hybrid mode:
 - ▶ In person: WDH 7-193 (9/27 and 11/22 online only)
 - ▶ Zoom: <https://umn-private.zoom.us/j/98057731209?pwd=d5zEAolm9Zglqa2lGG5bZqkLRzLmJl.1>
- ▶ TA: Jason Sriwijaya (sriwi001@umn.edu)

Important links

- ▶ Github
- ▶ Canvas
- ▶ Minnesota Supercomputing Institute (MSI) group: `ecp8506`
- ▶ Communications:
 - ▶ Emails
 - ▶ Slack channel: `ecp8506`

Grading

- ▶ Homework: 50%
 - ▶ Assignments
 - ▶ Quizzes
- ▶ Class participation 50%

Lots of experiments...

First time

- ▶ Rebuild this course around open-source R package `mrgsolve`.
- ▶ Work with HPC (MSI) for a graduate-level course.
- ▶ Large-scale academia/industry collaborations in teaching.

Objectives

- ▶ Understand the concepts of model-informed decision making using pharmacometric simulations.
- ▶ Know different simulation methods, and identify a method given scenarios.
- ▶ Learn relevant tools (`mrgsolve`) to perform pharmacometric simulations.
- ▶ Learn relevant tools (MSI/HPC, Github, `renv`) to ensure the efficiency, collaborative capability and reproducibility of pharmacometric works.

What to expect...

- ▶ **NOT** to teach pharmacometric model building/development.
- ▶ Focusing on what you can do when you have a pharmacometric model already.

Minnesota Supercomputing institute

- ▶ A core research facility at UMN
- ▶ Provides high-performance cluster (HPC) for computational works
 - ▶ Efficient
 - ▶ Collaborative
 - ▶ Reproducible

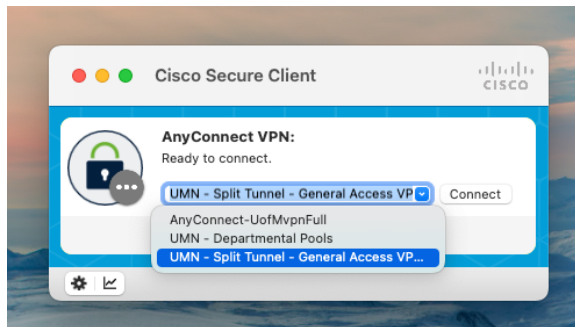
MSI Access

- ▶ Access to MSI resources is available to Principal Investigators (PIs). Individual can access MSI by
 - ▶ Participating a PI's research group
 - ▶ Participating a MSI class account (ecp8506, deadline **12/22/2024**)

VPN

MSI is accessible if you are

- ▶ You are connected to “eduroam” network on campus.
- ▶ You are off campus but connecting to the University’s Virtual Private Network (VPN).
 - ▶ do NOT select the channel named **“UMN - Departmental Pools”**.



Interactive HPC

- ▶ Several ways are available to interact with MSI
- ▶ In this course, we will use Open OnDemand RStudio Server



Notice for JupyterHub Users: During the June maintenance, the stand-alone Jupyter Notebooks service was retired. You have been redirected to our OnDemand service which can launch notebooks through an [interactive app](#).



OpenDemand provides an integrated, single access point for all of your HPC resources.

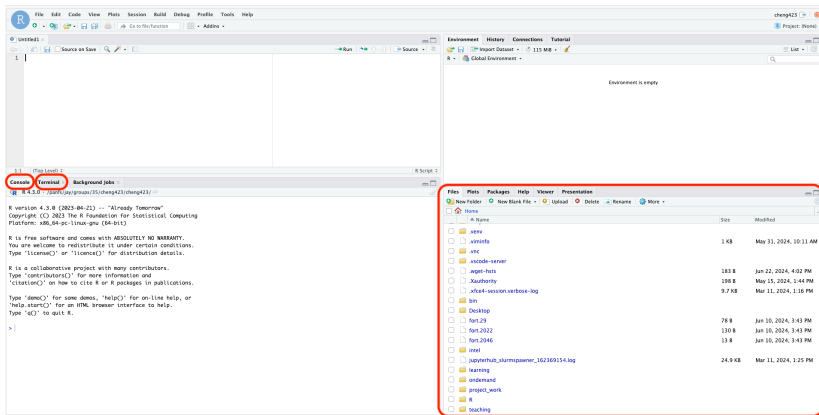
Message of the Day

Open OnDemand is a web-based portal for interactive access to MSI's compute clusters. You can access your MSI files, view your current jobs on the MSI clusters, and access a command line or interactive desktop on a cluster compute node, with configurable memory and compute resources. You also have access to a set of familiar servers, interactive development environments, and graphical user interfaces that have been adapted to use the Open OnDemand platform.

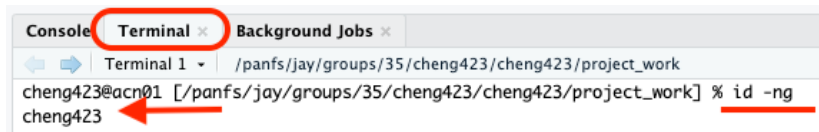
For more information about Open OnDemand at MSI, please visit <https://www.msi.umn.edu/content/using-openondemand>

For assistance please contact us at <https://www.msi.umn.edu/content/helpdesk>, help@msi.umn.edu, or (612)626-0802.

Access MSI Class Account



Check primary MSI group



The screenshot shows a terminal window with three tabs: 'Console', 'Terminal', and 'Background Jobs'. The 'Terminal' tab is active and has a red circle around its title. Below the tabs, the terminal shows the current directory as '/panfs/jay/groups/35/cheng423/cheng423/project_work'. The prompt is 'cheng423@acn01'. The command '% id -ng' has been entered, and the output 'cheng423' is displayed on the next line. A red arrow points from the output 'cheng423' to the left.

```
cheng423@acn01 [/panfs/jay/groups/35/cheng423/cheng423/project_work] % id -ng
cheng423
```

If output shows

- ▶ ecp8506, your primary group is ecp8506, storage available until 12/22/2024.
- ▶ Something else, you are involved in multiple groups. It's up to you to
 - ▶ Keep using the other group storage throughout the course
 - ▶ Following additional procedure to switch the primary group to ecp8506

The end

Next - Github and renv

Switch primary MSI group 1 (optional)

Console

Terminal x

Background Jobs x

R 4.3.0 · /panfs/jay/groups/37/ecp8506/cheng423/ ↗

R version 4.3.0 (2023-04-21) -- "Already Tomorrow"
Copyright (C) 2023 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)

R is free software and comes with ABSOLUTELY NO WARRANTY.
You are welcome to redistribute it under certain conditions.
Type 'license()' or 'licence()' for distribution details.

R is a collaborative project with many contributors.
Type 'contributors()' for more information and
'citation()' on how to cite R or R packages in publications.

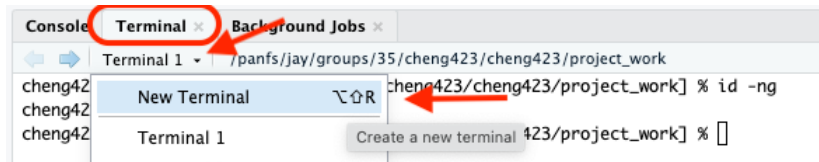
Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> setwd("/home/ecp8506/cheng423")

>



Switch primary MSI group 2 (optional)



Switch primary MSI group 3 (optional)



A terminal window titled 'Terminal 4' with the path '/panfs/jay/groups/37/ecp8506/cheng423'. The prompt is 'cheng423@acn01'. The first command is '% newgrp ecp8506', which is highlighted with a red arrow pointing to it from the text 'Switch primary group to "ecp8506"'. The second command is '% id -ng', which is highlighted with a red arrow pointing to it from the text 'Check primary group again, ensure changes happened as expected'. The output of the second command is 'ecp8506'.

```
Terminal 4 ▾ /panfs/jay/groups/37/ecp8506/cheng423
cheng423@acn01 [/panfs/jay/groups/37/ecp8506/cheng423] % newgrp ecp8506
cheng423@acn01 [/panfs/jay/groups/37/ecp8506/cheng423] % id -ng
ecp8506
```

Switch primary MSI group 4 (optional)

