

# ECP8506 Course Overview

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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

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- ▶ Assistant Professor at UMN ECP



- ▶ Contacts: [cheng423@umn.edu](mailto: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

## ▶ Primary

- ▶ Understand the concepts of model-informed decision making using pharmacometric simulations.
- ▶ Learn relevant tools (i.e., `mrgsolve`) to perform pharmacometric simulations.
- ▶ Know different simulation methods, and identify a method given scenarios.

## ▶ Secondary

- ▶ Learn other tools (e.g., 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 (i.e., simulate) 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 X101 - Introduction to the Minnesota Supercomputing Institute (MSI)

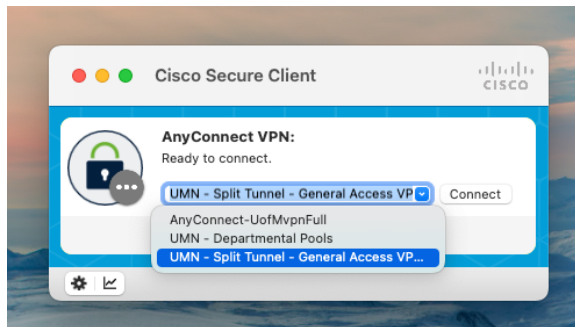
# MSI Access

- ▶ 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](mailto:help@msi.umn.edu), or (612)626-0802.

# Access MSI Class Account

[Home](#) / [My Interactive Sessions](#) / [RStudio Server](#)

## Interactive Apps

### Desktops

Desktop

Persistent Desktop

### GUIs

ANSYS Workbench

IGV

MATLAB

### IDEs

Abaqus

COMSOL Multiphysics

IDL

Mathematica

### Servers

Jupyter

RStudio Server

## RStudio Server

This app will launch [RStudio Server](#) an IDE for R. clusters.

Select class  
account "ecp8506"

### Account

ecp8506

### Resources

Interactive - 2 cores, 32 GB, 64 GB local scratch

### Time Limit

4 Hours

Shorter times will probably start faster

### R Version

R/4.3.0-openblas-rocky8

☒ Customize Environment

Let's keep R version consistent  
as 4.3.0 throughout the semester

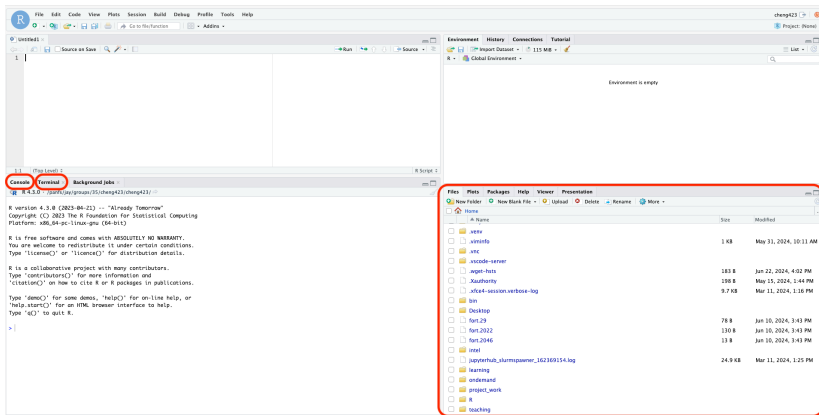
### Custom Environment

Enter commands (module load, source activate, etc) to create your desired environment.

☒ I would like to receive an email when the session starts

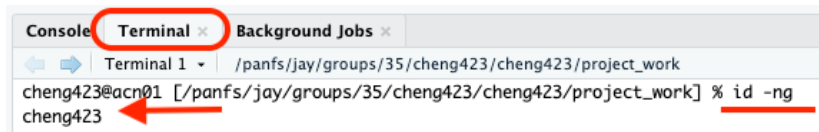
Launch

## 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. Another red arrow points from the prompt 'cheng423@acn01' to the left. The command 'id -ng' is underlined in red.

```
Console Terminal x Background Jobs x
Terminal 1 v /panfs/jay/groups/35/cheng423/cheng423/project_work
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 ×

Background Jobs ×

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.

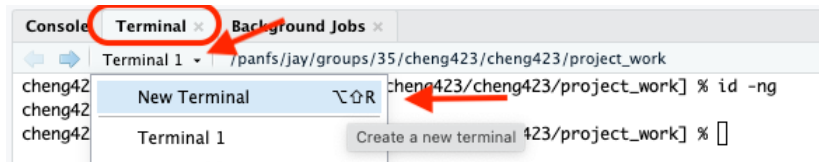
Type 'demo()' for some demos, 'help()' for on-line help, or  
'help.start()' for an HTML browser interface to help.  
Type 'q()' to quit R.

> 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 group to "ecp8506"

Check primary group again, ensure changes happened as expected

# Switch primary MSI group 4 (optional)

