

ECP8506 Course Overview

Shen Cheng

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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
 - ▶ B.S. in Biological Sciences, Soochow University
 - ▶ M.S. in Pharmacology, University of Michigan
 - ▶ Ph.D. in ECP (major in Pharmacometrics/minor in Biostatistics), University of Minnesota
 - ▶ Research Scientist, MetrumRG
- ▶ 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=d5zEAoIm9Zglqa2lGG5bZqkLRzLmJl.1>

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 (`mrqsolve`) 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

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

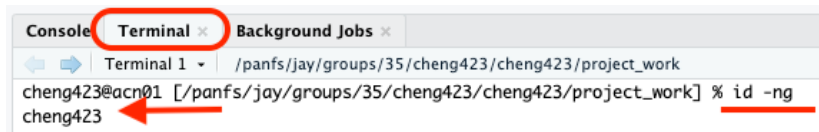
Custom Environment

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

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

Launch

Check primary MSI group



The screenshot shows a terminal window with three tabs: 'Console', 'Terminal', and 'Background Jobs'. The 'Terminal' tab is active and contains the following text:

```
Terminal 1 ▾ /panfs/jay/groups/35/cheng423/cheng423/project_work  
cheng423@acn01 [/panfs/jay/groups/35/cheng423/cheng423/project_work] % id -ng  
cheng423
```

Annotations in the image include a red circle around the 'Terminal' tab, a red arrow pointing from the 'id -ng' command to the output 'cheng423', and a red underline under the command 'id -ng'.

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.

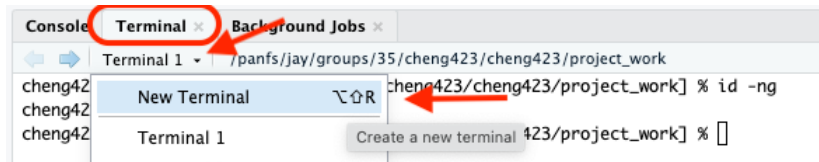
Type 'demo()' for some demos, 'help()' for on-line help, or
'help.start()' for an HTML browser interface to help.
Type 'q()' to quit R.

> 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 group to "ecp8506"

Check primary group again, ensure changes happened as expected

Switch primary MSI group 4 (optional)

