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



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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=d5zEAoIm9ZgIqa2IGG5bZqkLRzLmJI.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.

MSI

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)

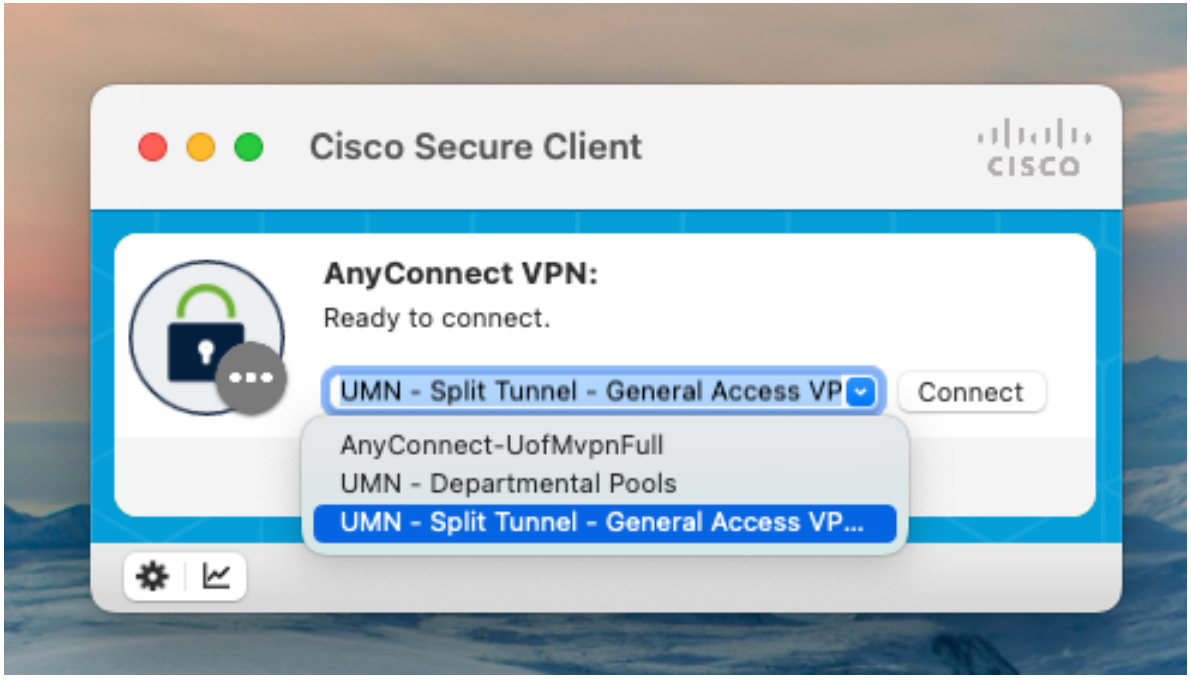
MSI Access

- 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

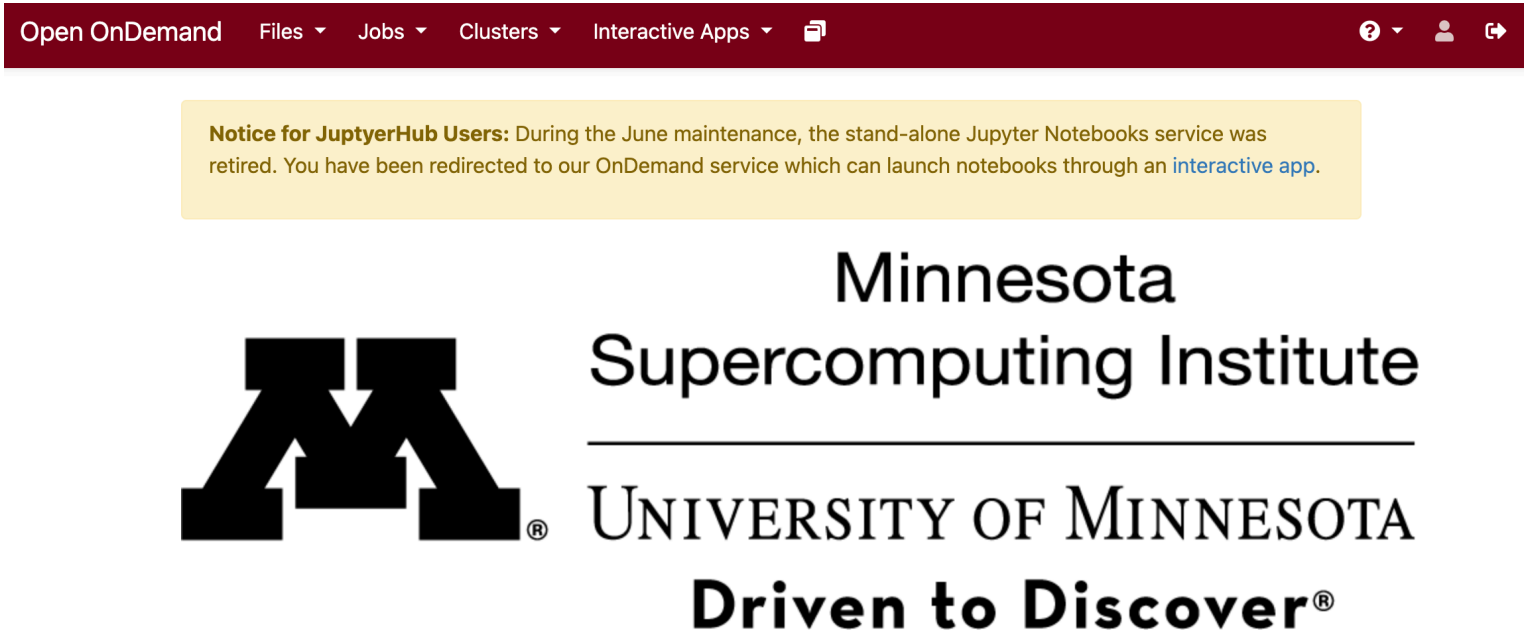
MSI is accessible if you are

- 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”**.

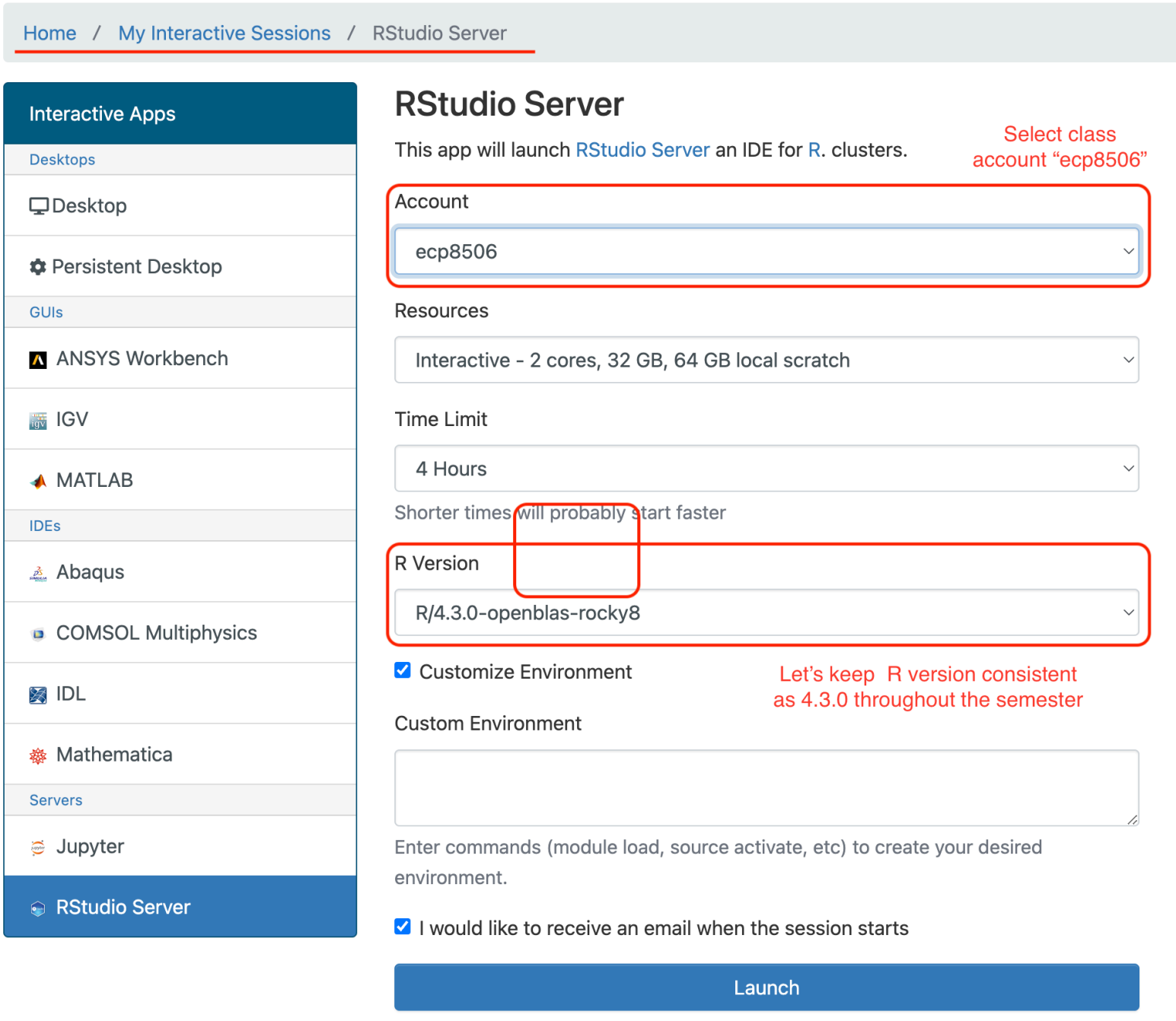


Interactive HPC

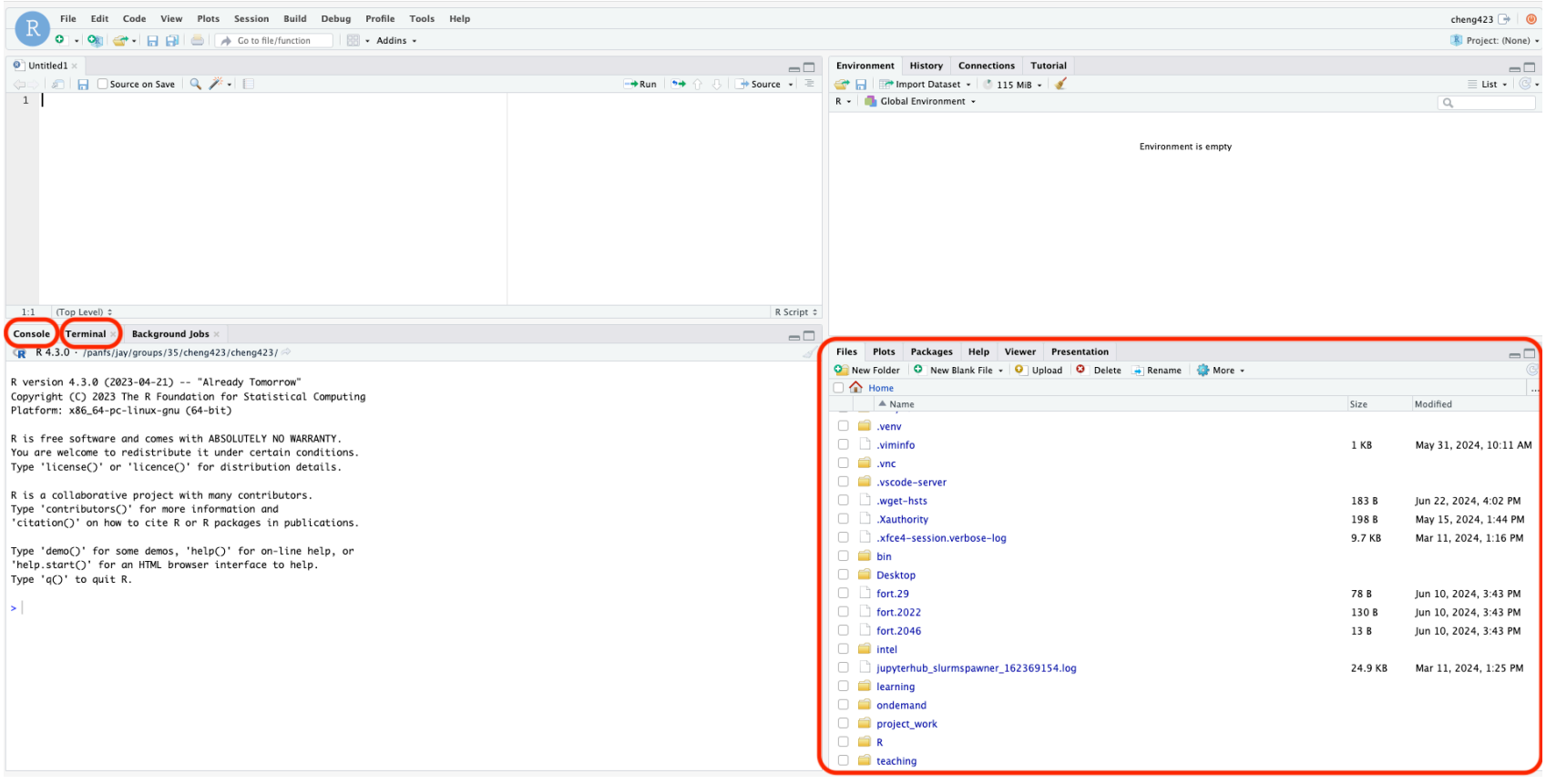
- Several ways are available to interact with MSI
- In this course, we will use Open Ondemand RStudio Server



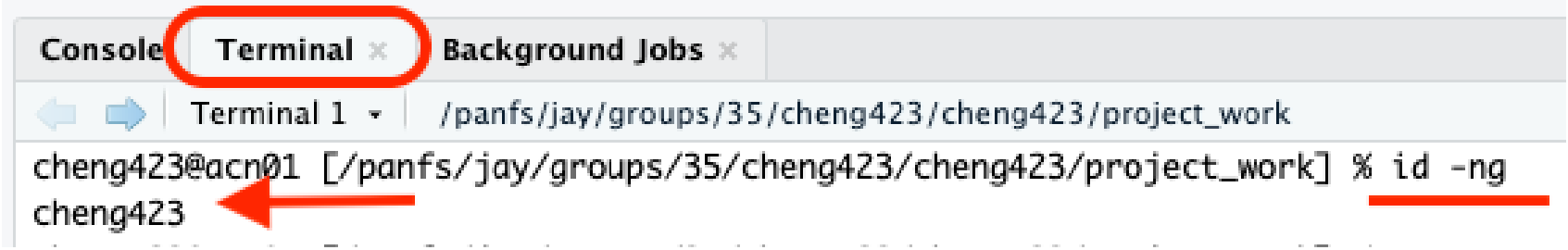
Access MSI Class Account



Access MSI Class Account



Check primary MSI group



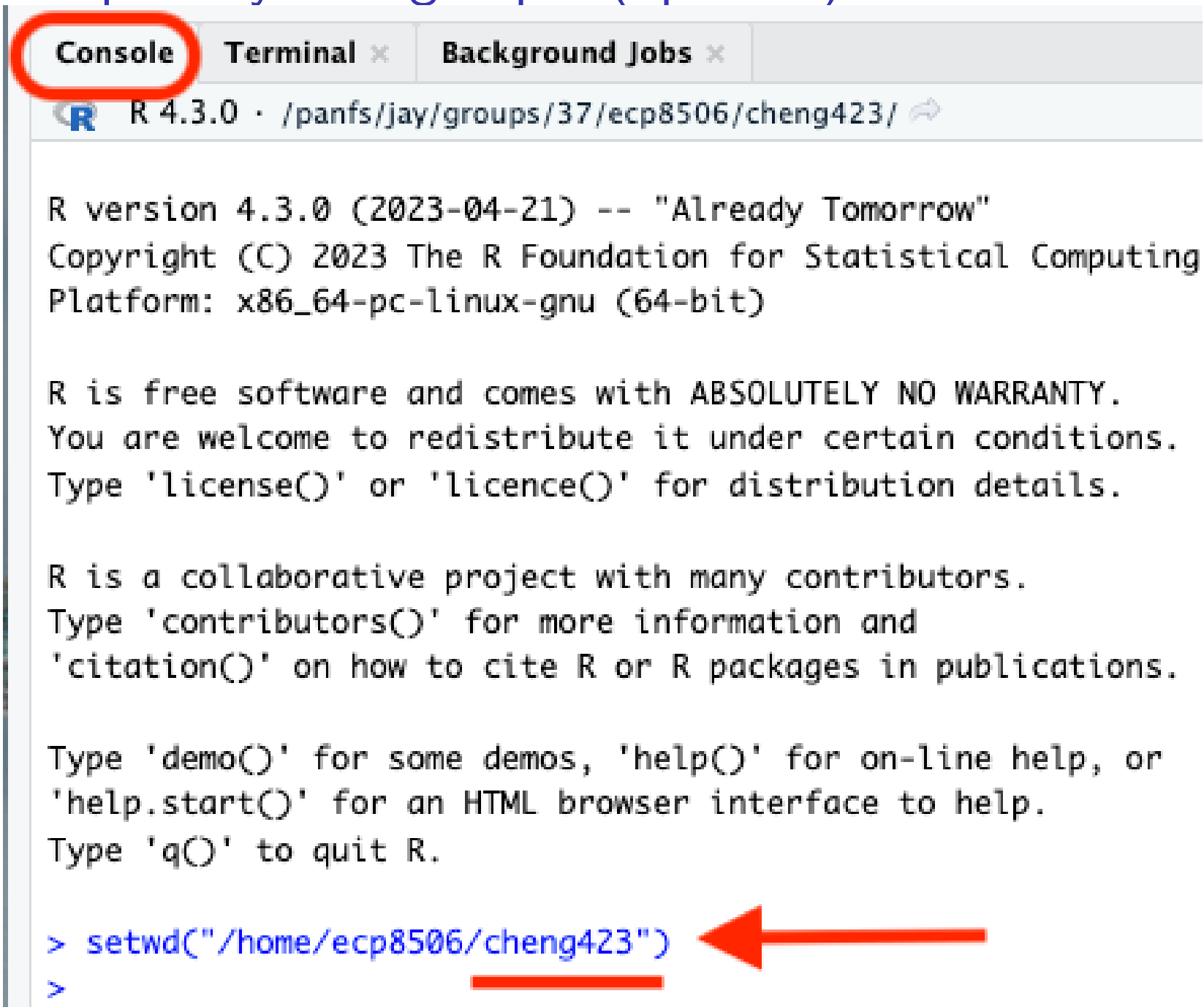
If output shows

- 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

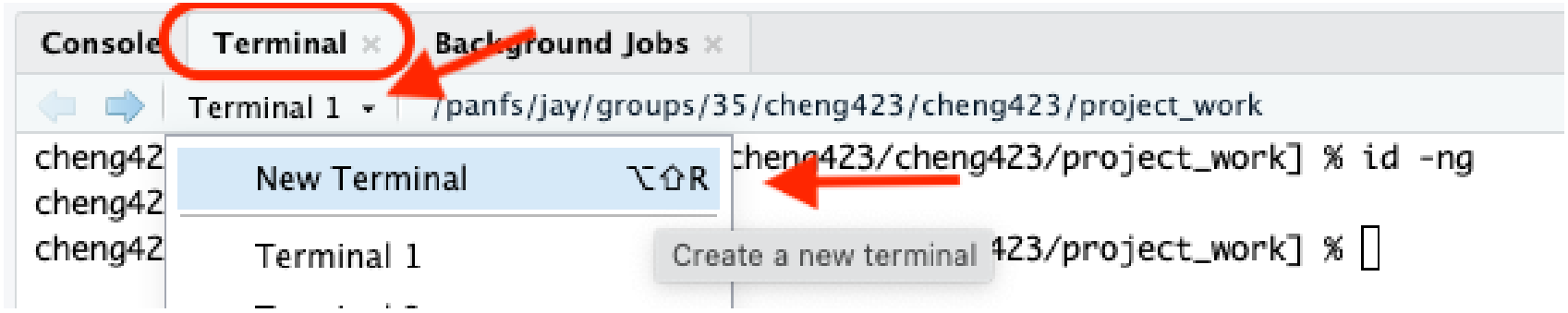
The end

Next - `Github` and `renv`

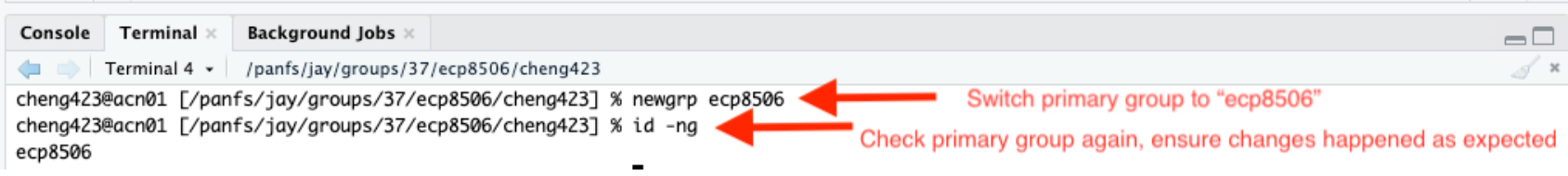
Switch primary MSI group 1 (optional)



Switch primary MSI group 2 (optional)



Switch primary MSI group 3 (optional)



Switch primary MSI group 4 (optional)