Parallel Computing in R

UCF Office of Research Cyberinfrastructure – November 12, 2025

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Office of Research Cyberinfrastructure's Mission

Our Mission:
Enable researchers through the effective use of research technology

Improve Research Computing and Data (RCD) Capabilities

Improve Technology Support for Researchers

CONTENTS

What is Parallel Processing?

Imagine there are **3 people**, we need to **urgently take them somewhere**.

What is Parallel Processing?

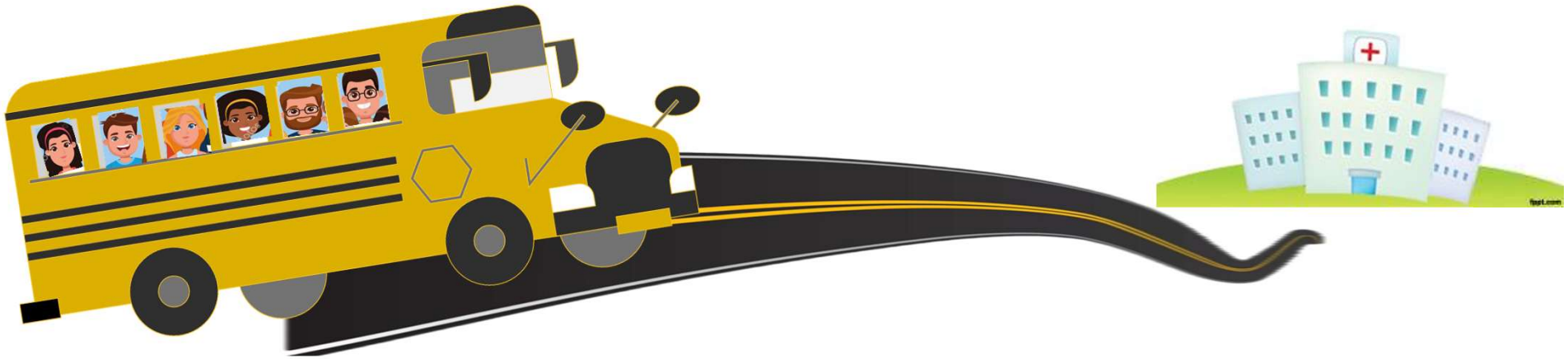
We can simply use a **car**.

What is Parallel Processing?

Imagine there are **10 people**, we need to **urgently take them somewhere**.

What is Parallel Processing?

We can use a **bus** this time.



What is Parallel Processing?

Now imagine we have **200** people, what is the **fastest way**?

What is Parallel Processing?

We can use a **multiple buses**, all working **at the same time**.

When to parallelize

- Our **goal** when doing parallel processing **reduce time-to-solution** by decomposing the work into **chunks that run simultaneously** on multiple cores/GPUs/nodes.

- Small Job

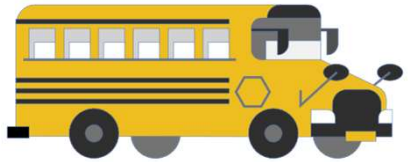
(small dataset, basic models, etc.)

Can be run on a **basic laptop CPU** using a **single core**

- Medium Job

(moderate dataset, heavier models, etc.)

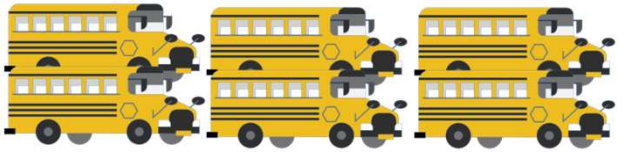
Can be done on a **powerful** laptop with **multi-core parallelization** on a single node.



- Heavy Job

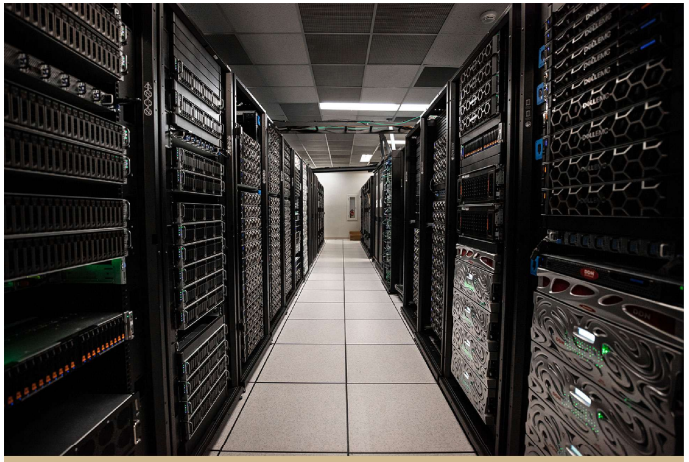
(very large dataset, LLM fine-tuning, etc.)

We need **super-computers** with powerful CPUs, utilizing **many cores / multiple CPUs in parallel.**



High Performance Computing (HPC)

- Parallel computing is the *technique* (splitting work to run at the same time). **HPC** is the *ecosystem* that uses those techniques at **large scale.**
- Use of **clustered CPUs/GPUs**, fast interconnects, and parallel software to run massive computations simultaneously.
- At UCF, **ARCC** houses two HPC clusters **Stokes (CPU)** and **Newton (GPU)**.
- **NSF ACCESS** and its resource providers deliver this HPC ecosystem to researchers, offering national-scale **clusters and supercomputers**.



High-Performance Computing systems inside the Data Center at Purdue University. These HPC systems are maintained and operated by the Rosen Center for Advanced Computing (RCAC).

HPC in R

Benefits

- R is suited for **Classical statistics workflows**, which benefit greatly from CPU parallelization—often simpler to parallelize than deep learning.
- **Scales** from a laptop to clusters with the same workflow and **minimal code changes**.
- Predictable speedups for independent tasks; easy to schedule lots of small jobs.

Limitations

- **GPU** in R is **niche**; most acceleration is CPU/threading, not ideal for deep learning tasks.
- There aren't many **direct parallel implementations** of specific statistical methods built into base R or CRAN packages.
- **Some** functions/packages just **won't run in parallel**.

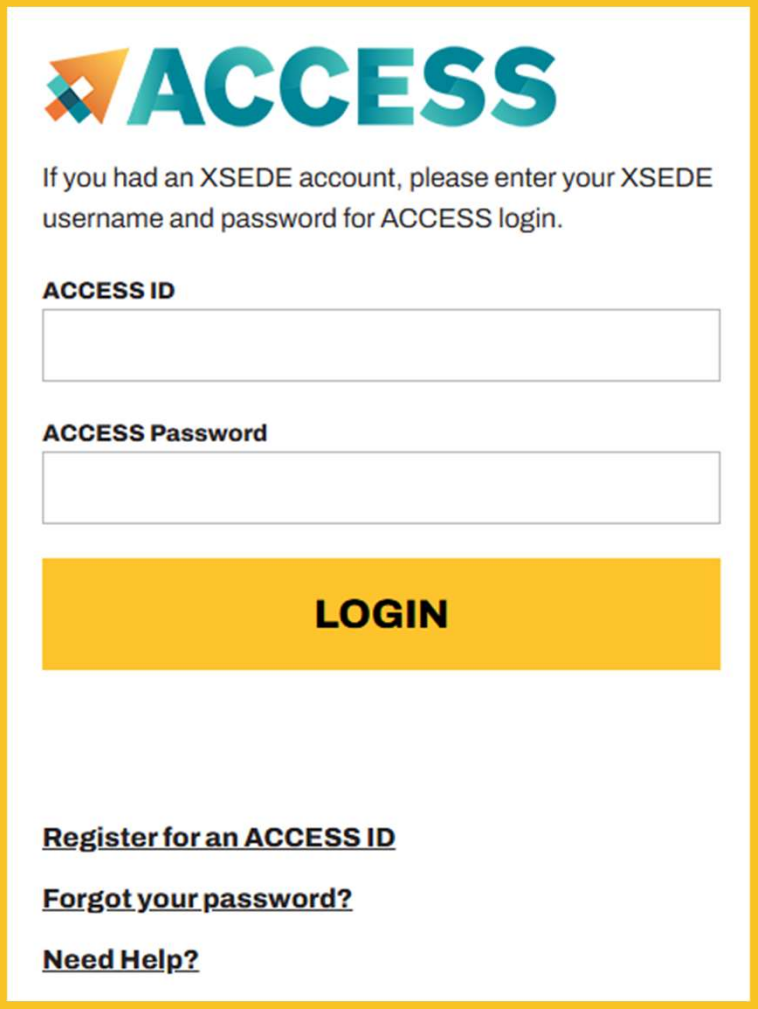
Accessing Purdue Anvil

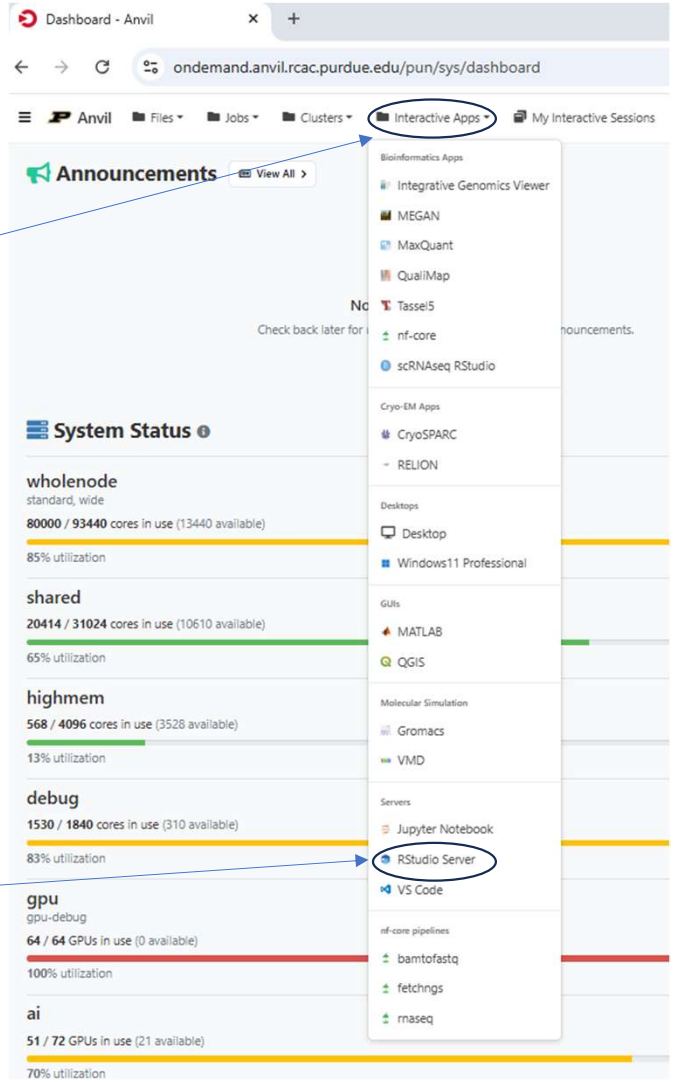
Step 1

https://ondemand.anvil.rcac.purdue.edu/

If not logged in already, log into ACCESS

(Make sure you have Duo authentication)





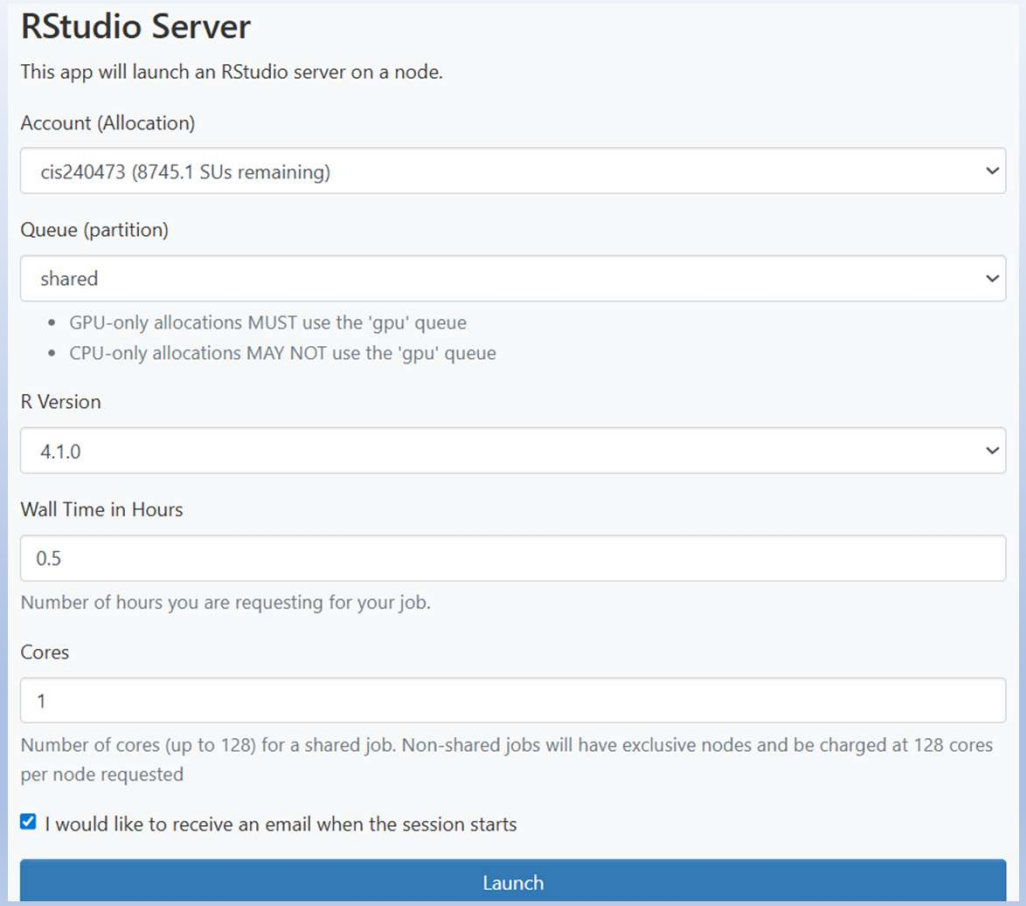
Purdue Anvil Open OnDemand (OOD)

OOD

Open OnDemand is an open-source web portal from the Ohio Supercomputing Center that lets users **access HPC resources through a browser** to manage files, submit jobs, and run graphical applications without installing software.

Interactive Application Menu

Dropdown lists all the **applications supported on Anvil** OOD. Clicking one of the applications will take you to a form through which you can **request the resources** you want to use.



Interactive RStudio Session

- **Account (Allocation):**
  The project or allocation that pays for your compute time (shows remaining Service Units).

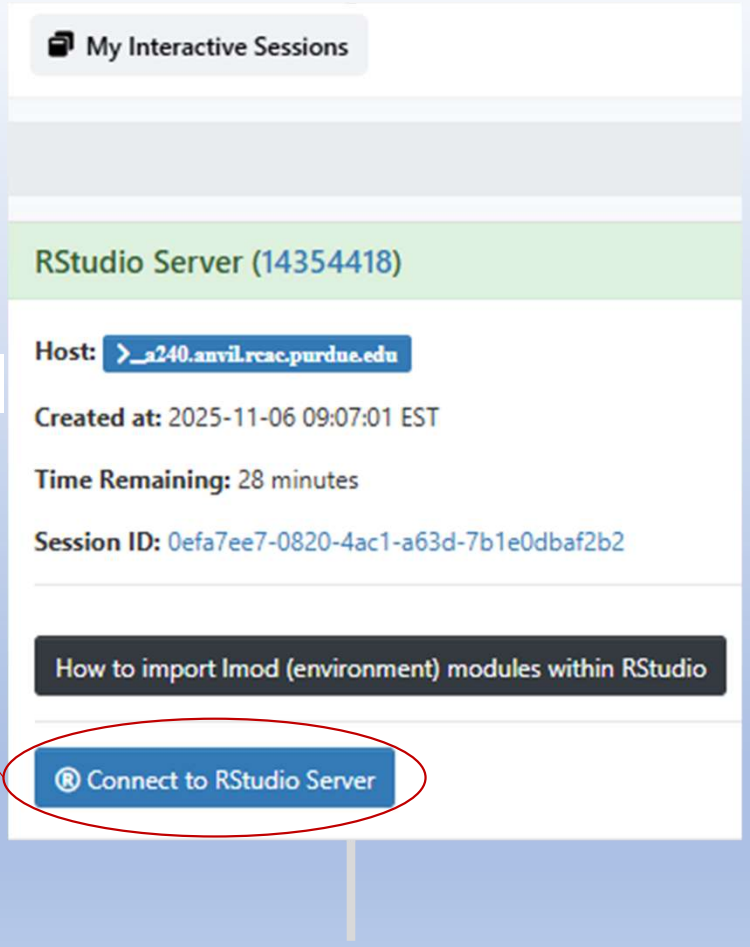
- **Queue (Partition):**
  shared – Runs on a shared CPU node
  wholenode – Gives you the entire node
  highmem – CPU nodes with **extra RAM** per node.
  gpu – Nodes with GPUs

- **Wall Time in Hours:**
  The maximum runtime for your session before it's automatically stopped.

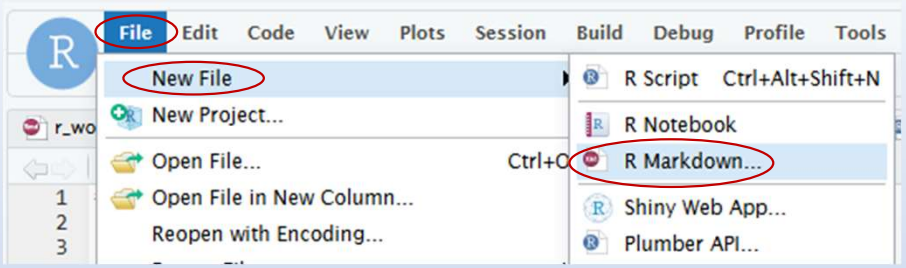
- **Cores:**
  Number of CPU cores to request (shared or exclusive use depending on queue).

Hands-On Practice (OOD)

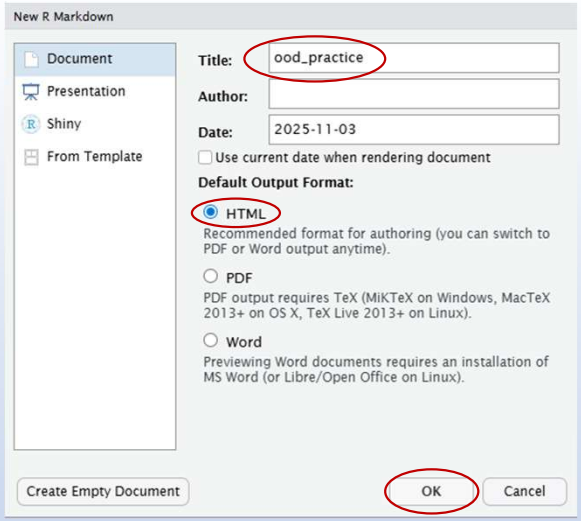
Connect to RStudio once session is ready



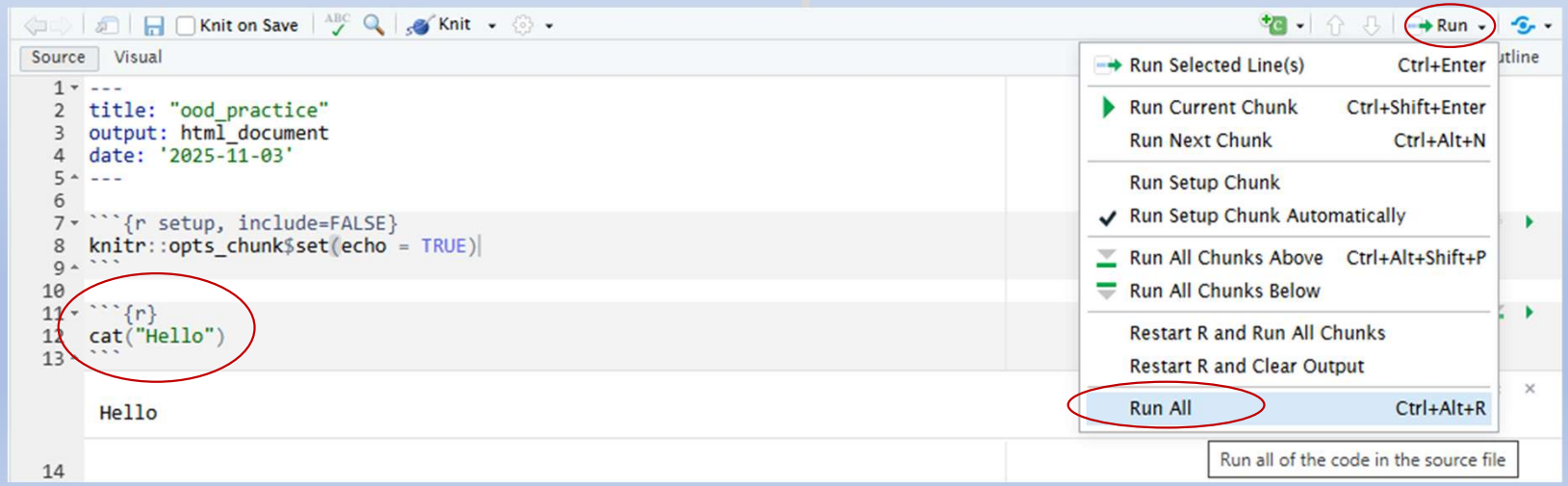
Step 1



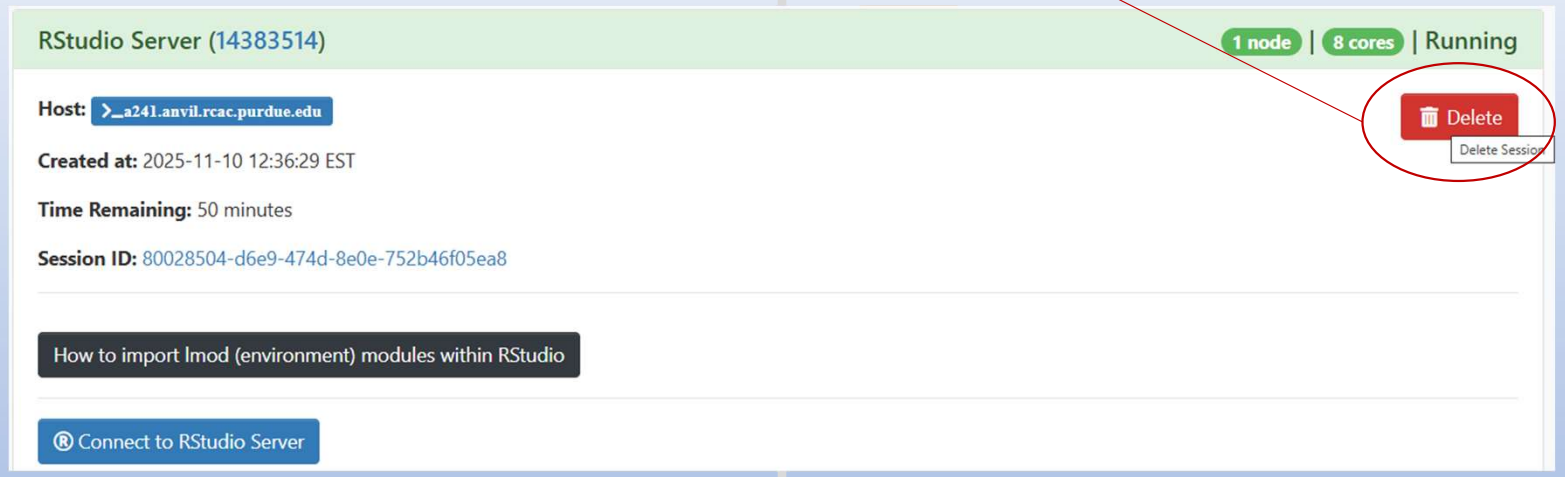
Step 2



Step 3



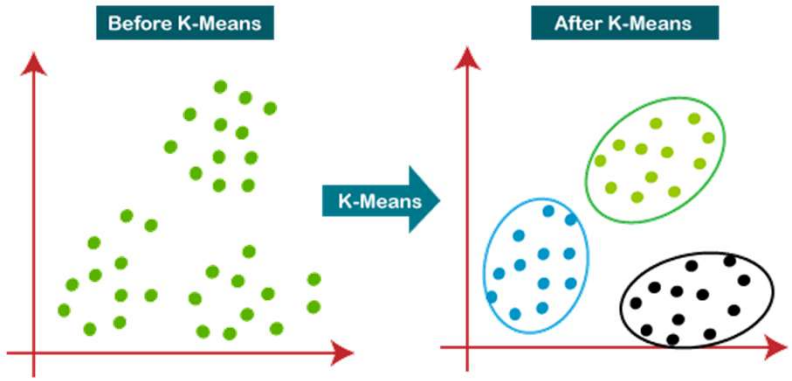
Delete once done to avoid using resources



Parallel K-means

K-Means Algorithm

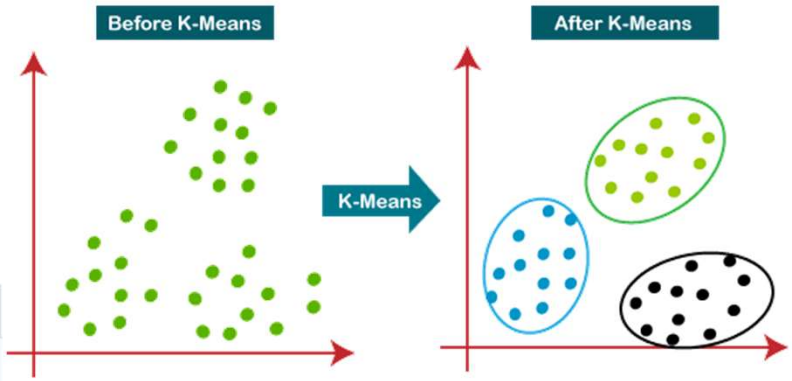
- K-means groups data into **K** clusters by similarity; you choose **K**, and the algorithm finds **centroids** (average points) for each group.
- It starts with **K** initial centroids and assigns every point to its **nearest** centroid.
- Then it **recomputes** each centroid as the mean of its assigned points and **repeats** assign → update until things stop changing much.



Task

- We have a synthetic dataset of ~ 500K patients
- We want to use the K-means Algorithm (in parallel) to group them based on their demographics
- Demographics are:

Race	String	`true`	Description of the patient's primary race.
Gender	String	`true`	Gender. `M` is male, `F` is female.
State	String	`true`	Patient's address state.
Healthcare_Expenses	Numeric	`true`	The total lifetime cost of healthcare to the patient (i.e. what the patient paid).
Healthcare_Coverage	Numeric	`true`	The total lifetime cost of healthcare services that were covered by Payers (i.e. what the insurance company paid).
Income	Numeric	`true`	Annual income for the Patient



```
library(parallel)
library(tictoc)
library(dplyr)
library(ggplot2)
library(fastDummies)
```

Libraries

- **parallel**
  - Built-in R package for multicore processing.
  - Provides functions to distribute work across CPU cores.
  - Ideal for running independent tasks simultaneously.

- **Tictoc:**
  - For timing

- **Dplyr, ggplot2:**
  - For visualizations.

- **fastDummies:**
  - To turn categorical variables into numeric dummy variables.

Parallel K-means Function

Goal: run many K-means initializations **in parallel** and keep the best solution.
Inputs: data (numeric matrix), **centers** (k), **n_cores** (workers), **n_starts** (restarts)
Output: a standard kmeans object (best run), identical to base R's kmeans()

- K-means is sensitive to initialization ⇒ we try *n_starts* independent runs.

- If n_cores is 1, we run basic kmeans()

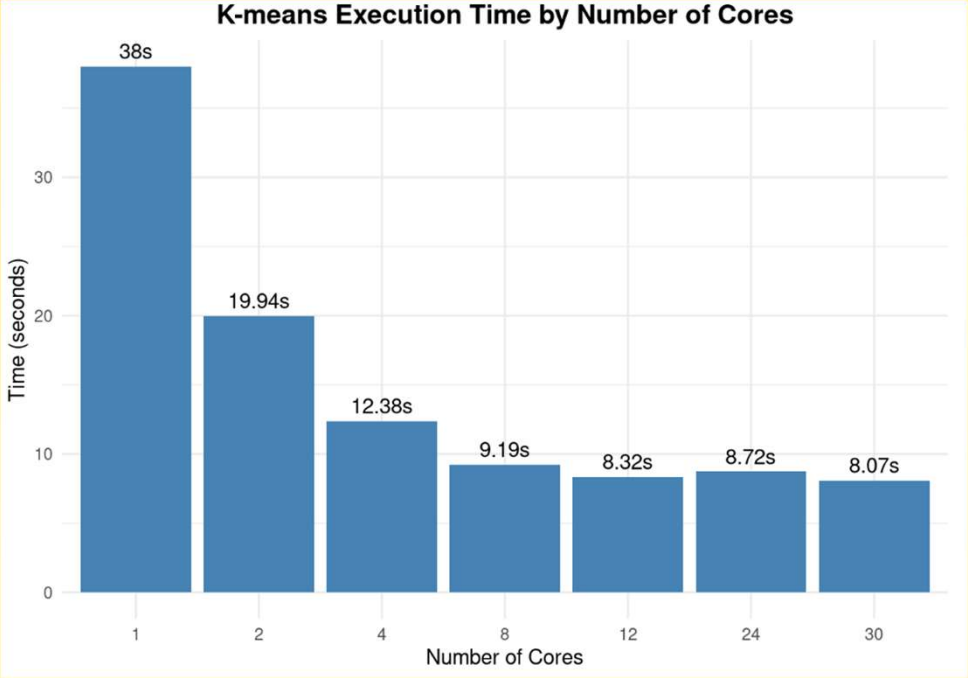
- ***makeCluster():***
- Launches *n_cores* independent R worker processes
- Each worker starts with a clean GlobalEnv

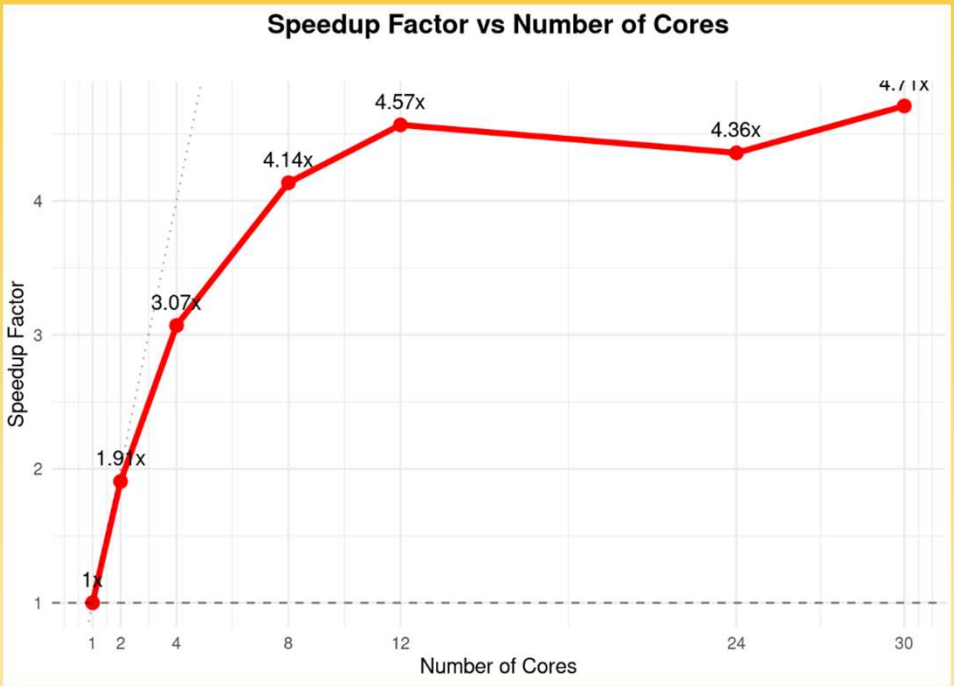
- ***clusterExport():***
- Copies objects from function environment to each worker's GlobalEnv

- ***parLapply():***
- Distributes *n_starts* tasks to workers

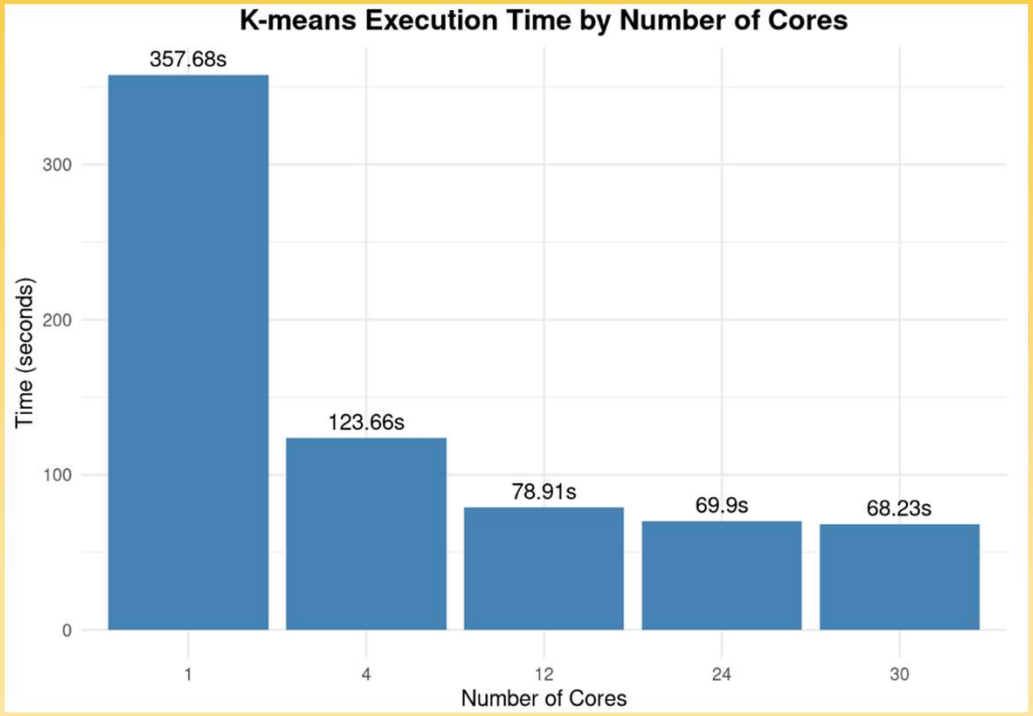
```r
# Function to run K-means with specified number of cores
parallel_kmeans <- function(data, centers = 10, n_cores = 1, n_starts = 25) {

  if (n_cores == 1) {
    # Sequential execution
    tryCatch({
      result <- kmeans(data, centers = centers, nstart = n_starts, iter.max = 100, algorithm = "Lloyd")
    }, error = function(e) {
      cat("Error in kmeans:", e$message, "\n")
      cat("Trying with fewer centers...\n")
      result <- kmeans(data, centers = min(5, centers), nstart = n_starts, iter.max = 100, algorithm = "Lloyd")
    })
  } else {
    # Parallel execution
    cl <- makeCluster(n_cores)

    # Export data to cluster
    clusterExport(cl, varlist = c("data", "centers"), envir = environment())

    # Run multiple K-means in parallel with error handling
    results <- parLapply(cl, 1:n_starts, function(i) {
      tryCatch({
        kmeans(data, centers = centers, nstart = 1, iter.max = 100, algorithm = "Lloyd")
      }, error = function(e) {
        # If error, try with fewer centers
        kmeans(data, centers = min(5, centers), nstart = 1, iter.max = 100, algorithm = "Lloyd")
      })
    })

    stopCluster(cl)

    # Select best result (lowest total within-cluster sum of squares)
    best_idx <- which.min(sapply(results, function(x) x$tot.withinss))
    result <- results[[best_idx]]
  }

  return(result)
}
```

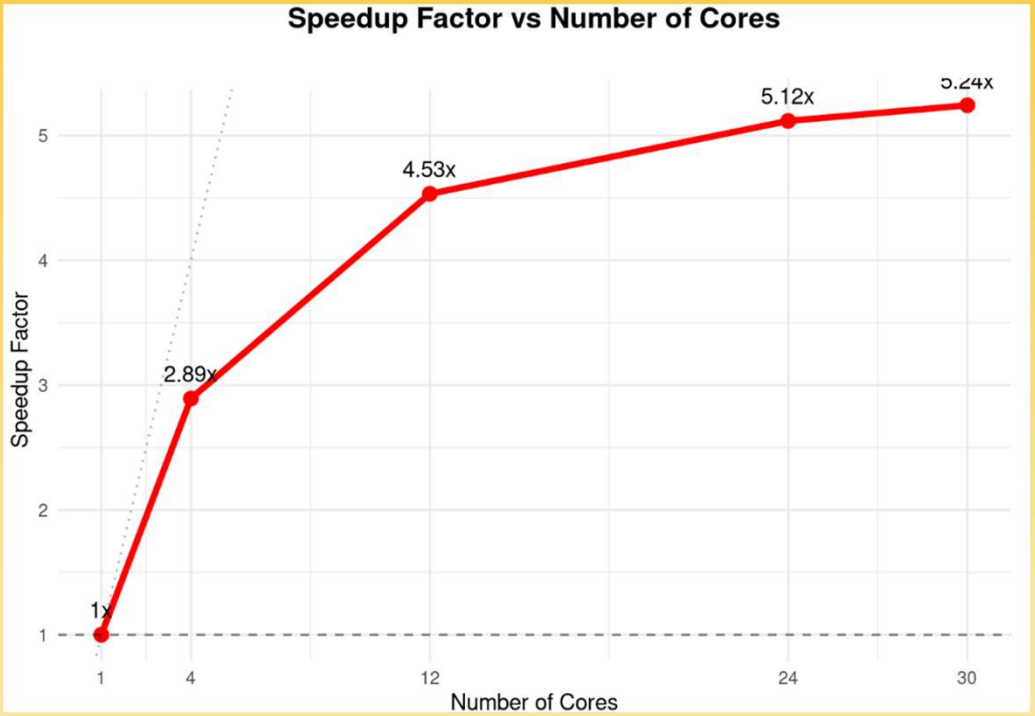
Performance





Performance
(on 10x larger dataset)

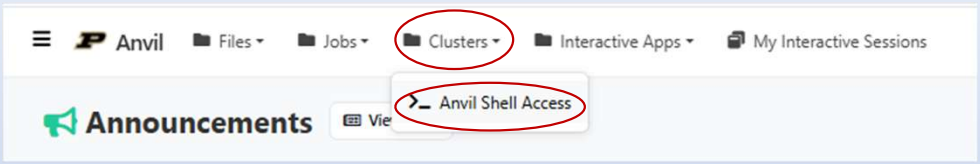




Hands-On Practice (Parallel K-means)

First, we get access to the files needed for the rest of the workshop

Step 1



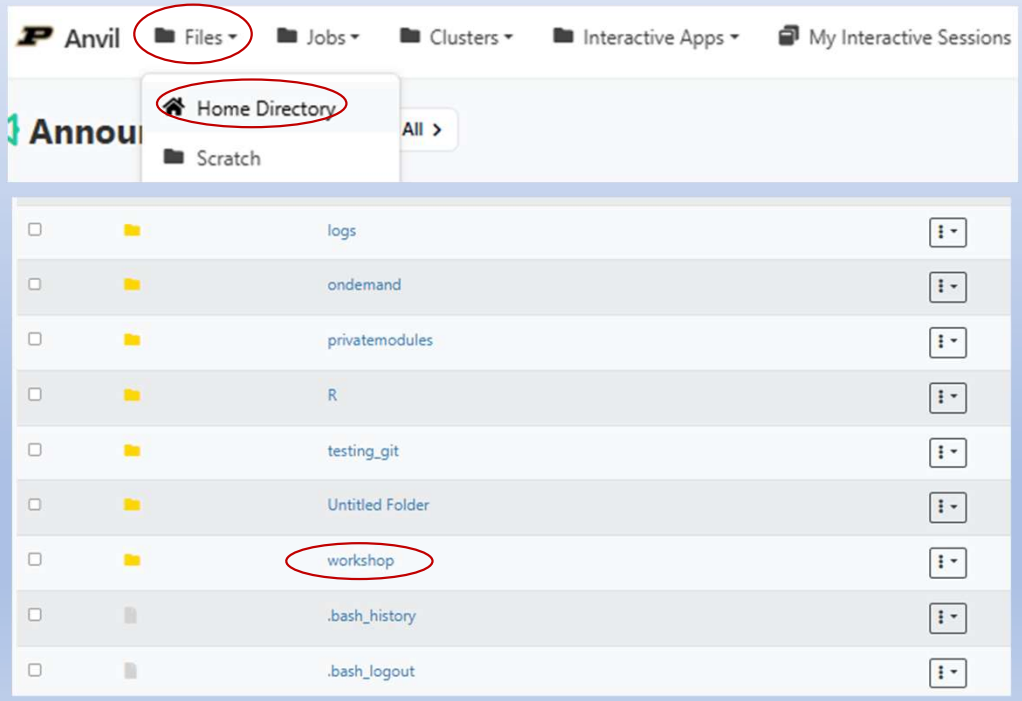
Step 2

Type command **git clone https://github.com/satyarforoughi/workshop**

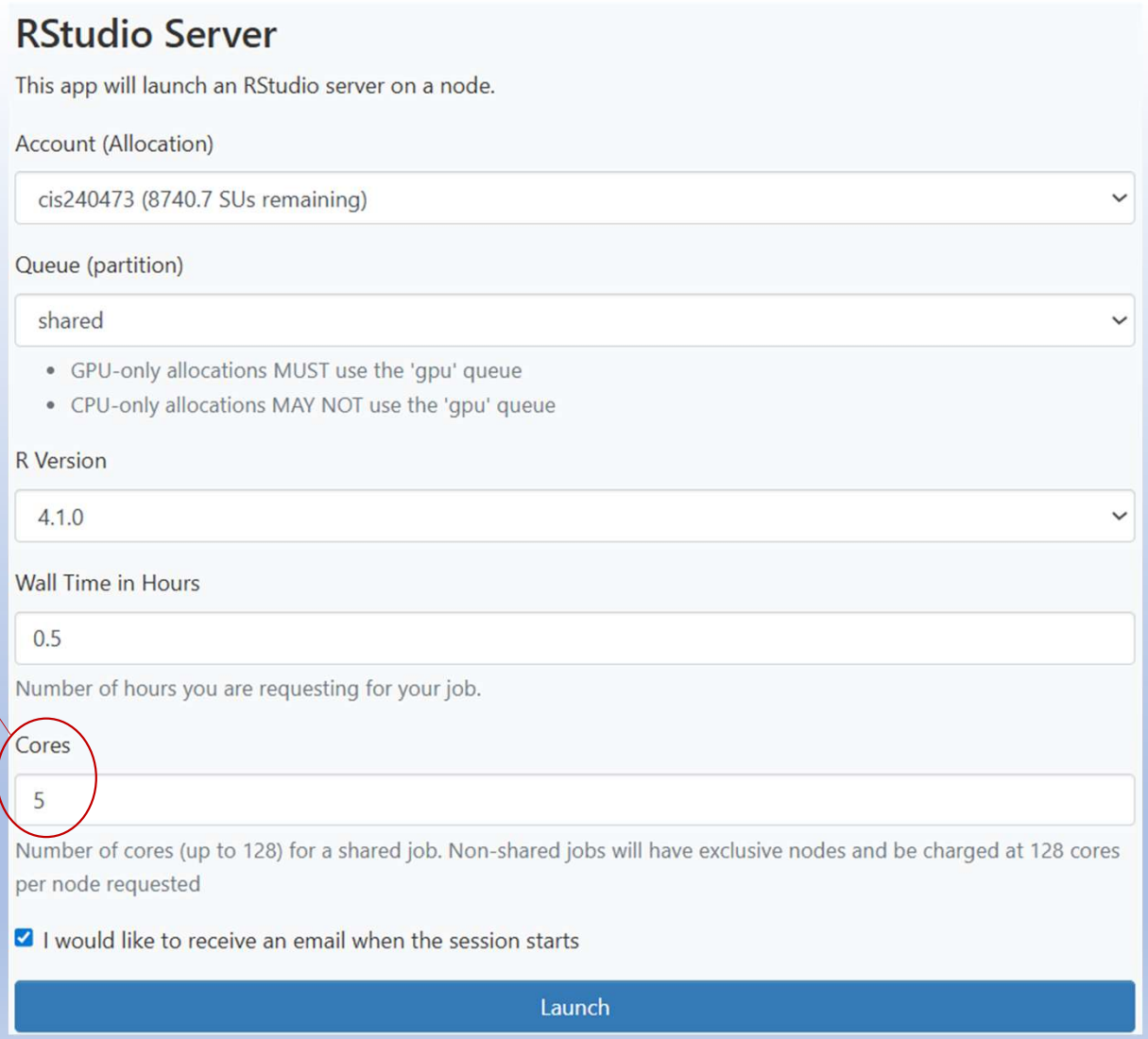
```
(base) x-sforoughi@login05.anvil:[~] $ git clone https://github.com/satyarforoughi/workshop
```

Checking

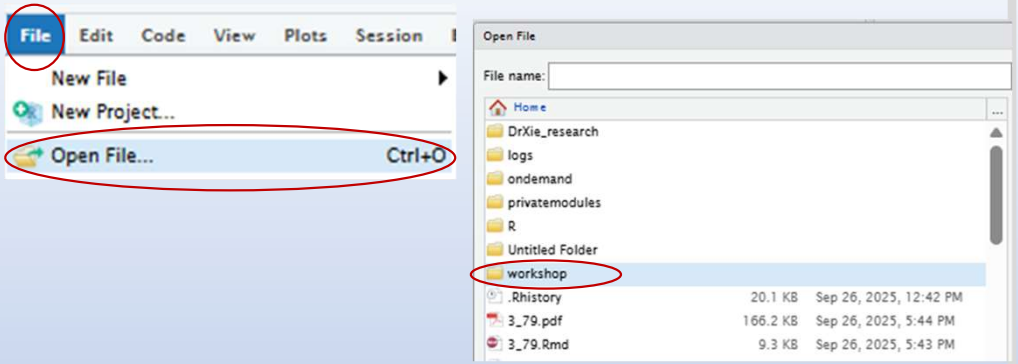
You should now see the folder “workshop” in Home Directory



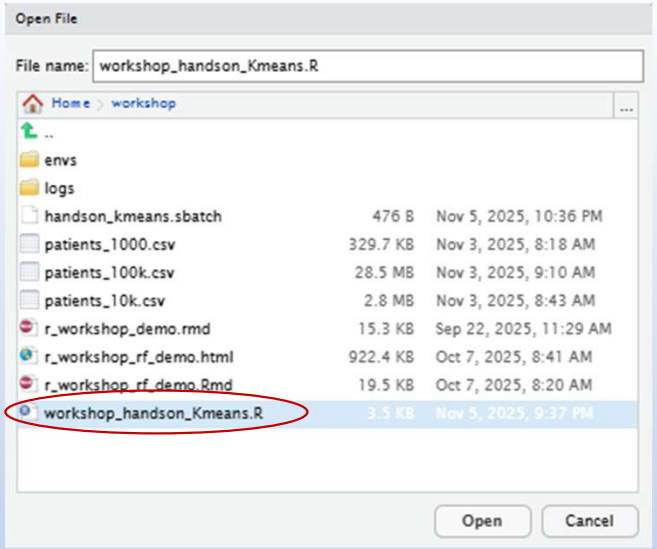
Request multiple cores



Step 1

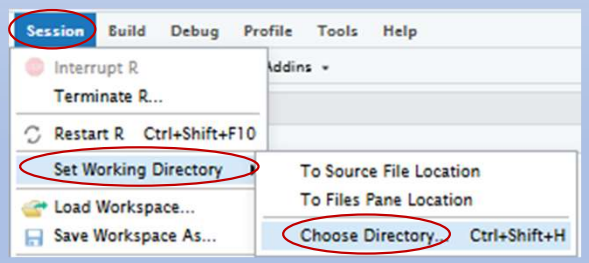


Step 2

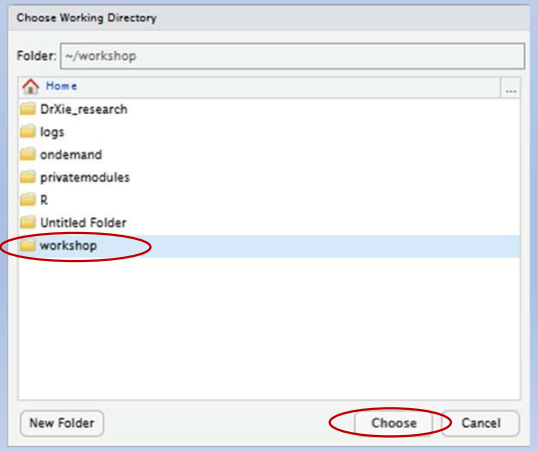


Set your session directory to the workshop folder

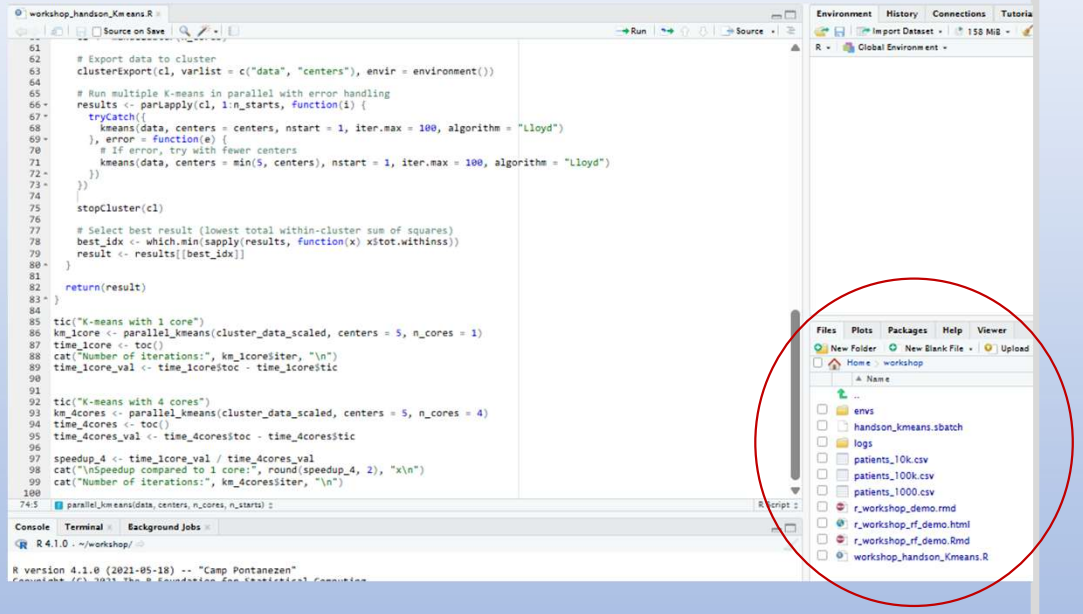
Step 3



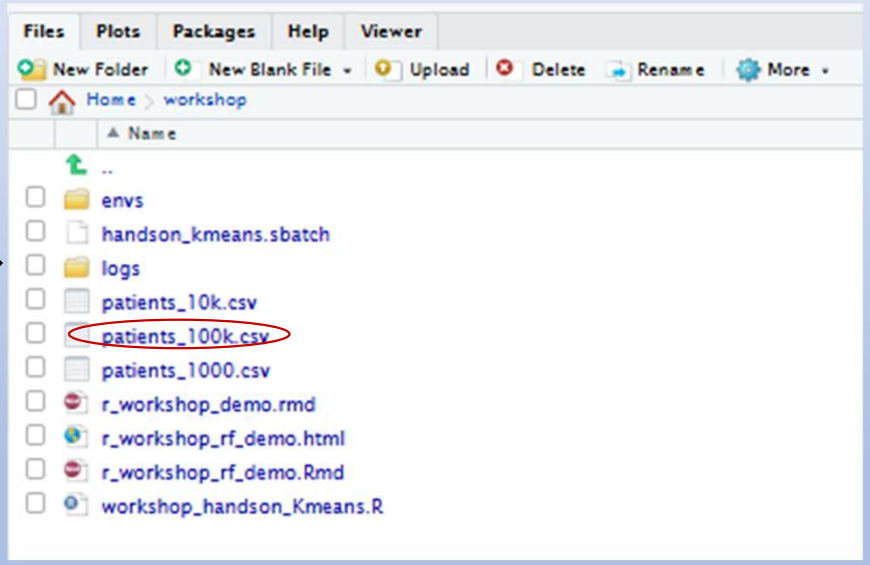
Step 4



Step 5



Make sure you see *patients_100k.csv* in files



Ctrl + Shift + Enter (Windows/Linux)
or ***Cmd + Shift + Enter*** (Mac)

To **run full script**

Using our parallel function and timing we compare using a **single core vs 4 cores** in parallel.

```
tic("K-means with 1 core")
km_1core <- parallel_kmeans(cluster_data_scaled, centers = 5, n_cores = 1)
time_1core <- toc()
cat("Number of iterations:", km_1core$iter, "\n")
time_1core_val <- time_1core$toc - time_1core$tic


tic("K-means with 4 cores")
km_4cores <- parallel_kmeans(cluster_data_scaled, centers = 5, n_cores = 4)
time_4cores <- toc()
time_4cores_val <- time_4cores$toc - time_4cores$tic

speedup_4 <- time_1core_val / time_4cores_val
cat("\nSpeedup compared to 1 core:", round(speedup_4, 2), "x\n")
cat("Number of iterations:", km_4cores$iter, "\n")
```

Output

```
Console   Terminal   Background Jobs
R 4.1.0 · ~/workshop/
> km_1core <- parallel_kmeans(cluster_data_scaled, centers = 5, n_cores = 1)

> time_1core <- toc()
K-means with 1 core: 11.198 sec elapsed

> cat("Number of iterations:", km_1core$iter, "\n")
Number of iterations: 17

> time_1core_val <- time_1core$toc - time_1core$tic

> tic("K-means with 4 cores")

> km_4cores <- parallel_kmeans(cluster_data_scaled, centers = 5, n_cores = 4)

> time_4cores <- toc()
K-means with 4 cores: 4.448 sec elapsed

> time_4cores_val <- time_4cores$toc - time_4cores$tic

> speedup_4 <- time_1core_val / time_4cores_val

> cat("\nSpeedup compared to 1 core:", round(speedup_4, 2), "x\n")

Speedup compared to 1 core: 2.52 x

> cat("Number of iterations:", km_4cores$iter, "\n")
Number of iterations: 11
>
```

Example 2

Changing parameters could also influence runtime.

```
tic("K-means with 1 core")
km_1core <- parallel_kmeans(cluster_data_scaled, centers = 3, n_cores = 1)
time_1core <- toc()
cat("Number of iterations:", km_1core$iter, "\n")
time_1core_val <- time_1core$toc - time_1core$tic


tic("K-means with 4 cores")
km_4cores <- parallel_kmeans(cluster_data_scaled, centers = 3, n_cores = 4)
time_4cores <- toc()
time_4cores_val <- time_4cores$toc - time_4cores$tic

speedup_4 <- time_1core_val / time_4cores_val
cat("\nSpeedup compared to 1 core:", round(speedup_4, 2), "x\n")
cat("Number of iterations:", km_4cores$iter, "\n")
```

Changing number of centers

```
> tic("K-means with 1 core")
> km_1core <- parallel_kmeans(cluster_data_scaled, centers = 3, n_cores = 1)
> time_1core <- toc()
K-means with 1 core: 5.93 sec elapsed
> cat("Number of iterations:", km_1core$iter, "\n")
Number of iterations: 30
> time_1core_val <- time_1core$toc - time_1core$tic
>
>
> tic("K-means with 4 cores")
> km_4cores <- parallel_kmeans(cluster_data_scaled, centers = 3, n_cores = 4)
> time_4cores <- toc()
K-means with 4 cores: 3.035 sec elapsed
> time_4cores_val <- time_4cores$toc - time_4cores$tic
>
> speedup_4 <- time_1core_val / time_4cores_val
> cat("\nSpeedup compared to 1 core:", round(speedup_4, 2), "x\n")

Speedup compared to 1 core: 1.95 x
> cat("Number of iterations:", km_4cores$iter, "\n")
Number of iterations: 22
```

Example 3

What happens if we try to use 8 cores?

```
### 5 vs 8 ###
tic("K-means with 5 cores")
km_5core <- parallel_kmeans(cluster_data_scaled, centers = 5, n_cores = 5)
time_5core <- toc()
cat("Number of iterations:", km_5core$iter, "\n")
time_5core_val <- time_5core$toc - time_5core$tic


tic("K-means with 8 cores")
km_8cores <- parallel_kmeans(cluster_data_scaled, centers = 5, n_cores = 8)
time_8cores <- toc()
time_8cores_val <- time_8cores$toc - time_8cores$tic

speedup_8 <- time_5core_val / time_8cores_val
cat("\nSpeedup compared to 5 cores:", round(speedup_8, 2), "x\n")
cat("Number of iterations:", km_8cores$iter, "\n")
```

5 vs 8 cores

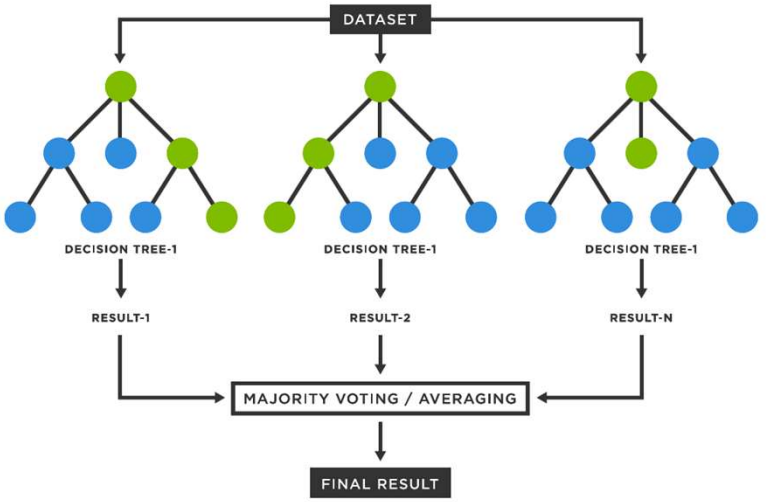
```
> tic("K-means with 5 cores")
> km_5core <- parallel_kmeans(cluster_data_scaled, centers = 5, n_cores = 5)
> time_5core <- toc()
K-means with 5 cores: 4.248 sec elapsed
> cat("Number of iterations:", km_5core$iter, "\n")
Number of iterations: 21
> time_5core_val <- time_5core$toc - time_5core$tic
>
>
> tic("K-means with 8 cores")
> km_8cores <- parallel_kmeans(cluster_data_scaled, centers = 5, n_cores = 8)
> time_8cores <- toc()
K-means with 8 cores: 4.565 sec elapsed
> time_8cores_val <- time_8cores$toc - time_8cores$tic
>
> speedup_8 <- time_5core_val / time_8cores_val
> cat("\nSpeedup compared to 5 cores:", round(speedup_8, 2), "x\n")

Speedup compared to 5 cores: 0.93 x
> cat("Number of iterations:", km_8cores$iter, "\n")
Number of iterations: 37
```

Parallel Random Forest

Random Forest Algorithm

- A Random Forest is like asking **many decision trees** the same question and then taking a **majority vote** (for categories) or an **average** (for numbers).

- Each tree learns from a **slightly different slice** of the data and looks at **random subsets of features**, so they don’t all make the same mistakes.



Task

- We have a synthetic dataset of ~ 500K patients
- We want to use a Random Forest model (in parallel) to predict their total hospital encounters from 2020 – 2025 based on their attributes (until 2020).
- Attributes are:

Race	String	`true`	Description of the patient's primary race.
Gender	String	`true`	Gender. `M` is male, `F` is female.
State	String	`true`	Patient's address state.
Healthcare_Expenses	Numeric	`true`	The total lifetime cost of healthcare to the patient (i.e. what the patient paid).
Healthcare_Coverage	Numeric	`true`	The total lifetime cost of healthcare services that were covered by Payers (i.e. what the insurance company paid).
Income	Numeric	`true`	Annual income for the Patient
Total Conditions	Numeric	`true`	Total diagnosed conditions before 2020.

```
library(parallel)
library(randomForest)
library(ranger)
library(tictoc)
library(dplyr)
library(ggplot2)
```

Libraries

- **randomForest**
  - Classic R implementation of the random forest algorithm.
- **ranger:**
  - Pre-built library for running RF in parallel.
- **Parallel, tictoc, Dplyr, ggplot2:**
  - Same as before.

“Manual” Parallel RF Function

Goal: build a Random Forest by **splitting trees across cores** and then **combining** the sub-forests.
Inputs: X (feature matrix), y (target), n_cores (workers), ntree (total trees), classification (TRUE/FALSE)
Output: a standard **randomForest** model (combined from per-core sub-forests).

clusterEvalQ():
- Executes given expression on each worker; here, library(randomForest).

clusterExport():
- Copies X, y, trees_per_core, classification to each worker’s GlobalEnv so the worker function can see them.

do.call(randomForest::combine()):
- Merges sub-forests into one final Random Forest model.

makeCluster(), parLapply():
- Same as before.

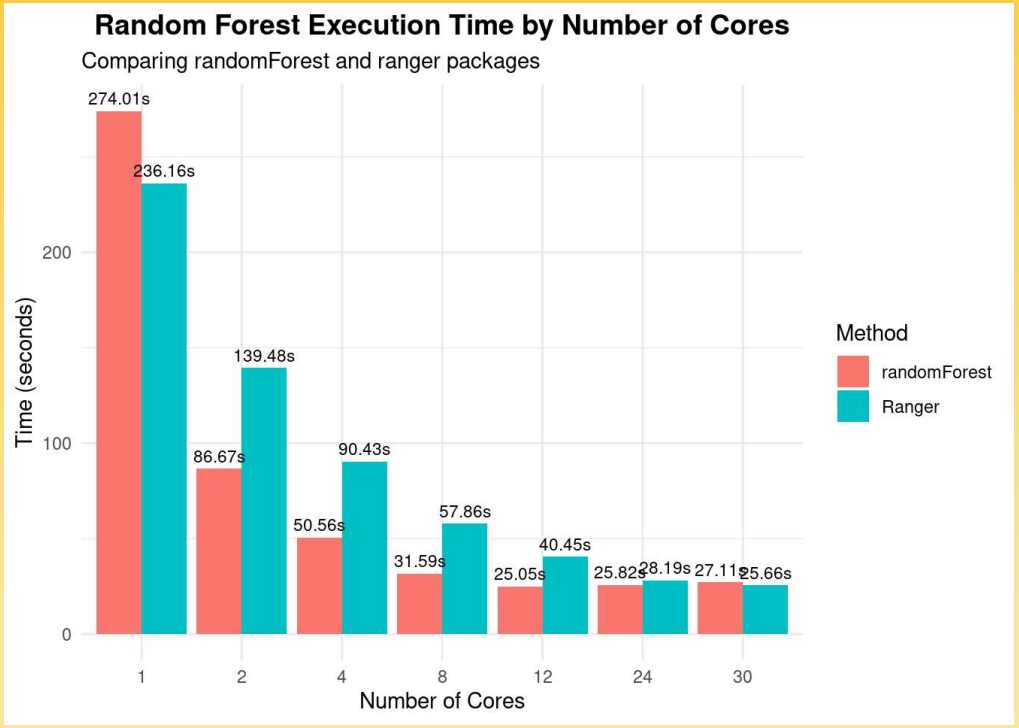
```r
# Function to run Random Forest with specified number of cores using randomForest package
parallel_rf_manual <- function(X, y, n_cores = 1, ntree = 500, classification = FALSE) {

  if (n_cores == 1) {
    # Sequential execution
    if (classification) {
      model <- randomForest(x = X, y = y, ntree = ntree, importance = TRUE)
    } else {
      model <- randomForest(x = X, y = y, ntree = ntree, importance = TRUE)
    }
  } else {
    # Parallel execution - split trees across cores
    trees_per_core <- ceiling(ntree / n_cores)

    # Create cluster
    cl <- makeCluster(n_cores)

    # Export necessary objects and load library on each worker
    clusterEvalQ(cl, library(randomForest))
    clusterExport(cl, varlist = c("X", "y", "trees_per_core", "classification"),
                  envir = environment())

    # Train Random Forest models in parallel
    rf_list <- parLapply(cl, 1:n_cores, function(i) {
      set.seed(i * 1000)  # Different seed for each worker
      if (classification) {
        randomForest(x = X, y = y, ntree = trees_per_core, importance = FALSE)
      } else {
        randomForest(x = X, y = y, ntree = trees_per_core, importance = FALSE)
      }
    })

    stopCluster(cl)

    # Combine forests using randomForest's combine function
    # Explicitly use randomForest::combine to avoid conflicts with dplyr
    model <- do.call(randomForest::combine, rf_list)
  }

  return(model)
}
```

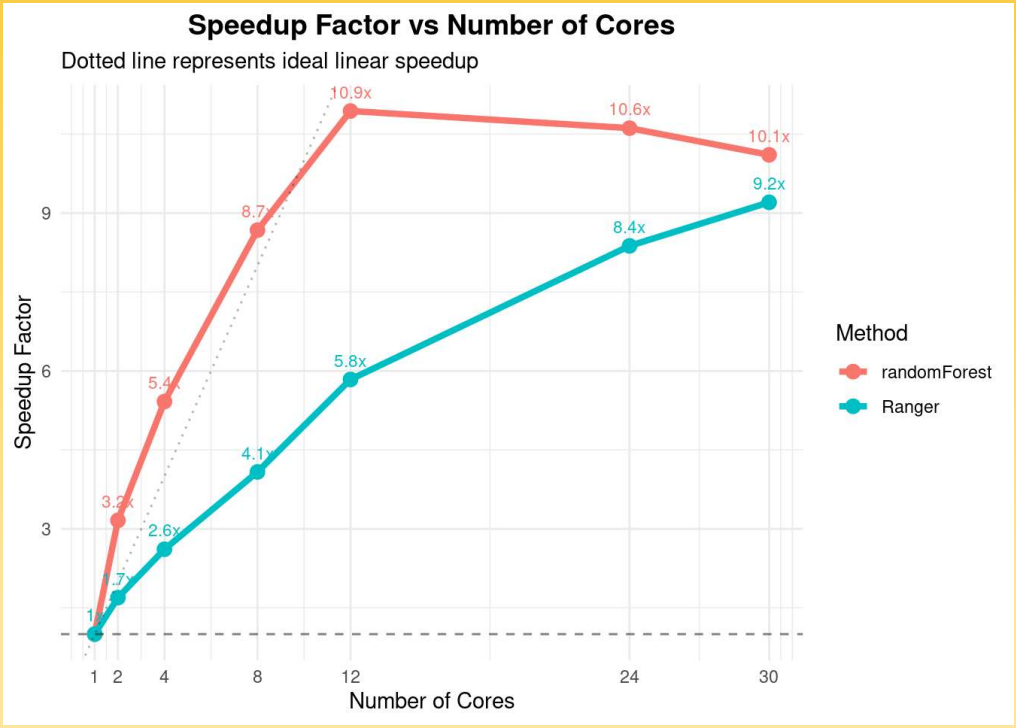
Using ranger

- The ranger library already has an implementation of random forest for parallel computing.
- We just put our data into the correct format
- Choose whether we want regression or classification

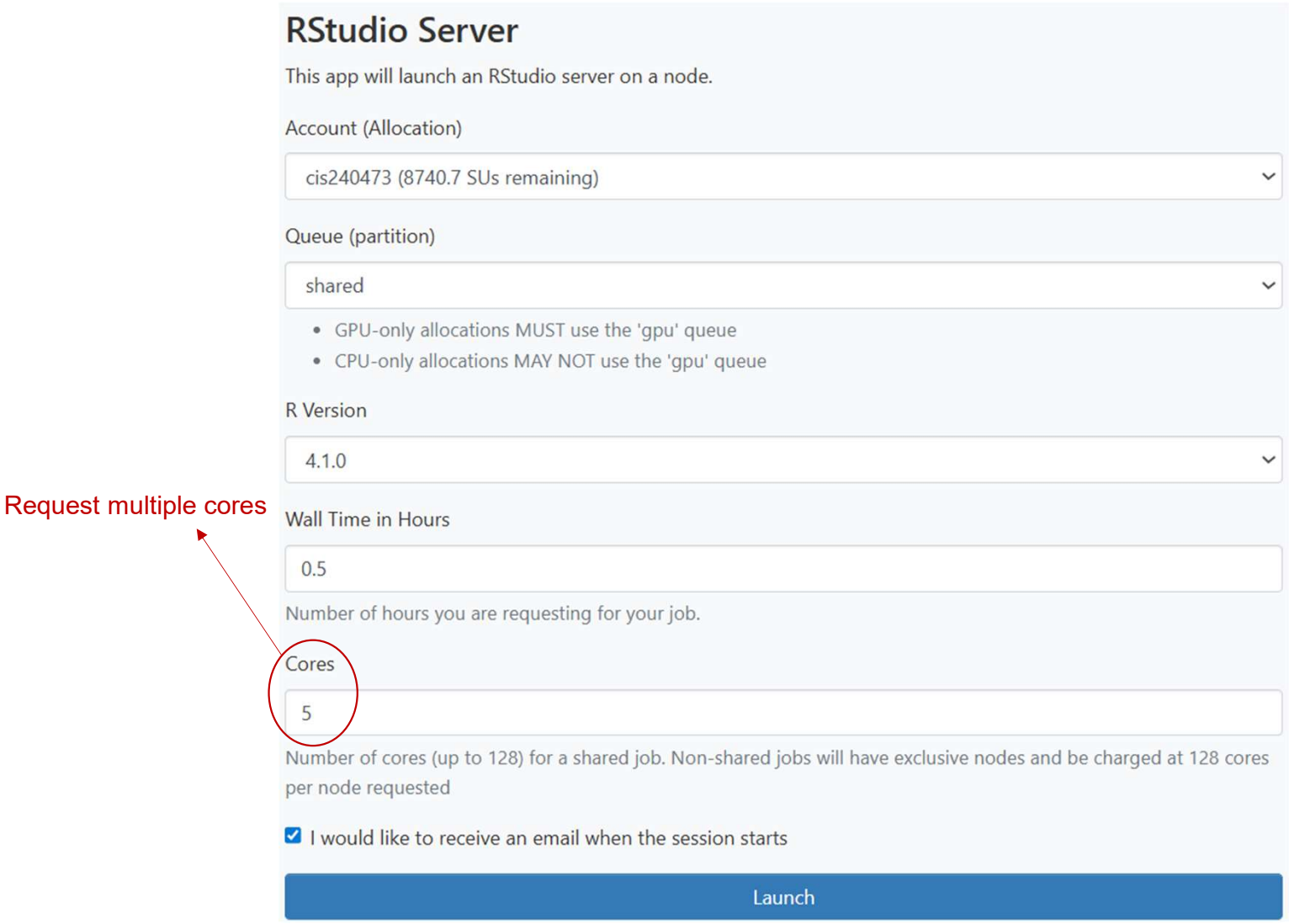
```r
# Function to run Random Forest using ranger (has built-in parallel support)
parallel_rf_ranger <- function(X, y, n_cores = 1, num_trees = 500, classification = FALSE) {

  # Combine X and y for ranger
  data_combined <- cbind(X, target = y)

  if (classification) {
    model <- ranger(target ~ .,
                    data = data_combined,
                    num.trees = num_trees,
                    importance = "impurity",
                    num.threads = n_cores,
                    classification = TRUE)
  } else {
    model <- ranger(target ~ .,
                    data = data_combined,
                    num.trees = num_trees,
                    importance = "impurity",
                    num.threads = n_cores)
  }

  return(model)
}
```

Performance

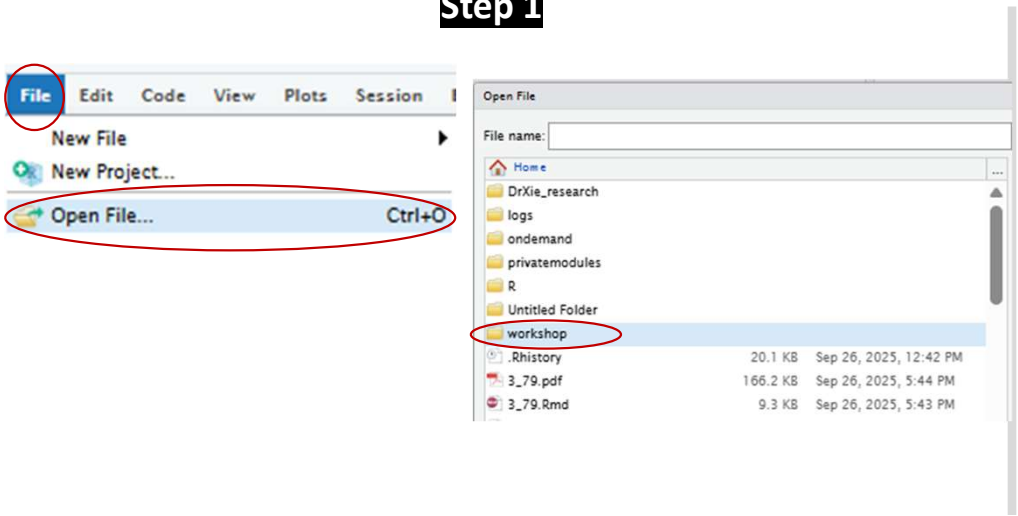




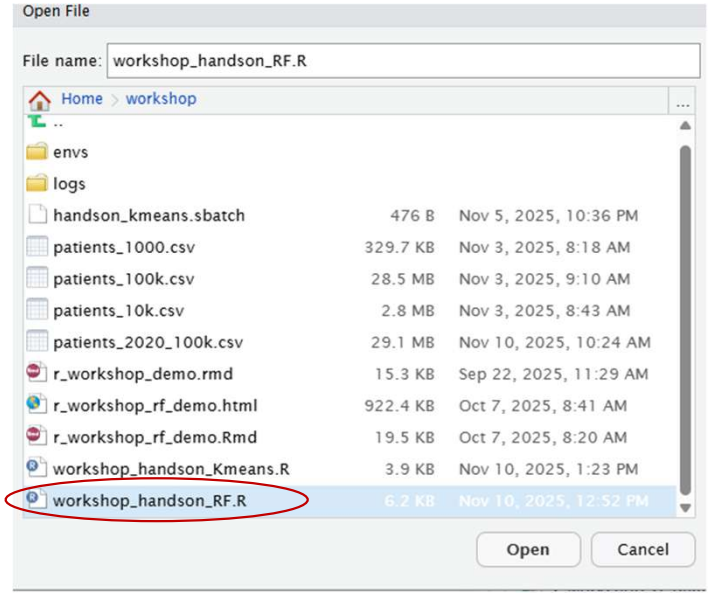
Hands-On Practice (Parallel RF)


RStudio Server
This app will launch an RStudio server on a node.
Account (Allocation)
cis240473 (8740.7 SUs remaining)
Queue (partition)
shared
GPU-only allocations MUST use the 'gpu' queue
CPU-only allocations MAY NOT use the 'gpu' queue
R Version
4.1.0
Request multiple cores
Wall Time in Hours
0.5
Number of hours you are requesting for your job.
Cores
5
Number of cores (up to 128) for a shared job. Non-shared jobs will have exclusive nodes and be charged at 128 cores per node requested
I would like to receive an email when the session starts
Launch

Step 1

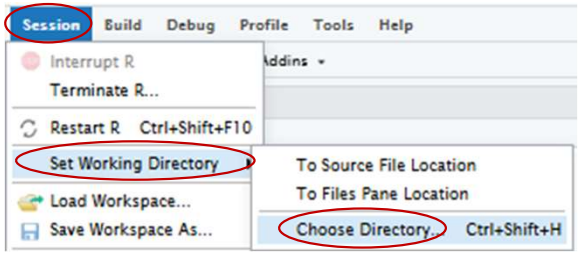


Step 2

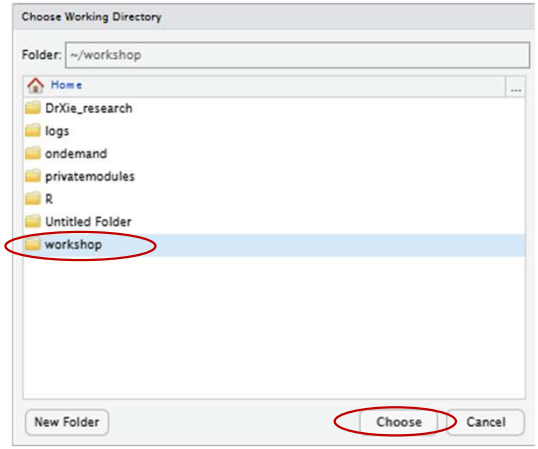


Set your session directory to the workshop folder

Step 3



Step 4



Ctrl + Shift + Enter (Windows/Linux)
or ***Cmd + Shift + Enter*** (Mac) ➡ To **run full script**

Using our parallel function and timing we compare using a **single core vs 4 cores** in parallel for both **manual** and **ranger library**.

```
tic("Random Forest Classification with 1 core (randomForest)")
rf_1core <- parallel_rf_manual(X_train_large, y_train_class_large,
                               n_cores = 1, ntree = 200, classification = TRUE)
time_1core <- toc()
time_1core_val <- time_1core$toc - time_1core$tic
# Evaluate model
pred_1core <- predict(rf_1core, X_test)
accuracy_1core <- mean(pred_1core == y_test_class)
cat("\nAccuracy:", round(accuracy_1core * 100, 2), "%\n")

tic("Random Forest Classification with 4 cores (randomForest)")
rf_4cores <- parallel_rf_manual(X_train_large, y_train_class_large,
                                n_cores = 4, ntree = 200, classification = TRUE)
time_4cores <- toc()
time_4cores_val <- time_4cores$toc - time_4cores$tic

speedup_4 <- time_1core_val / time_4cores_val
cat("\nSpeedup compared to 1 core:", round(speedup_4, 2), "x\n")
pred_4cores <- predict(rf_4cores, X_test)
accuracy_4cores <- mean(pred_4cores == y_test_class)
cat("Accuracy:", round(accuracy_4cores * 100, 2), "%\n")
```

```
cat("\n=== RANGER PACKAGE COMPARISON ===\n")
# Test with different core counts using ranger
ranger_times <- c()
ranger_cores <- c()

for (n_cores in c(1, 4)) {
  tic(paste("Ranger with", n_cores, "cores"))
  rf_ranger <- parallel_rf_ranger(X_train_large, y_train_class_large,
                                  n_cores = n_cores, num_trees = 200,
                                  classification = TRUE)
  time_ranger <- toc()
  ranger_times <- c(ranger_times, time_ranger$toc - time_ranger$tic)
  ranger_cores <- c(ranger_cores, n_cores)

  # Calculate accuracy
  pred_ranger <- predict(rf_ranger, data = cbind(X_test, target = y_test_class))$predictions
  accuracy_ranger <- mean(pred_ranger == y_test_class)
  cat("Accuracy:", round(accuracy_ranger * 100, 2), "%\n\n")
}
```

Output

```
> time_1core <- toc()
Random Forest Classification with 1 core (randomForest): 20.865 sec elapsed
> cat("\nAccuracy:", round(accuracy_1core * 100, 2), "%\n")

Accuracy: 52.17 %

> tic("Random Forest Classification with 4 cores (randomForest)")
> time_4cores <- toc()
Random Forest Classification with 4 cores (randomForest): 4.734 sec elapsed
Speedup compared to 1 core: 4.41 x

> pred_4cores <- predict(rf_4cores, X_test)

> accuracy_4cores <- mean(pred_4cores == y_test_class)

> cat("Accuracy:", round(accuracy_4cores * 100, 2), "%\n")
Accuracy: 51.95 %


Ranger with 1 cores: 14.728 sec elapsed
Accuracy: 51.86 %

Ranger with 4 cores: 4.518 sec elapsed
Accuracy: 52.45 %
```

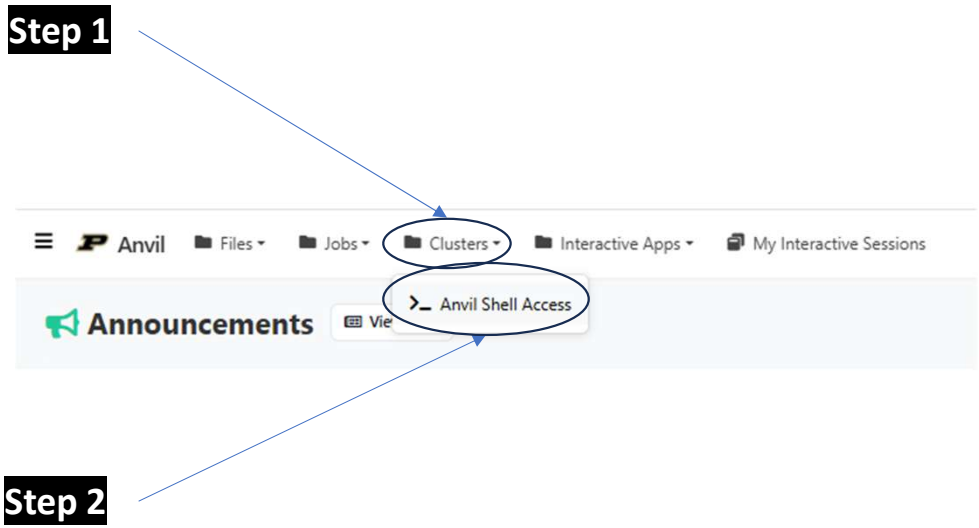
Command-Line Interface

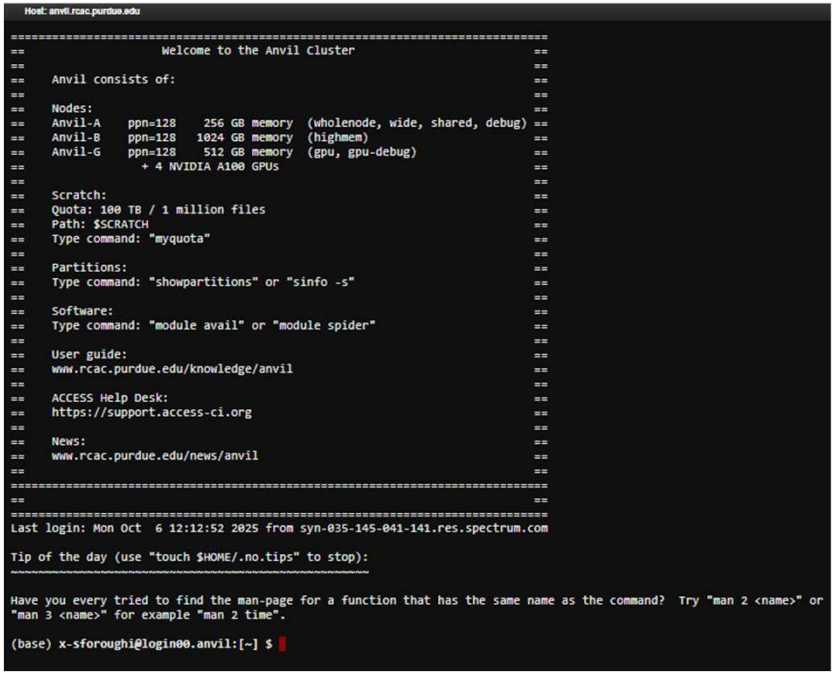
Command-Line Interface (CLI)

- The **CLI** is a text-based terminal where you run commands, and scripts for **full control** and reproducibility.
- Rather than waiting for an “interactive” session, such as OOD, we can utilize a **Slurm scheduler**.
- **Slurm** is the workload manager (scheduler) that allocates resources and runs your jobs on compute nodes. You **request resources** (CPUs, memory, GPUs, time) and Slurm **queues and dispatches** your job when those resources are available.

Hands-On Practice (CLI)

Accessing Terminal





Creating Folders and Files

- We create a **folder** in our home directory where our script **will install** the necessary **packages**

```
(base) x-sforoughi@login01.anvil:[~] $ mkdir -p ~/R/workshop_libs
```

- Change directory to workshop folder

```
(base) x-sforoughi@login01.anvil:[~] $ cd workshop
(base) x-sforoughi@login01.anvil:[workshop] $
```

Writing Slurm File

Similar to OOD

Folders to write outputs and errors

Load R

Set library folder

Run R script

```
#!/bin/bash
#SBATCH --account=cis240473
#SBATCH --partition=shared
#SBATCH --cpus-per-task=5
#SBATCH --time=00:30:00
#SBATCH --job-name=kmeans_cli
#SBATCH --output=logs/%x_%j.out
#SBATCH --error=logs/%x_%j.err

# Create logs dir if doesn't already exist
mkdir -p logs

echo "Job started at $(date)"
echo "This is being ran from $(pwd)"

module load r/4.4.1
export R_LIBS_USER=/home/$(whoami)/R/workshop_libs

Rscript workshop_handson_Kmeans.R

echo "Job completed at $(date)"
```

Creating Folders and Files

- **Run** the Slurm file

```
(base) x-sforoughi@login01.anvil:[workshop] $ sbatch handson_kmeans.sbatch
```

- **Check status** of your job iteratively

```
(base) x-sforoughi@login01.anvil:[workshop] $ watch squeue -u $USER
```

Cntrl + C to quit

- Once done, look at **output** and **error** files in logs

```
(base) x-sforoughi@login01.anvil:[workshop] $ cat logs/kmeans_cli_14352226.out
```

```
(base) x-sforoughi@login01.anvil:[workshop] $ cat logs/kmeans_cli_14352226.err
```

Thank You!

RESOURCES AND CONTACT INFO

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nandan.tandon@ucf.edu