

# KATANA FOR R

Fonti Kar

Workshop materials: <a href="https://github.com/UNSW-codeRs/katana4R">https://github.com/UNSW-codeRs/katana4R</a>

If you haven't already, please:

- Request for Katana access (takes a few days to process)
  - https://research.unsw.edu.au/katana
- Download and install FileZilla from <a href="https://filezilla-project.org/">https://filezilla-project.org/</a>



# OUTLINE

- What is Katana?
- The Workflow
- File transfer with FileZilla
- Job scripts
- Shell terminal, Katana on Demand
- Using screen
- Submitting your job

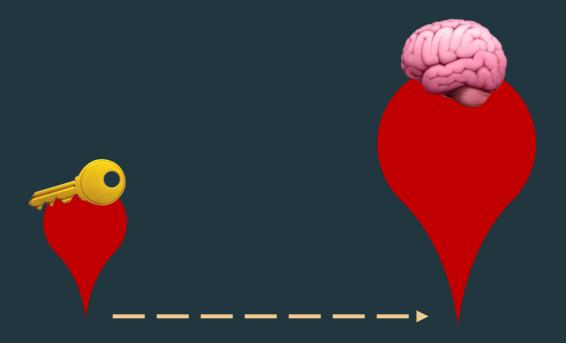


# HI! THIS IS KATANA.



Log in node

# HI! THIS IS KATANA.

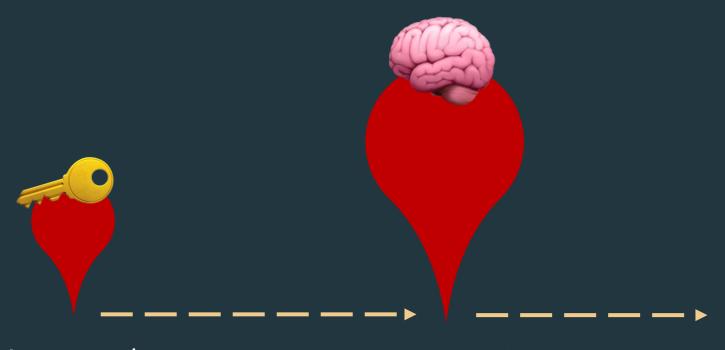


Log in node

Head node

Acquire resources
Directed to a computing node

### HI! THIS IS KATANA.





Log in node

Head node

Acquire resources

Directed to a computing node

Computing node(s) / cluster

UNSW wide / research center You get allocated to a node within a cluster\*

# WHEN DO I NEED KATANA?

- Time-consuming analyses
- Many iterative processes
- Computer is having a hard time.



### WHAT DO I NEED FOR KATANA?

ullet Get access. Apply with UNSW IT Service  $\overline{f V}$ 



Download and install FileZilla



Project hygiene



Self-contained workflow



Shell Terminal / Katana On Demand (KOD)



### WHAT DO I NEED FOR KATANA?

Get access. Apply with UNSW IT Service  $\sqrt{\phantom{a}}$ 



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Self-contained workflow



Shell Terminal / Katana On Demand (KOD)



### THE WORKFLOW

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#### 1. Write a job script:

- How much computational resources you require
- R version you need
- Which .R script to run
  - 2. Upload data, .R script + job script:
  - FileZilla
  - Katana Data Mover

#### 3. Submit job script via Shell Terminal

- Check the status of job
- Delete the job
- Run more jobs

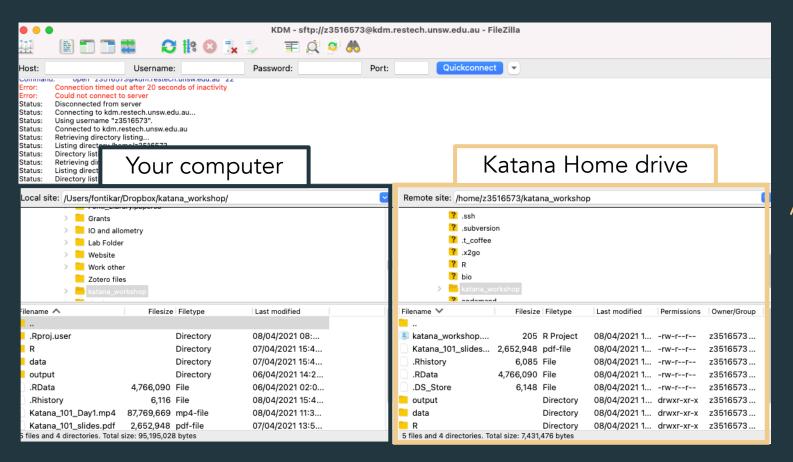


- 4. Download outputs from your job:
- FileZilla
- Katana Data Mover



### FILE TRANSFER WITH FILEZILLA 5

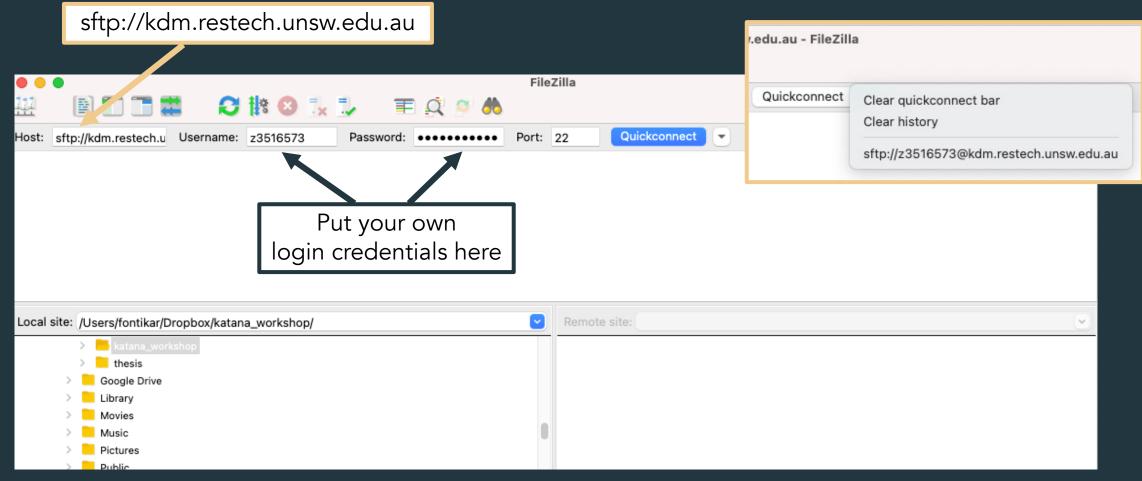
- Best way to move files between Katana and your computer
- Files are moved to via the Katana Data Mover server kdm.restech.unsw.edu.au



/home/z1234567



via Quickconnect



Set up once and find the KDM in drop down menu\*



#### Storage on Katana

Name of directory	File path	Backed up?	Storage limit	Best for
Home drive	/home/z1234567	Υ	10GB	Code, small data (<1GB)
Global scratch	/srv/scratch/z1234567	Ν	16TB	Shared data, or big data

# **EXERCISE**

- 1. Using FileZilla, Create a **pbs/** folder on Katana in <u>HOME</u> directory
- 2. Upload **katana\_workshop** to <u>GLOBAL SCRATCH</u>

Name of directory	File path	Backed up?	Storage limit	Best for
Home drive	/home/z1234567	Υ	10GB	Code, small data (<1GB)
Global scratch	/srv/scratch/z1234567	N	16TB	Shared data, or big data

### REQUESTING COMPUTATIONAL RESOURCES



#### WALL TIME - How long you need Katana for

- Biggest constraint
- <12 hrs can run anywhere, shorter wait
- >12 hrs can run on BEES only nodes



#### RAM MEMORY - How much working memory you need

- Important for spatial analyses e.g. raster data
- Lots of data? Need more memory for faster access



#### CPU CORES - How much processing power you need

- Less of an issue if working with a single model + simple tabulated data
- Can you optimise your code to run in parallel?

### REQUESTING COMPUTATIONAL RESOURCES





#### Every project's needs are different

- Get to know your analyses
- Monitor computer activity (Task Manager, Activity Monitor)

#### Trial-and-error

• Test your analysis out with less data or fewer iterations

If in doubt, start with defaults and work from there

Budgeting for slightly more but not too much



### JOB SCRIPTS Hear Let Me compy your The widely the wide



- The instructions you leave with Katana so your job(s) can run autonomously
- Simple .txt file (Notepad, Text Editor, Sublime Text 3) with .pbs suffix
- Upload\* using FileZilla in a pbs/ folder **/**



Self-contained workflow



- Resources you need (nodes, CPU, RAM, wall time)
- R version you need
- File path to the relevant working directory
- Which .R script to run

- 1. Resources you need (nodes, CPU, RAM, wall time)
- 2. R version you need
- 3. File path to the relevant working directory
- 4. Which .R script to run

All scripts must begin with #!/bin/bash

```
#!/bin/bash *
   #PBS -N job_name
   #PBS -l select=1:ncpus=1:mem=1gb
   #PBS -l walltime=1:00:00
   #PBS -M your.name@student.unsw.edu.au
   #PBS -m ae
   #Clear Katana workspace
   module purge
   #Loading R version
   module add R/4.0.2
14
   #Navigate to working direction
   cd /srv/scratch/z123456/katana_workshop
   #Run R code
   Rscript R/script_name.R
```

- 1. Resources you need (nodes, CPU, RAM, wall time)
- 2. R version you need
- 3. File path to the relevant working directory
- 4. Which .R script to run

Give your job a short, informative name e.g. growth\_glm\_logit

```
#!/bin/bash
   #PBS -N job_name
   #PBS -l select=1:ncpus=1:mem=1gb
   #PBS -l walltime=1:00:00
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```

- 1. Resources you need (nodes, CPU, RAM, wall time)
- 2. R version you need
- 3. File path to the relevant working directory
- 4. Which .R script to run

select: Number of nodes
ncpu: Number of CPU processors
mem: Amount of RAM memory

walltime: Length of job (hours)

```
#!/bin/bash
   #PBS -N job_name
    #PBS -l select=1:ncpus=1:mem=1gb
   #PBS -l walltime=1:00:00
   #PBS -M your.name@student.unsw.edu.au
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```

- 1. Resources you need (nodes, CPU, RAM, wall time)
- 2. R version you need
- 3. File path to the relevant working directory
- 4. Which .R script to run

Email for Katana to reach you

```
#!/bin/bash
   #PBS -N job_name
   #PBS -l select=1:ncpus=1:mem=1gb
   #PBS -l walltime=1:00:00
   #PBS -M your.name@student.unsw.edu.au
   #PBS -m ae
   #Clear Katana workspace
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    cd /srv/scratch/z123456/katana_workshop
   #Run R code
   Rscript R/script_name.R
```

- 1. Resources you need (nodes, CPU, RAM, wall time)
- 2. R version you need
- 3. File path to the relevant working directory
- 4. Which .R script to run

When should Katana to email you?

a = when job aborts with error

e = when job ends naturally

```
#!/bin/bash
   #PBS -N job_name
   #PBS -l select=1:ncpus=1:mem=1gb
   #PBS -l walltime=1:00:00
   #PBS -M your.name@student.unsw.edu.au
   #PBS -m ae
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    cd /srv/scratch/z123456/katana_workshop
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   Rscript R/script_name.R
```

- 1. Resources you need (nodes, CPU, RAM, wall time)
- 2. R version you need
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- 4. Which .R script to run

Clearing Katana's global environment. Ensures you are working on a clean slate

```
#!/bin/bash
   #PBS -N job_name
   #PBS -l select=1:ncpus=1:mem=1gb
   #PBS -l walltime=1:00:00
   #PBS -M your.name@student.unsw.edu.au
   #PBS -m ae
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```

- 1. Resources you need (nodes, CPU, RAM, wall time)
- 2. R version you need
- 3. File path to the relevant working directory
- 4. Which .R script to run

#### Loads the R version you need\*

Tip: In Katana, type module avail R/ into terminal to see what R versions are available

```
#!/bin/bash
   #PBS -N job_name
   #PBS -l select=1:ncpus=1:mem=1gb
   #PBS -l walltime=1:00:00
   #PBS -M your.name@student.unsw.edu.au
   #PBS -m ae
   #Clear Katana workspace
   module purge
   #Loading R version
   module add R/4.0.2
14
   #Navigate to working direction
    cd /srv/scratch/z123456/katana_workshop
17
   #Run R code
   Rscript R/script_name.R
```

- 1. Resources you need (nodes, CPU, RAM, wall time)
- 2. R version you need
- 3. File path to the relevant working directory
- 4. Which .R script to run

Change directory to global scratch to set it as a working directory

```
#!/bin/bash
   #PBS -N job_name
   #PBS -l select=1:ncpus=1:mem=1gb
   #PBS -l walltime=1:00:00
   #PBS -M your.name@student.unsw.edu.au
   #PBS -m ae
   #Clear Katana workspace
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```

- 1. Resources you need (nodes, CPU, RAM, wall time)
- 2. R version you need
- 3. File path to the relevant working directory
- 4. Which .R script to run

Run specified R script within R/ folder

```
#!/bin/bash
   #PBS -N job_name
   #PBS -l select=1:ncpus=1:mem=1gb
   #PBS -l walltime=1:00:00
   #PBS -M your.name@student.unsw.edu.au
   #PBS -m ae
   #Clear Katana workspace
   module purge
   #Loading R version
   module add R/4.0.2
14
   #Navigate to working direction
   cd /srv/scratch/z123456/katana_workshop
   #Run R code
Rscript R/script_name.R
```

### FILE PATHS IN . pbs + .R MUST BE RELATIVE

#### .pbs

```
#!/bin/bash
   #PBS -N job name
   #PBS -l select=1:ncpus=1:mem=1qb
   #PBS -l walltime=1:00:00
   #PBS -M your.name@student.unsw.edu.au
   #PBS -m ae
   #Clear Katana workspace
10
   module purge
11
12
   #Loading R version
13
   module add R/4.0.2
14
15
   #Navigate to working direction
    cd /srv/scratch/z123456/katana_workshop
16
17
18
   #Run R code
  Rscript R/script_name.R
```

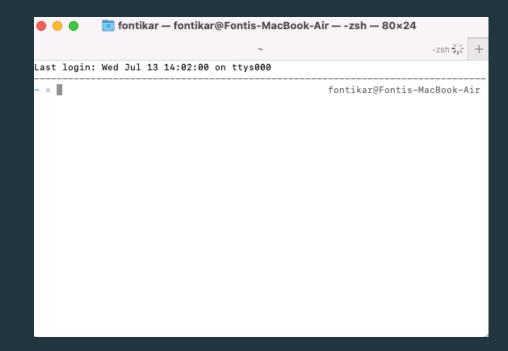
#### .R

```
# Install/load any packages
install.packages("pacman")
# Installs and library() if package is not available
pacman::p_load(readr, dplyr, purrr)
# Read in data
plant <- read_csv("data/Plant_height.csv")</pre>
# Exclude Hero/Shrub
 plant %
   fi?cer(! growthform == "Herb/Shrub" &
             growthform == "Shrub/Tree" &
          ! growthform == "Fern") -> plant_processed
# Split data as a list
plant_ls <- split(plant_processed, plant_processed$growthform)
# Run model for each growth form and output the coefficients
plant_output <- plant_ls %>%
  "ap(~ lm(loght ~ temp, data = .)) %>%
  map(~ rummary(.))
# Save the model ow nut
saveRDS(plant_output, "output/growthform_lm_output")
```

# SHELL TERMINAL

- Windows: Windows Terminal App
- Mac: Terminal zsh
- Katana on Demand:
  - https://kod.restech.unsw.edu.au
  - Caveats: Access via UNSW network or VPN

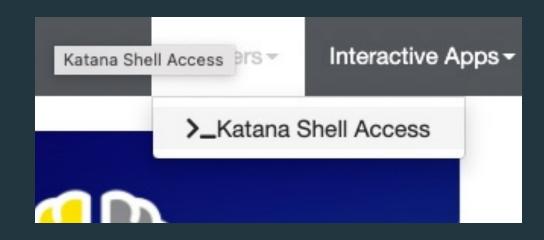




### KATANA ON DEMAND (KOD)

https://kod.restech.unsw.edu.au

- Click on Clusters
- Click on \_Katana Shell Access
- Enter your credentials
- You're at the head node of Katana!



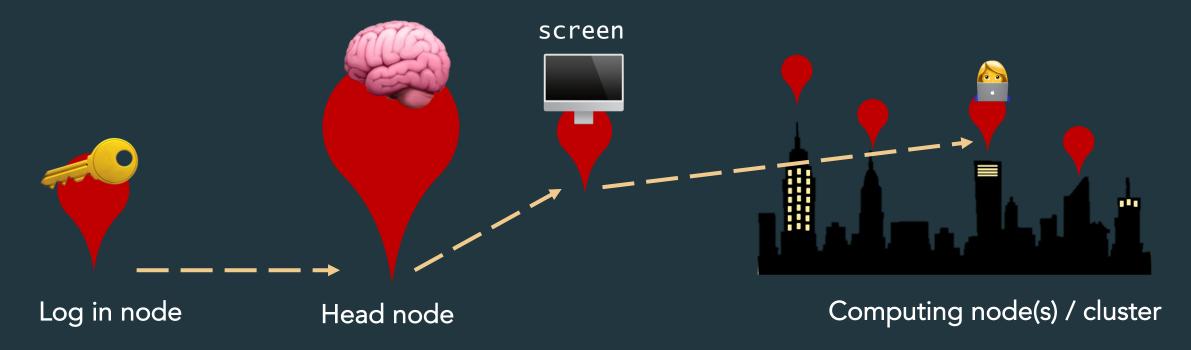
# EXERCISE ?

- 1. Make a copy of the pbs\_jobscript\_template
- 2. Change the email and zID and save it for future use!
- 3. Edit your own .pbs script
  - Request 30 mins, 1GB RAM, 1 CPU
  - Leave module add/ as template
  - Navigate to /srv/scratch/katana\_workshop
  - Rscript R/growthform\_lm\_analysis.R
- 4. Upload your .pbs script to HOME/pbs/

Cino, ix a co.

### SUBMITTING YOUR JOB

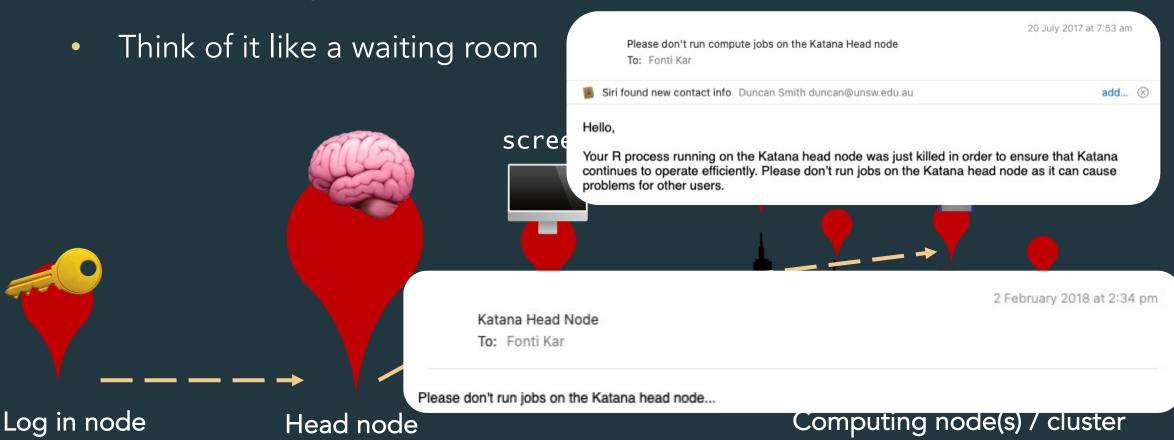
- screen is a program that allows you to submit jobs to Katana •
- Think of it like a waiting room



### SUBMITTING YOUR JOB



screen is a program that allows you to submit jobs to Katana •



### screen CHEATSHEET

screen				
Function	Keystrokes [ ] = enter together	Example		
Create new screen	screen -S name_of_screen	[z3516573@katana1 ~]\$ screen -S test		
Detach from screen	[Ctrl a] d	[detached from 11723.test]		
Reattach to screen	screen —r name_of_screen screen —r #prefix screen —r —d name_of_screen *for attached screens	[z3516573@katana1 ~]\$ screen -r test [z3516573@katana1 ~]\$ screen -r 117		
List all screens	screen —ls	[z3516573@katana1 ~]\$ screen -ls There are screens on: 6968.test (Detached) 11723.test (Detached)		
Delete a screen	screen —X —S name_of_screen quit	[[z3516573@katana1 ~]\$ <u>s</u> creen -X -S 69 quit		

### KATANA CHEATSHEET

Katana

Function	Keystrokes	Example	
Submit your job	qsub pbs/job_script_name.pbs	[z3516573@katana1 ~]\$ qsub pbs/my_job_script.pbs	
Check on the status of job(s)	qstat -u \$USER qstat -u z123456 qstat -su \$USER for more det	[z3516573@katana1 ~]\$ qstat -u \$USER ailed info	
Delete a job	qdel JOBID	Job ID Username Queue :	
Reduce resources *only for queued jobs	qalter —l select=1:ncpus=4:mem=5: JOBID [z3516573@katana	12mb a1 ~]\$ qalter -l select=1:ncpus=4:mem=4 1134122	

lexis Oile:

- 1. Log into Katana OnDemand <a href="https://kod.restech.unsw.edu.au">https://kod.restech.unsw.edu.au</a>
- 2. Go to Clusters > \_Katana Shell Access, enter credentials
- 3. Create a new screen
- 4. Queue your .pbs job and detach
- 5. Check status
- 6. Alter your RAM memory to 2GB

```
@katana1 ~]$ screen -S test

@katana1 ~]$ qsub pbs/my_job_script.pbs

[Ctrl a] d
```

@katana1 ~]\$ qstat -u \$USER

@katana1 ~]\$ qalter -l

### SO, YOU WANT TO BYPASS KOD?

• Shell is platform and OS specific <sup>=</sup>

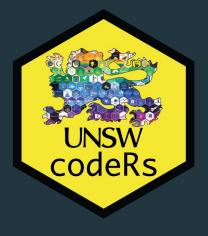


- Katana access via secure shell (ssh)
  - e.g ssh z123456@katana1.restech.unsw.edu.au
  - Two servers katana1 and katana2
  - lf you just type katana@unsw.edu.au = random 🥸



Idea: Find people using the same OS and set it up together if you are super keen!

### WE MADE IT FOLKS.



#### Want more?

- Coding and R workshops in T2 <a href="http://environmentalcomputing.net/">http://environmentalcomputing.net/</a>
- Drop-in help sessions, tutorials + nerdy events https://unsw-coders.netlify.app/

#### Need help?

- https://research.unsw.edu.au/katana
- https://unsw-restech.github.io/help\_and\_support.html
- Hacky Hour https://research.unsw.edu.au/hacky-hour