

Questions for the course "Introduction to running R, Python, and Julia in HPC", 17-19 October 2023

WEDNESDAY, 18 October 2023, Julia

1. Please note the following:
2. Add your questions below, numbering them continuously.
3. Be careful in case someone else is writing at the same time.
4. Please **DO NOT** delete your questions even when they have been answered, as we are planning to use them to improve our material.
5. Do not share any sensitive information as this document is accessible to anyone with the correct link.
6. You can start a **new line within a question by pressing <SHIFT> + <ENTER>**.
7. General information / summary:
8. Hostnames for login nodes (the main course project is at UPPMAX):
 - a. UPPMAX – rackham
 - i. **SSH:** rackham.uppmax.uu.se
 - ii. **ThinLinc:** rackham-gui.uppmax.uu.se
 - iii. **From webbrowser:** <https://rackham-gui.uppmax.uu.se/>
 - b. HPC2N - Kebnekaise
 - i. **SSH:** kebnekaise.hpc2n.umu.se
 - ii. **ThinLinc:** kebnekaise-t1.hpc2n.umu.se
 - iii. **From webbrowser:** <https://kebnekaise-t1.hpc2n.umu.se:300/>
9. Course project at UPPMAX: NAISS2023-22-914
10. Storage area for the course project at UPPMAX: /proj/naiss2023-22-914
11. Course project at HPC2N: hpc2n2023-110
12. Storage area for the course project at HPC2N:
/proj/nobackup/hpc2n2023-110
13. Zoom ONLY for the parallel sessions: <https://umu.zoom.us/j/64351885207?pwd=RVpwYnFRdINLQkM5WWR0VWsrSzUwQT09>

Q/A Julia

14. println("Hello World!"), Why do you use println?
 - a. That gives a new line after the print
 - b. Look in screen!
15. Editors:
 - a. Nano easiest
 - b. vim if you are used to itexit
 - c. emacs if you are used to it

- d. mobaxterm has a built in editor
 - e. Gedit graphical
16. If i run `julia serial-sum.jl 4 8` in the julia env it gives `errjuliaor` (syntax: extra token "4" after end of expression)? The other way round works
- a. You should run from **batch env (\$)**, exit julia REPL first!
 - b. Interesting that 8 4 did work, though
17. In julia, when writing 'ls' i got this message: **ERROR:** `UndefVarError: ls not defined`
- a. 'ls' will work in the shell mode, use ';'
 - But it seemed like Pedro was not in shell mode when giving command 'ls'?
 - b. Go back to julian mode with `<backspace>`
 - c. He is using shell mode now.
 - Yes now, but not before. Never mind, I'll sort it out:)
18. **Note:** `]` is for package mode
19. **NOTE:** As it happened to me (Björn) you may see after some time with installing packages that your disk quota is full. This happens when you install in the `$HOME` area. It may be better to put your files to a project area.
20. In the beginning when using the command `'Pkg.add("DFTK")'` (after `'using Pkg'`) the only package failed to download was DFTK. Cannot continue from there.
- a. Kebnekaise or Rackham? Rackham.
 - b. What was the error?

```

Precompiling project...
  × MPI
  × DFTK
46 dependencies successfully precompiled in 148 seconds. 59 already precompiled.
2 dependencies errored. To see a full report either run `import Pkg; Pkg.precompile()` or load the packages

```

When using command `'import Pkg; Pkg.precompile()'` as instructed i get:

```

[julia> import Pkg; Pkg.precompile()
Precompiling project...
  × DFTK
  0 dependencies successfully precompiled in 9 seconds. 106 already precompiled.

ERROR: The following 1 direct dependency failed to precompile:
DFTK [acf6eb54-70d9-11e9-0013-234b7a5f5337]

```

... and more error text.

Seems like library 'libmpi' could not be loaded and it errored from there. Says there is no such file or directory.

I loaded and started julia from `/home/<user>/R-python-julia-HPC/Exercises` : is this incorrect?

- c. Can you try "using Pkg" "Pkg.add("DFTK")" as I did?

Yes, I get:

Resolving package versions...

No Changes to ``/domus/h1/<user>/julia/environments/v1.8/Project.toml``

No Changes to ``/domus/h1/<user>/julia/environments/v1.8/Manifest.toml``

- d. What is the output of `LOAD_PATH` ? (Björn)

"4-element Vector{String}:

"@"

"@v#.#"

"@stdlib"

"/sw/comp/julia/1.8.5/rackham/lib/glob_pkg/environments/v1.8"

i. LOOKS OK

- e. I think the issue can come from the "/sw/comp/..." environment, can you try the following: exit() the julia session, and start a new one
- f. Then,
- g. empty!(LOAD_PATH)
- h. push!(LOAD_PATH, "@")
- i. push!(LOAD_PATH, "@v#.#")
- j. push!(LOAD_PATH, "@stdlib")
- k. After, this try the "using Pkg" and add the package DFTK
Thanks! Did as stated, and after Pkg.add("DFTK") i got the "No changes" responses again. Should I try activating my-first-env again and add DFTK in there?
- l. Yes, if the initial installation of DFTK worked, let me know
Had to install MPIPreferences by 'add MPIPreferences' in Pkg mode. Then 'using MPIPreferences', then MPIPreferences.use_system_binary – and then redo adding DFTK.
Now it works.

21. For DFTK it needed MPI to precompile.

- a. On UPPMAX follow: https://www.uppmx.uu.se/support/user-guides/julia-user-guide/#tocjump_22751075665337883_13
- b. In other words do this in terminal and restart julia
For julia/1.8.5:
- c. \$ module load gcc/11.3.0 openmpi/4.1.3

22. This; #SBATCH --time=00:10:00 # Asking for 10 minutes. If you specific the time and later it take longer time. Will it be terminated automatically?

- a. Terminated, yes
- b. So better overestimate the times a little bit

23. PLACEHOLDER

24. After command 'vim name.jl', and after creating whatever function in the new window – how save and exit from there? I tried ending with ':wq' and then pushing enter, did not work.

- a. <esc> :wq
- b. This is why vim is not recommended for non-vim users in a course. We should have been more clear!
Okay. Yes could have been clearer, thanks, but no worries ofc. What use otherwise?
- Thanks, see the editors below now.
- c. Follow-up question: do you write e.g. Nano in shell mode in julia, like 'Nano name.jl' instead of vim then?
- d. Yes.
 - i. I did not know you could start from the REPL shell! Otherwise you do it from the bash shell
sorry, which one of these is the shell mode in julia?

25. Editors:

- a. Nano easiest — ^ means <ctrl>
 - b. vim if you are used to it
 - c. emacs if you are used to it
 - d. mobaxterm has a built in graphical editor
 - e. Gedit graphical (installed on both centres!)
26. When will XQuartz, that the instructions stated was good to download for graphics in terminal, be useful?
- a. For Jupyter and RStudio, and if you used the terminal. But you must have logged in with -X or -Y (ordinary dash/hyphen)
 - i. Like ssh -X <username>@centre-address
 - b. Otherwise ThinLinc is good
27. I did this Submitted batch job 8495841 on cluster snowy and got this: scontrol show job 8495841 ---> slurm_load_jobs error: Invalid job id specified
- a. **On Snowy: add - -M snowy on the scontrol line**
28. In running julia in batch mode. I'm unsure how to access this 'batch mode' – do I do this after accessing rackham/uppmax and then my directory?
Do I write these lines:
- ```
#!/bin/bash -l
#SBATCH -A naiss2023-22-914
#SBATCH --time=00:10:00
#etc....
```
- straight into terminal or do I need to load something before, to activate batch mode?
- a. You need to have it in a script file
  - b. Than sbatch <filename>
29. When having stared jupiter etc. How when finished exit the code running in julia and get back to terminal?
- a. <ctrl> - C works, that is how I do it but there may be some other way. Does that work for you? Thank you! That worked.
30. PLACEHOLDER
31. PLACEHOLDER
32. PLACEHOLDER
33. PLACEHOLDER
34. Recordings for today are now uploaded to the same playlist as yesterday, on HPC2N's YouTube channel: <https://www.youtube.com/watch?v=aCSMEGgITG8&list=PL6jMHLEmPVLxdCIIWrzseYkGoCCXjrukM>
35. Evaluation survey for today: <https://forms.office.com/e/bDAFJwXRK9>