

# R on HPC



Jan 2020

# R

- Versions: 3.0.2, 3.1.2, 3.2.5, 3.5.0, 3.6.0 (module avail R)
- Intel version (MKL) : 3.2.3 3.4.3

```
[ccevg@atlas8-c01 ~]$ module avail R
```

```
----- /app1/modules/centos6.3 -----  
R-3.0.2      R-3.0.2_test R-3.1.2      R-3.2.5      R-3.5.0      R-3.6.0
```

```
----- /app1/modules/centos6.3-intel -----  
R-3.2.3_intel R-3.4.3_intel
```

# R - serial job

Can submit to serial/short,  
depending on required runtime

```
#!/bin/bash
#PBS -q serial
#PBS -l select=1:ncpus=1:mem=10GB
#PBS -j oe
#PBS -N Job_Name
cd $PBS_O_WORKDIR
source /etc/profile.d/modules.sh
module load R-3.2.5
```

Rscript Rcode.r

Use openmp queue for high  
memory

```
#!/bin/bash
#PBS -q openmp
#PBS -l select=1:ncpus=1:mem=80GB
#PBS -j oe
#PBS -N Job_Name
cd $PBS_O_WORKDIR
source /etc/profile.d/modules.sh
module load R-3.2.5
```

Rscript Rcode.r

# R - parallel

- using third party packages
  - doParallel / foreach / BiocParallel
- can choose 1 node of any parallel queue
  - select=1
- For multi node parallelism
  - pdbMPI / snow

```
#!/bin/bash

#PBS -P Project_Name_of_Job
#PBS -q paralle124
#PBS -l select=1:ncpus=24:mpiprocs=24:mem=160GB
#PBS -j oe
#PBS -N Job_Name
### -N Job_Name: set filename for standard output/error
message.

cd $PBS_O_WORKDIR; ## This line is needed, do not modify.

##--- Put your exec/application commands below ---
##--- For example:
source /etc/profile.d/rec_modules.sh
module load R-3.2.5; module list

### np=$( cat ${PBS_NODEFILE} |wc -l ); ### get number of CPUs
Rscript your_parallel_R.r
```

# Installing R packages -1

- Only on **atlas8** login node
- Load the relevant R module (ex: R-3.5.0)
- Install them using `install.packages()`

```
[ccev@atlas8-c01 ~]$ module load R-3.5.0
[ccev@atlas8-c01 ~]$ R

R version 3.5.0 (2018-04-23) -- "Joy in Playing"
Copyright (C) 2018 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.

  Natural language support but running in an English locale

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.

> install.packages('caret')█
```

# Install R packages -2

Choose NUS mirror site for repo

- Singapore (Singapore) [https]
- Singapore (Singapore) [http]

```
Selection: 66
Other CRAN mirrors

 1: Argentina (La Plata)           2: Belgium (Antwerp) [https]
 3: Canada (BC) [https]           4: Canada (MB) [https]
 5: Canada (NS) [https]          6: Canada (ON)
 7: China (Beijing) [https]      8: China (Hefei) [https]
 9: El Salvador                   10: France (Paris 1)
11: Iran [https]                 12: Italy (Milano)
13: Korea (Seoul 2)             14: Mexico (Texcoco)
15: New Zealand [https]         16: Portugal (Lisbon)
17: Portugal (Porto)            18: Singapore (Singapore) [https]
19: South Africa (Cape Town)     20: South Africa (Johannesburg)
21: Taiwan (Chungli) [https]    22: Taiwan (Taipei)
23: Thailand                    24: USA (IN) [https]
25: USA (MO)                   26: USA (NC)
```

```
Installing package into '/home/svu/ccevg/R/x86_64-pc-linux-gnu-library/3.5'
(as 'lib' is unspecified)
--- Please select a CRAN mirror for use in this session ---
Secure CRAN mirrors

 1: 0-Cloud [https]              2: Algeria [https]
 3: Australia (Canberra) [https] 4: Australia (Melbourne 1) [https]
 5: Australia (Melbourne 2) [https] 6: Australia (Perth) [https]
 7: Austria [https]             8: Belgium (Ghent) [https]
 9: Brazil (PR) [https]         10: Brazil (RJ) [https]
11: Brazil (SP 1) [https]       12: Brazil (SP 2) [https]
13: Bulgaria [https]           14: Chile [https]
15: China (Hong Kong) [https]   16: China (Guangzhou) [https]
17: China (Lanzhou) [https]     18: China (Shanghai) [https]
19: Colombia (Cali) [https]     20: Czech Republic [https]
21: Denmark [https]            22: Ecuador (Cuenca) [https]
23: Ecuador (Quito) [https]     24: Estonia [https]
25: France (Lyon 1) [https]     26: France (Lyon 2) [https]
27: France (Marseille) [https] 28: France (Montpellier) [https]
29: Germany (Erlangen) [https] 30: Germany (Göttingen) [https]
31: Germany (Münster) [https]   32: Germany (Regensburg) [https]
33: Greece [https]             34: Hungary [https]
35: Iceland [https]            36: Indonesia (Jakarta) [https]
37: Italy (Padua) [https]       38: Japan (Tokyo) [https]
39: Japan (Yonezawa) [https]    40: Korea (Busan) [https]
41: Korea (Gyeongseong-do) [https] 42: Korea (Seoul 1) [https]
43: Korea (Ulsan) [https]      44: Malaysia [https]
45: Mexico (Mexico City) [https] 46: Morocco [https]
47: Norway [https]             48: Philippines [https]
49: Serbia [https]            50: Spain (Madrid) [https]
51: Sweden [https]            52: Switzerland [https]
53: Turkey (Denizli) [https]    54: Turkey (Mersin) [https]
55: UK (Bristol) [https]       56: UK (London 1) [https]
57: USA (CA 1) [https]         58: USA (IA) [https]
59: USA (KS) [https]           60: USA (MI 1) [https]
61: USA (MI 2) [https]         62: USA (OR) [https]
63: USA (TN) [https]          64: USA (TX 1) [https]
65: Uruguay [https]           66: (other mirrors)
```

# Installing R packages -3

Bioconductor packages can be installed using the default way on atlas8 login node

Some packages depend on system libraries and need to compile from source. Such requests should be escalated to NUSIT HPC (via [nTouch](#))