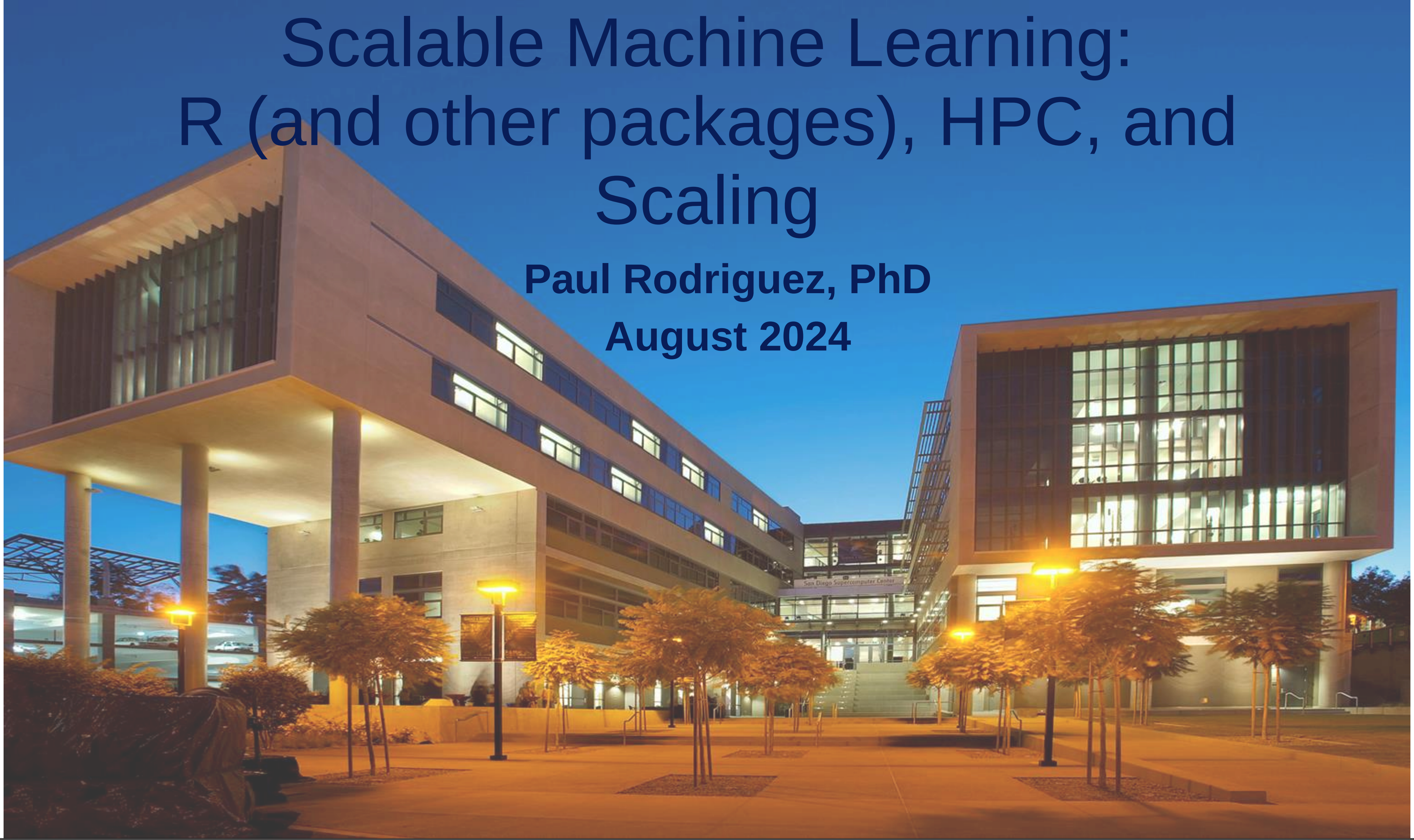


Scalable Machine Learning: R (and other packages), HPC, and Scaling

Paul Rodriguez, PhD

August 2024

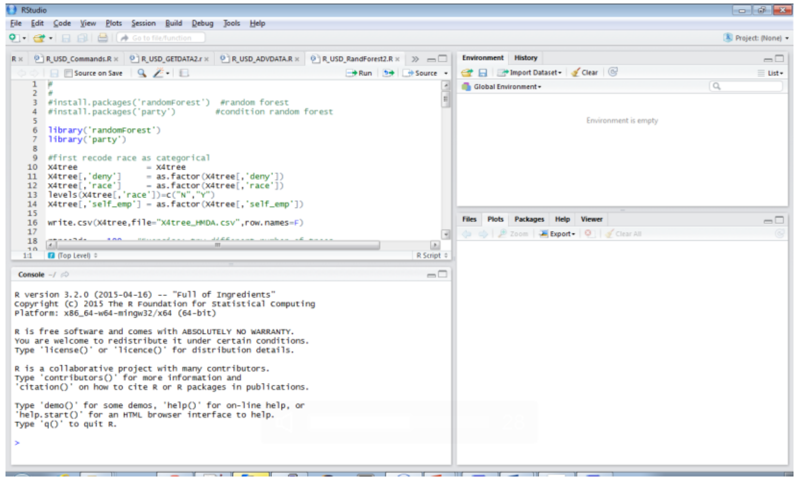
Outline

- R and Scaling
- Parallel R
- Embarrassingly Parallel R
- A big data exploration of R

Rstudio: an integrated development environment

Edit window to Build scripts

R console



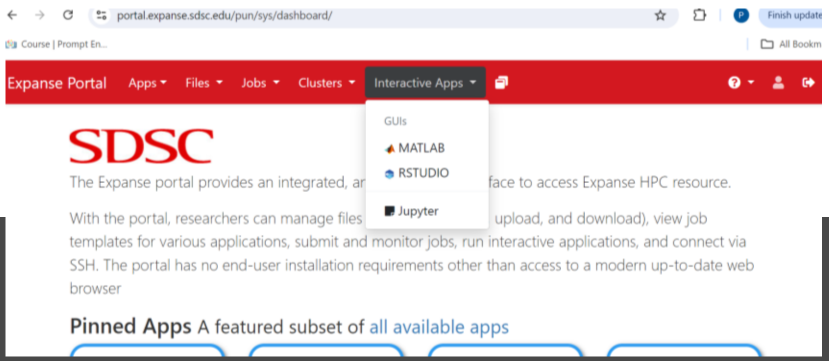
```
#
#
#install.packages('randomForest')  #random forest
#install.packages('party')         #condition random forest

library('randomForest')
library('party')

#first recode race as categorical
X4tree               = X4tree
X4tree[,'deny']      = as.factor(X4tree[,'deny'])
X4tree[,'race']      = as.factor(X4tree[,'race'])
levels(X4tree[,'race'])=c("N","Y")
X4tree[,'self_emp'] = as.factor(X4tree[,'self_emp'])

write.csv(X4tree,file="X4tree_HMDA.csv",row.names=F)
```

```
R version 3.2.0 (2015-04-16) -- "Full of Ingredients"
Copyright (C) 2015 The R Foundation for Statistical Computing
Platform: x86_64-w64-mingw32/x64 (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.

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.

>
```

Environment Information on variables and command history

Plots, help docs, package lists

Rstudio is available thru expanse portal



The Expanse portal provides an integrated, ar face to access Expanse HPC resource.

With the portal, researchers can manage files upload, and download), view job templates for various applications, submit and monitor jobs, run interactive applications, and connect via SSH. The portal has no end-user installation requirements other than access to a modern up-to-date web browser

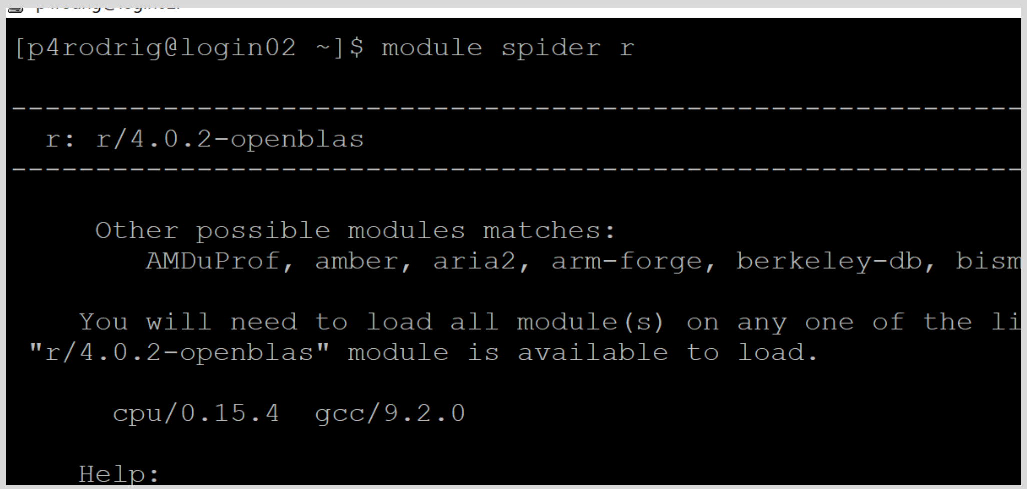
Pinned Apps A featured subset of all available apps

R interactively on Expanse command line

1. Get an interactive compute node:

2. Try

$ module spider r *(this tells you what modules you need)*



```
[p4rodrig@login02 ~]$ module spider r

------------------------------------------------------------------------
  r: r/4.0.2-openblas
------------------------------------------------------------------------

     Other possible modules matches:
        AMDuProf, amber, aria2, arm-forge, berkeley-db, bism

    You will need to load all module(s) on any one of the li
 "r/4.0.2-openblas" module is available to load.

      cpu/0.15.4  gcc/9.2.0

    Help:
```

3. Enter

$ module load cpu/0.15.4
$ module load gcc/9.2.0
$ module load r/4.0.2-openblas

$ R

```
R version 4.0.2 (2020-06-22) -- "Taking Off Again"
Copyright (C) 2020 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (64-bit)
…..
Type 'q()' to quit R.

>
```

R strengths for HPC (IMHO)

- **Data Wrangling –**

- **Particular statistical procedure implementations -**
  Imputation methods (for missing data)
  Sampling methods
  Instrument Variable (2 stage) Regression
  Matching subjects for pairwise analysis
  Generalized Linear Model (e.g. logistic regression)
  MCMC routines (but Stan is likely better package)
  Some ML models (e.g. randomForest, LASSO)

R strengths for HPC (IMHO)

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  Some ML models (e.g. randomForest, LASSO)

Inferential Stats, Experimental Studies

Data Science, Machine Learning

R Scaling In a nutshell

- R uses BLAS/LAPACK math libraries for operations on vectors

  [Same for Matlab and Python]

- R packages provide multicore, out-of-core, multinode, or distributed data (SparkR) options

  [Same for Matlab and Python]

- Some ML model implementations may be built to use parallel backends (review the available options)

Consider Scaling Regression Computations

- **Linear Model:** $Y = X * B$

  where Y=outcomes , X=data matrix

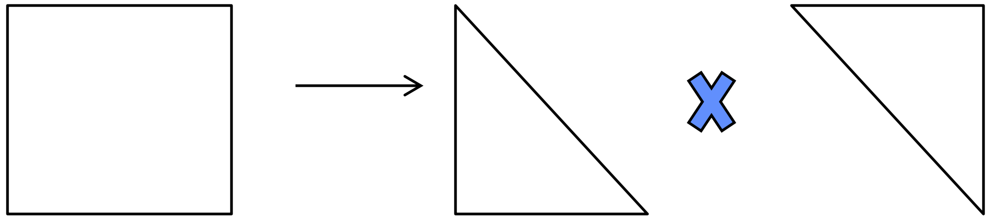
- **Solutions:**

  take "inverse" $of\ X * Y = B$ (time consuming)

  use derivatives to search for solutions (very general)

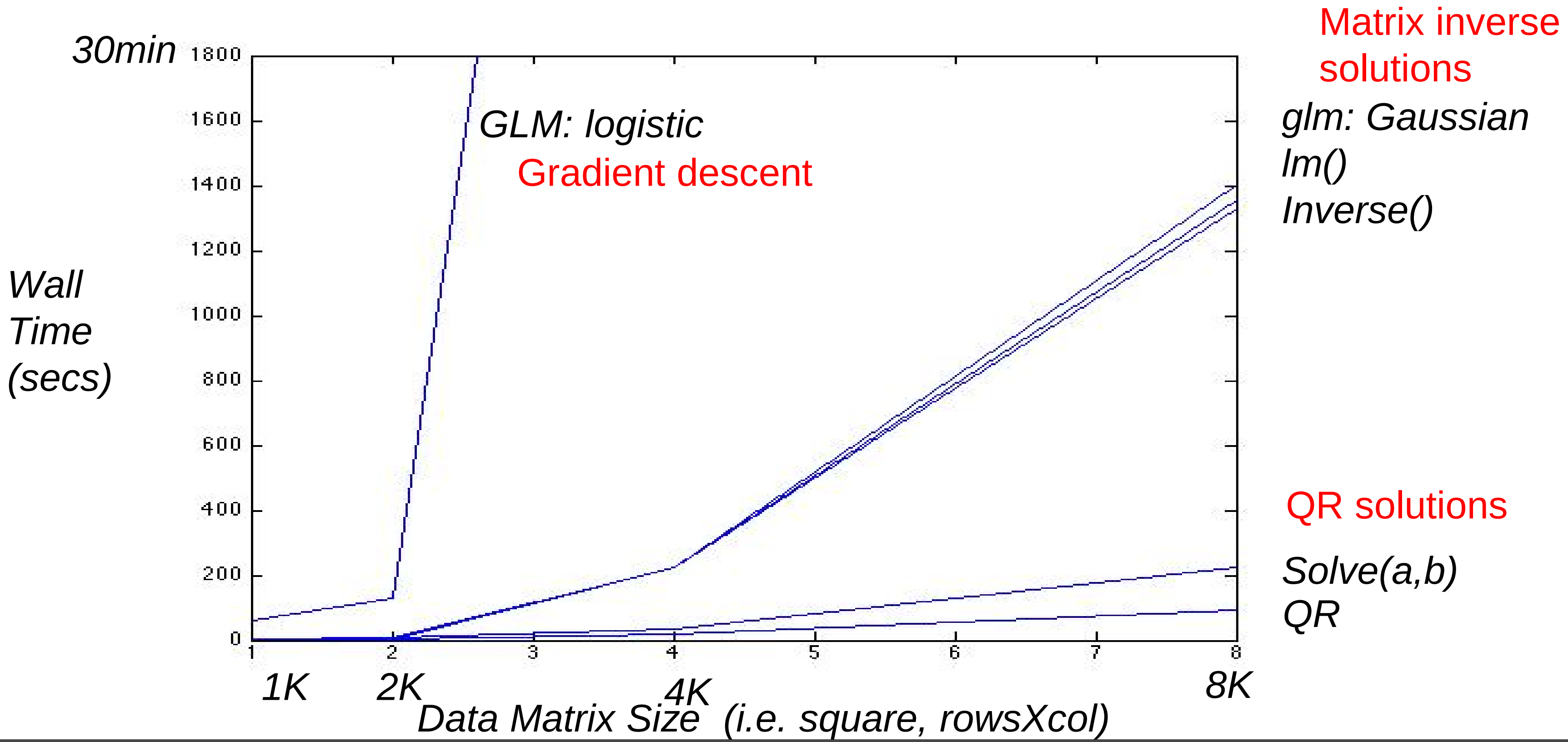
- **Or, less obvious:**

  QR decomposition of *X* into triangular matrices (quicker but more memory)



Solving Linear Systems
Performance with R, 1 compute node

R:
glm(Y~X,family=gaussian) #gaussn regrssn (like lm)
glm(Y~X,family=binomial) # logistic regrssn (Y=0 or 1)



R multicore processing

- ‘doParallel’ package – provides the back end to the ‘for each’ parallel processing command

- uses threads across CPU cores to pass data & commands

- It also works for multinode (runs on top of RMPI)

See https://cran.r-project.org/web/packages/doParallel/vignettes/gettingstartedParallel.pdf

R multicore coding

```
install.packages(doParallel)
library(doParallel)
registerDoParallel(cores=24)
```

1. allocate workers

R multicore coding

```
install.packages(doParallel)
library(doParallel)
registerDoParallel(cores=24)

    my_data_frame = …..

    my_results = foreach(
```

1. allocate workers

2. Make ‘foreach’ loop

R multicore coding

```
install.packages(doParallel)
library(doParallel)
registerDoParallel(cores=24)

    my_data_frame = …..

    my_results = foreach(i=1:24,.combine=rbind)
```

1. allocate workers

2. Make ‘foreach’ loop

3. specify how to combine results

R multicore coding

```
install.packages(doParallel)
library(doParallel)
registerDoParallel(cores=24)

    my_data_frame = …..

    my_results = foreach(i=1:24,.combine=rbind) %dopar%
      {   …
```

1. allocate workers

2. Make ‘foreach’ loop

3. specify how to combine results

4. %dopar% runs it across cores, (%do% runs it serially)

R multicore coding

```
install.packages(doParallel)
library(doParallel)
registerDoParallel(cores=24)

    my_data_frame = …..

    my_results = foreach(i=1:24,.combine=rbind) %dopar%
      {   …
               your code here

           return(  a variable or object )
    })
```

1. allocate workers

2. Make ‘foreach’ loop

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R multicore coding

```
install.packages(doParallel)
library(doParallel)
registerDoParallel(cores=24)

     my_data_frame = …..

     my_results = foreach(i=1:24,.combine=rbind) %dopar%
        {   …
                 your code here

             return(  a variable or object )
     })
```

1. allocate workers

2. Make ‘foreach’ loop

3. specify how to combine results

4. %dopar% runs it across cores, (%do% runs it serially)

BEWARE: foreach will copy data to every core if it seems necessary

R multinode: parallel backend

```
library(doParallel)

cl <- makeCluster(48)
registerDoParallel(cl)
```

1. allocate cluster as parallel backend

R multinode: parallel backend

```
library(doParallel)

cl <- makeCluster(48)
registerDoParallel(cl)

my_data_frame = …..

results = foreach(i=1:48,.combine=rbind) %dopar%
  {   … your code here


        return(  a variable or object )
})
stopCluster(cl)
```

1. allocate cluster as parallel backend

2. %dopar% puts loops across cores and nodes

R multinode: parallel backend

```
library(doParallel)

cl <- makeCluster(48)
registerDoParallel(cl)

my_data_frame = …..

results = foreach(i=1:48,.combine=rbind) %dopar%
  {   … your code here


        return(  a variable or object )
})
stopCluster(cl)
```

1. allocate cluster as parallel backend

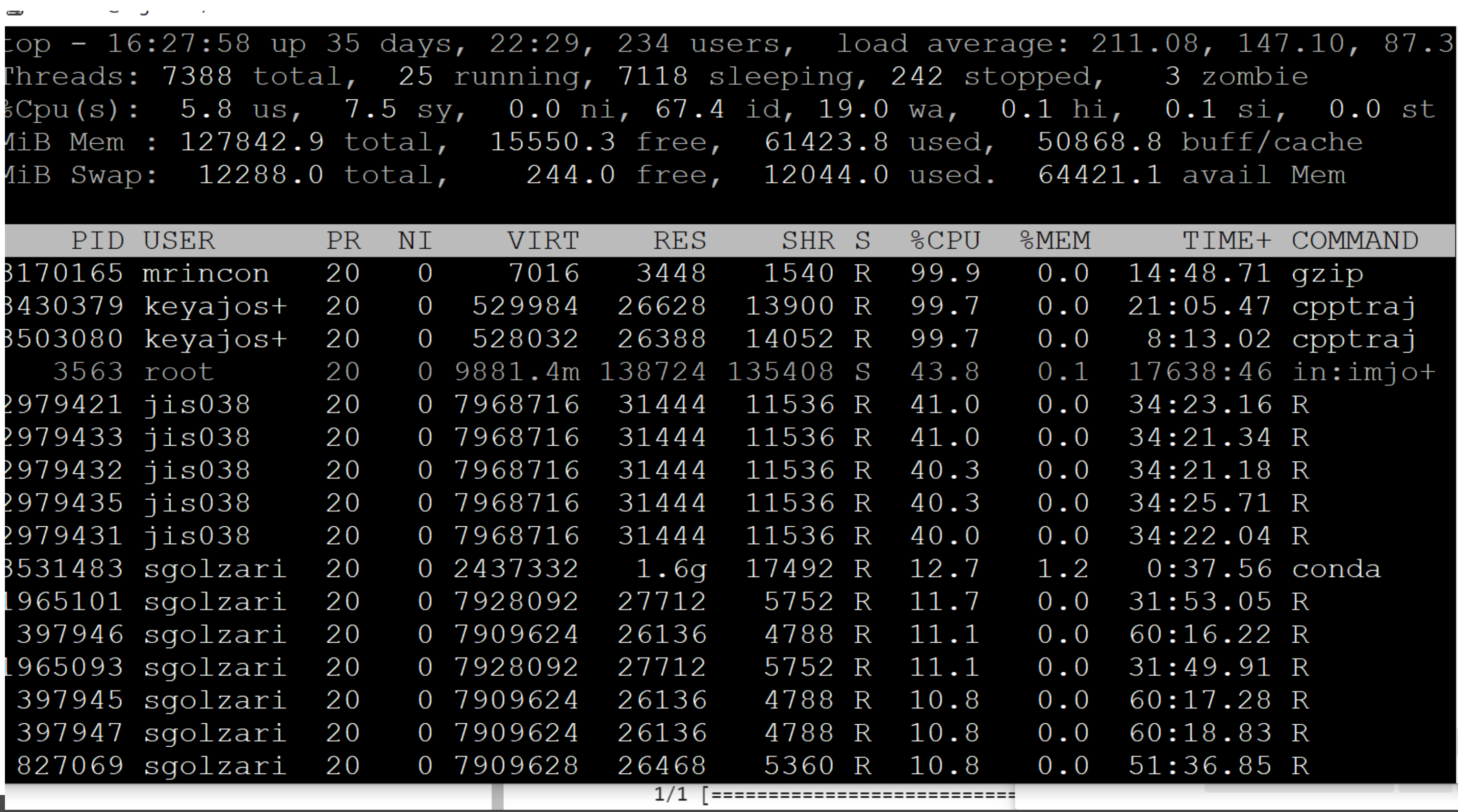
**2.
%dopar% puts loops across cores and nodes**

BEWARE: copying data across nodes is higher communication costs

Speaking of R and memory…

Recall the other day Marty noticed, someone was running R (using $top)

Several R processing going, and only 16Gb free memory left!



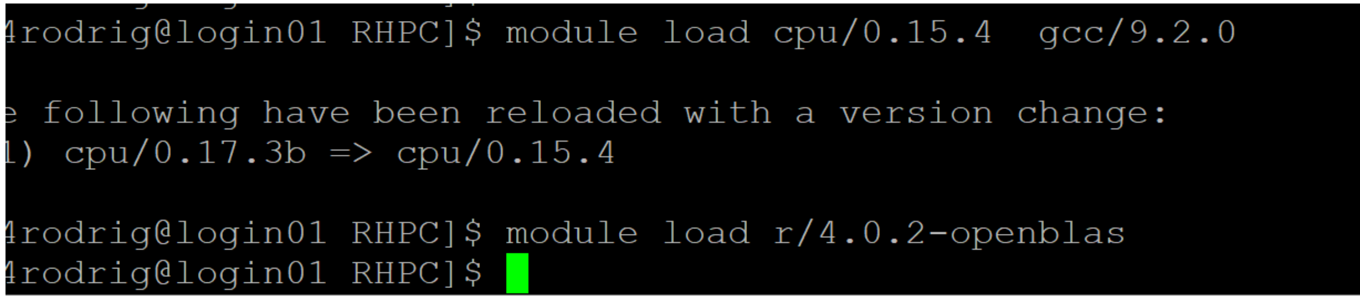
```
top - 16:27:58 up 35 days, 22:29, 234 users,  load average: 211.08, 147.10, 87.3
Threads: 7388 total,  25 running, 7118 sleeping, 242 stopped,   3 zombie
%Cpu(s):  5.8 us,  7.5 sy,  0.0 ni, 67.4 id, 19.0 wa,  0.1 hi,  0.1 si,  0.0 st
MiB Mem : 127842.9 total,  15550.3 free,  61423.8 used,  50868.8 buff/cache
MiB Swap:  12288.0 total,    244.0 free,  12044.0 used.  64421.1 avail Mem

    PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM     TIME+ COMMAND
3170165 mrincon   20   0    7016   3448   1540 R  99.9   0.0  14:48.71 gzip
3430379 keyajos+  20   0  529984  26628  13900 R  99.7   0.0  21:05.47 cpptraj
3503080 keyajos+  20   0  528032  26388  14052 R  99.7   0.0   8:13.02 cpptraj
   3563 root      20   0 9881.4m 138724 135408 S  43.8   0.1  17638:46 in:imjo+
2979421 jis038    20   0 7968716  31444  11536 R  41.0   0.0  34:23.16 R
2979433 jis038    20   0 7968716  31444  11536 R  41.0   0.0  34:21.34 R
2979432 jis038    20   0 7968716  31444  11536 R  40.3   0.0  34:21.18 R
2979435 jis038    20   0 7968716  31444  11536 R  40.3   0.0  34:25.71 R
2979431 jis038    20   0 7968716  31444  11536 R  40.0   0.0  34:22.04 R
3531483 sgolzari  20   0 2437332   1.6g  17492 R  12.7   1.2   0:37.56 conda
1965101 sgolzari  20   0 7928092  27712   5752 R  11.7   0.0  31:53.05 R
 397946 sgolzari  20   0 7909624  26136   4788 R  11.1   0.0  60:16.22 R
1965093 sgolzari  20   0 7928092  27712   5752 R  11.1   0.0  31:49.91 R
 397945 sgolzari  20   0 7909624  26136   4788 R  10.8   0.0  60:17.28 R
 397947 sgolzari  20   0 7909624  26136   4788 R  10.8   0.0  60:18.83 R
 827069 sgolzari  20   0 7909628  26468   5360 R  10.8   0.0  51:36.85 R
                                     1/1 [==========================
```

Exercise: Testing R parallel, command line

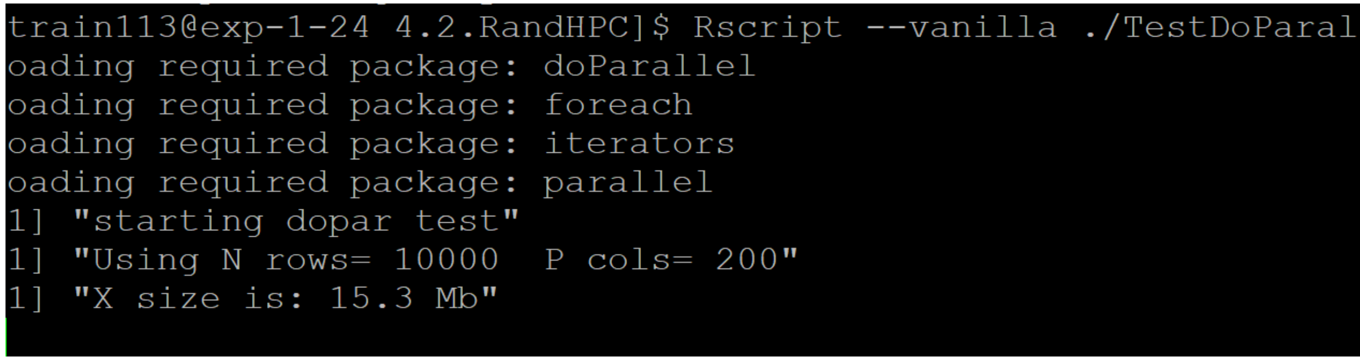
- commands

1. Log into expanse terminal
2. $ srun-compute
3. $ cd github repo: _r_on_HPC   folder
4. $ 'module spider r' to see what to load
5. $ R   (run one time)
6. > install.packages("doParallel")

   (say 'yes' for local install)
7. $ Rscript –vanilla TestDoParallel_v1.R



```
4rodrig@login01 RHPC]$ module load cpu/0.15.4   gcc/9.2.0

e following have been reloaded with a version change:
1) cpu/0.17.3b => cpu/0.15.4

4rodrig@login01 RHPC]$ module load r/4.0.2-openblas
4rodrig@login01 RHPC]$ 
```



```
train113@exp-1-24 4.2.RandHPC]$ Rscript --vanilla ./TestDoParal
oading required package: doParallel
oading required package: foreach
oading required package: iterators
oading required package: parallel
1] "starting dopar test"
1] "Using N rows= 10000  P cols= 200"
1] "X size is: 15.3 Mb"
```

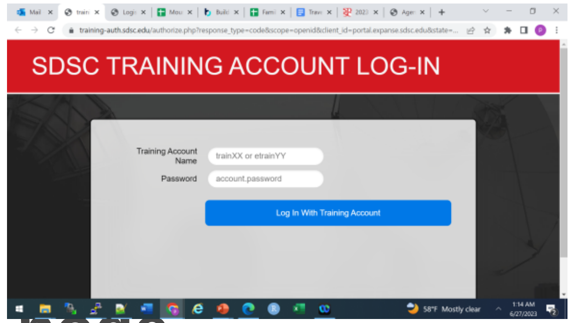
Also start a 2nd terminal and ssh into that compute node and run $ top –u $USER - how's memory usage?

In top, enter H to see threads, enter f -> down arrow -> space -> esc to toggle cupid

Exercise: Testing R parallel in portal (homework)

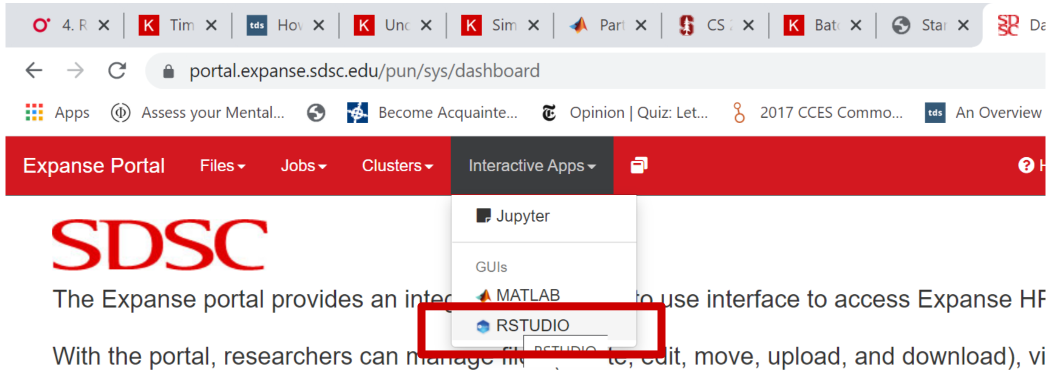
1. **Log into expanse portal and start R studio**

   goto URL: *https://portal.expanse.sdsc.edu/training*



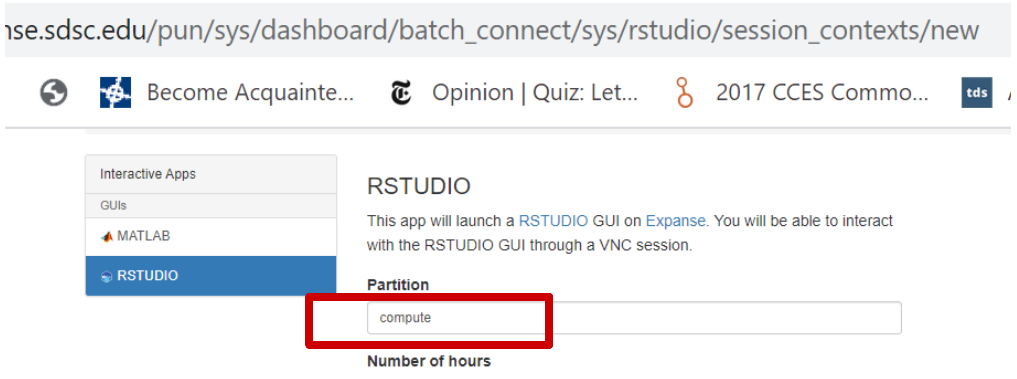
2. **Also log into expanse command line and ssh to compute node**

3. **run 'top –u username' to see performance**
   - look for tradeoffs in memory vs execution as matrix size varies (see next slides)



The Expanse portal provides an integ… …o use interface to access Expanse HF

With the portal, researchers can manage fil… …te, edit, move, upload, and download), vi

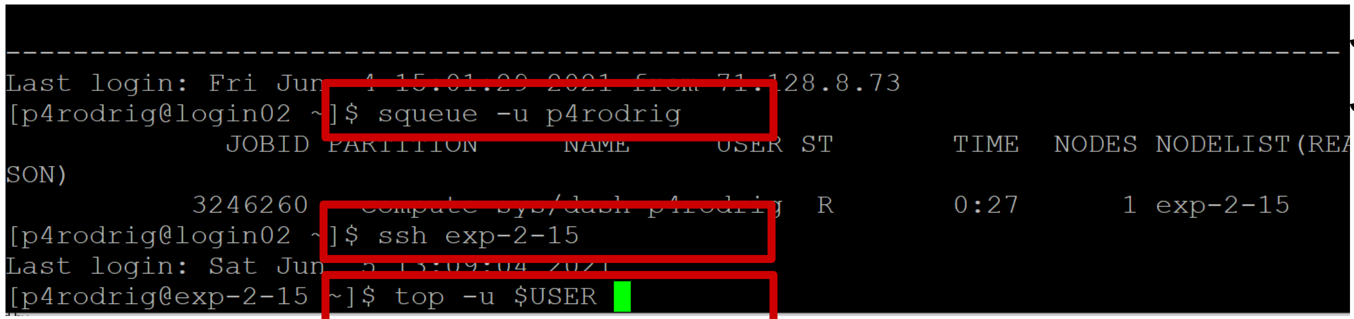


RSTUDIO

This app will launch a RSTUDIO GUI on Expanse. You will be able to interact with the RSTUDIO GUI through a VNC session.

Partition: compute

Number of hours



```
---------------------------------------------------------------
Last login: Fri Jun  4 15:01:29 2021 from 71.128.8.73
[p4rodrig@login02 ~]$ squeue -u p4rodrig
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REA
SON)
           3246260   compute sys/dash p4rodrig  R       0:27      1 exp-2-15
[p4rodrig@login02 ~]$ ssh exp-2-15
Last login: Sat Jun  5 13:09:04 2021
[p4rodrig@exp-2-15 ~]$ top -u $USER
```

1 Open portal ->
  Interactive Apps ->
    Rstudio

Enter
Node: “compute”
Cores: “64”
Memory: 124 Gb
(other fields defaults ok)

2 Also login to Expanse terminal window

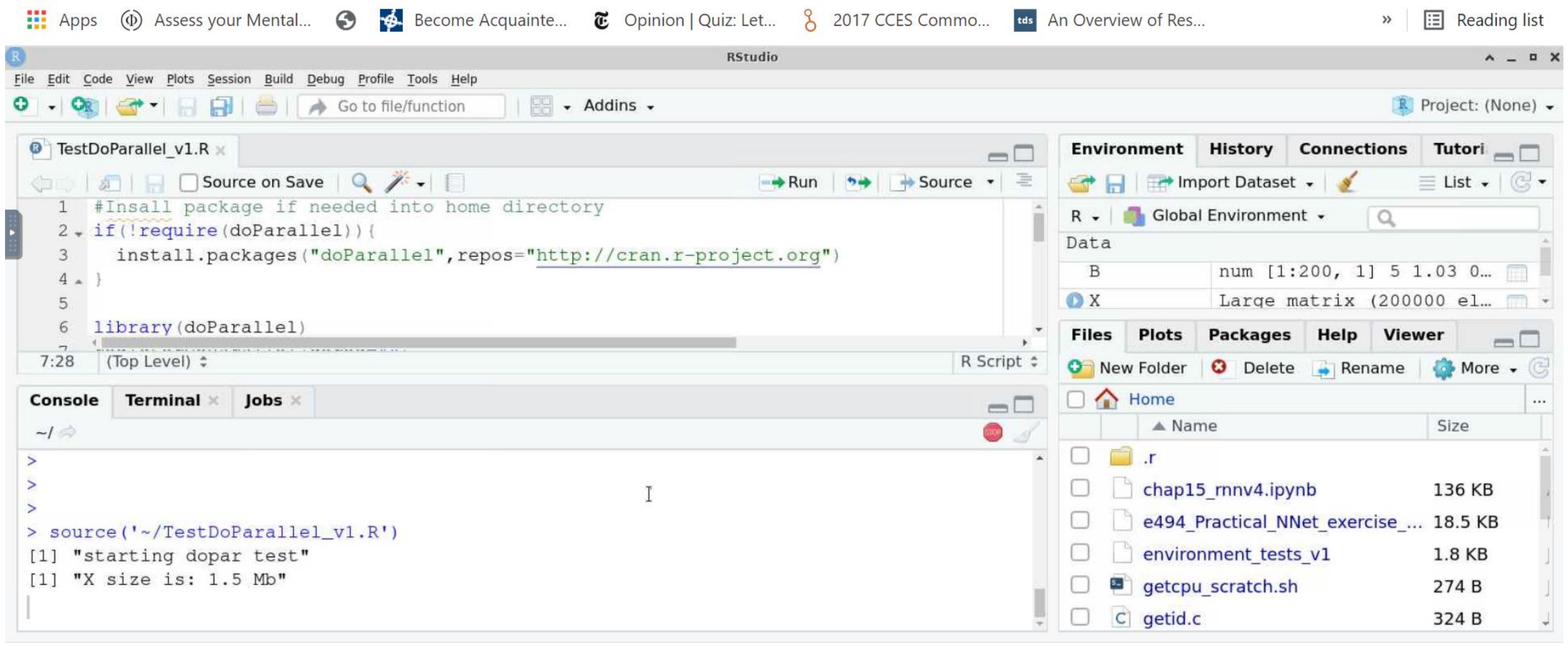
$ squeue –u $USER
$ ssh exp-##-##
$ top –u $USER

‘H’ will toggle threads
‘f’ , downarrow to P, space, esc.

3 Open the 'Test_doParallel ' Rscript

Select 'source' to run the whole script, it will install 'doParallel' package (if the R installation doesn't have it already)

look for # <<< ----- comments to change data parameters



```
#Insall package if needed into home directory
if(!require(doParallel)){
  install.packages("doParallel",repos="http://cran.r-project.org")
}

library(doParallel)
```

```
>
>
>
> source('~/TestDoParallel_v1.R')
[1] "starting dopar test"
[1] "X size is: 1.5 Mb"
```

```
Data
  B     num [1:200, 1] 5 1.03 0...
  X     Large matrix (200000 el...
```

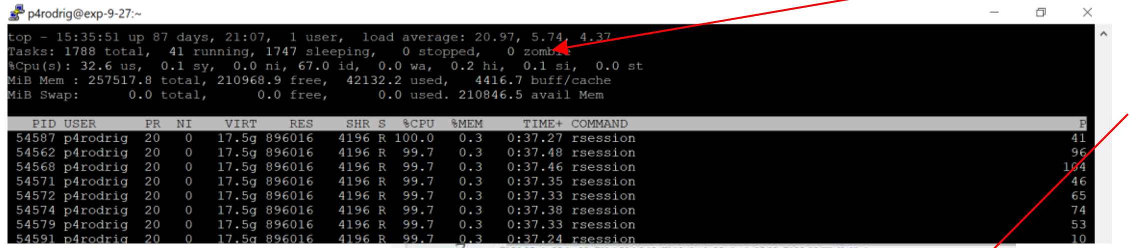
Name	Size
.r	
chap15_rnnv4.ipynb	136 KB
e494_Practical_NNet_exercise_...	18.5 KB
environment_tests_v1	1.8 KB
getcpu_scratch.sh	274 B
getid.c	324 B

Review the top output

Notice the elapsed time and memory size

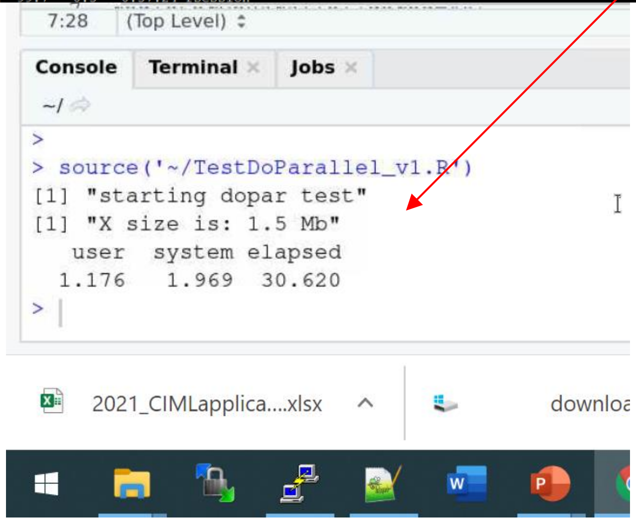
Change the NxP matrix size and rerun

(start with N=10K, P=2K)

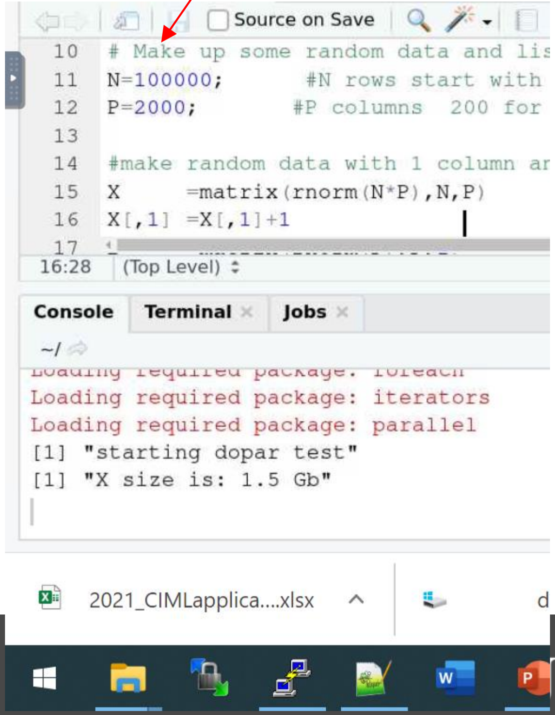


p4rodrig@exp-9-27:~

```
top - 15:35:51 up 87 days, 21:07,  1 user,  load average: 20.97, 5.74, 4.37
Tasks: 1788 total,  41 running, 1747 sleeping,   0 stopped,   0 zomb
%Cpu(s): 32.6 us,  0.1 sy,  0.0 ni, 67.0 id,  0.0 wa,  0.2 hi,  0.1 si,  0.0 st
MiB Mem : 257517.8 total, 210968.9 free,  42132.2 used,   4416.7 buff/cache
MiB Swap:      0.0 total,      0.0 free,      0.0 used. 210846.5 avail Mem

  PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM     TIME+ COMMAND                P
54587 p4rodrig  20   0   17.5g 896016   4196 R 100.0   0.3   0:37.27 rsession              41
54562 p4rodrig  20   0   17.5g 896016   4196 R  99.7   0.3   0:37.48 rsession              96
54568 p4rodrig  20   0   17.5g 896016   4196 R  99.7   0.3   0:37.46 rsession             104
54571 p4rodrig  20   0   17.5g 896016   4196 R  99.7   0.3   0:37.35 rsession              46
54572 p4rodrig  20   0   17.5g 896016   4196 R  99.7   0.3   0:37.33 rsession              65
54574 p4rodrig  20   0   17.5g 896016   4196 R  99.7   0.3   0:37.38 rsession              74
54579 p4rodrig  20   0   17.5g 896016   4196 R  99.7   0.3   0:37.33 rsession              53
54591 p4rodrig  20   0   17.5g 896016   4196 R  99.7   0.3   0:37.24 rsession              10
```



```
>
> source('~/TestDoParallel_v1.R')
[1] "starting dopar test"
[1] "X size is: 1.5 Mb"
   user  system elapsed
  1.176   1.969  30.620
>
```

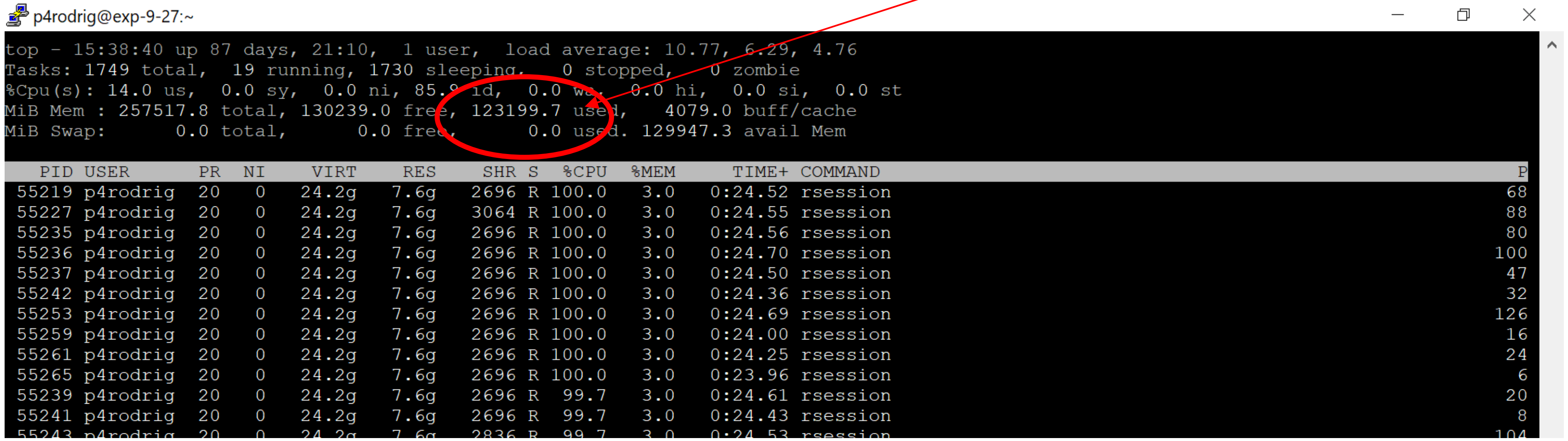


```
# Make up some random data and lis
N=100000;       #N rows start with
P=2000;       #P columns  200 for

#make random data with 1 column ar
X      =matrix(rnorm(N*P),N,P)
X[,1]  =X[,1]+1
```

```
Loading required package: iterators
Loading required package: parallel
[1] "starting dopar test"
[1] "X size is: 1.5 Gb"
```

Try this at home:

Let N=100K , P=2000
Notice the memory used is close to 124Gb we asked for



p4rodrig@exp-9-27:~

```
top - 15:38:40 up 87 days, 21:10,  1 user,  load average: 10.77, 6.29, 4.76
Tasks: 1749 total,  19 running, 1730 sleeping,   0 stopped,   0 zombie
%Cpu(s): 14.0 us,  0.0 sy,  0.0 ni, 85.9 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
MiB Mem : 257517.8 total, 130239.0 free, 123199.7 used,   4079.0 buff/cache
MiB Swap:      0.0 total,      0.0 free,      0.0 used. 129947.3 avail Mem

  PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM     TIME+ COMMAND                                   P
55219 p4rodrig  20   0   24.2g   7.6g   2696 R 100.0   3.0   0:24.52 rsession                                 68
55227 p4rodrig  20   0   24.2g   7.6g   3064 R 100.0   3.0   0:24.55 rsession                                 88
55235 p4rodrig  20   0   24.2g   7.6g   2696 R 100.0   3.0   0:24.56 rsession                                 80
55236 p4rodrig  20   0   24.2g   7.6g   2696 R 100.0   3.0   0:24.70 rsession                                100
55237 p4rodrig  20   0   24.2g   7.6g   2696 R 100.0   3.0   0:24.50 rsession                                 47
55242 p4rodrig  20   0   24.2g   7.6g   2696 R 100.0   3.0   0:24.36 rsession                                 32
55253 p4rodrig  20   0   24.2g   7.6g   2696 R 100.0   3.0   0:24.69 rsession                                126
55259 p4rodrig  20   0   24.2g   7.6g   2696 R 100.0   3.0   0:24.00 rsession                                 16
55261 p4rodrig  20   0   24.2g   7.6g   2696 R 100.0   3.0   0:24.25 rsession                                 24
55265 p4rodrig  20   0   24.2g   7.6g   2696 R 100.0   3.0   0:23.96 rsession                                  6
55239 p4rodrig  20   0   24.2g   7.6g   2696 R  99.7   3.0   0:24.61 rsession                                 20
55241 p4rodrig  20   0   24.2g   7.6g   2696 R  99.7   3.0   0:24.43 rsession                                  8
55243 p4rodrig  20   0   24.2g   7.6g   2836 R  99.7   3.0   0:24.53 rsession                                104
```

If you ask for 248Gb will it run?
What if you use only 24 cores?

Parallezing for loops
(pseudo code)

R with
doParallel

```
makecluster
registercluster

foreach with dopar,




combine results
```

Parallezing for loops
(pseudo code)

R with doParallel	Matlab with parallel toolbox

makecluster
registercluster
	parcluster('local')
	parpool()

foreach with dopar,	*parfor* *or* *'spmd' with distributed arrays*
combine results	gather array

Parallezing for loops

(pseudo code)

R with doParallel	Matlab with parallel toolbox	Python with dask.distributed

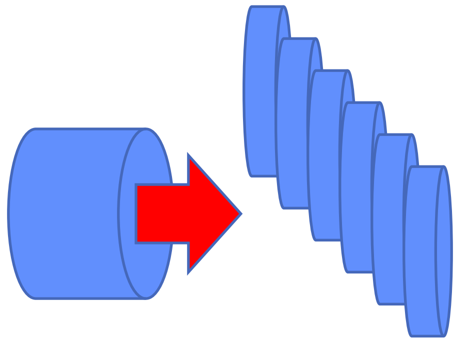
makecluster
registercluster
	parcluster('local')
	parpool()
		Import delayed, Client
		Client(numwkrs)

foreach with dopar,	*parfor*
	or
	'spmd' with distributed arrays
		for i in range(numwkrs):
		  A=delayed(my_func)(i)
		  Acombine.append(A)

combine results	gather array	Acombined.compute()

An option for (embarrassingly) Parallel R

1. Split up data into N parts

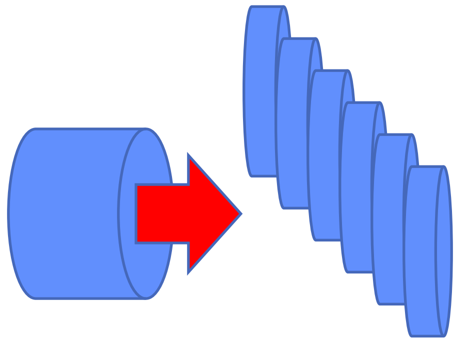


An option for (embarrassingly) Parallel R

1. Split up data into N parts

2. In slurm batch script:

    mpirun …   my-perl-script



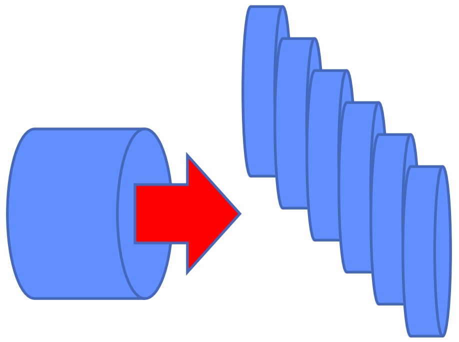
My-perl-script:
get cpu-id & pass it to R

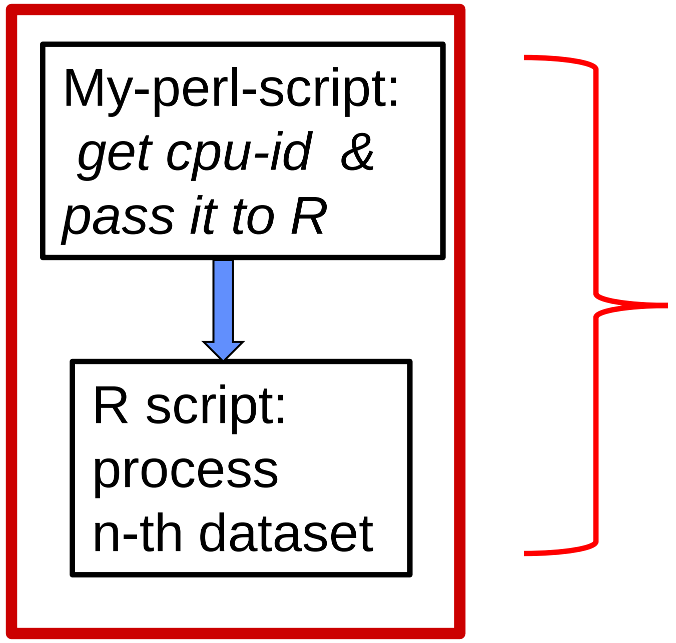
R script:
process
n-th dataset

An option for (embarrassingly) Parallel R

1. Split up data into N parts

2. In slurm batch script:
   mpirun … my-perl-script





This gets distributed across nodes and cores by slurm & mpi parameters

Slurm parameters: one R instance per core across all nodes

Normal batch job info

```
…
#SBATCH --partition=compute
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=128
#SBATCH --cpus-per-task=1

module load slurm
module load cpu
module load gcc
module load intel-mpi



mpirun -genv I_MPI_PIN_DOMAIN=omp:compact ./get_mpirank_runcmd.pl
```

2 x128 = 256 mpi ranks

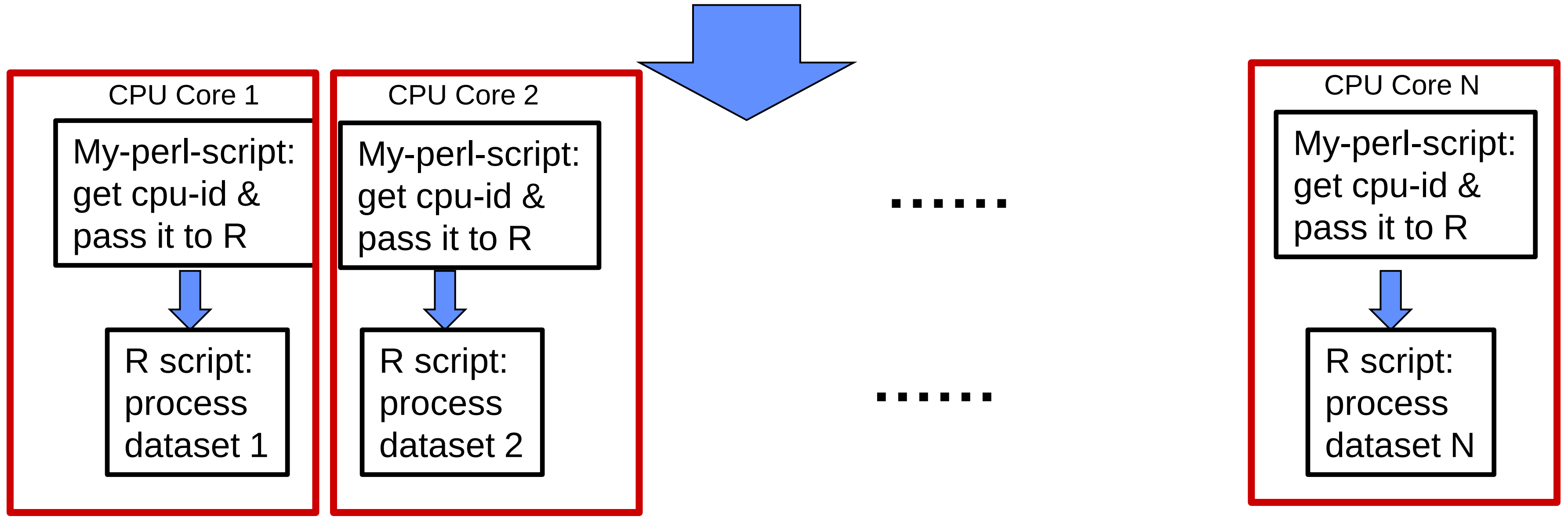
256 perl script/R instances
1 core each

(based on /cm/shared/examples/sdsc/mpi-openmp-hybrid/hybrid-slurm.sb)

one R instance per core across all nodes

. In slurm batch script:

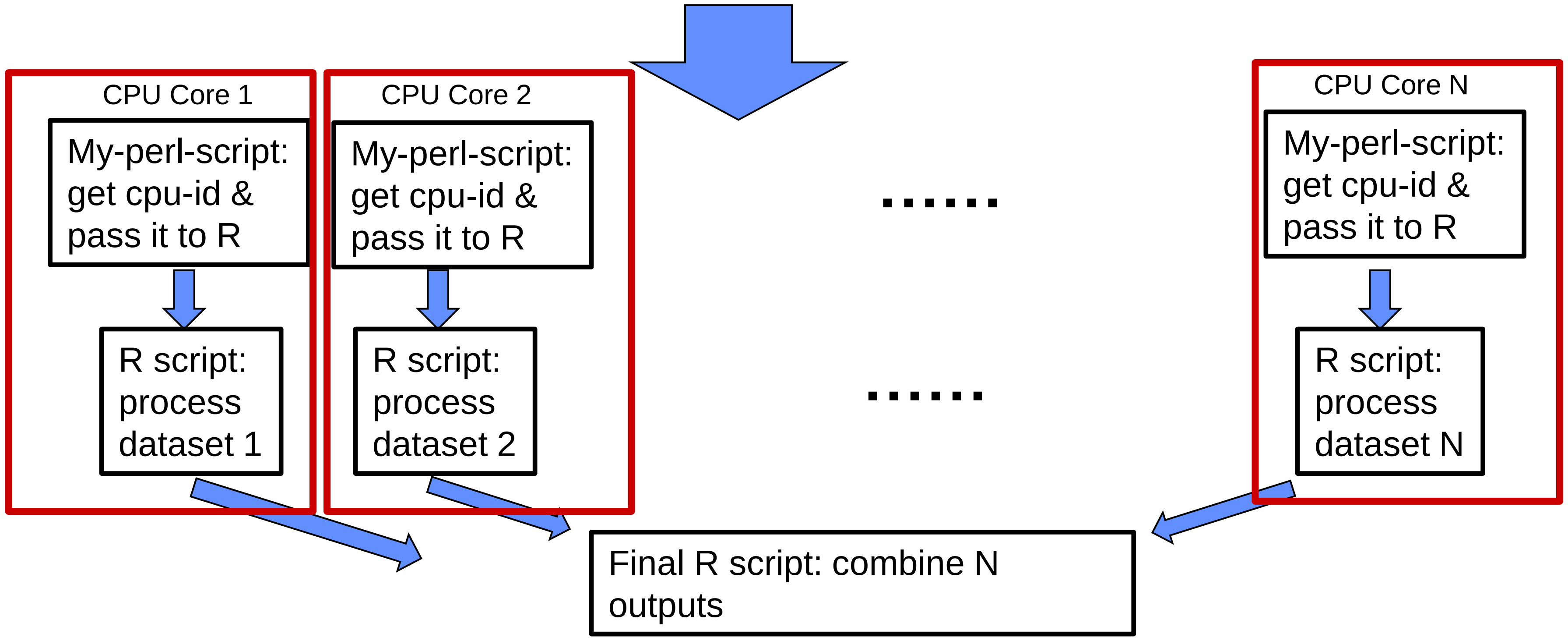
```
mpirun …    my-perl-script
```


CPU Core 1
My-perl-script: get cpu-id & pass it to R
R script: process dataset 1
CPU Core 2
My-perl-script: get cpu-id & pass it to R
R script: process dataset 2
……
……
CPU Core N
My-perl-script: get cpu-id & pass it to R
R script: process dataset N

one R instance per core across all nodes

In slurm batch script:

mpirun … my-perl-script



CPU Core 1
My-perl-script: get cpu-id & pass it to R
R script: process dataset 1
CPU Core 2
My-perl-script: get cpu-id & pass it to R
R script: process dataset 2
……
……
CPU Core N
My-perl-script: get cpu-id & pass it to R
R script: process dataset N
Final R script: combine N outputs

More programming but perhaps more useful

Slurm parameters: one R instance per node with 128 cores per R instance

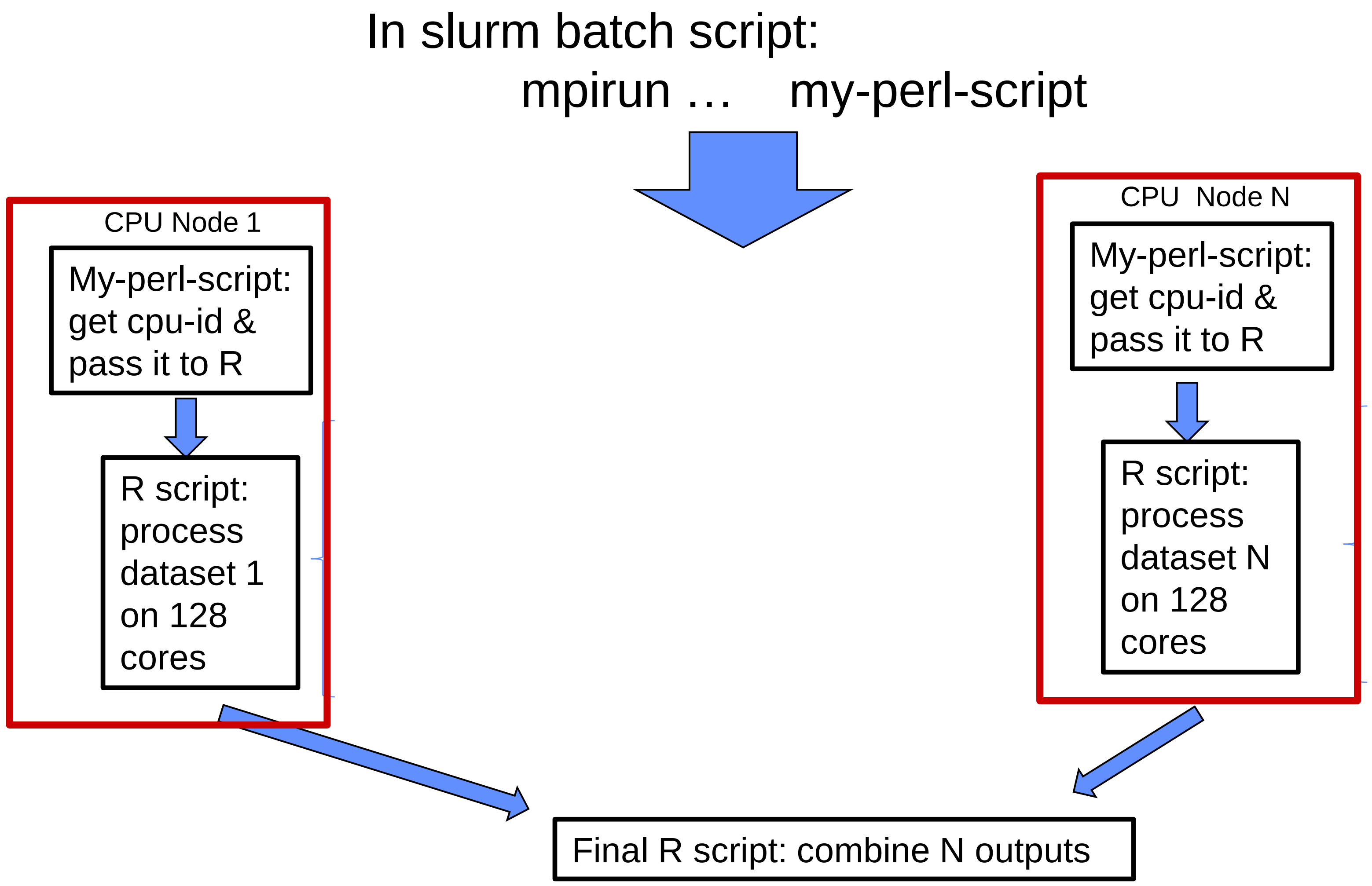
Normal batch job info

```
…
#SBATCH --partition=compute
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=128

module load slurm
module load cpu
module load gcc
module load intel-mpi

module load r

mpirun -genv I_MPI_PIN_DOMAIN=omp:compact ./get_mpirank_runcmd.pl
```

2 x1 = 2 mpi ranks

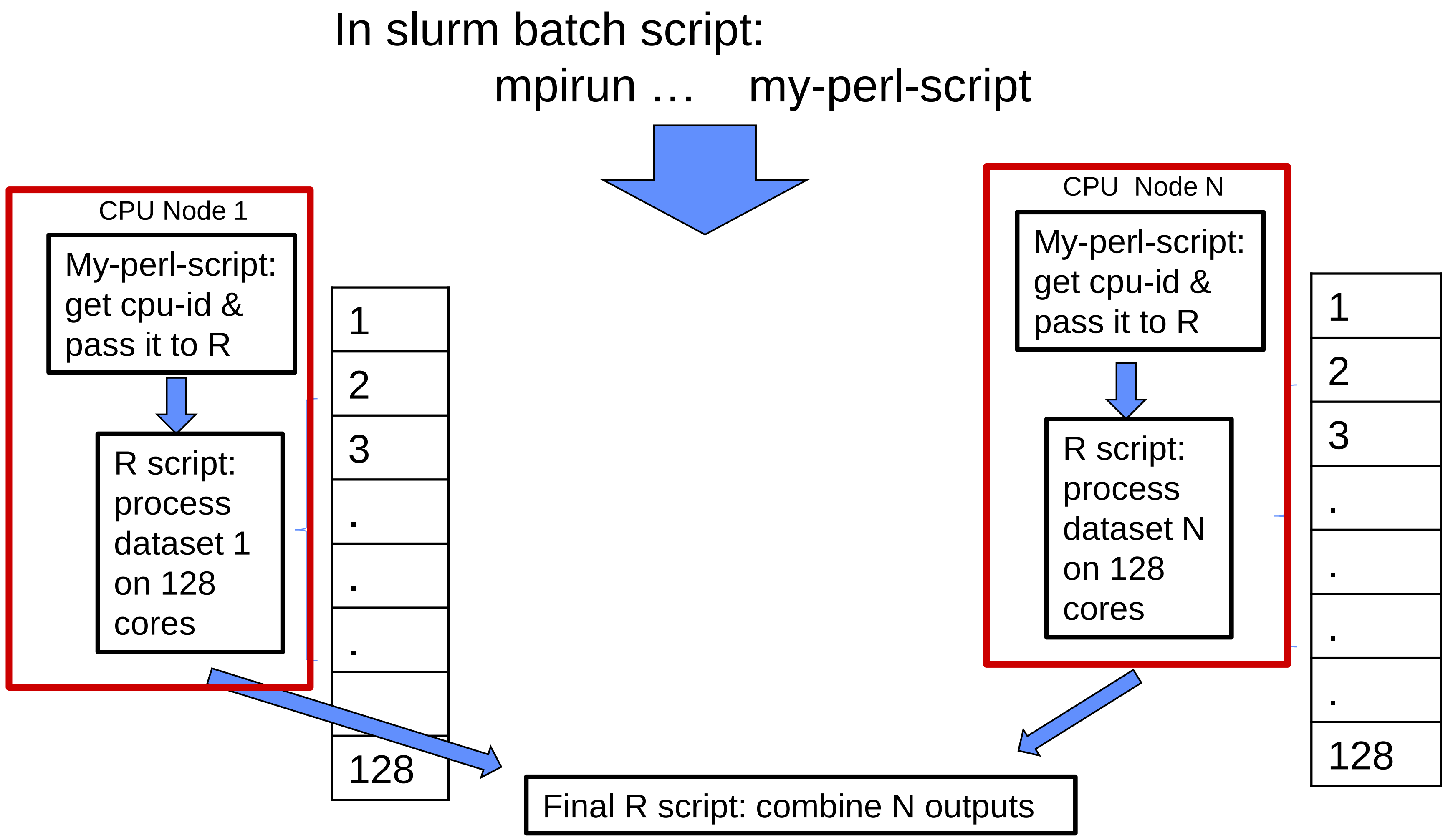
2 perl script/R instances
128 cores each
(doParallel can use them)

Example: One R instance per node, doParallel across all cores in each node



In slurm batch script:
mpirun … my-perl-script
CPU Node 1
My-perl-script: get cpu-id & pass it to R
R script: process dataset 1 on 128 cores
CPU Node N
My-perl-script: get cpu-id & pass it to R
R script: process dataset N on 128 cores
Final R script: combine N outputs

Example: One R instance per node, doParallel across all cores in each node


In slurm batch script:
mpirun … my-perl-script
CPU Node 1
My-perl-script: get cpu-id & pass it to R
R script: process dataset 1 on 128 cores
1
2
3
.
.
.
128
CPU Node N
My-perl-script: get cpu-id & pass it to R
R script: process dataset N on 128 cores
1
2
3
.
.
.
.
128
Final R script: combine N outputs

Big Data exploration

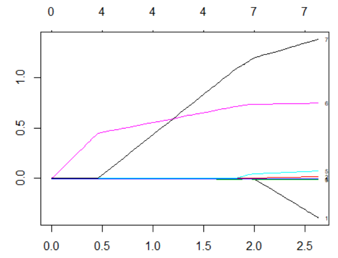
- Run R ‘biglasso’ with a dataset too big for RAM
- Create large CSV file (117Gb) of X data matrix and Y outcomes:
  Y=X*B + noise (where X is 100K x50K)
- Explore other packages with out-of-core dataset functions:
  Matlab, Dask-ML, Spark, Keras
- Beware: lasso implementations can differ;
  also, Y,X,B should be ‘nice’

Lasso Regression

- **Penalized Loss function** $L = \boldsymbol{MSE} + \boldsymbol{\lambda} \sum |b_{\boldsymbol{i}}|$

- **Recall: using penalty term is the same as using a constraint (constrained optimization)**

  find min $\boldsymbol{MSE}\ such\ that \sum |bi| < S$



- **Different implementations may:**
  - use different fit methods (ie forward stepwise, coordinate descent, gradient descent,…)
  - might parallelize by splitting up data, computations, or vectorizing
  - read/load data more or less efficiently

Considerations

- All packages have special functions to handle out of core dataset
- Sometimes better to have Y,X together; sometimes two files are better

- All were run as Expanse batch jobs, not through notebook/portal

- All were set up run on 1 compute node (248Gb RAM) and use scratch (ssd) space. (Large memory nodes are available on Expanse, but not tested)

- Mostly default parameters used; Little optimization performed; Not a benchmark study!

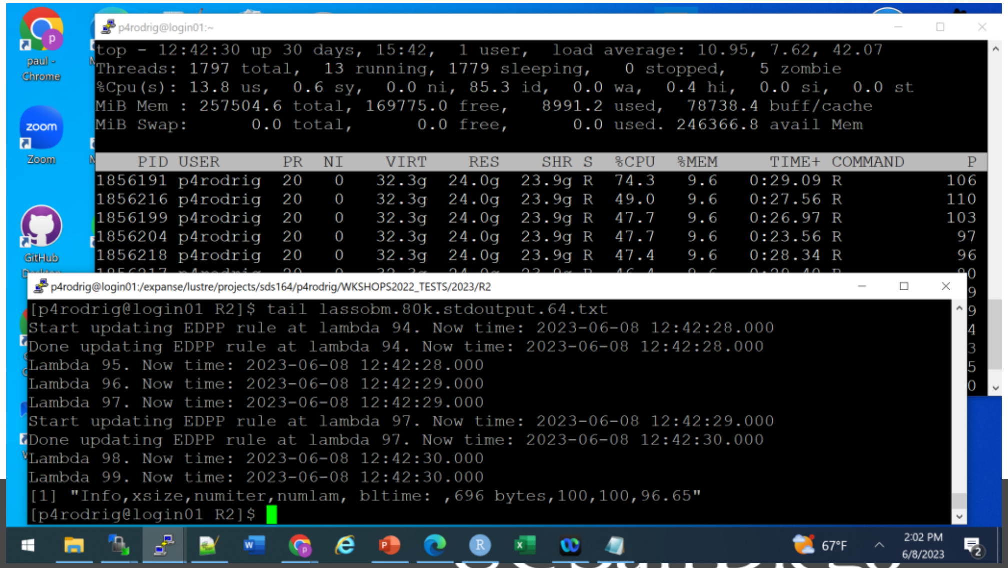
R

- **R – biglasso (bigmatrix) package to set up file backed dataframe**

https://cran.rstudio.com/web/packages/biglasso/

Issue: setting up the path for the file backend was hard – ended up just running out of scratch SSD as working directory;

Outcome: R copies everything into binary file (the backend) and got results in about 2hours



p4rodrig@login01:~

```
top - 12:42:30 up 30 days, 15:42,  1 user,  load average: 10.95, 7.62, 42.07
Threads: 1797 total,  13 running, 1779 sleeping,   0 stopped,   5 zombie
%Cpu(s): 13.8 us,  0.6 sy,  0.0 ni, 85.3 id,  0.0 wa,  0.4 hi,  0.0 si,  0.0 st
MiB Mem : 257504.6 total, 169775.0 free,   8991.2 used,  78738.4 buff/cache
MiB Swap:      0.0 total,      0.0 free,      0.0 used. 246366.8 avail Mem

    PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM     TIME+ COMMAND   P
1856191 p4rodrig  20   0   32.3g  24.0g  23.9g R  74.3   9.6   0:29.09 R       106
1856216 p4rodrig  20   0   32.3g  24.0g  23.9g R  49.0   9.6   0:27.56 R       110
1856199 p4rodrig  20   0   32.3g  24.0g  23.9g R  47.7   9.6   0:26.97 R       103
1856204 p4rodrig  20   0   32.3g  24.0g  23.9g R  47.7   9.6   0:23.56 R        97
1856218 p4rodrig  20   0   32.3g  24.0g  23.9g R  47.4   9.6   0:28.34 R        96
```

p4rodrig@login01:/expanse/lustre/projects/sds164/p4rodrig/WKSHOPS2022_TESTS/2023/R2

```
[p4rodrig@login01 R2]$ tail lassobm.80k.stdoutput.64.txt
Start updating EDPP rule at lambda 94. Now time: 2023-06-08 12:42:28.000
Done updating EDPP rule at lambda 94. Now time: 2023-06-08 12:42:28.000
Lambda 95. Now time: 2023-06-08 12:42:28.000
Lambda 96. Now time: 2023-06-08 12:42:29.000
Lambda 97. Now time: 2023-06-08 12:42:29.000
Start updating EDPP rule at lambda 97. Now time: 2023-06-08 12:42:29.000
Done updating EDPP rule at lambda 97. Now time: 2023-06-08 12:42:30.000
Lambda 98. Now time: 2023-06-08 12:42:30.000
Lambda 99. Now time: 2023-06-08 12:42:30.000
[1] "Info,xsize,numiter,numlam, bltime: ,696 bytes,100,100,96.65"
[p4rodrig@login01 R2]$
```

R code highlights

Use biglasso package

Y data fits in memory so just read it in

X data will be setup with file-backed memory

biglasso() arguments look like the glmnet LASSO implementation

```
library(biglasso)
….
Y.bm=read.big.matrix(inputYfile,sep = ",")
X.bm=setupX(inputXfile,sep=",",
                         type="double",
                         backingfile    = "x.bin",
                         descriptorfile = "x.desc")
….

bl_results=biglasso( X.bm, Y.bm,
                         row.idx = 1:nrow(X.bm),
                         penalty = c("lasso"),
                         family = c("gaussian"),
                         ncores = numcores,  …
```

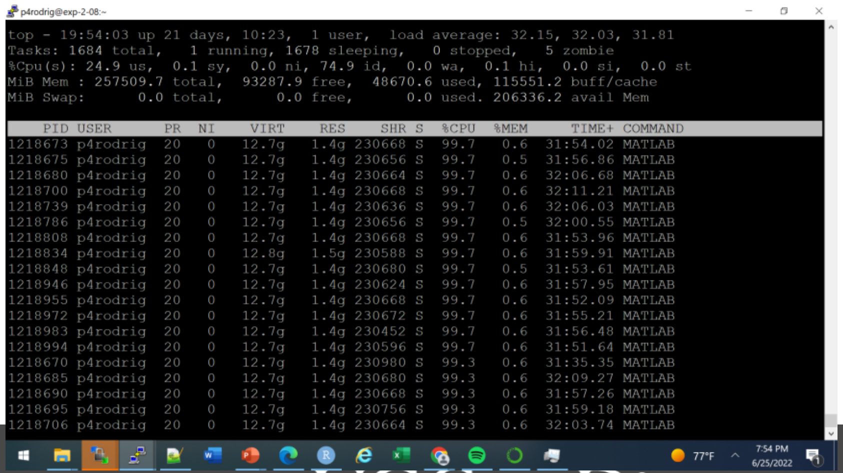
Matlab

- Matlab – has tall table functions to read in large CSV file; but lasso needs tall array

I found a ‘table2array’ function that helped set up the data

But matlab tall arrays are not intended to run with too much memory, or too many columns, b/c lasso uses correlation matrix

in the variable selection algorithm



```
top - 19:54:03 up 21 days, 10:23,  1 user,  load average: 32.15, 32.03, 31.81
Tasks: 1684 total,   1 running, 1678 sleeping,   0 stopped,   5 zombie
%Cpu(s): 24.9 us,  0.1 sy,  0.0 ni, 74.9 id,  0.0 wa,  0.1 hi,  0.0 si,  0.0 st
MiB Mem : 257509.7 total,  93287.9 free,  48670.6 used, 115551.2 buff/cache
MiB Swap:      0.0 total,      0.0 free,      0.0 used. 206336.2 avail Mem

    PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM     TIME+ COMMAND
1218673 p4rodrig  20   0   12.7g   1.4g 230668 S  99.7   0.6  31:54.02 MATLAB
1218675 p4rodrig  20   0   12.7g   1.4g 230656 S  99.7   0.5  31:56.86 MATLAB
1218680 p4rodrig  20   0   12.7g   1.4g 230664 S  99.7   0.6  32:06.68 MATLAB
1218700 p4rodrig  20   0   12.7g   1.4g 230668 S  99.7   0.6  32:11.21 MATLAB
1218739 p4rodrig  20   0   12.7g   1.4g 230636 S  99.7   0.6  32:06.03 MATLAB
1218786 p4rodrig  20   0   12.7g   1.4g 230656 S  99.7   0.5  32:00.55 MATLAB
1218808 p4rodrig  20   0   12.7g   1.4g 230668 S  99.7   0.6  31:53.96 MATLAB
1218834 p4rodrig  20   0   12.8g   1.5g 230588 S  99.7   0.6  31:59.91 MATLAB
1218848 p4rodrig  20   0   12.7g   1.4g 230680 S  99.7   0.5  31:53.61 MATLAB
1218946 p4rodrig  20   0   12.7g   1.4g 230624 S  99.7   0.6  31:57.95 MATLAB
1218955 p4rodrig  20   0   12.7g   1.4g 230668 S  99.7   0.6  31:52.09 MATLAB
1218972 p4rodrig  20   0   12.7g   1.4g 230672 S  99.7   0.6  31:55.21 MATLAB
1218983 p4rodrig  20   0   12.7g   1.4g 230452 S  99.7   0.6  31:56.48 MATLAB
1218994 p4rodrig  20   0   12.7g   1.4g 230596 S  99.7   0.6  31:51.64 MATLAB
1218670 p4rodrig  20   0   12.7g   1.4g 230980 S  99.3   0.6  31:35.35 MATLAB
1218685 p4rodrig  20   0   12.7g   1.4g 230680 S  99.3   0.6  32:09.27 MATLAB
1218690 p4rodrig  20   0   12.7g   1.4g 230668 S  99.3   0.6  31:57.26 MATLAB
1218695 p4rodrig  20   0   12.7g   1.4g 230756 S  99.3   0.6  31:59.18 MATLAB
1218706 p4rodrig  20   0   12.7g   1.4g 230664 S  99.3   0.6  32:03.74 MATLAB
```

Dask-ml

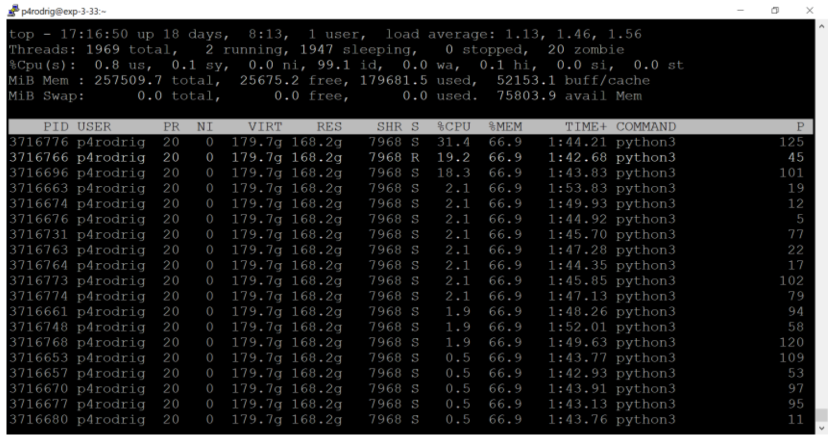
- **Dask-ML – worked easily with distributed dataframe, built on top of sklearn,**

read_csv uses a ‘blocksize’ parameter

repeatedly calls sklearn ‘partial-fit’ functions that iterate 1 time for ‘batch’ processing

worked better with Y&X in one dataframe

I stopped it after 4hrs, but it was running



```
top - 17:16:50 up 18 days,  8:13,  1 user,  load average: 1.13, 1.46, 1.56
Threads: 1969 total,   2 running, 1947 sleeping,   0 stopped,  20 zombie
%Cpu(s):  0.8 us,  0.1 sy,  0.0 ni, 99.1 id,  0.0 wa,  0.1 hi,  0.0 si,  0.0 st
MiB Mem : 257509.7 total,  25675.2 free, 179681.5 used,  52153.1 buff/cache
MiB Swap:      0.0 total,      0.0 free,      0.0 used.  75803.9 avail Mem

    PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM     TIME+ COMMAND            P
3716776 p4rodrig  20   0  179.7g 168.2g   7968 S  31.4  66.9   1:44.21 python3          125
3716766 p4rodrig  20   0  179.7g 168.2g   7968 R  19.2  66.9   1:42.68 python3           45
3716696 p4rodrig  20   0  179.7g 168.2g   7968 S  18.3  66.9   1:43.83 python3          101
3716663 p4rodrig  20   0  179.7g 168.2g   7968 S   2.1  66.9   1:53.83 python3           19
3716674 p4rodrig  20   0  179.7g 168.2g   7968 S   2.1  66.9   1:49.93 python3           12
3716676 p4rodrig  20   0  179.7g 168.2g   7968 S   2.1  66.9   1:44.92 python3            5
3716731 p4rodrig  20   0  179.7g 168.2g   7968 S   2.1  66.9   1:45.70 python3           77
3716763 p4rodrig  20   0  179.7g 168.2g   7968 S   2.1  66.9   1:47.28 python3           22
3716764 p4rodrig  20   0  179.7g 168.2g   7968 S   2.1  66.9   1:44.35 python3           17
3716773 p4rodrig  20   0  179.7g 168.2g   7968 S   2.1  66.9   1:45.85 python3          102
3716774 p4rodrig  20   0  179.7g 168.2g   7968 S   2.1  66.9   1:47.13 python3           79
3716661 p4rodrig  20   0  179.7g 168.2g   7968 S   1.9  66.9   1:48.26 python3           94
3716748 p4rodrig  20   0  179.7g 168.2g   7968 S   1.9  66.9   1:52.01 python3           58
3716768 p4rodrig  20   0  179.7g 168.2g   7968 S   1.9  66.9   1:49.63 python3          120
3716653 p4rodrig  20   0  179.7g 168.2g   7968 S   0.5  66.9   1:43.77 python3          109
3716657 p4rodrig  20   0  179.7g 168.2g   7968 S   0.5  66.9   1:42.93 python3           53
3716670 p4rodrig  20   0  179.7g 168.2g   7968 S   0.5  66.9   1:43.91 python3           97
3716677 p4rodrig  20   0  179.7g 168.2g   7968 S   0.5  66.9   1:43.13 python3           95
3716680 p4rodrig  20   0  179.7g 168.2g   7968 S   0.5  66.9   1:43.76 python3           11
```

Spark

- **Spark – uses distributed dataframe with pyspark.ml.regression package**

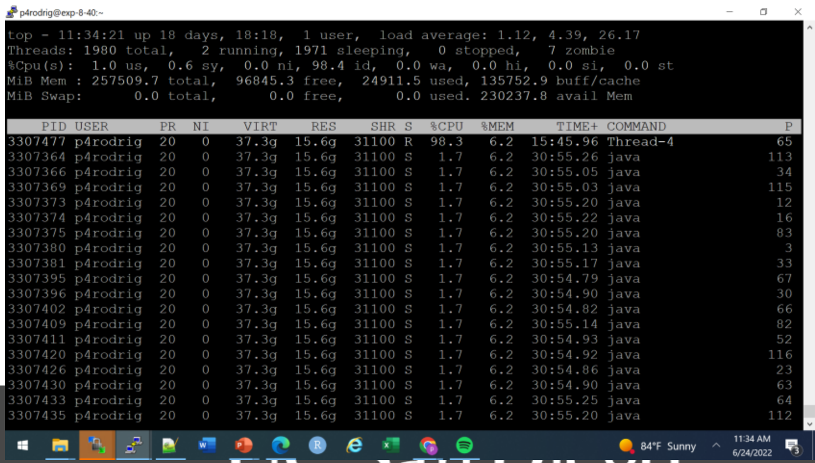
Use the vector assembler options to get Y and 'features' all in one dataframe

Got some help on spark session options:

device & executor memory, eg: local[64], 8Gb, 2Gb

Local[64], 50 min in, 1 iteration

I stopped it after 4 hrs; it was running



```
top - 11:34:21 up 18 days, 18:18,  1 user,  load average: 1.12, 4.39, 26.17
Threads: 1980 total,   2 running, 1971 sleeping,   0 stopped,   7 zombie
%Cpu(s):  1.0 us,  0.6 sy,  0.0 ni, 98.4 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
MiB Mem : 257509.7 total,  96845.3 free,  24911.5 used, 135752.9 buff/cache
MiB Swap:      0.0 total,      0.0 free,      0.0 used. 230237.8 avail Mem

    PID USER      PR  NI    VIRT    RES    SHR S  %CPU  %MEM     TIME+ COMMAND                    P
3307477 p4rodrig  20   0   37.3g  15.6g  31100 R  98.3   6.2  15:45.96 Thread-4                  65
3307364 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:55.26 java                     113
3307366 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:55.05 java                      34
3307369 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:55.03 java                     115
3307373 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:55.20 java                      12
3307374 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:55.22 java                      16
3307375 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:55.20 java                      83
3307380 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:55.13 java                       3
3307381 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:55.17 java                      33
3307395 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:54.79 java                      67
3307396 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:54.90 java                      30
3307402 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:54.82 java                      66
3307409 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:55.14 java                      82
3307411 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:54.93 java                      52
3307420 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:54.92 java                     116
3307426 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:54.86 java                      23
3307430 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:54.90 java                      63
3307433 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:55.25 java                      64
3307435 p4rodrig  20   0   37.3g  15.6g  31100 S   1.7   6.2  30:55.20 java                     112
```

Keras

- Keras - set up a tensorflow dataset with data generator (to reading batches at a time from csv file); a little tricky to get shapes right;

I set up a 1 layer linear neural network with a L1 regularizer on weights

runs, 1000 epochs in 1 hour+ (on cpu)

I did not set up convergence options like other Lasso implementations

Final Considerations, R and other packages

- Start with small data with interactive session or notebook – maybe even just use a smaller sample?

- All packages generally work as documented, but

- All packages require working through some implementation issues or environment options for the session/job/execution

A note on installing R Packages (into your own directories)

- **In R (might help to be on interactive node):**

  install.packages(‘package-name’)

  (see https://cran.r-project.org/ for package lists and reviews)

- **Sometimes you have to be explicit:**

  install.packages('ggmap',

  repos='http://cran.us.r-project.org',dependencies=TRUE)

  If compiling is required and you get an error, call support

  Packages are put into your /home/user/R directory

End