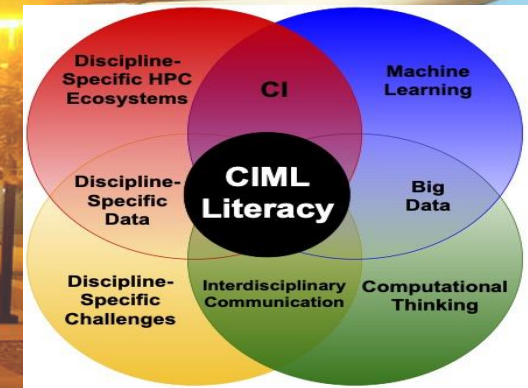


Scalable Machine Learning: R (and other packages), HPC, and Scaling

July 2022

Paul Rodriguez, PhD
(SDSC)



Outline

- **R and Scaling**
- **Parallel R**
- **Embarassingly Parallel R**
- **A big data exploration of R**

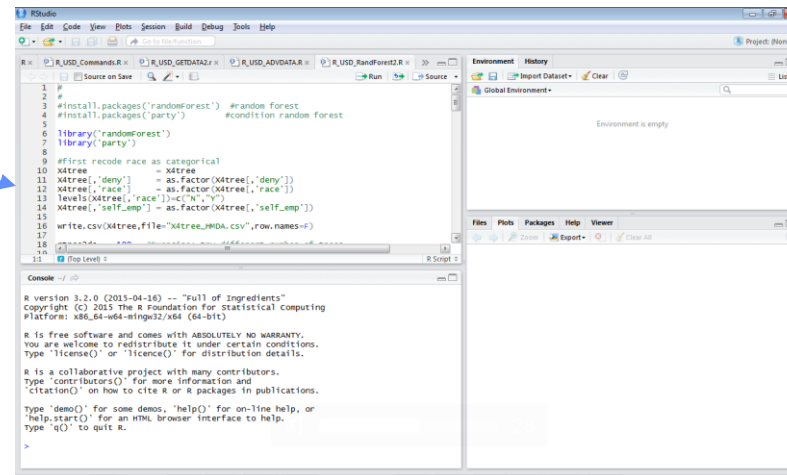
A typical R development workflow

- R studio: An Integrated development environment for R

Menu tab

*Edit window to
Build scripts*

R console



*Environment
Information on
variables and
command history*

*Plots, help
docs, package
lists*

Typical R code workflow

#READ DATA

```
X = read.csv('hmda_aer.csv', header=T, stringsAsFactors=T)
```

#SUBSET DATA

```
indices_2keep = which(X[, 's13'] %in% c(3,4,5))  
X = X[unique(indices_2keep),]
```

#CREATE/TRANSFORM VARIABLES

```
pi_rat = as.numeric(X[, 's46']/100) #debt2income ratio
```

#RUN MODEL and SHOW RESULTS

```
lm_result = lm(deny~pi_rat) #lm is 'linear model'  
summary(lm_result)
```

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
 - MCMC routines (but Stan is likely better package)
 - Generalized Linear Model
 - Some ML model (e.g. randomForest)

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)

R Scaling In a nutshell

- R sessionInfo() command shows math libraries

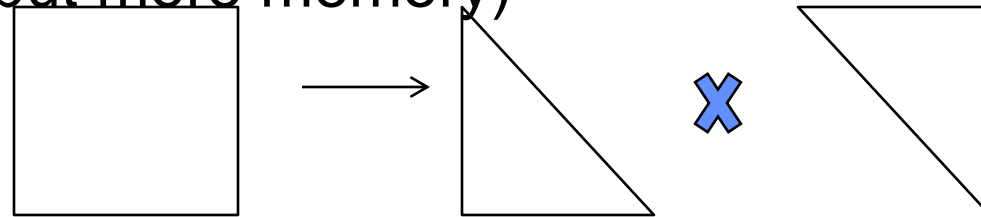
```
> sessionInfo()
R version 4.0.2 (2020-06-22)
Platform: x86_64-pc-linux-gnu (64-bit)
Running under: CentOS Linux 8 (Core)

Matrix products: default
BLAS/LAPACK: /cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/gcc-9.2.0/openblas
grrcfayp3br6kmcnelbgrepqmadwv43e/lib/libopenblas_zenp-r0.3.10.so

locale:
 [1] LC_CTYPE=en_US.UTF-8      LC_NUMERIC=C
 [3] LC_TIME=en_US.UTF-8      LC_COLLATE=en_US.UTF-8
 [5] LC_MONETARY=en_US.UTF-8  LC_MESSAGES=en_US.UTF-8
```

Consider Regression Computations

- **Linear Model:** $Y = X * B$
where Y =outcomes , X =data matrix
- **Algebraically, we could:**
take “inverse” of $X * Y = B$ (time consuming)
use derivatives to search for solutions (very general)
- **Or, better:**
QR decomposition of X into triangular matrices (easier to solve but more memory)



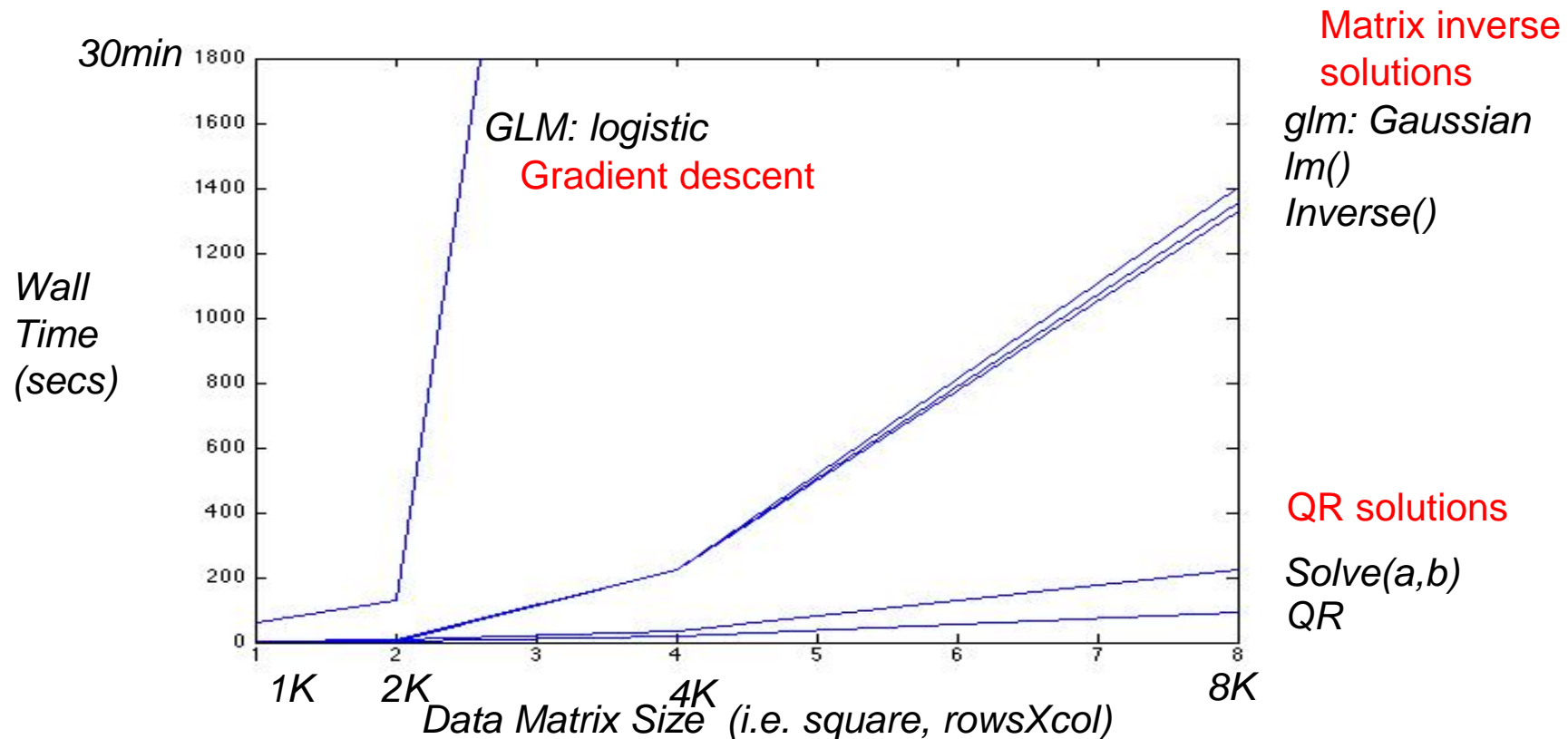
Solving Linear Systems

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)



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- Embarassingly Parallel R
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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 

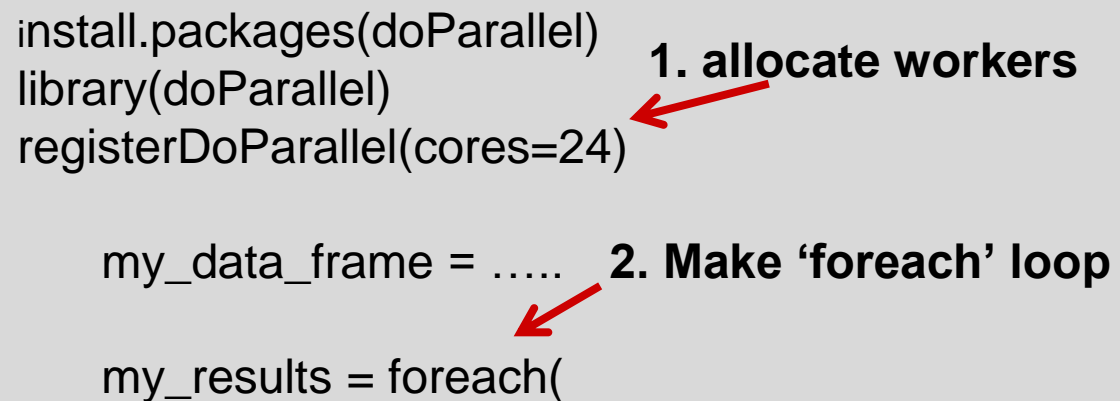
R multicore coding

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

1. allocate workers

2. Make 'foreach' loop


```
my_data_frame = .....
my_results = foreach(
```



R multicore coding

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

1. allocate workers



```
my_data_frame = .....
```

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) %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

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)
```

1. allocate workers

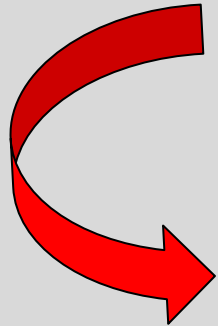
```
my_data_frame = .....
```

2. Make 'foreach' loop

```
my_results = foreach(i=1:24,.combine=rbind) %dopar%
{ ...
  your code here
  return( a variable or object )
}
```

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 its 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)
```


**1. allocate cluster as
parallel backend**



```
my_data_frame = .....
```

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

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



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

R multinode: parallel backend

```
library(doParallel)
```

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


**1. allocate cluster as
parallel backend**



```
my_data_frame = .....
```

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

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



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

```
})
```

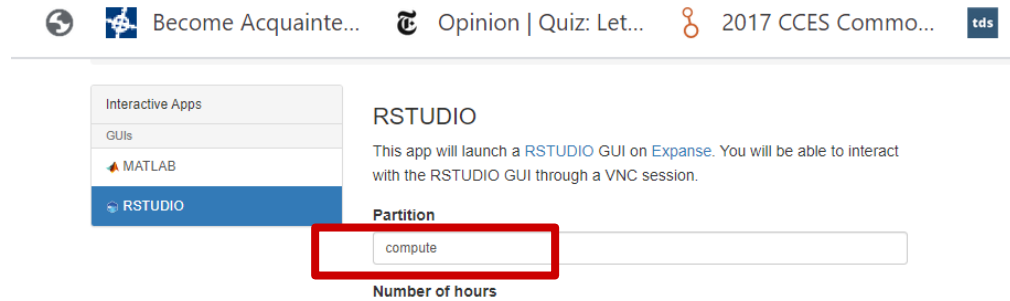
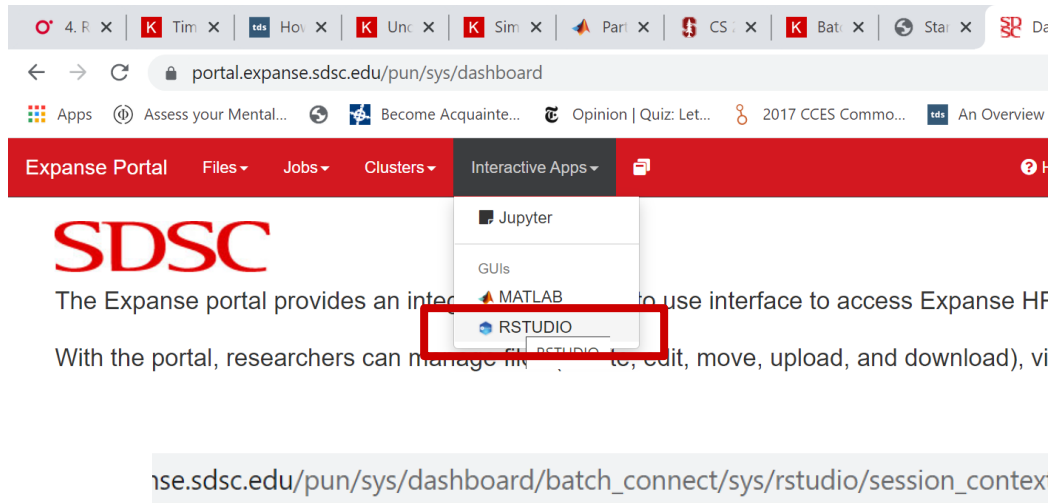
```
stopCluster(cl)
```



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

Testing/Evaluating R parallel

- **Exercise: 'TestdoParallel' R script**
 1. **Log into expanse portal and start R studio**
 2. **Also log into expanse command line and ssh to compute node**
 3. **run 'top -u username' to see performance**
 - Enter 'H' to see threads; Enter f, toggle 'P' to see cpu ids
 - look for tradeoffs in memory vs execution as matrix size varies (see next slides)



```

-----
Last login: Fri Jun  4 15:01:29 2021 from 71.128.8.73
[p4rodrig@login02 ~]$ queue -u p4rodrig
      JOBID PARTITION    NAME             USER  ST      TIME  NODES NODELIST(REASON)
      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:
login.expance

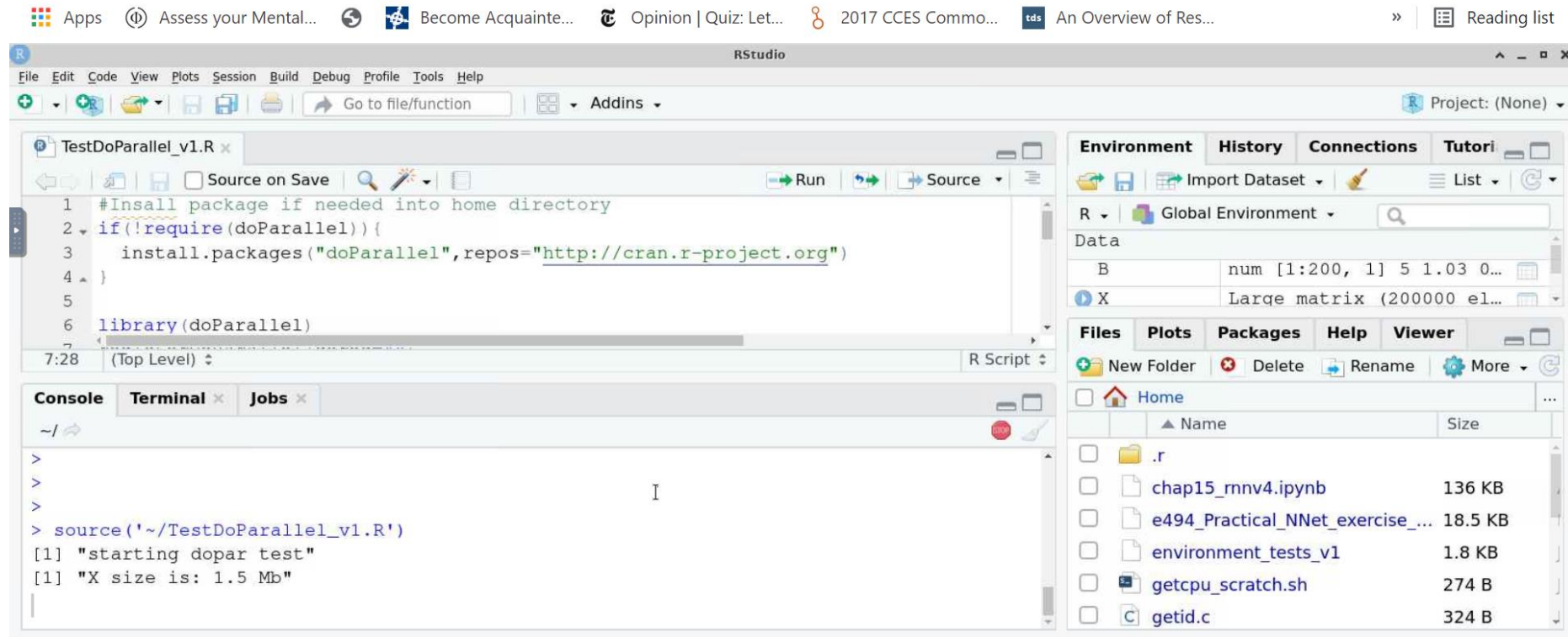
`$ queue -u $USER`
`$ ssh exp-##-##`
`$ top -u $USER`

'H' will toggle threads

'f', highlight P, space, esc
will toggle last cpuid

Open the 'Test_doParallel' Rscript

Select 'source' to run the whole script



The screenshot displays the RStudio environment with the following components:

- Top Bar:** Includes browser tabs for 'Apps', 'Assess your Mental...', 'Become Acquainte...', 'Opinion | Quiz: Let...', '2017 CCES Commo...', 'tds An Overview of Res...', and a 'Reading list' icon.
- Menu Bar:** Standard RStudio menus: File, Edit, Code, View, Plots, Session, Build, Debug, Profile, Tools, Help.
- Toolbar:** Icons for file operations and a 'Go to file/function' search bar.
- Source Editor:** Displays the script 'TestDoParallel_v1.R' with the following code:

```
1 #Install package if needed into home directory
2 if(!require(doParallel)){
3   install.packages("doParallel", repos="http://cran.r-project.org")
4 }
5
6 library(doParallel)
```

The status bar at the bottom of the editor shows '7:28 (Top Level)' and 'R Script'.
- Environment Panel:** Shows the 'Global Environment' with two objects:
 - B:** A numeric vector of length 200, with values ranging from 0 to 5.
 - X:** A large matrix of size 200,000 by 1.
- Files Panel:** Shows the file explorer for the home directory, listing files such as '.r', 'chap15_rnnv4.ipynb' (136 KB), 'e494_Practical_NNet_exercise_...' (18.5 KB), 'environment_tests_v1' (1.8 KB), 'getcpu_scratch.sh' (274 B), and 'getid.c' (324 B).
- Console:** Shows the execution of the script with the following output:

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

Review the top output

```
p4rodrig@exp-9-27:~  
top - 15:35:51 up 87 days, 21:07, 1 user, load average: 20.97, 5.76, 4.37  
Tasks: 1788 total, 41 running, 1747 sleeping, 0 stopped, 0 zombie  
%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  
54587 p4rodrig  20   0   17.5g   896016  4196 R 100.0   0.3   0:37.27 rsession  
54562 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.48 rsession  
54568 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.46 rsession  
54571 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.35 rsession  
54572 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.33 rsession  
54574 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.38 rsession  
54579 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.33 rsession  
54591 p4rodrig  20   0   17.5g   896016  4196 R  99.7   0.3   0:37.24 rsession
```

Notice the elapsed time and memory size

Change the $N \times P$ matrix size and rerun

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

```
7:28 (Top Level)   
Console Terminal x Jobs x  
~/   
>   
> source('~/TestDoParallel_v1.R')  
[1] "starting dopar test"  
[1] "X size is: 1.5 Mb"  
      user system elapsed  
1.176   1.969  30.620  
> |
```

```
10 # Make up some random data and lis  
11 N=100000;      #N rows start with  
12 P=2000;        #P columns 200 for  
13  
14 #make random data with 1 column ar  
15 X =matrix(rnorm(N*P),N,P)  
16 X[,1] =X[,1]+1  
17  
16:28 (Top Level)   
Console Terminal x Jobs x  
~/   
Loading required package: foreach  
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, 85.8 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

Matlab with parallel toolbox

parcluster('local')
parpool()

parfor
or
'spmd' with
distributed arrays

gather array

Python with dask.distributed

Import delayed, Client
Client(numwks)

for i in range(numwks):
 A=delayed(my_func)(i)
 Acombine.append(A)

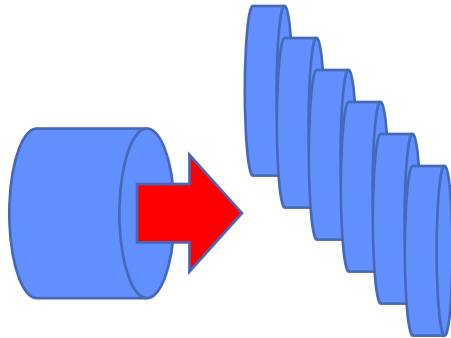
Acombined.compute()

Outline

- R and Scaling
- Parallel R
- **Embarassingly Parallel R**
- A big data exploration of R

An option for (embarrassingly) Parallel R

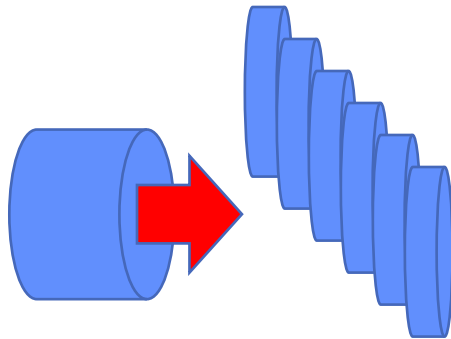
1. Split up data into N parts



An option for (embarrassingly) Parallel R

1. Split up
data into N
parts

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



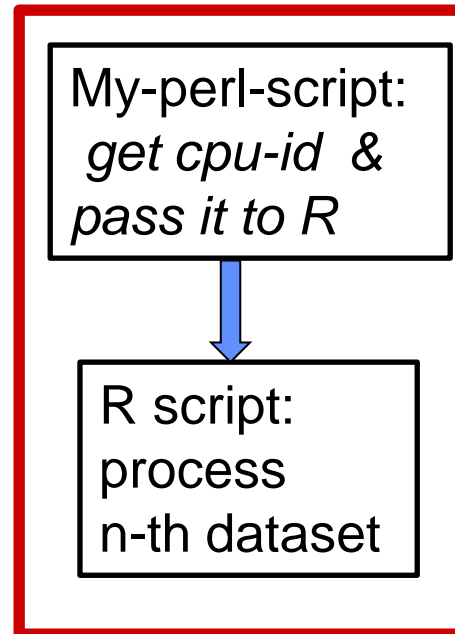
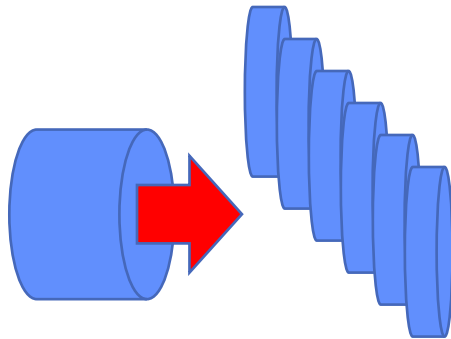
My-perl-script:
*get cpu-id &
pass it to R*

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
```

2 x 128 = 256 mpi ranks

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

256 perl script/R instances
1 core each

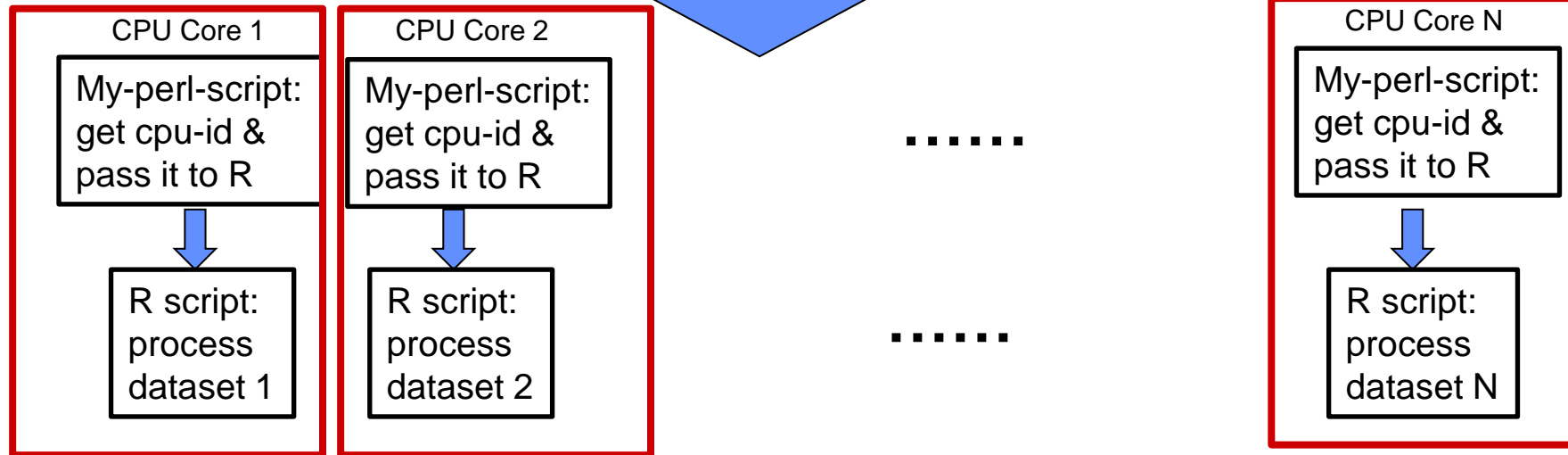
```
mpirun -genv I_MPI_PIN_DOMAIN=omp:compact ./get_mpirank_runcmd.pl
```

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

one R instance per core across all nodes

1. Split up
data into N
parts

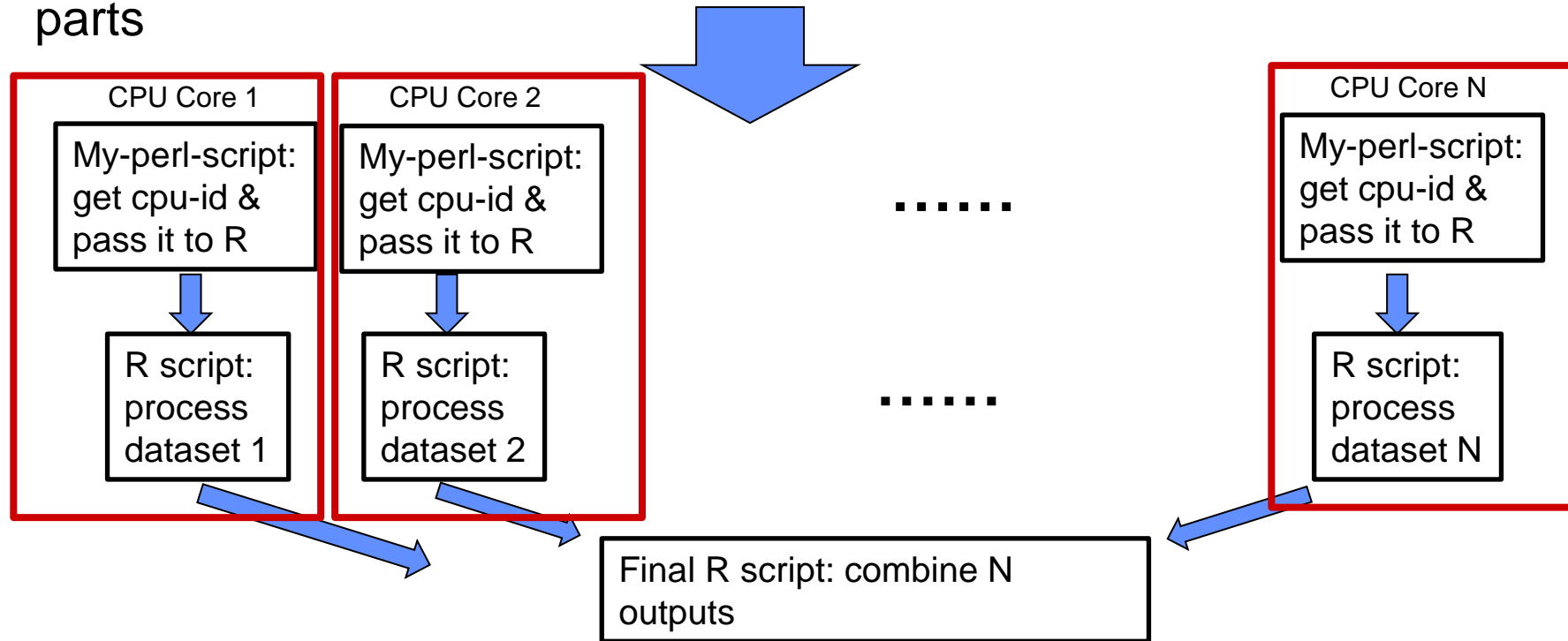
2. In slurm batch script:
`mpirun ... my-perl-script`



one R instance per core across all nodes

1. Split up
data into N
parts

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



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
```

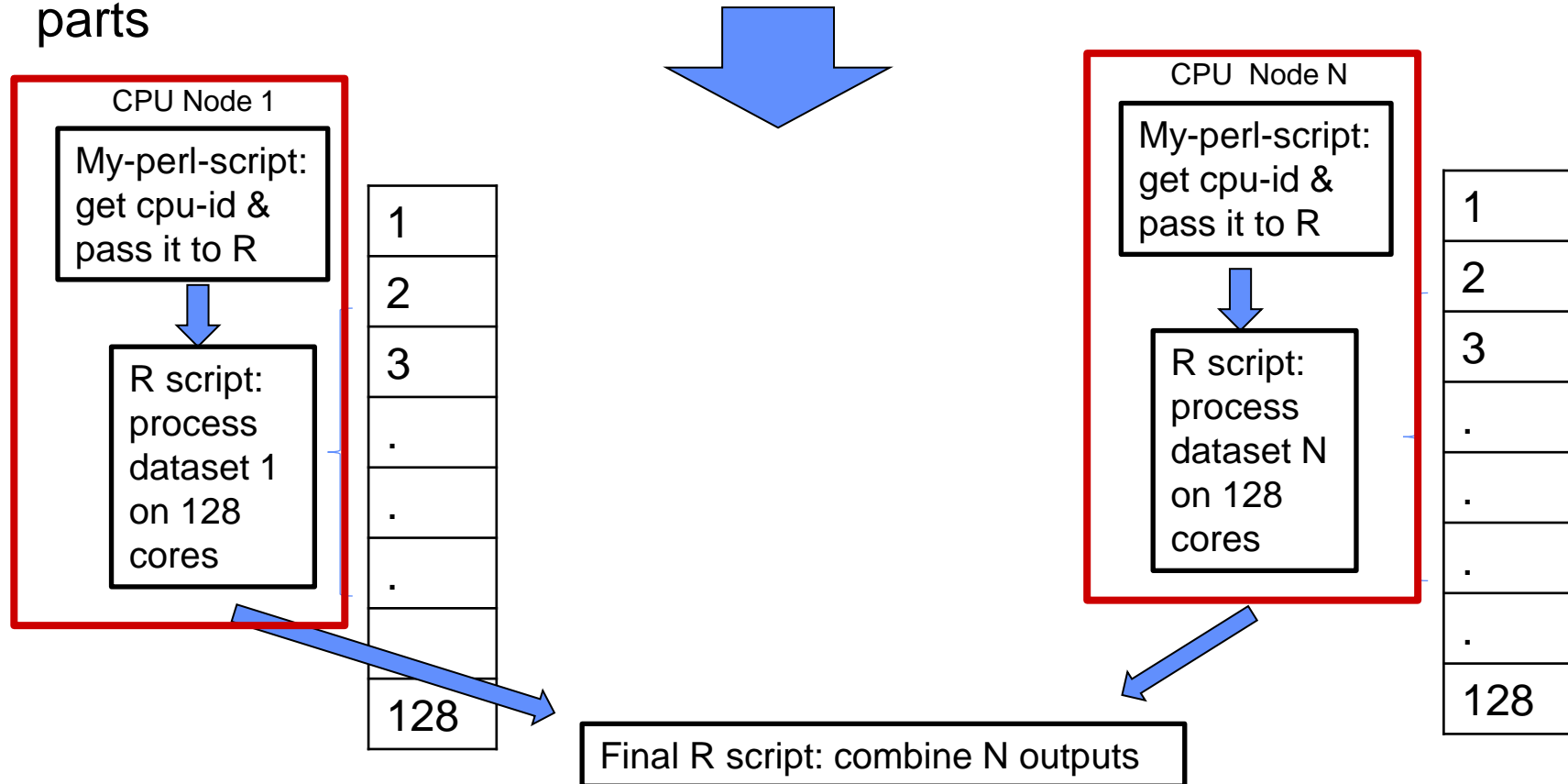
2 x 1 = 2 mpi ranks

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

1. Split up
data into N
parts

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



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- R and Scaling
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- **A big data exploration of R**

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:
 $Y = X * B + \text{noise}$ (where X is 100K x 50K)
- 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** $L = MSE + \lambda \sum |b_i|$
- **Recall: using penalty term is the same as using a constraint (constrained optimization)**

find min MSE such that $\sum |b_i| < S$

- **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: the file backend for the big data object path option was hard to get right – ended up just running out of scratch SSD as working directory;

copies everything into binary file and descriptor file and got results in about 2hours

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 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, ...
```

Batch script for R biglasso, highlights

.....

```
#SBATCH --partition=compute
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=64
#SBATCH -A account
... etc
```

```
module load slurm
module load cpu
module load gcc/9.2.0
module load r
```

```
cp Xmatrix_100000_50000.csv /scratch/$USER/job_${SLURM_JOB_ID}/Xinput.csv
cp Ymatrix_100000_1.csv /scratch/$USER/job_${SLURM_JOB_ID}/Yinput.csv
```

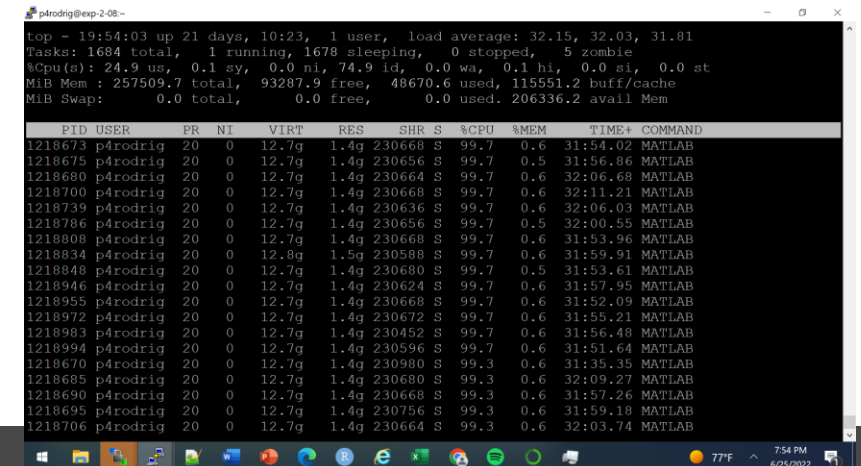
```
Rscript --vanilla path-2-your-script/rLassov2.R
    /scratch/$USER/job_${SLURM_JOB_ID}/Xinput.csv
    /scratch/$USER/job_${SLURM_JOB_ID}/Yinput.csv 64 TRUE > save_std_output.txt
```

Matlab

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

I recalled a 'table2array' function that helped

But matlab kept failing with worker getting disconnected after 1 or 2 hours of processing; might be a memory issue



```
p4rodrig@exp-2-08:~$ top
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

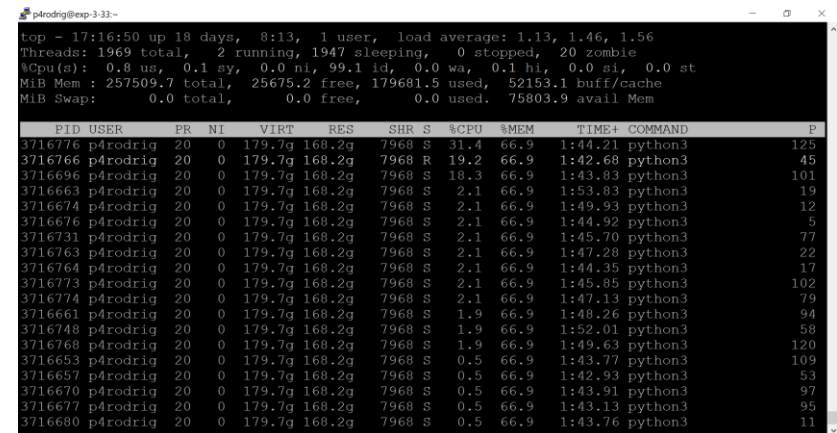
- Dask-ML – worked easily with distributed dataframe, built on top of sklearn,

`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



The image shows a terminal window with the following content:

```
p4rodrig@exp-3-33:~$ 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

I stopped it after 4 hrs; it was running

Local[64], 50 min in, 1 iteration

```
p4rodrig@exp-6-40:~$ 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

Some notes

- **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**

How to use R directly on Expanse

1. Get an interactive compute node:

2. Try

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

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.

>

```
[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:
```


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

Other R package possibilities:

- Rspark - R interface to Spark
- R Keras – R interface to Keras
- pdbR - distributed matrix support (better for dense matrices vs Spark)
- Rgputools – GPU support

THE END