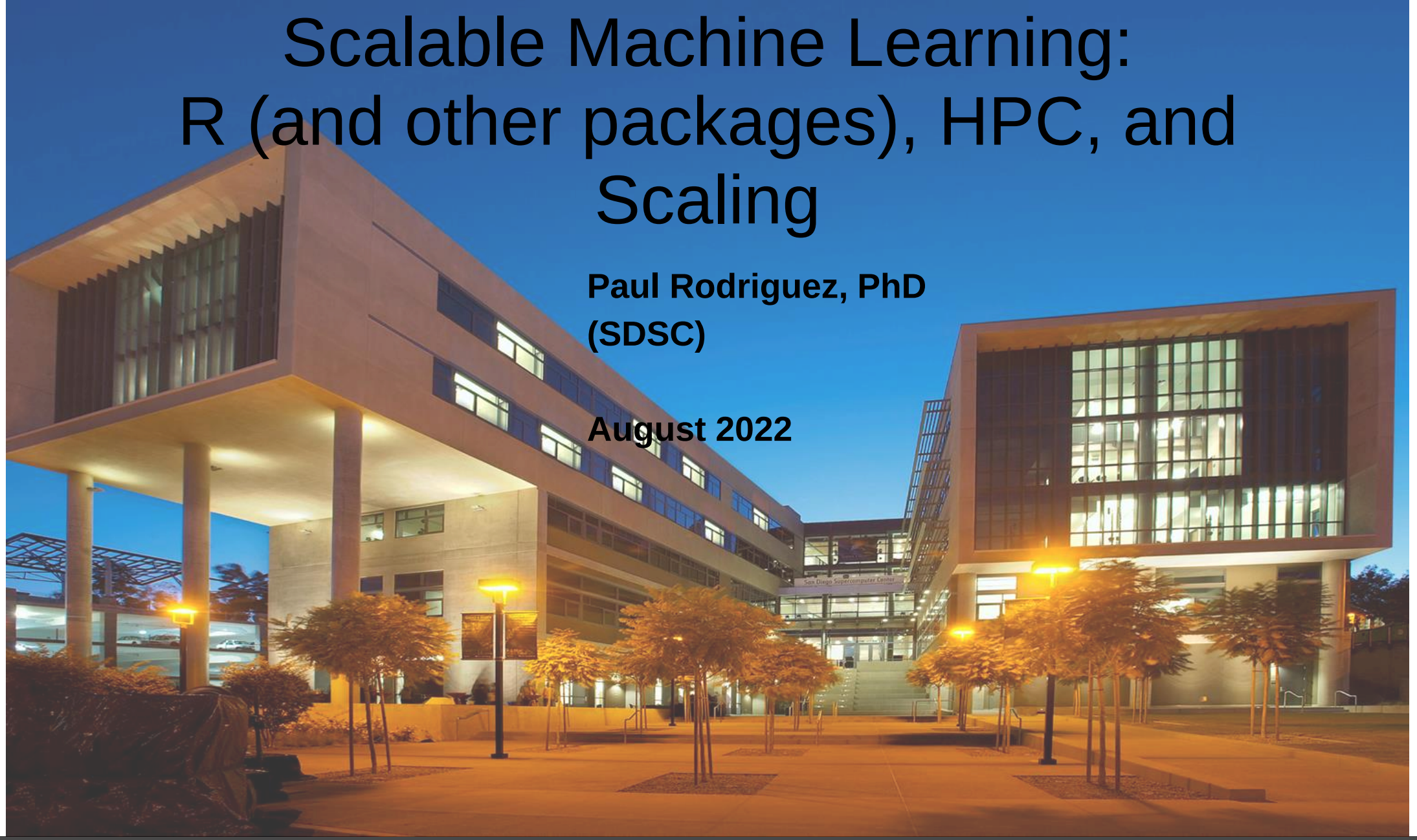
# Scalable Machine Learning: R (and other packages), HPC, and Scaling



**Paul Rodriguez, PhD**
**(SDSC)**

**August 2022**

# Outline

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

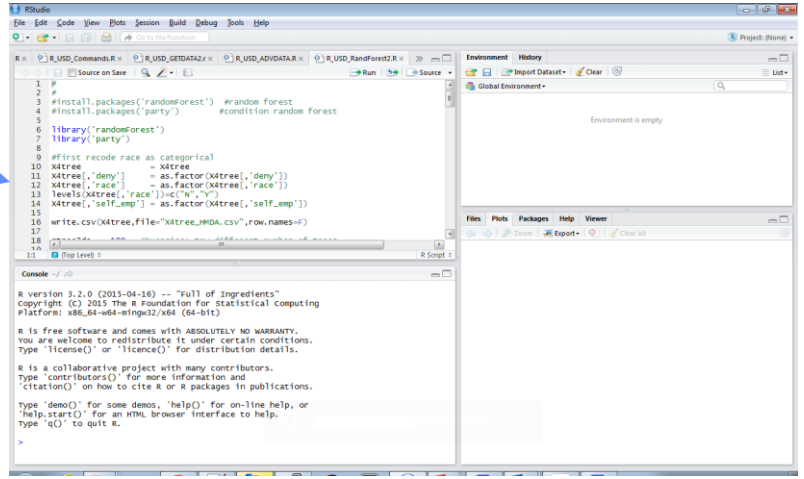
# A typical R development workflow

- **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 ‘linearmodel’
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

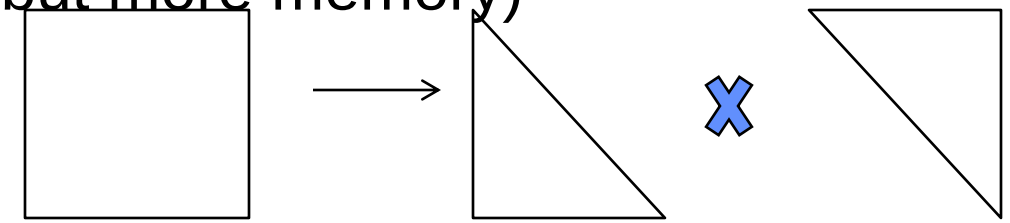
- **Algebraically, we could**:

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

  use derivatives to search for solutions (very general)

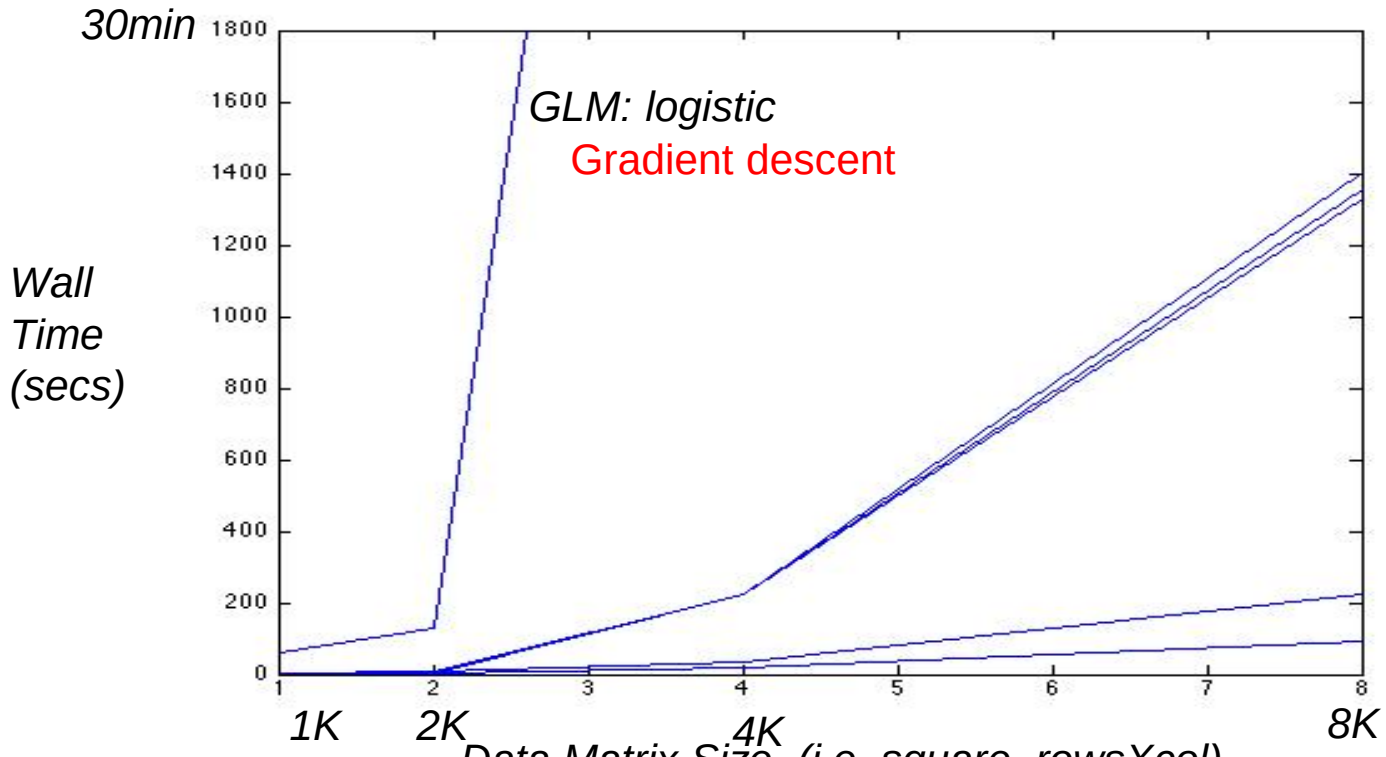
- **Or, better:**

  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)*




Matrix inverse solutions

*glm: Gaussian*
*lm()*
*Inverse()*

QR solutions

*Solve(a,b)*
*QR*

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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)

    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)
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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**

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**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 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)

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

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library(doParallel)

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


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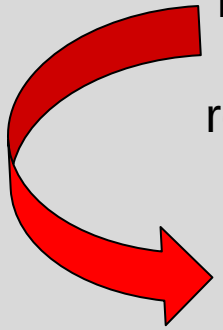
 stopCluster(cl)
```

**1. allocate cluster as parallel backend**

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

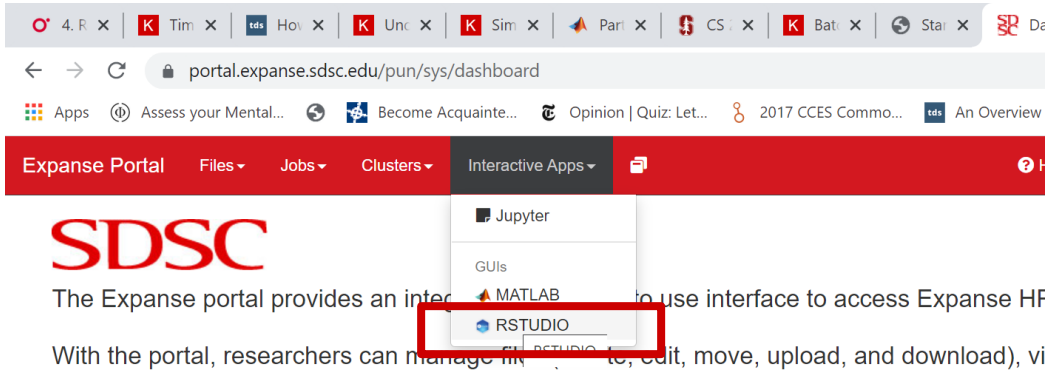


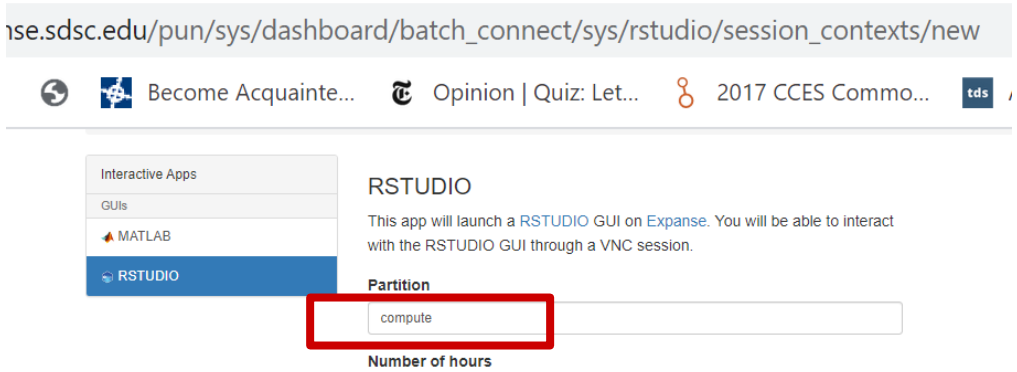
**BEWARE: foreach will copy data to every core in every node if its seems necessary**

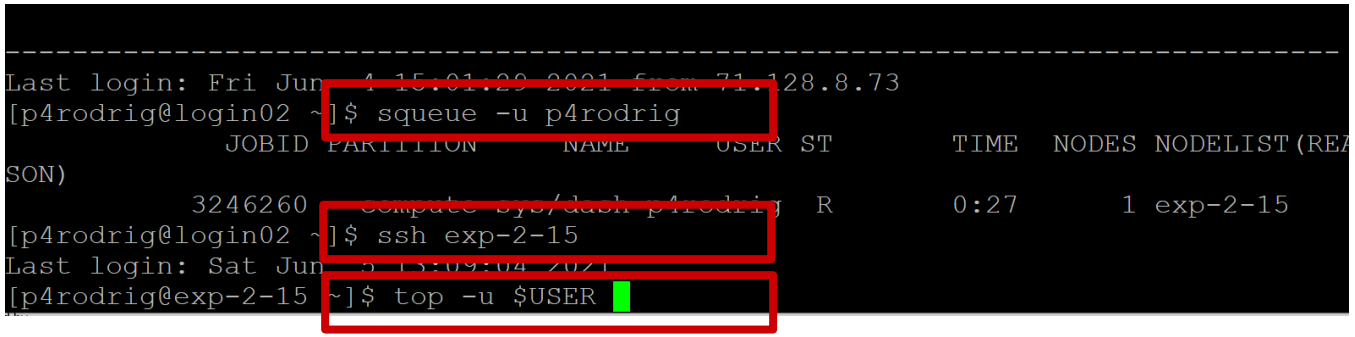
# Testing/Evaluating R parallel

- **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)




*1*
*Open portal ->*
*Interactive Apps ->*
*Rstudio*

*Enter*
*Node: "compute"*
*Cores: "64"*
*Memory: 124 Gb*
*(other fields defaults ok)*

*2*
*Also login:*
*login.expanse*

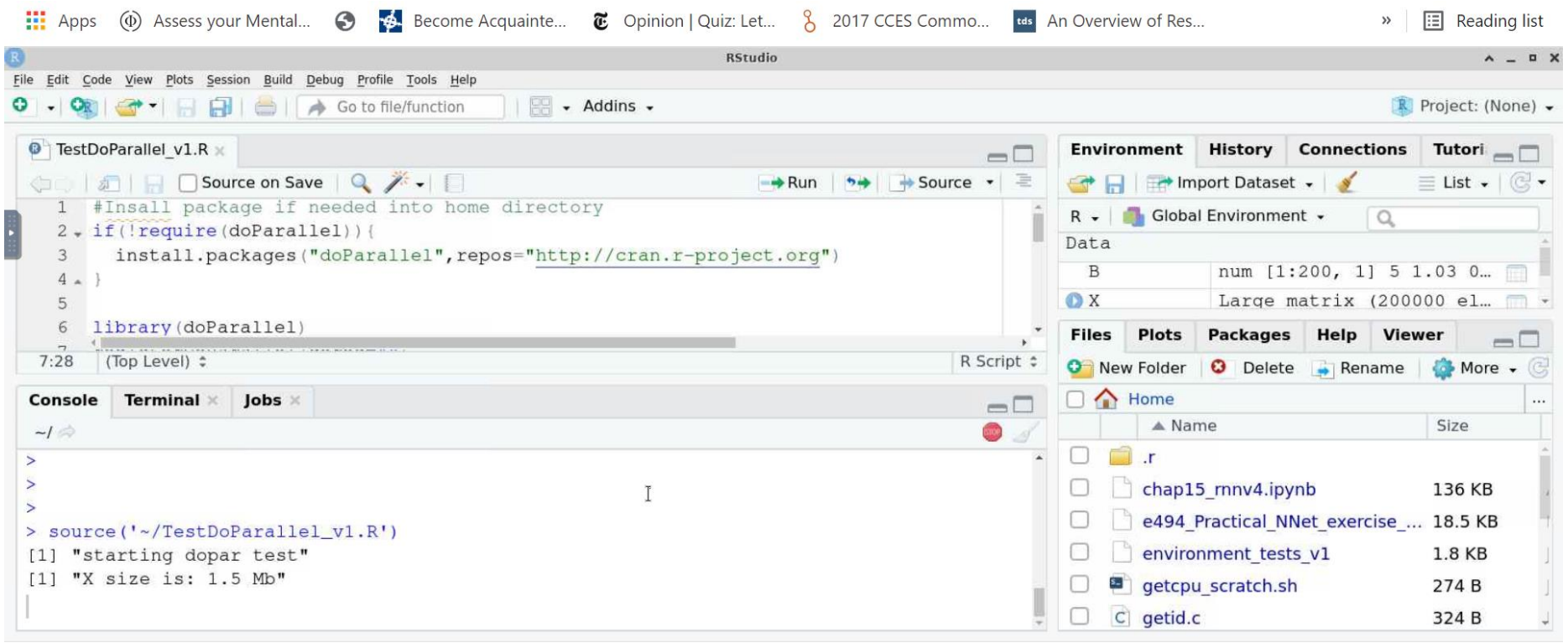
*$ squeue –u $USER*
*$ ssh exp-##-##*
*$ top –u $USER*

*'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*

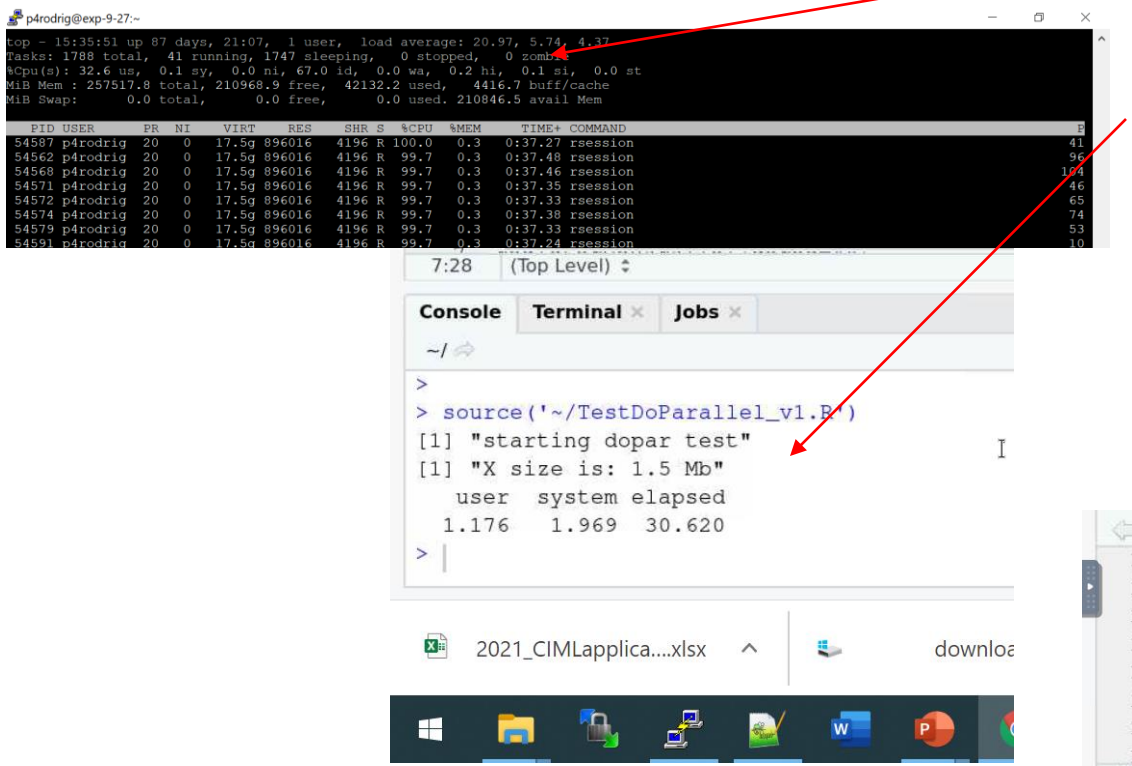


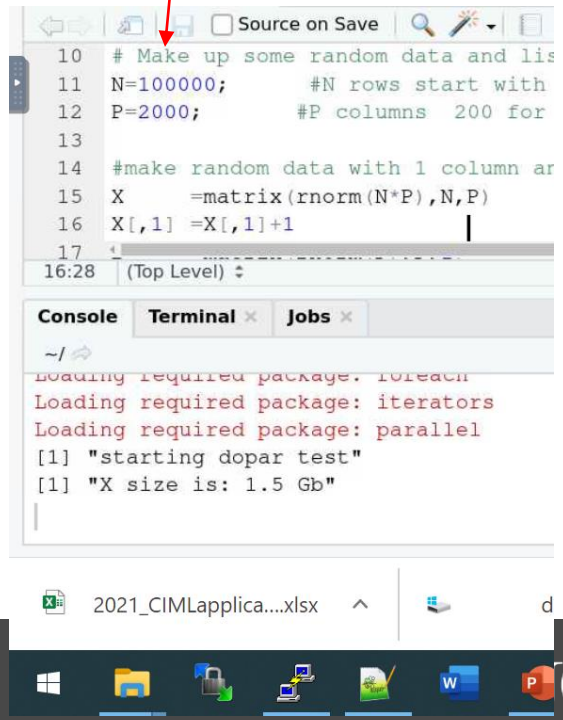
*Review the top output*

*Notice the elapsed time and memory size*

*Change the NxP matrix size and rerun*

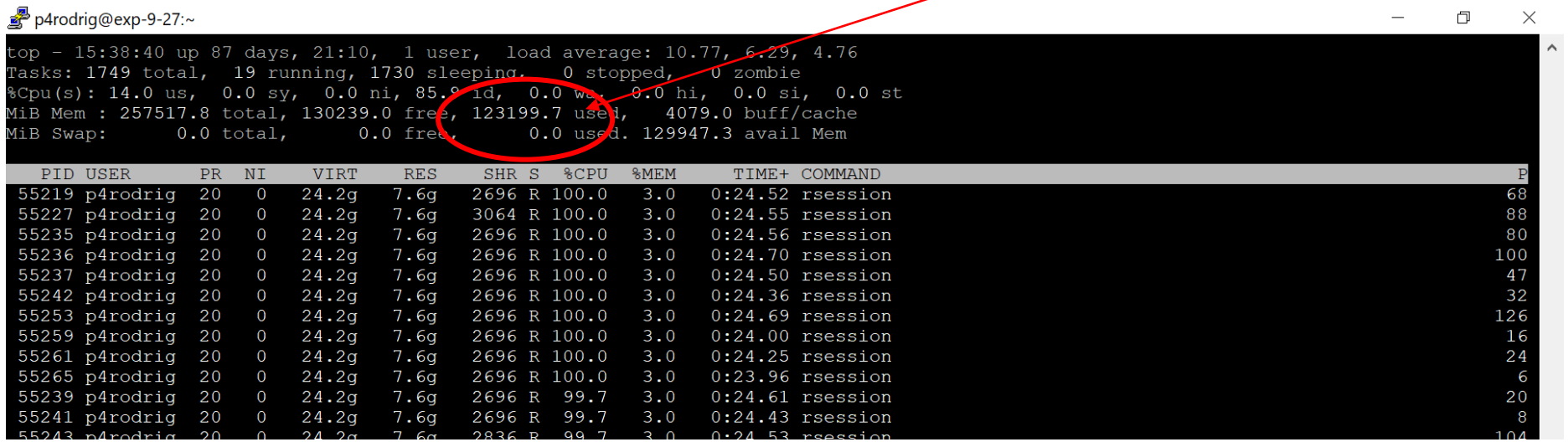
*(start with N=10K, P=2K)*



*Try this at home:*

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




*If you ask for 246Gb will it run?*
*What if you use only 24 cores?*

# Parallezing for loops

## (pseudo code)

| R with doParallel | Matlab with parallel toolbox | Python with dask.distributed |
|---|---|---|
| *makecluster*<br>*registercluster* | *parcluster('local')*<br>*parpool()* | Import delayed, Client<br>Client(numwkrs) |
| *foreach with dopar,* | *parfor*<br>*or*<br>*'spmd' with distributed arrays* | for i in range(numwkrs):<br>A=delayed(my_func)(i)<br>Acombine.append(A) |
| *combine results* | gather array | Acombined.compute() |

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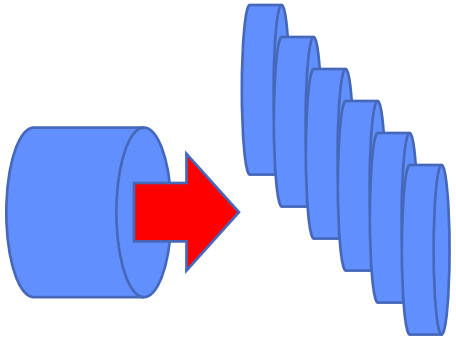
# An option for (embarrassingly) Parallel R

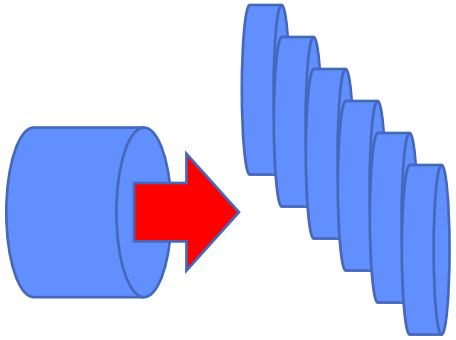
1. Split up data into N parts

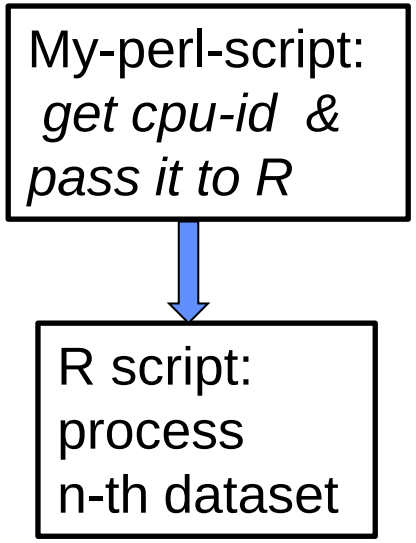


# An option for (embarrassingly) Parallel R

1. Split up data into N parts

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





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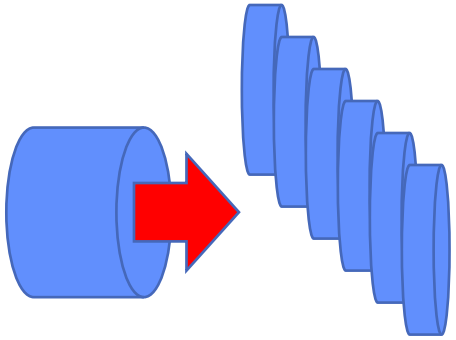
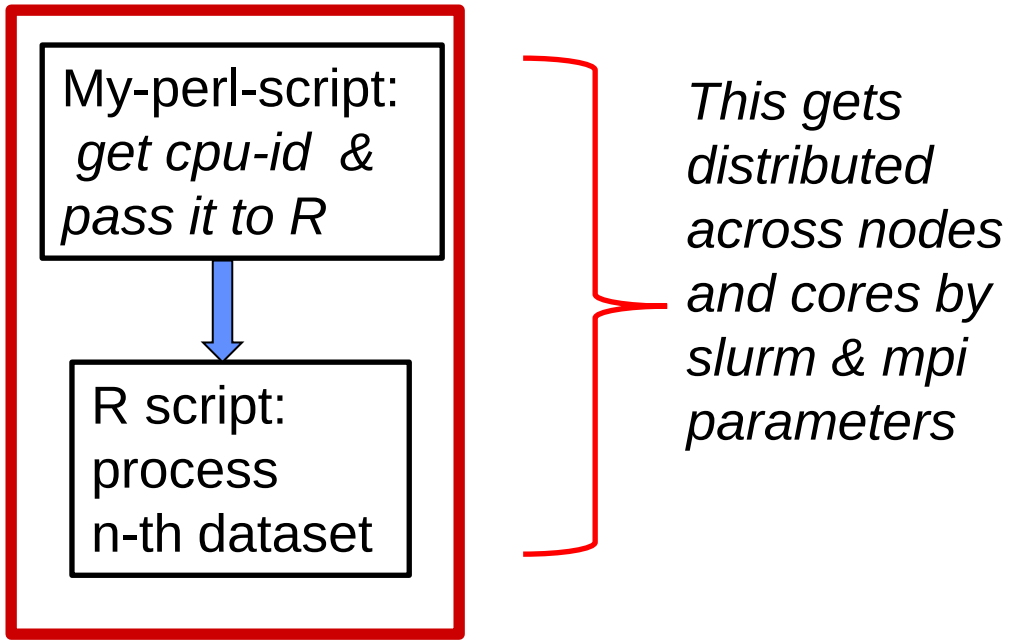




# Slurm parameters: one R instance per core across all nodes

*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

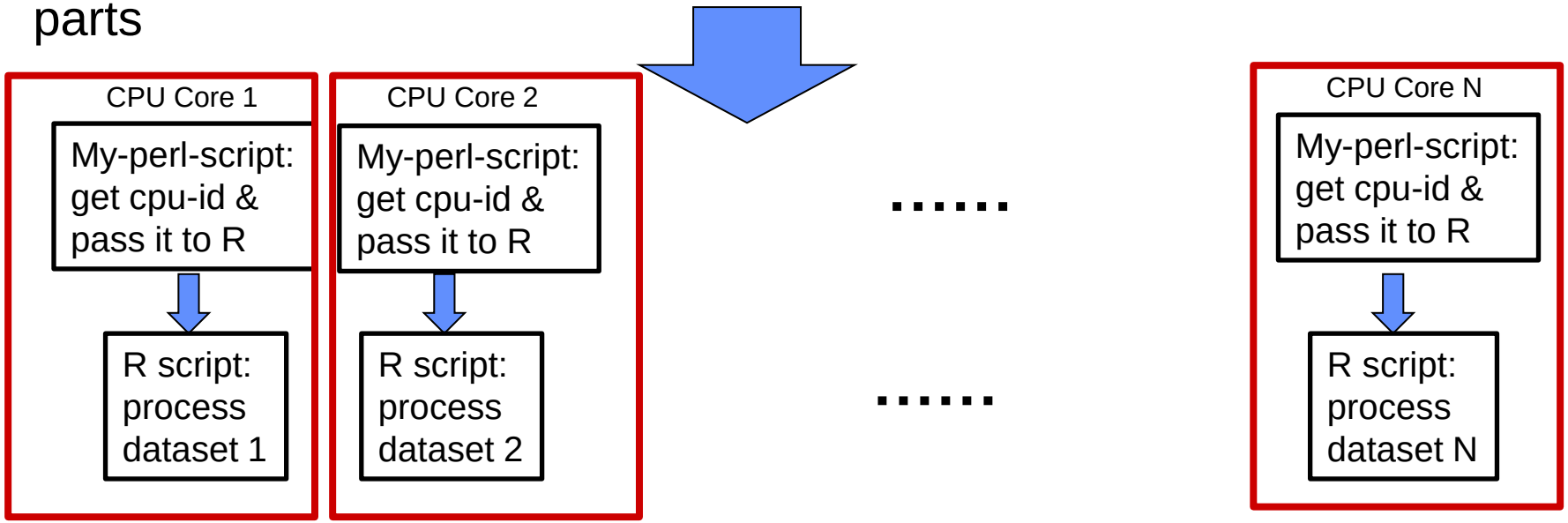
*(based on /cm/shared/examples/sdsc/mpi-openmp-hybrid/hybrid-slurm.sb)*

# one R instance per core across all nodes

1. Split up data into N parts

2. In slurm batch script:

mpirun … my-perl-script



# one R instance per core across all nodes

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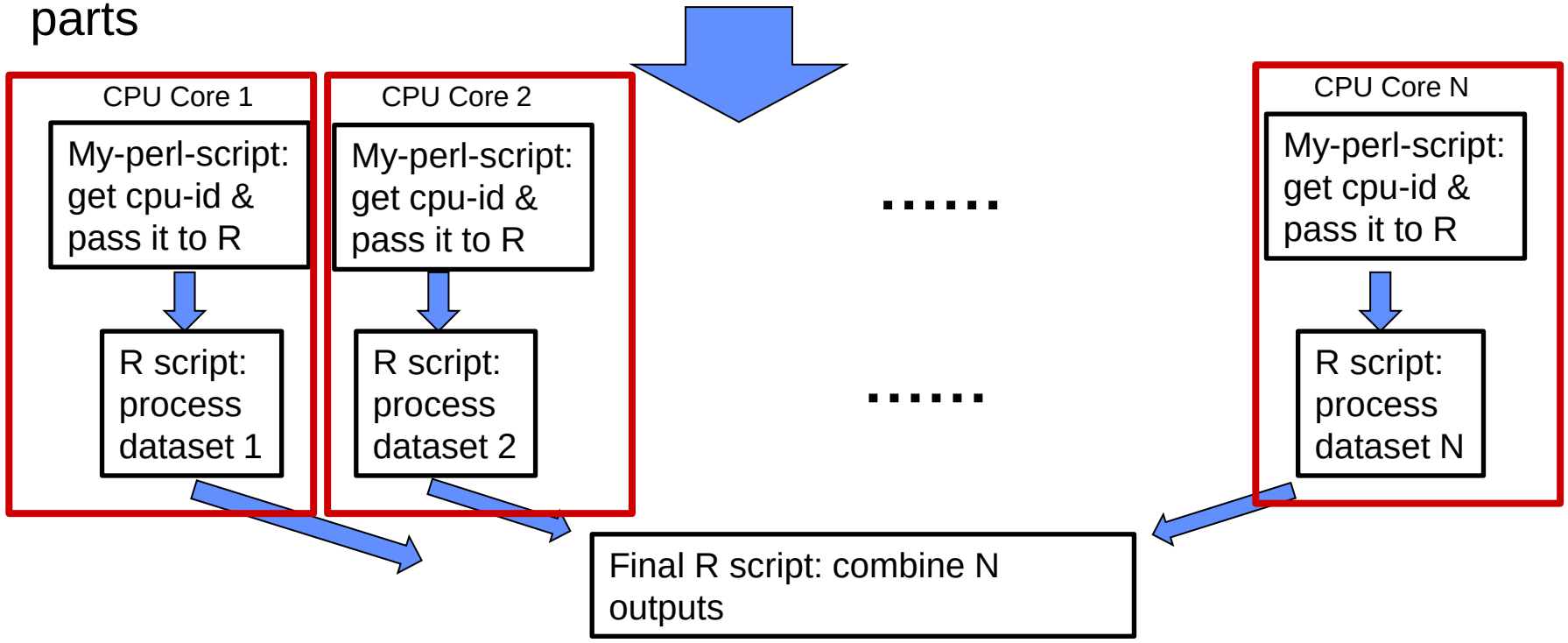
2. In slurm batch script:

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 x1 = 2 mpi ranks

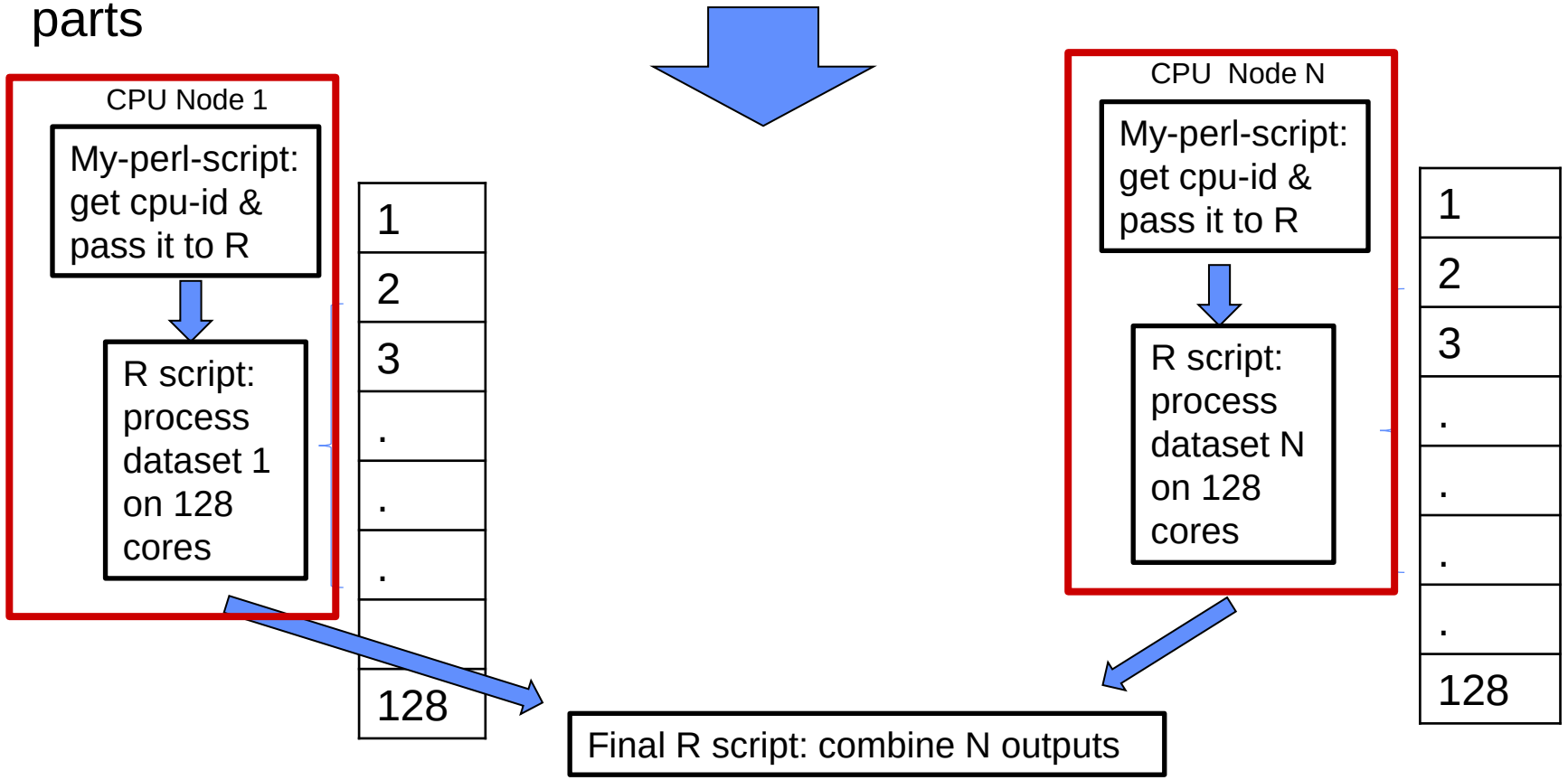
2 perl script/R instances
128 cores each
(doParallel can use them)

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

1. Split up data into N parts

2. In slurm batch script:

mpirun … my-perl-script



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# 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** $L = \boldsymbol{MSE} + \boldsymbol{\lambda} \sum |b_i|$

- **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: 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

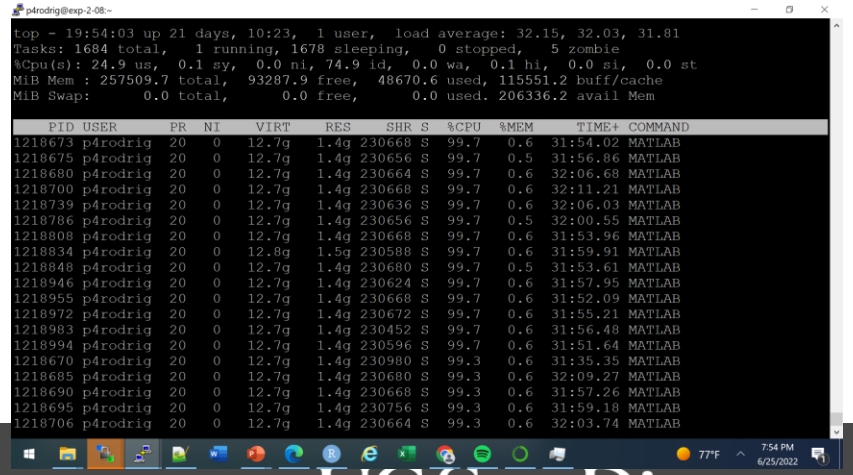
Rscript --vanilla path-2-your-script/rLassov2.R
        /scratch/$USER/job_$SLURM_JOB_ID/Xinput.csv
       /scratch/$USER/job_$SLURM_JOB_ID/Yinput.csv 64 TRUE > save_std_output.txt
```

# 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



# Dask-ml

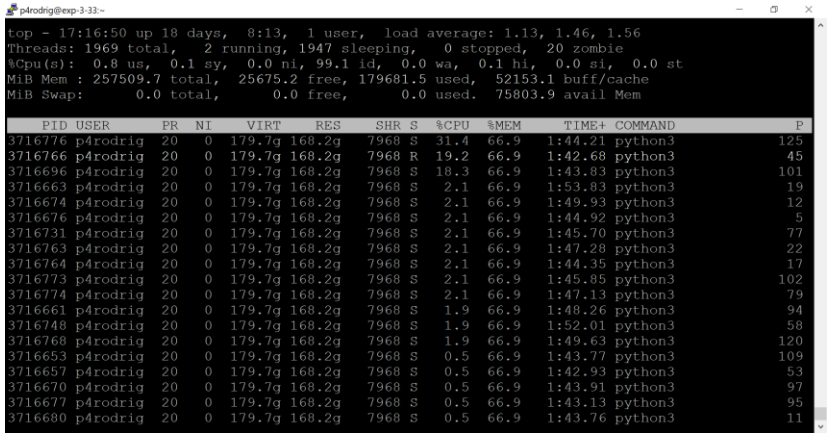
- Dask-ML – worked easily with distributed dataframe, built on top of sklearn,

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



# Spark

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

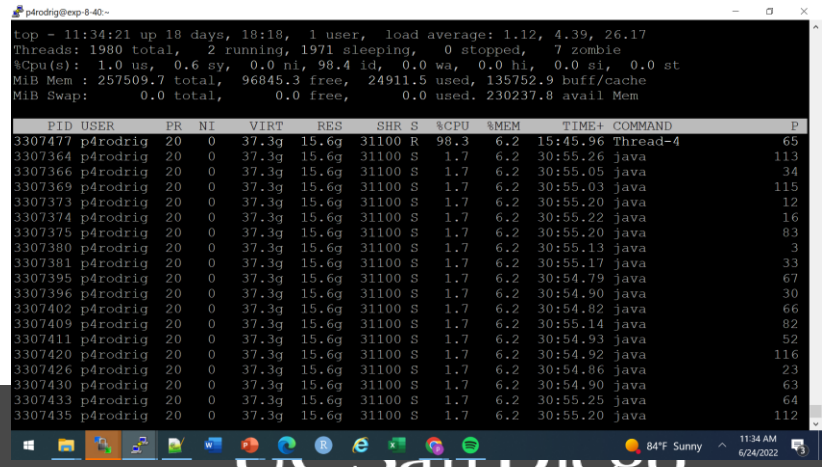
**Use the vector assembler options to get Y and ‘features’ all in one dataframe**

**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*



# 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**

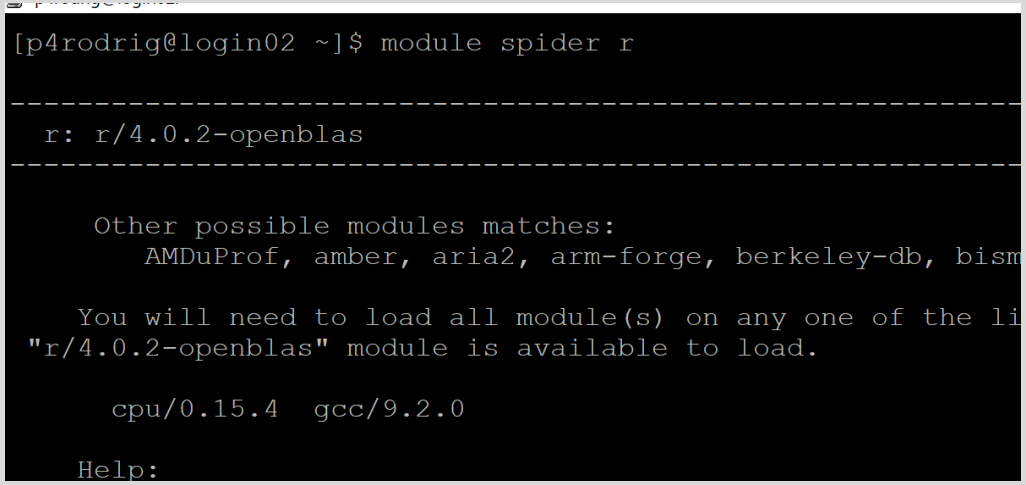
# Some notes

- 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.

>

# 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*