CIML

R and Scaling on HPC

Paul Rodriguez

R, Scaling R, Parallel R

- A Glimpse of R (recap)
- R and Scaling
- Parallel options for R
- doParallel demo on Expanse portal

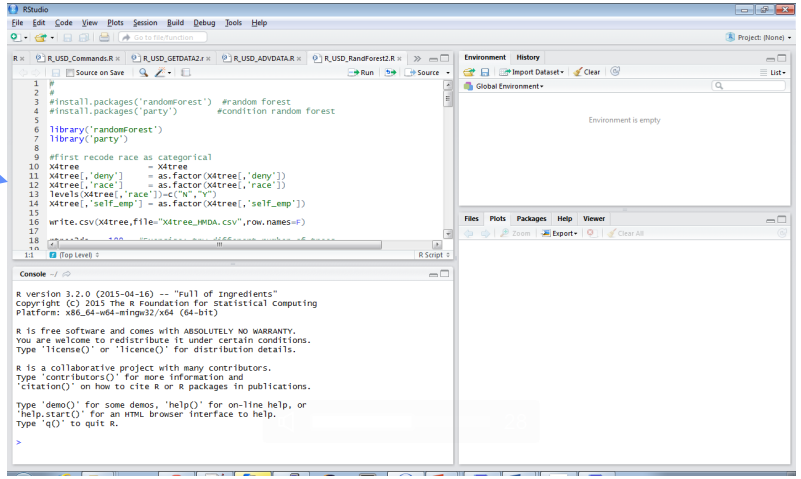
A typical R development workflow

- 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

R commands in brief

- A typical R code workflow:

```
#READ DATA (housing mortage cases)
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
race              = as.numeric(X[,'s13'] %in% c(3,4)) #make race values 1-4 into values 0 or 1
deny              = as.numeric(X[,'s7']==3)            #make deny values into 0 or 1,
                                                            1 only for deny='3'
#RUN MODEL and SHOW RESULTS
lm_result         =lm(deny~race+pi_rat)          #lm is 'linearmodel'
summary(lm_result)
```

R strengths for HPC

- Data Wrangling

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- Sampling/bootstrap methods

R strengths for HPC

- **Data Wrangling**
- **Sampling/bootstrap methods**
- **Particular Statistical procedures that you won't find implemented anywhere else, e.g.**

  Multiple Imputation methods,

  Instrument Variable (2 stage) Regression

  Matching subjects for pairwise analysis

  MCMC routines

Scaling, practically

- **Scaling (with or without more data):**
  - more complex analysis (ie optimizations)
  - more sampling (ie more trees in Random Forest)

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  - more complex analysis (ie optimizations)
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- **Sometimes easy to parallelize (like with sampling)**

- **Sometimes too much communication between parts (matrix inversion)**

R Scaling In a nutshell

- R takes advantage of math libraries for vector operations

```
> 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
```

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- R takes advantage of math libraries for vector operations
- R packages provide multicore, multimode, or distributed data (SparkR) options

R Scaling In a nutshell

- **R takes advantage of math libraries for vector operations**
- **R packages provide multicore, multinode, or distributed data (SparkR) options**
- **However, model implementations not necessarily built to use parallel backends**
  - Some models more amenable to parallel versions

Consider Regression Computations

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

  where Y=outcomes , X=data matrix

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  - use derivatives to search for solutions (very general)

Consider Regression Computations

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

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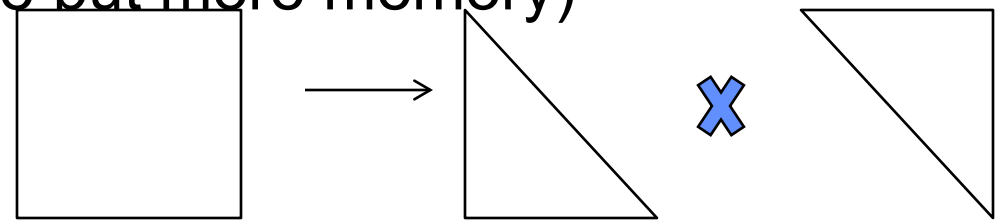
- **Algebraically, we could**:
  - take "inverse" $of\ X * Y = B$ (time consuming)
  - use derivatives to search for solutions (very general)

- **Or, better:**
  - QR decomposition of *X* into triangular matrices (easier to solve but more memory)



Consider Regression models in R

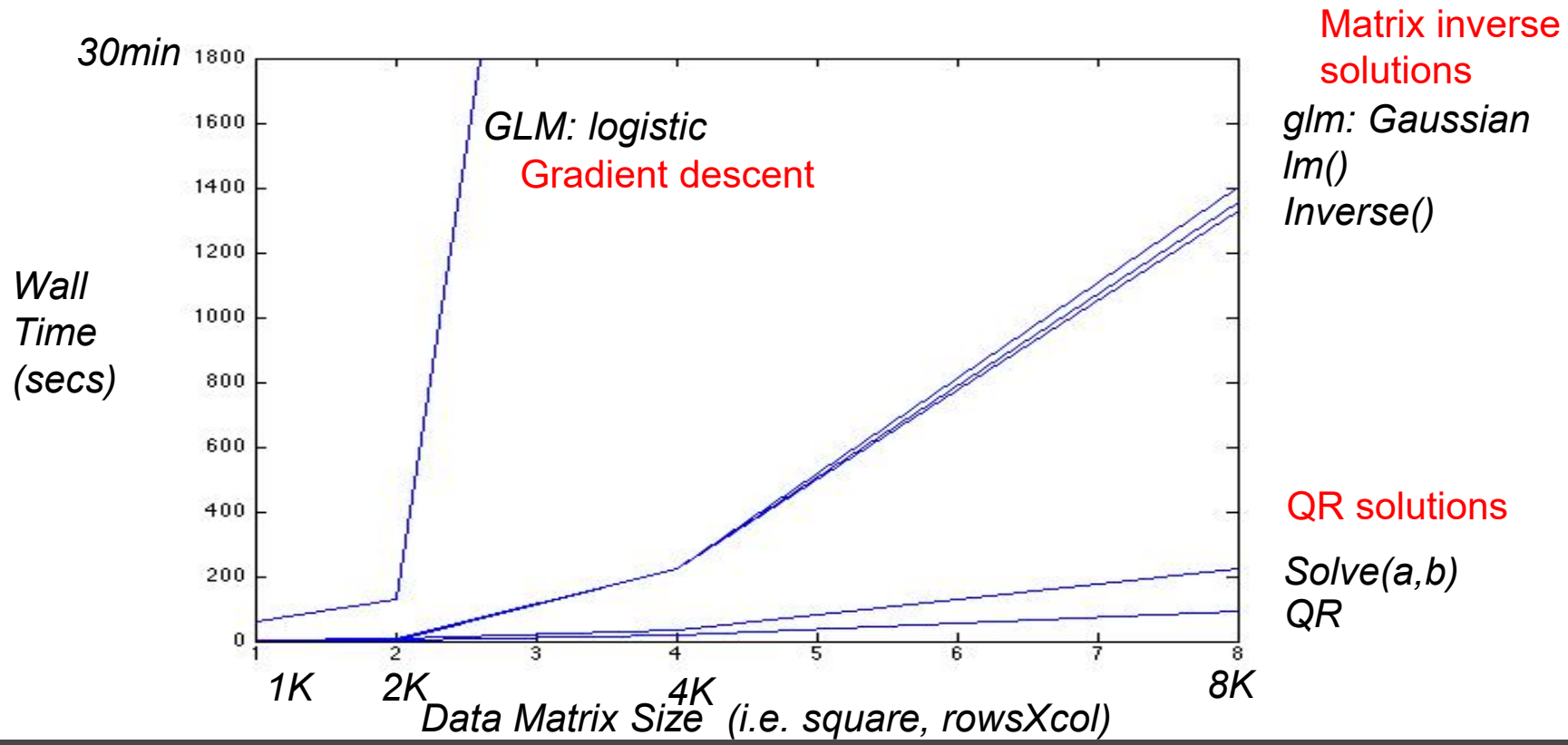
- **Related Models and Functions :**

lm() Linear Model

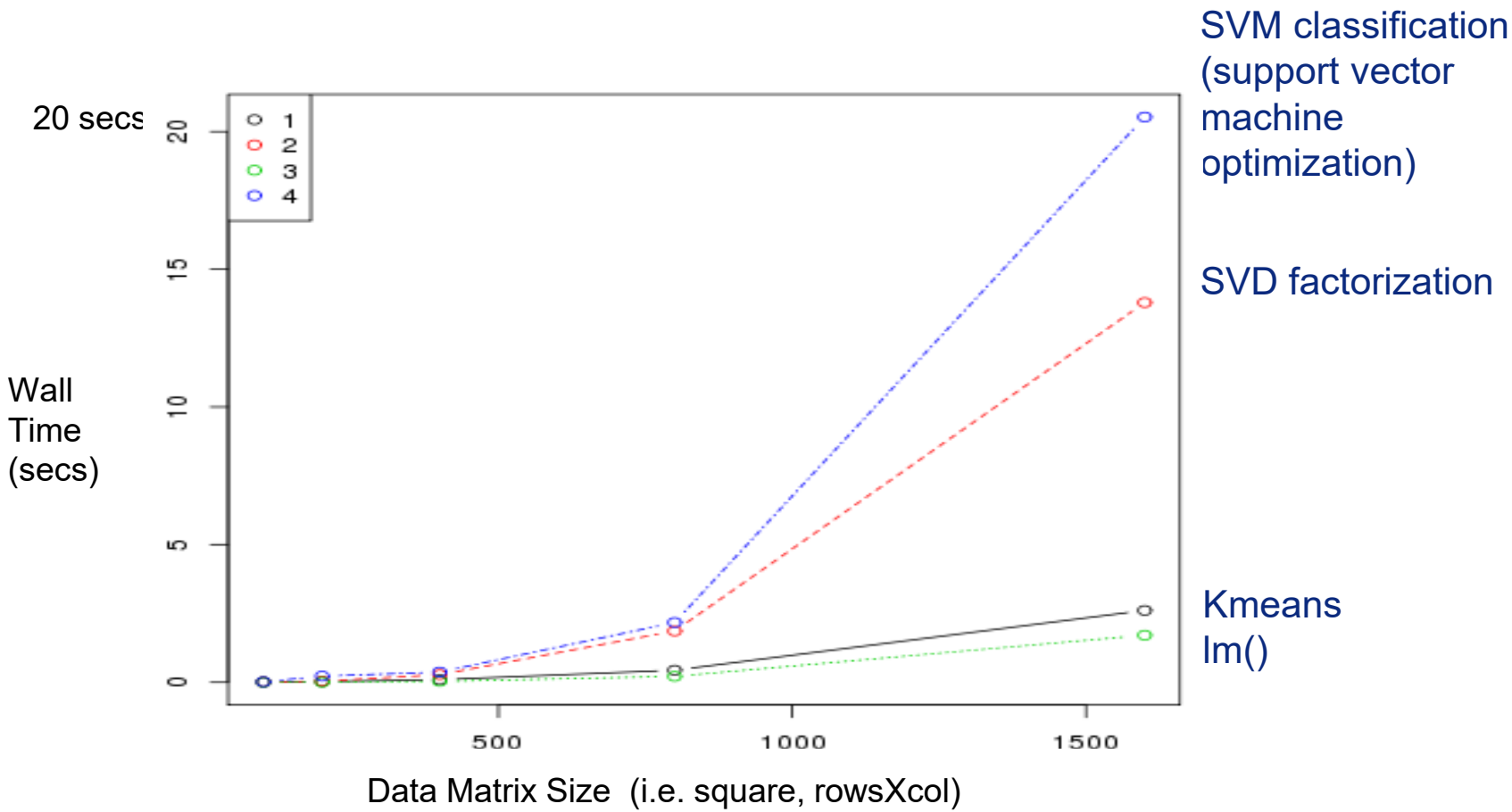
glm() Generalized Linear Model
(logistic regression,
LASSO version from Hastie et al.,etc)

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)



Machine learning models: Performance on 1 compute node



R multicore processing

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- ‘doParallel’ package – provides the back end to the ‘for each’ parallel processing command
- uses threads across cpu cores to pass data & commands
- Updates and combines the previous ‘snow’ and ‘multicore’ packages, so that is also works for multinode (and it’s similar to doMPI, both run 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)
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    my_data_frame = …..

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```

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install.packages(doParallel)
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      {   …
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BEWARE: foreach will copy data it thinks is need to every core

R multinode: parallel backend

```
library(doParallel)

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

1. allocate cluster as parallel backend

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stopCluster(cl)
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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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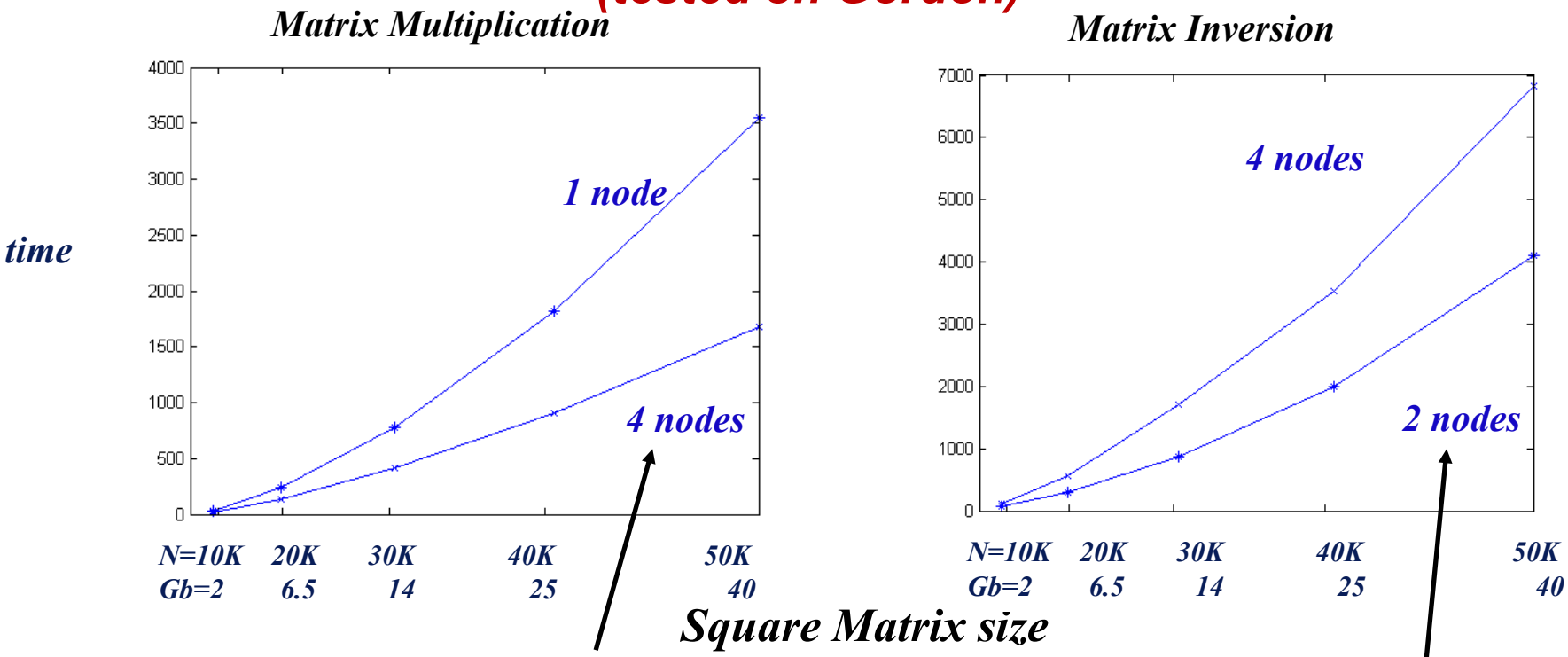
Multiple Compute Nodes not always help

(tested on Gordon)

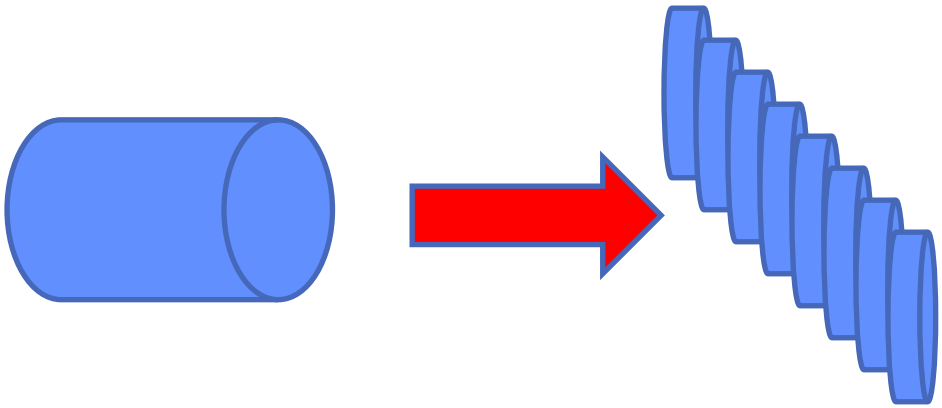


multinodes: more nodes is less time for multiplication,

less nodes is better for inversion

An option for (embarrassingly) Parallel R

1. Split up data into N parts



An option for (embarrassingly) Parallel R

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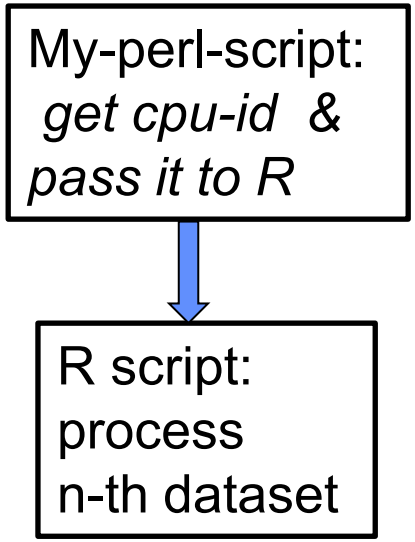
2. In slurm batch script:

mpirun … my-perl-script



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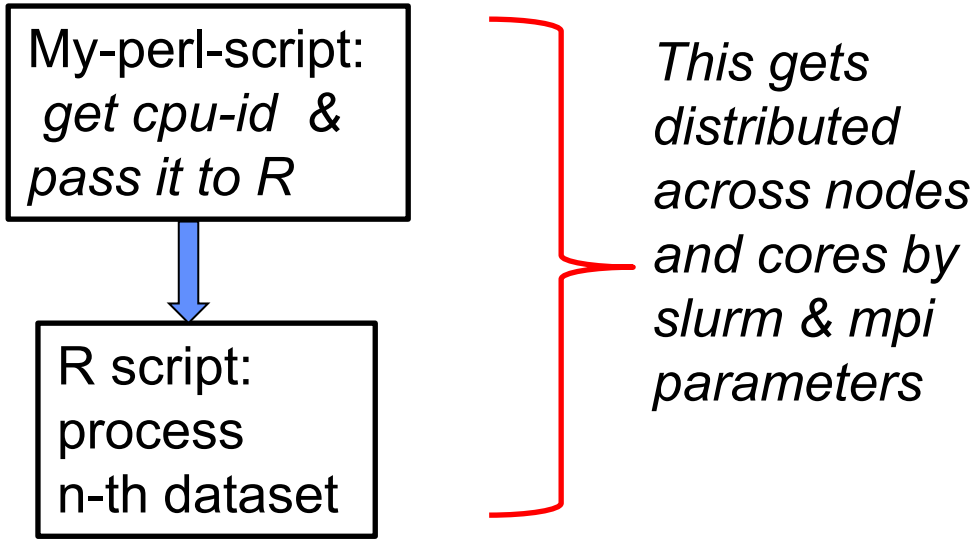

Slurm parameters: one R instance per core across all nodes

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

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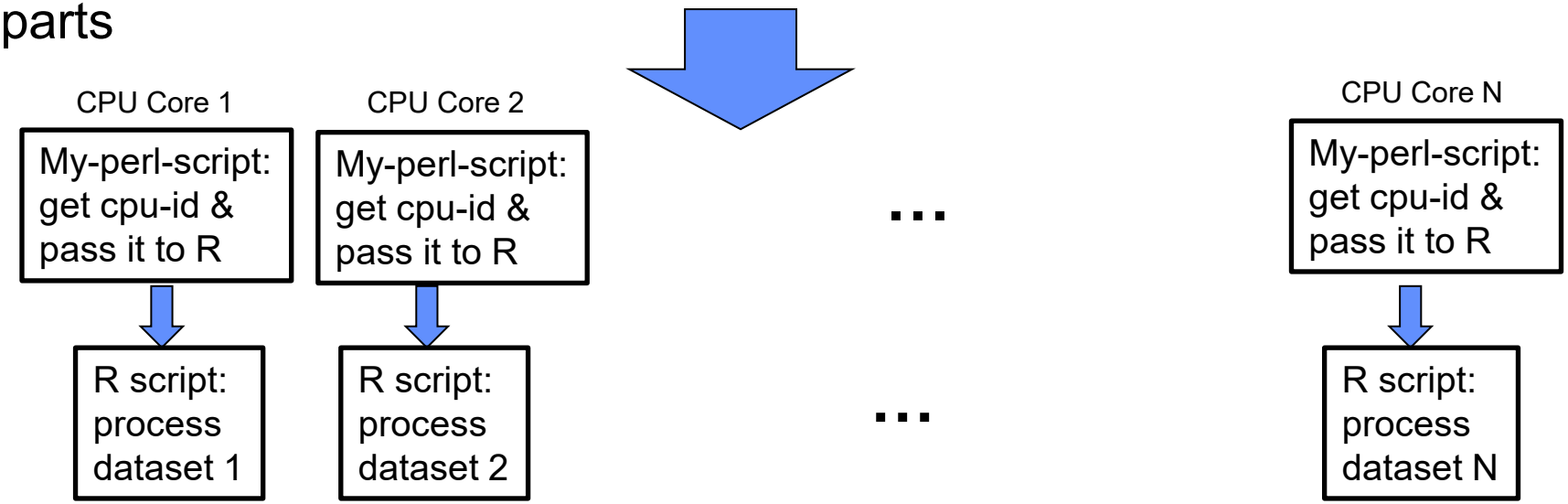

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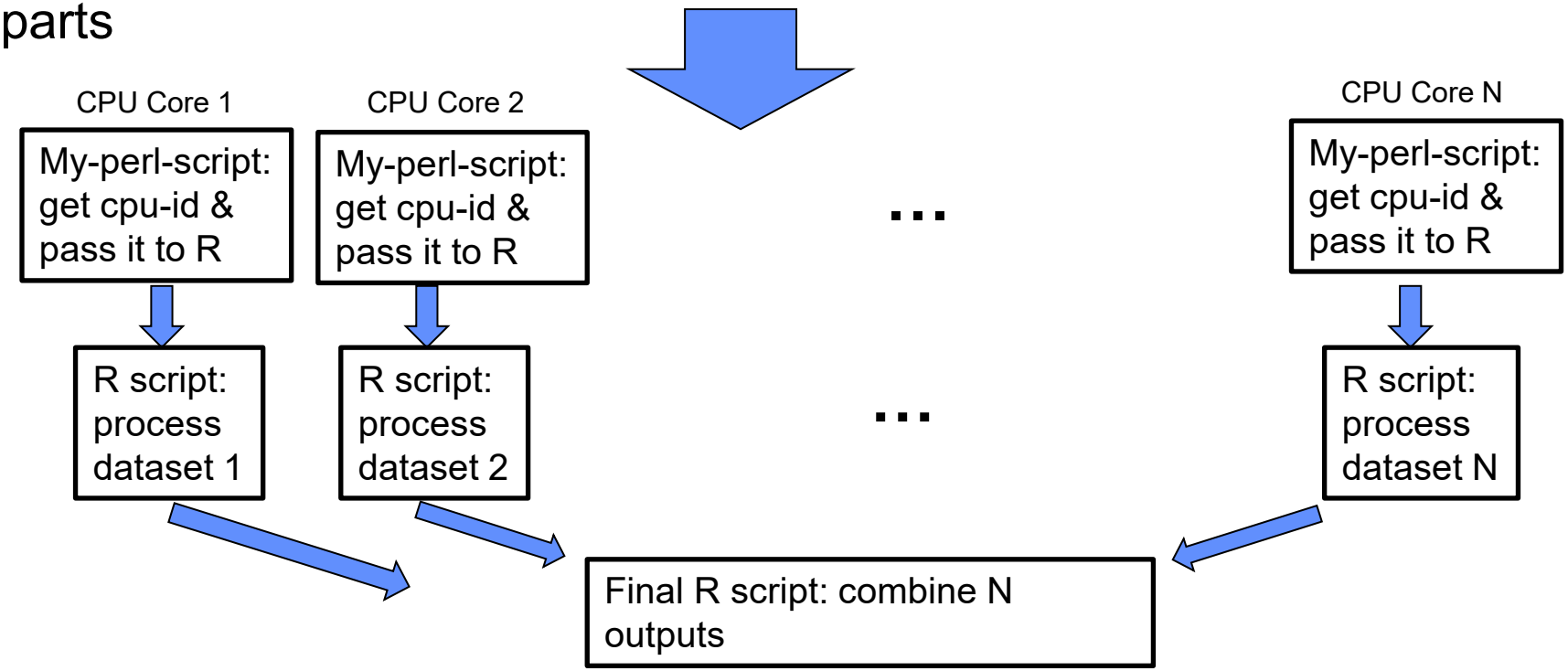


More programming but perhaps more useful

Slurm parameters: one R instance per nodes 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

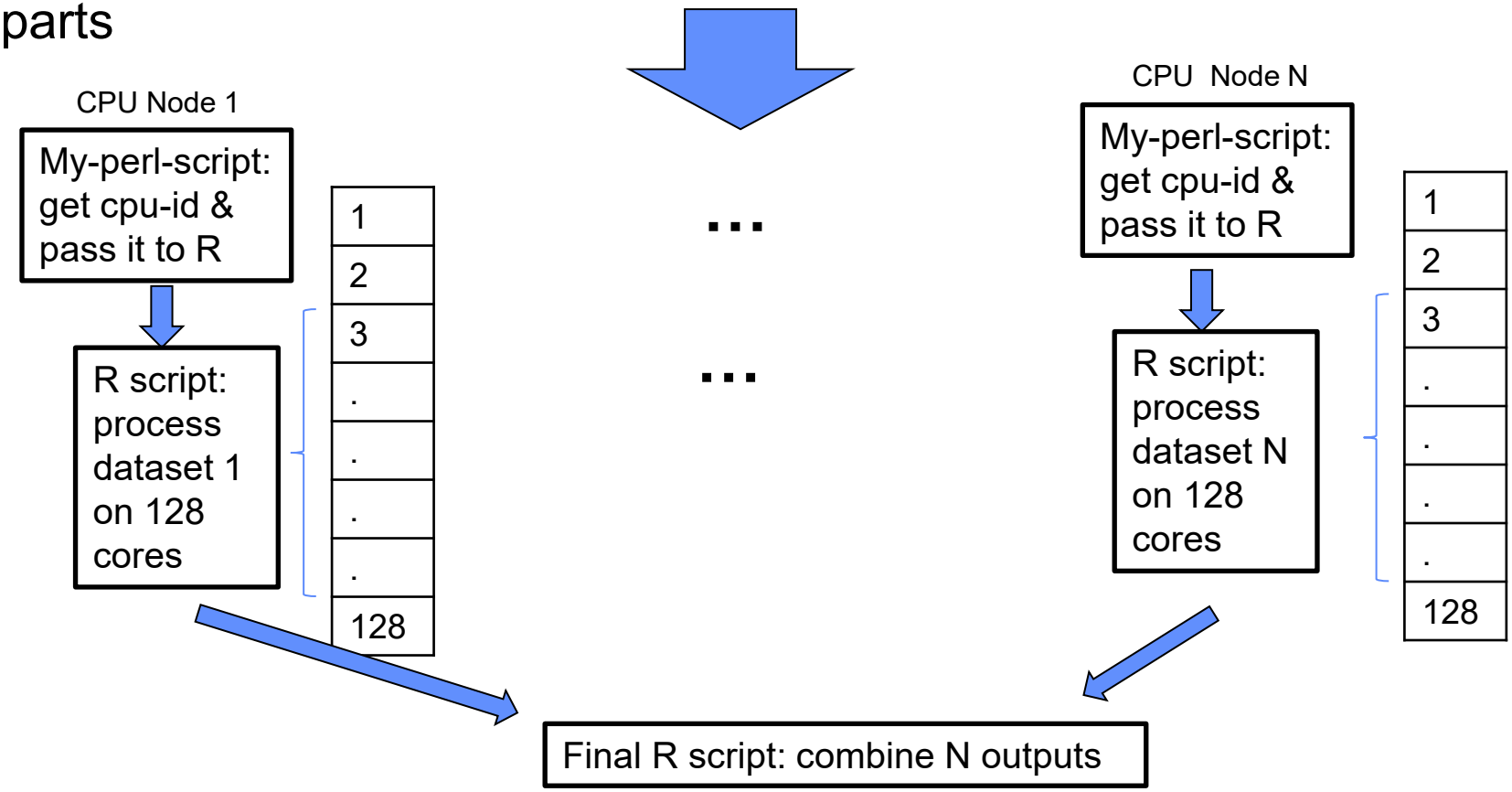
2 perl script/R instances
128 cores each
(doParallel can use them)

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



Example: scaling MCMC

Distributed Markov Chain Monte Carlo for Bayesian Hierarchical Models, Frederico Bumbaca, UCIrvine,

- *MCMC searches parameter space through long sequences of updates to get complete probability distribution*
- *Individual sequences are not parallelizable, but sometimes parameters can be 'partitioned'*
- *Used the R package, "bayesm"*
- *Ran on SDSC Comet with embarrasing parallelization*

# Individuals	Cores	Individ per Core	Total Minutes (I/O time)
100 million	**1,7282 (max)**	**~ 58K**	**206 (38)**

Another MCMC option: Stan program

R or Python interface, with many options

Stan script → translated into C++ code and compiled

If you take log likelihood:

$$P(data, parameters) = \prod P(data_i, parameters)$$

$$\log P(data, parameters) = \sum_{i}^{N} \log P(data_i, parameters)$$

then Stan will partition the data across cores.

(P() is calculated 1000's of times in a sequential chain)

Other R packages:

Also, for big data or big matrix

- Rspark - R interface to Spark (upcoming session)
- pdbR - distributed matrix support (better for dense matrices vs Spark)

Also:

- R openMP, Rmpi –
- Ff, bigmemory – map data to files
- Rgputools – GPU support

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)*

```
[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.

>

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

- **In R:**

  install.packages('package-name')

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

- **Sometimes on Comet, you had 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

- **pause**

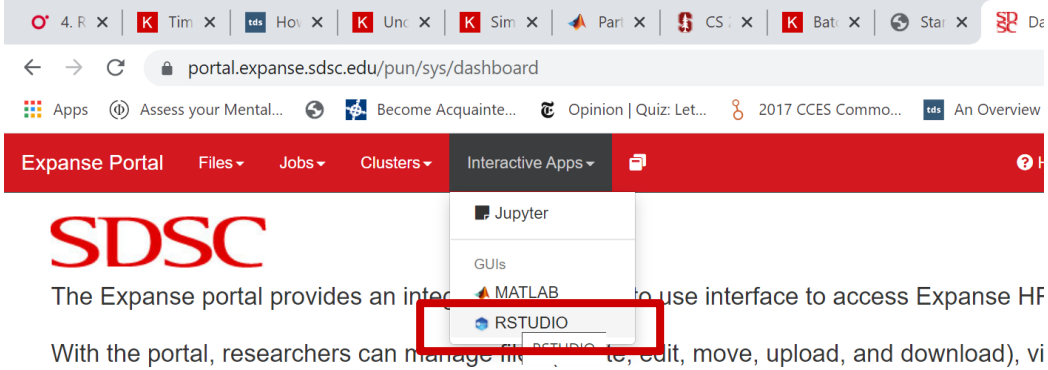
TestdoParallel R script

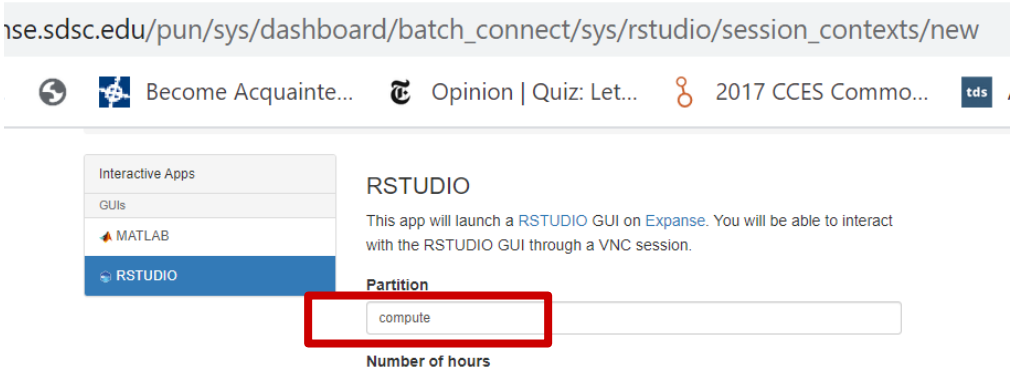
1 start Rstudio from portal (use shared and say <48 cores)
and run script
(it repeatedly does a regression)

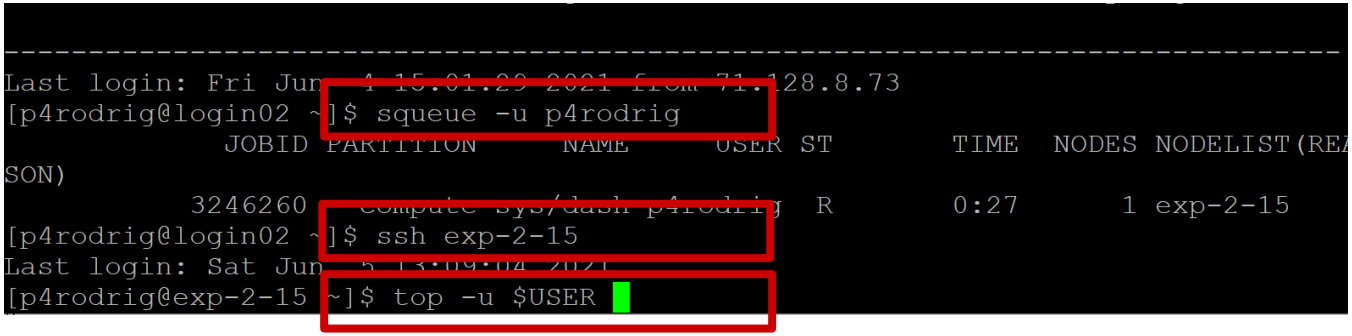
2 review execution using ‘top’ utility

3 vary the NxP matrix size or number of cores

Goal: look for tradeoffs in memory vs execution
e.g. If N gets too large then use less cores







Open portal ->
Interactive Apps ->
Rstudio

Enter
Node: "compute"
Cores: "64"
(other fields defaults ok)

Also login:
login.expanse

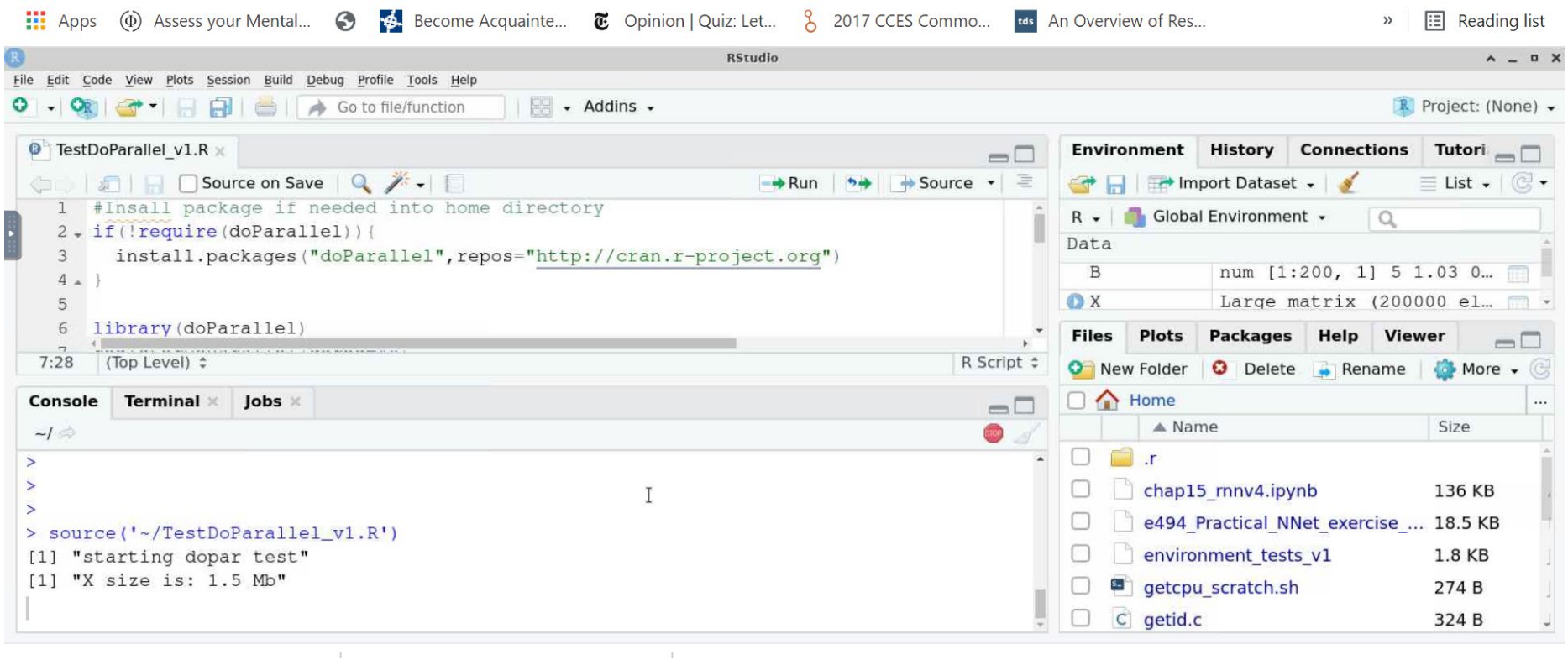
$ squeue –u $USER
$ ssh exp-##-##
$ top –u $USER

'H' will toggle threads

'fP' will toggle last cpuid

Open the 'Test_doParallel ' Rscript

Select 'source' to run the whole script



```
,  load average: 0.00, 0.03, 0.26
eeping,   0 stopped,   0 zombie
id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
 15384.5 used,   2560.7 buff/cache
     0.0 used. 239374.2 avail Mem

  SHR S  %CPU  %MEM     TIME+ COMMAND
3592 S   1.0   0.1   0:16.39 rstudio
3760 R   1.0   0.0   0:01.34 top
0676 S   0.7   0.0   0:21.31 Xvnc
9828 S   0.7   0.1   0:06.58 Compositor
9828 S   0.3   0.1   0:19.86 QtWebEngineProc
9828 S   0.3   0.1   0:01.71 Chrome_ChildIOT
3492 S   0.3   0.1   0:00.04 rsession
3492 S   0.3   0.1   0:00.03 rsession
3492 S   0.3   0.1   0:00.04 rsession
3492 S   0.3   0.1   0:00.03 rsessio
3492 S   0.3   0.1   0:00.04 rsessio
3484 S   0.3   0.1   0:00.03 rsessio
8180 S   0.0   0.0   0:00.03 systemd
   0 S   0.0   0.0   0:00.00 (sd-pam
2852 S   0.0   0.0   0:00.00 slurm_s
0676 S   0.0   0.0   0:00.37 Xvnc
0676 S   0.0   0.0   0:00.19 Xvnc
0676 S   0.0   0.0   0:00.11 Xvnc
```

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

2021_CIMLapplica....xlsx downloa

Review the top output

Notice the elapsed time and memory size

Change the NxP matrix size and rerun

```
Source on Save
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
16:28  (Top Level)
Console  Terminal  Jobs
~/
Loading required package: iterators
Loading required package: parallel
[1] "starting dopar test"
[1] "X size is: 1.5 Gb"
```

2021_CIMLapplica....xlsx d

THE END