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

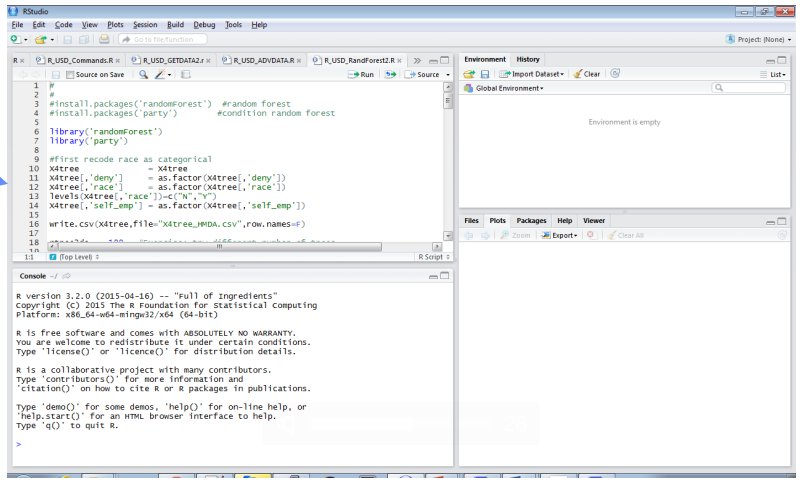
A typical R development workflow

- 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

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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

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  - more complex analysis (ie optimizations)
  - more sampling (ie more trees in Random Forest)

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- **Sometimes easy to parallelize (like with sampling)**

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

R Scaling In a nutshell

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- **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

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

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  - use derivatives to search for solutions (very general)

Consider Regression Computations

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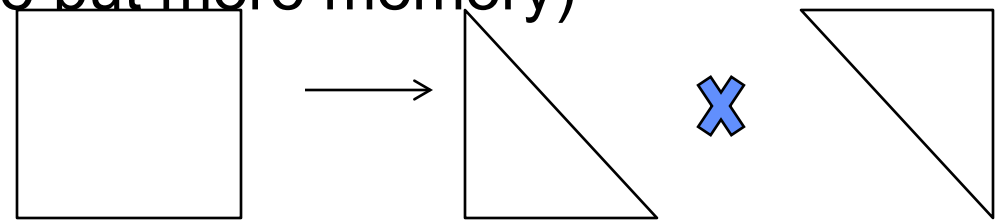
  where Y=outcomes , X=data matrix

- **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)



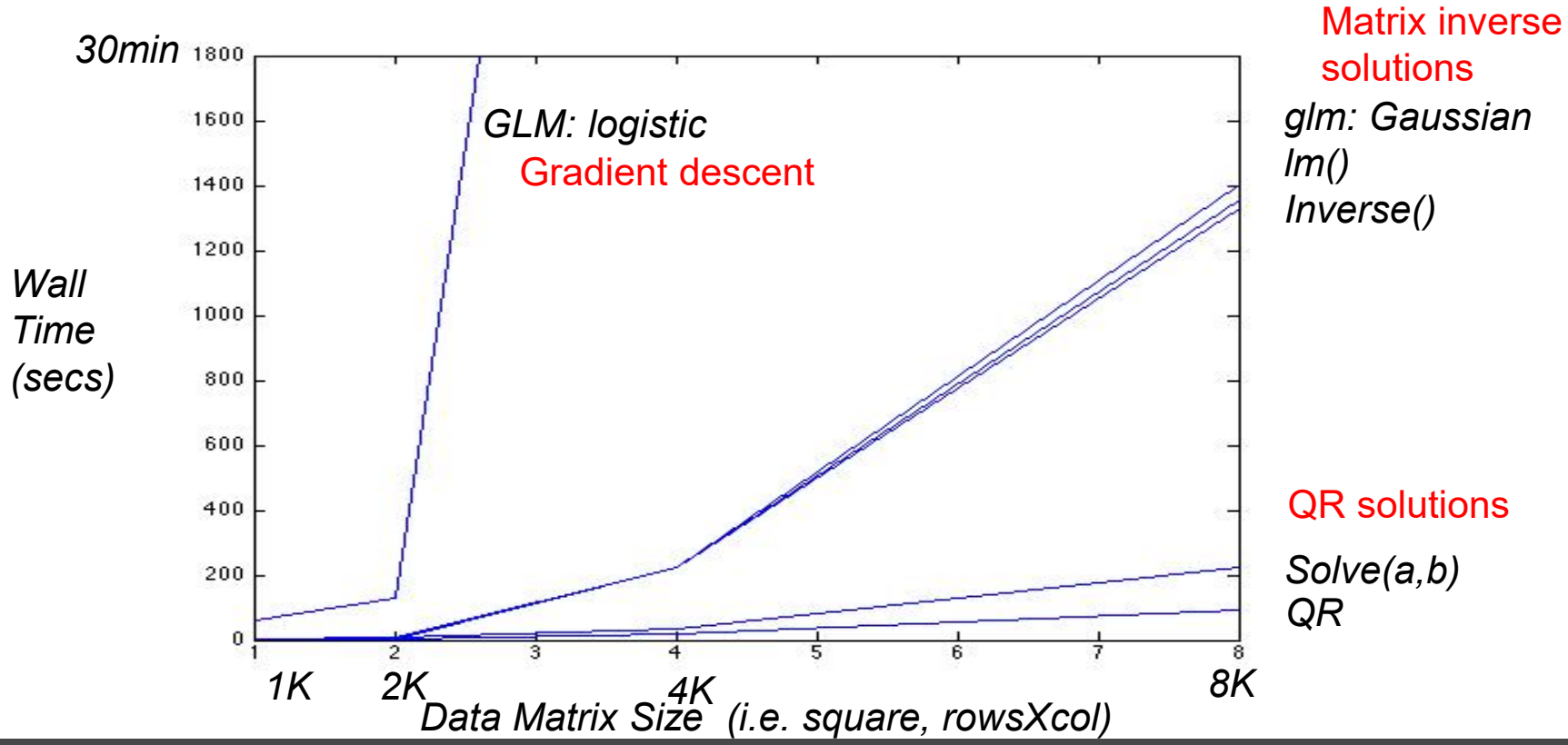
Consider Regression models in R

- **Related Models and Functions :**

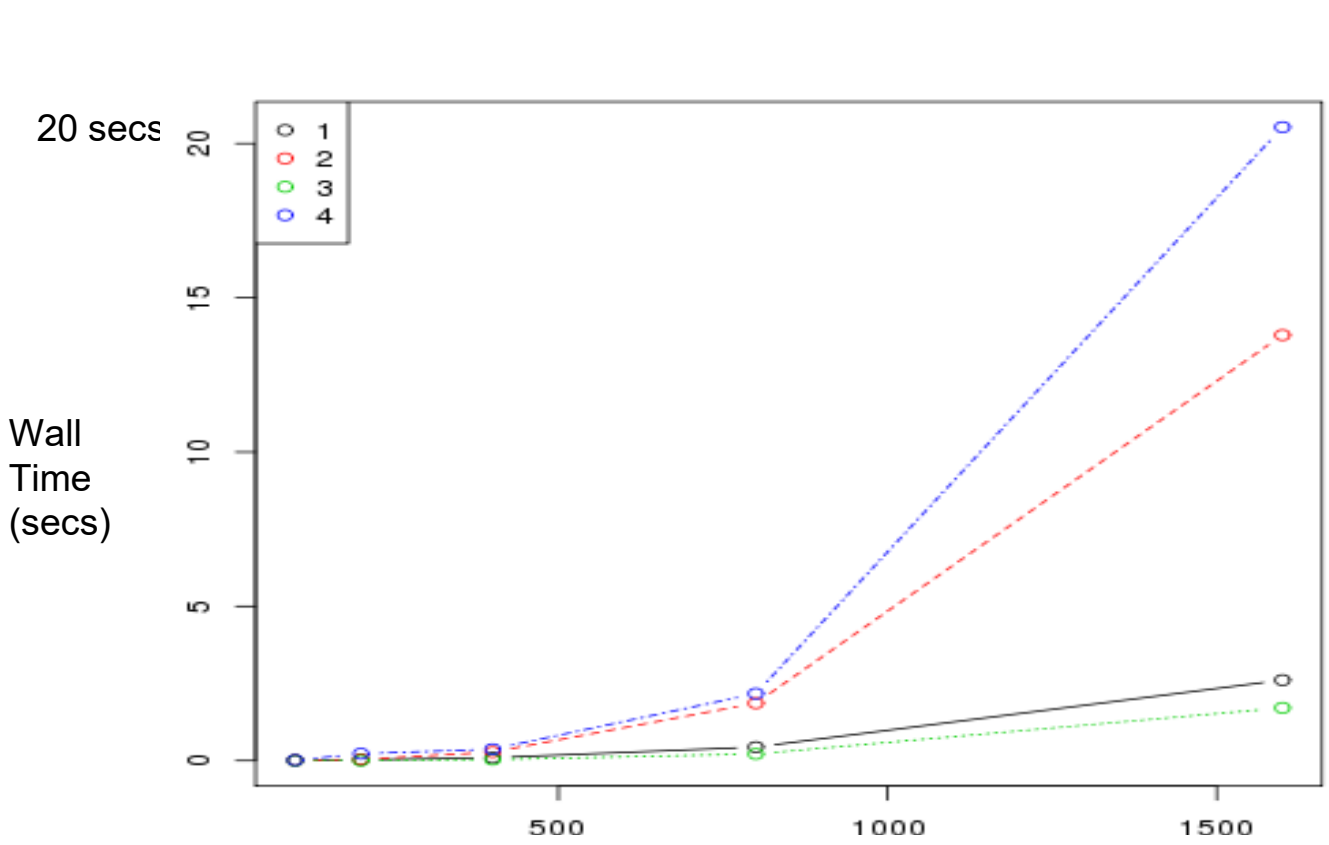
lm() Linear Model
glm() Generalized Linear Model
(logistic regression,
LASSO version from Hastie et al.,etc)

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



SVM classification (support vector machine optimization)

SVD factorization

Kmeans
lm()

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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

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install.packages(doParallel)
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    my_data_frame = …..

    my_results = foreach(
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1. allocate workers

2. Make ‘foreach’ loop

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install.packages(doParallel)
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      {   …
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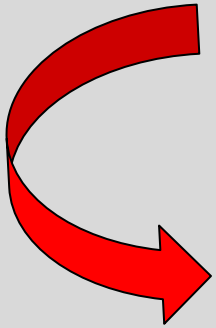

BEWARE: foreach will copy data it thinks is need to every core

R multinode: parallel backend

```
library(doParallel)

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

1. allocate cluster as parallel backend

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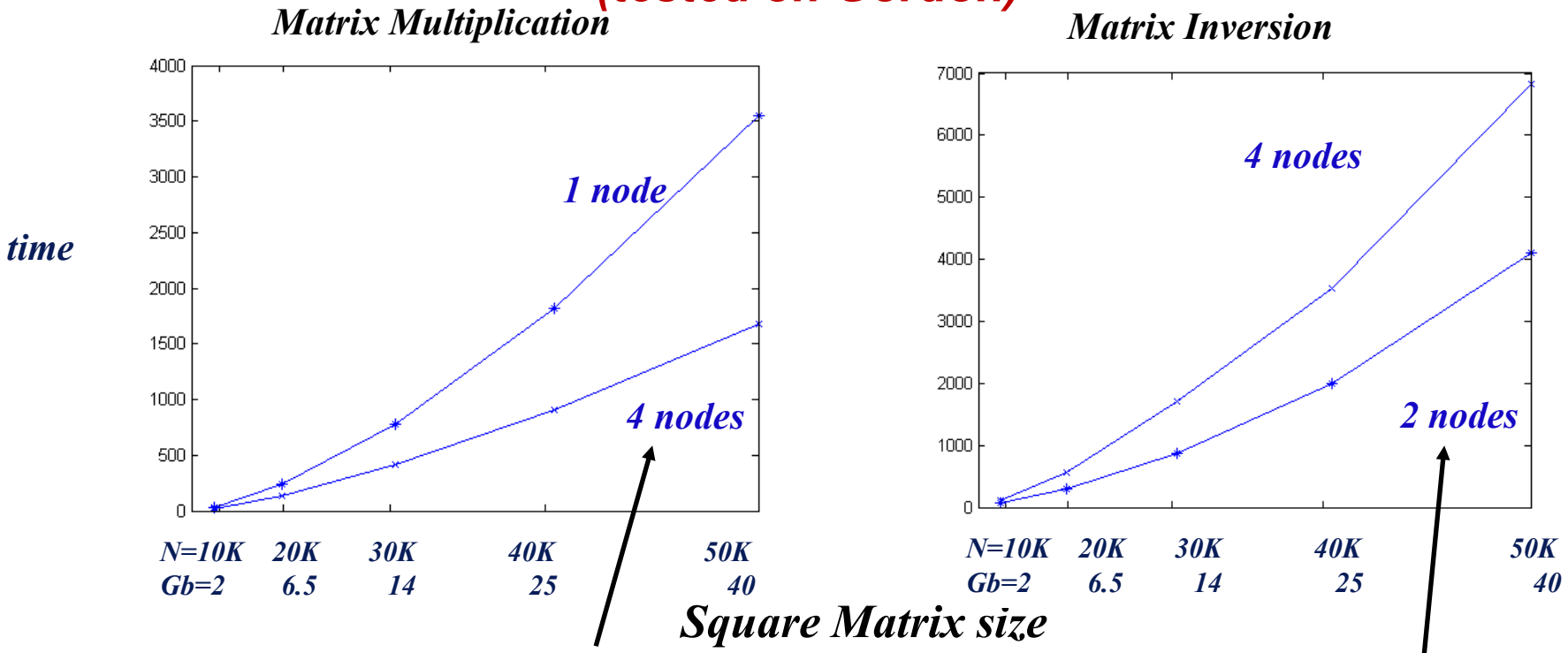
BEWARE: foreach will copy data it thinks is need to every core and node

Multiple Compute Nodes not always help

(tested on Gordon)

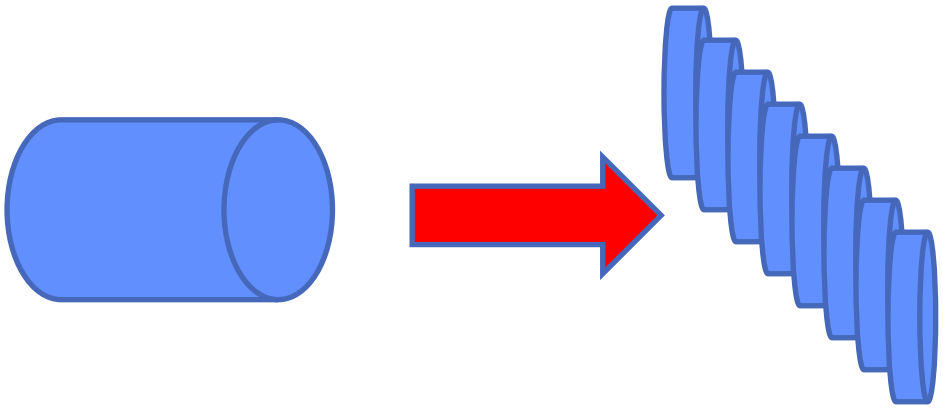


multinodes: more nodes is less time for multiplication,

less nodes is better for inversion

An option for (embarrassingly) Parallel R

1. Split up data into N parts



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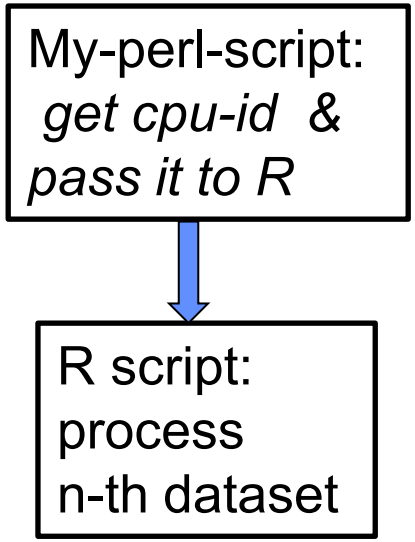
2. In slurm batch script:
   mpirun … my-perl-script



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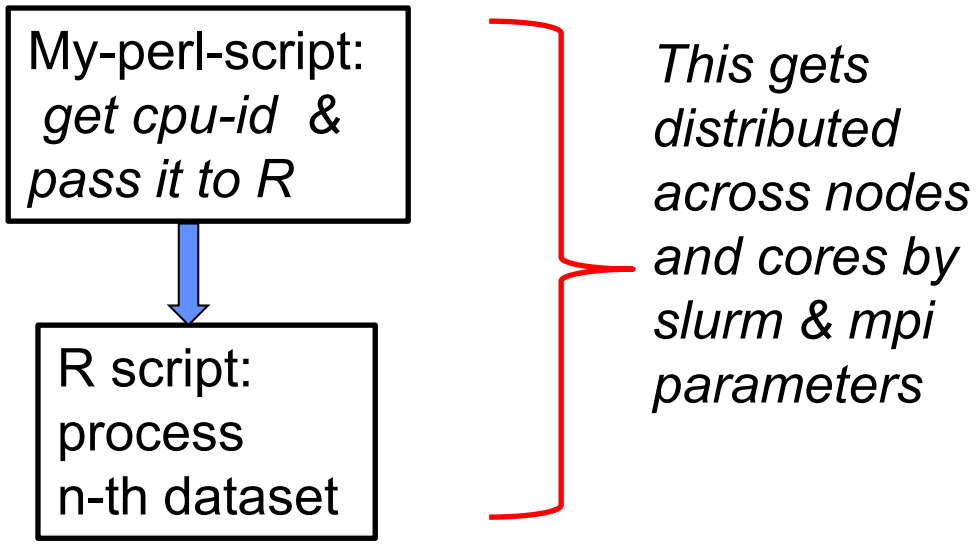

Slurm parameters: one R instance per core across all nodes

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)

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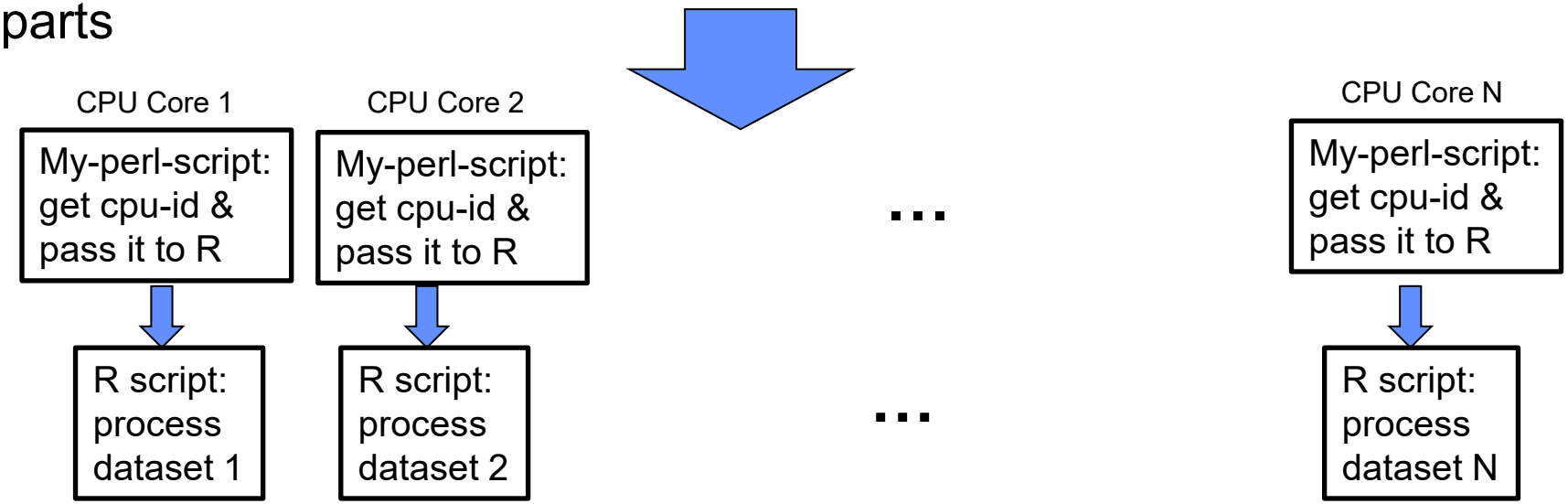

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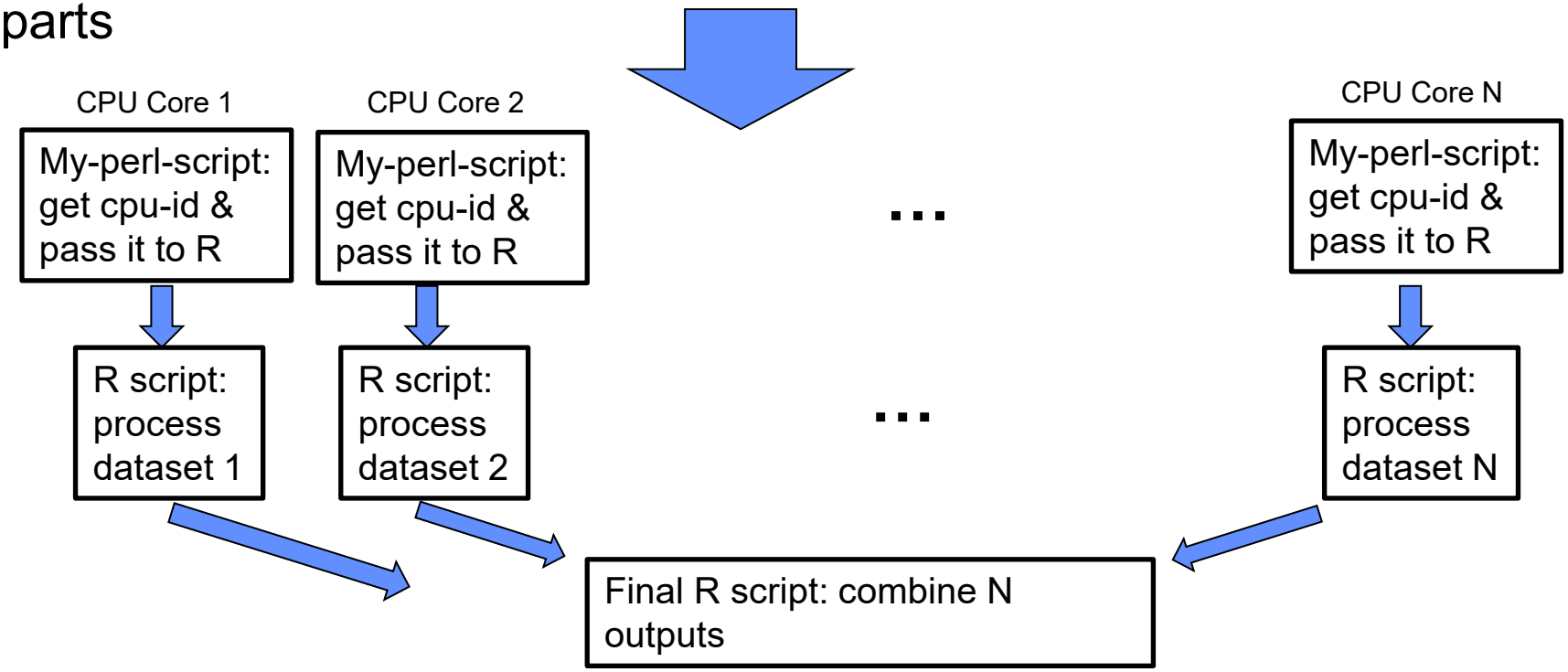

More programming but perhaps more useful

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

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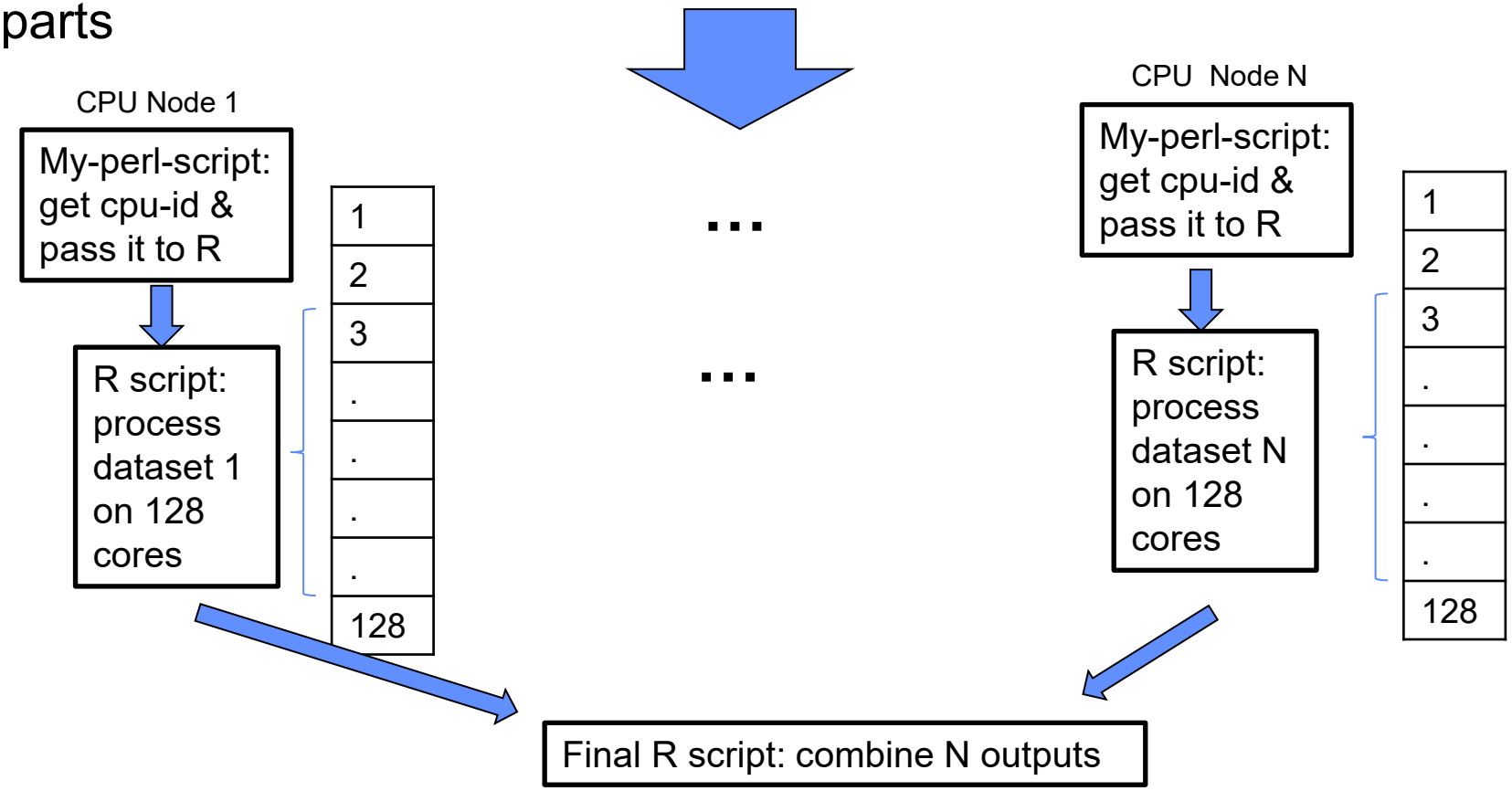
2. In slurm batch script:

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)*

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

$ 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:
```

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**

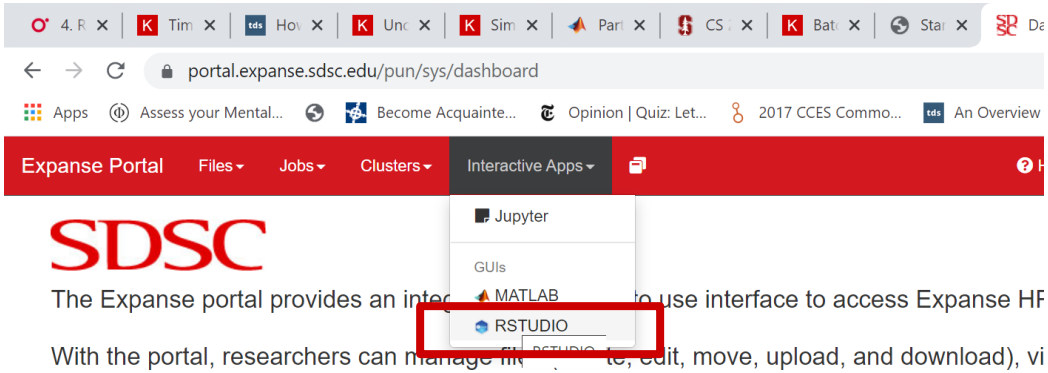
TestdoParallel R script

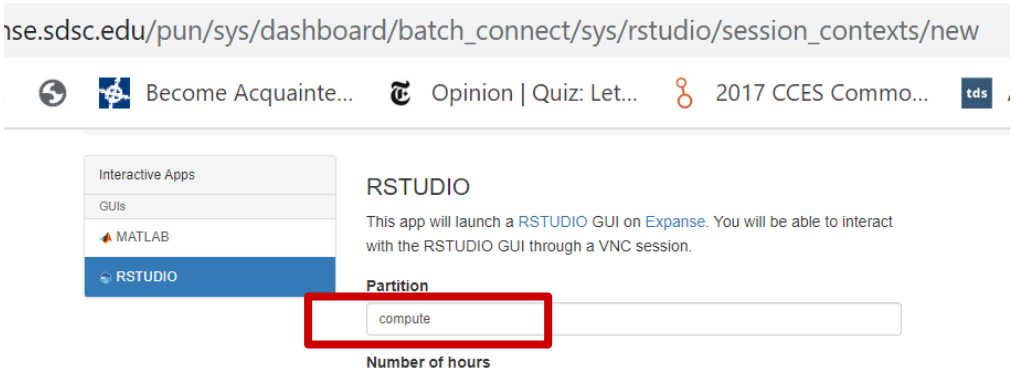
1 start Rstudio from portal and run script
(it repeatedly does a regression)

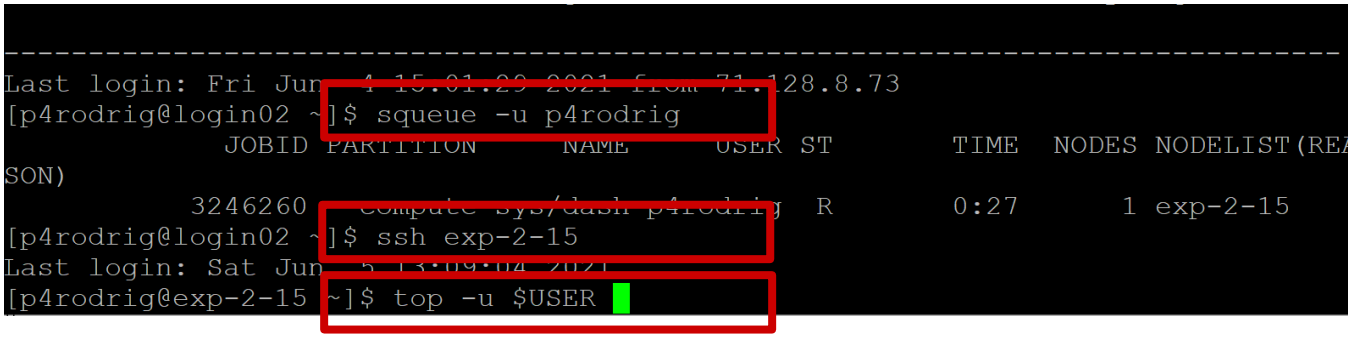
2 review execution using ‘top’ utility

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

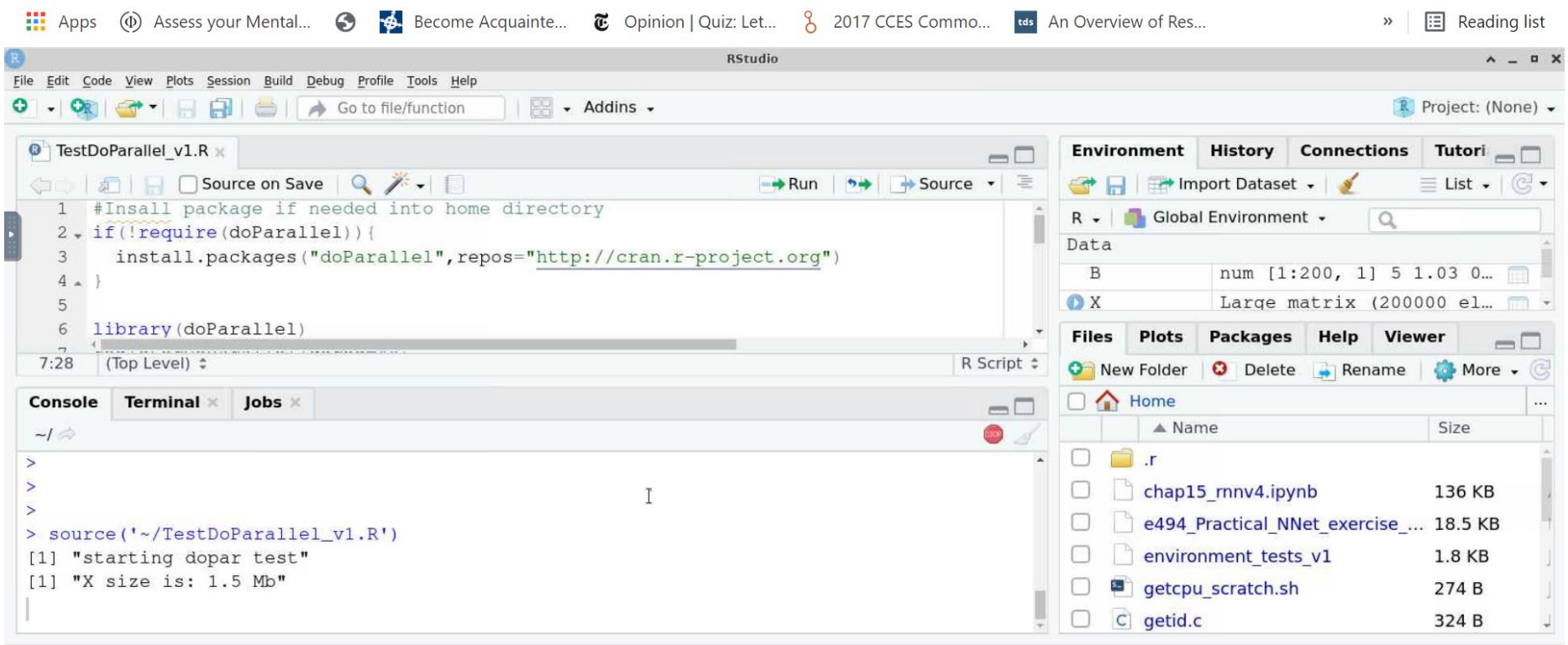
$ squeue –u $USER
$ ssh exp-##-##
$ top –u $USER

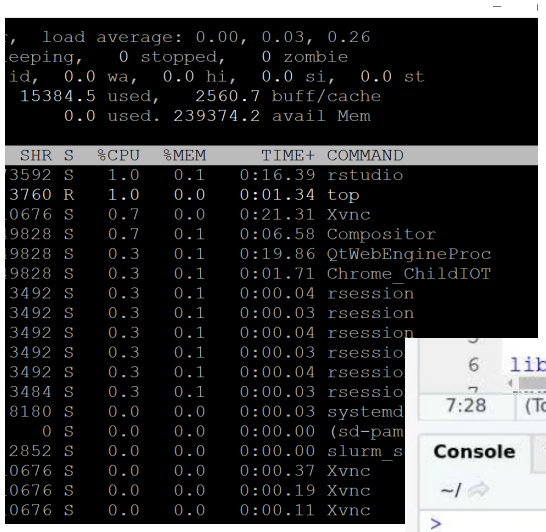
'H' will toggle threads

'fP' will toggle last cpuid

Open the 'Test_doParallel ' Rscript

Select 'source' to run the whole script

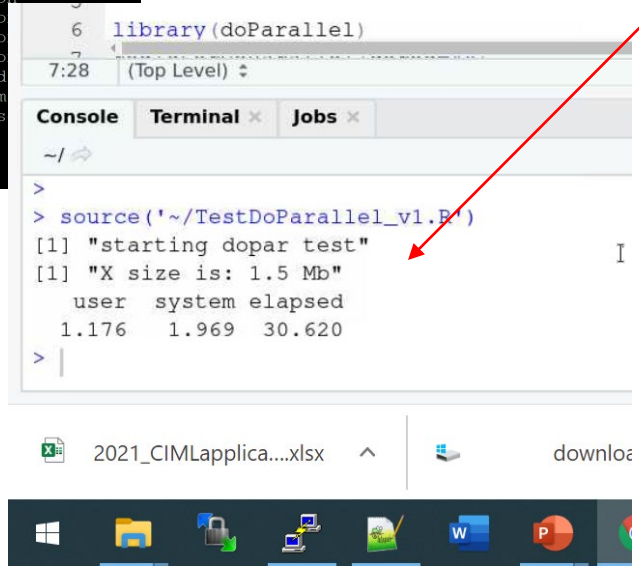


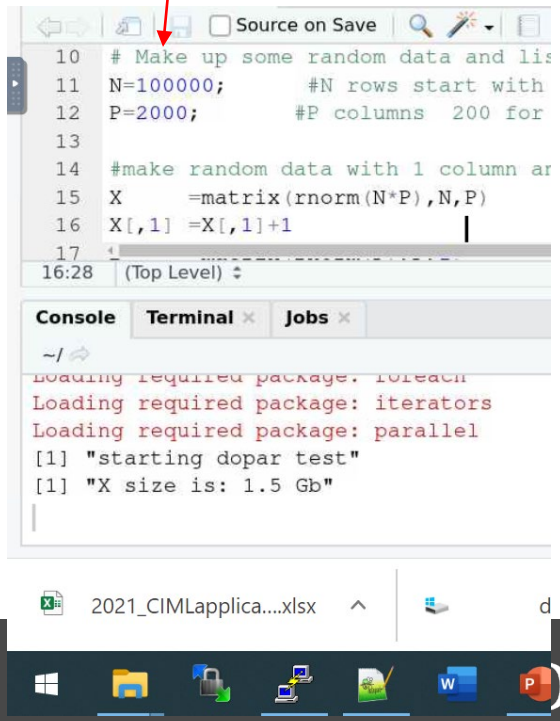


Review the top output

Notice the elapsed time and memory size

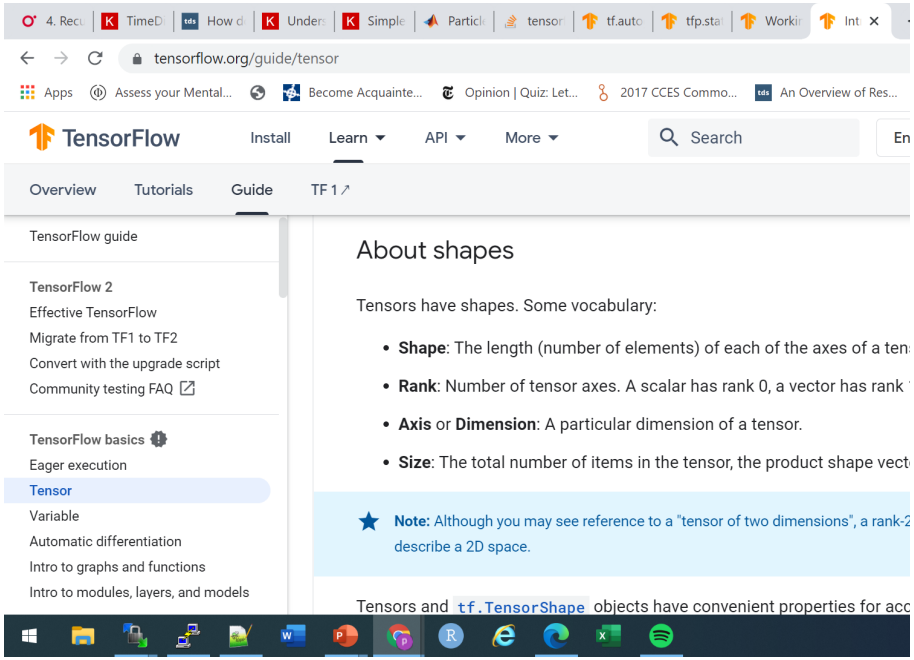
Change the NxP matrix size and rerun

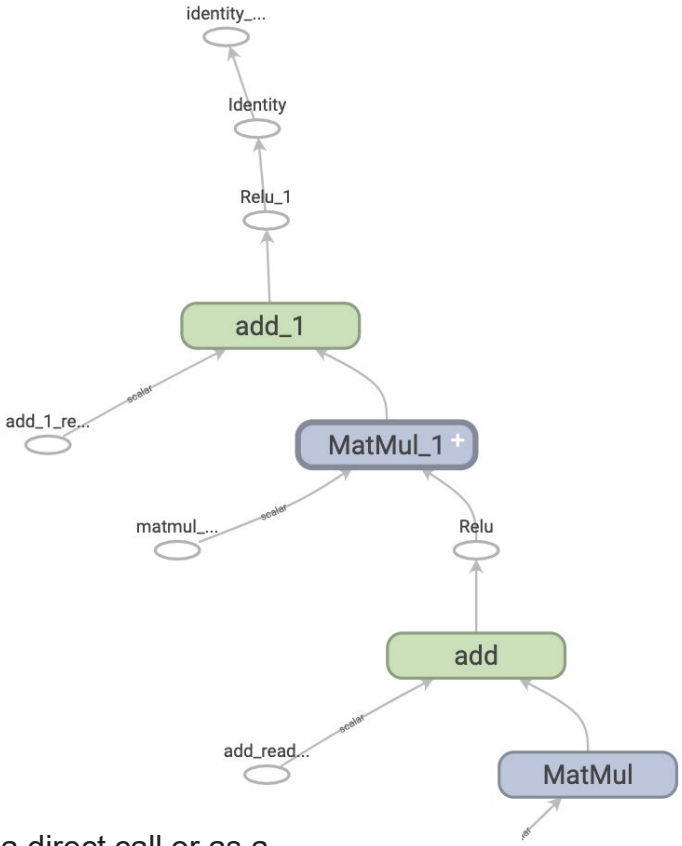




THE END

Graphs are data structures that contain a set of tf.Operation objects, which represent units of computation; and tf.Tensor objects, which represent the units of data that flow between operations. They are defined in a tf.Graph context. Since these graphs are data structures, they can be saved, run, and restored all without the original Python code.
This is what a TensorFlow graph representing a two-layer neural network looks like when visualized in TensorBoard.





You create and run a graph in TensorFlow by using tf.function, either as a direct call or as a decorator. tf.function takes a regular function as input and returns a Function. **A Function is a Python callable that builds TensorFlow graphs from the Python function. You use a Function in the same way as its Python equivalent.**