Data Science with R and pbdR at ORNL: From the CADES Cloud to the OLCF

Part 1: R and the Cloud

Drew Schmidt and George Ostrouchov
6/18/2018

Outline

(10:00-12:00) Part 1: R and the Cloud

- Basic R information
- Profiling
- Running R services in openstack

(12:00-1:00) Break for Lunch/Q&A

(1:00-3:00) Part 2: pbdR and the OLCF

- Distributed computing with pbdR
- Several applications on OLCF resources

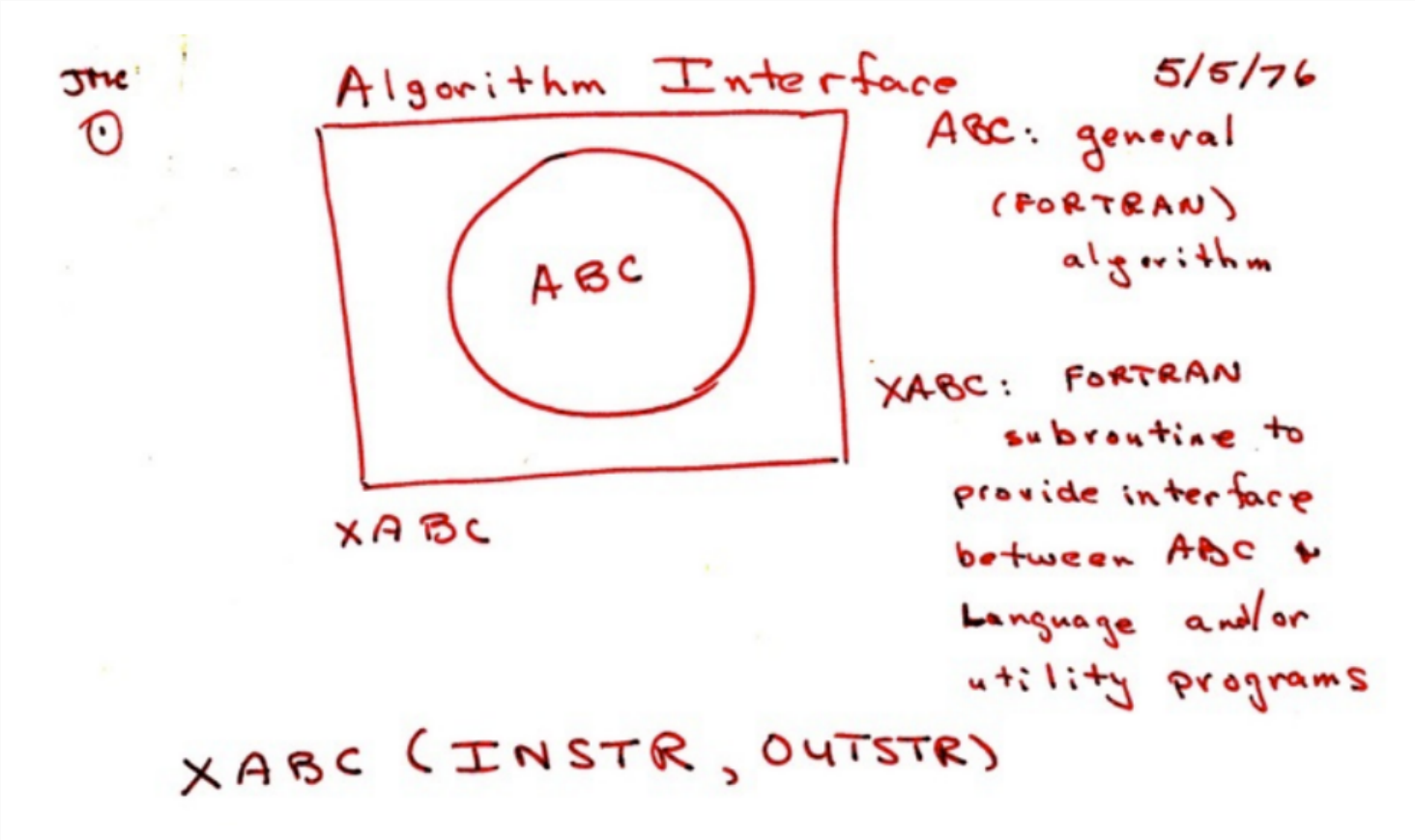
Some R Basics

What is R?

> R is part programming language and part data analysis package.
>
> --me

> R is a shockingly dreadful language for an exceptionally useful data analysis environment.
>
> from aRrgh: a newcomer's (angry) guide to R

What is R?



From http://datascience.la/john-chambers-user-2014-keynote/

What is R?

Variable naming like C

```
x <- 1
_nope <- 2
3_alsono <- 3
```

```
## Error: <text>:2:1: unexpected input
## 1: x <- 1
## 2: _
##    ^
```

What is R?

Variable naming like C

```
x <- 1
_nope <- 2
3_alsono <- 3
```

```
## Error: <text>:2:1: unexpected input
## 1: x <- 1
## 2: _
##    ^
```

lol jk

```
`this variable name has spaces` <- 1
`🐱` <- "cat"
ls()
```

```
## [1] "\U0001f431"                    "this variable name has spaces"
```

What is R?

A very stupid language

```
T
```

```
## [1] TRUE
```

```
F
```

```
## [1] FALSE
```

```
T <- FALSE
F <- TRUE
T
```

```
## [1] FALSE
```

```
F
```

```
## [1] TRUE
```

IEEE Spectrum

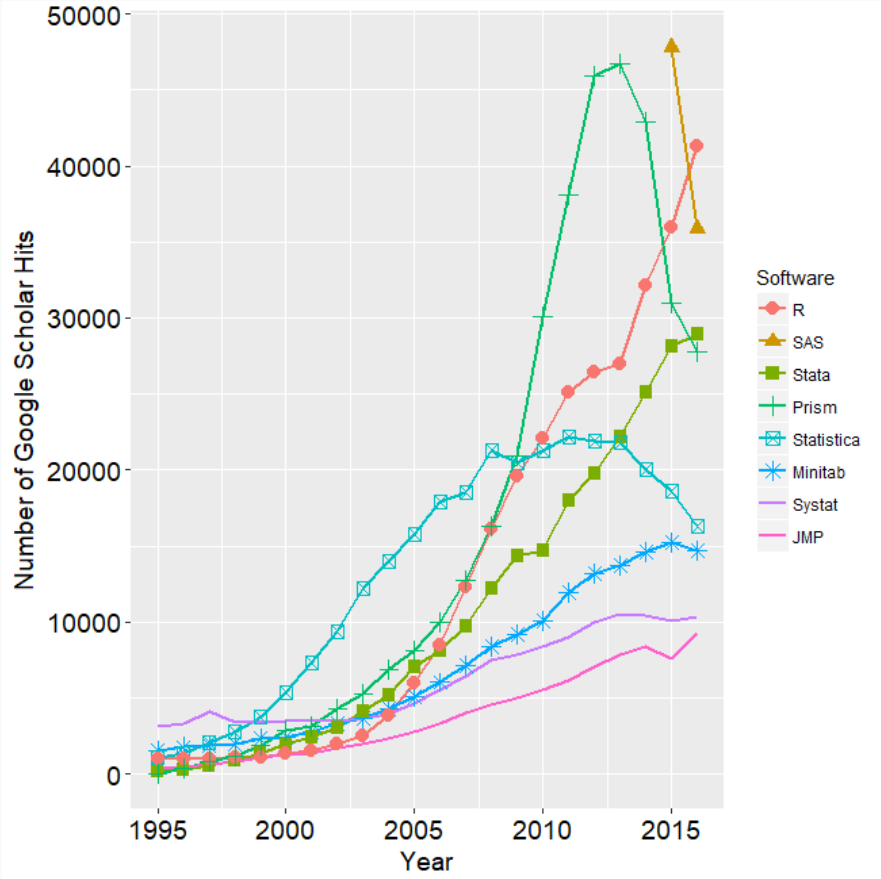
2015

Language Rank	Types	Spectrum Ranking
1. Java		100.0
2. C		99.3
3. C++		95.5
4. Python		93.4
5. C#		92.4
6. PHP		84.7
7. Javascript		84.4
8. Ruby		78.8
9. R		74.2
10. MATLAB		72.9

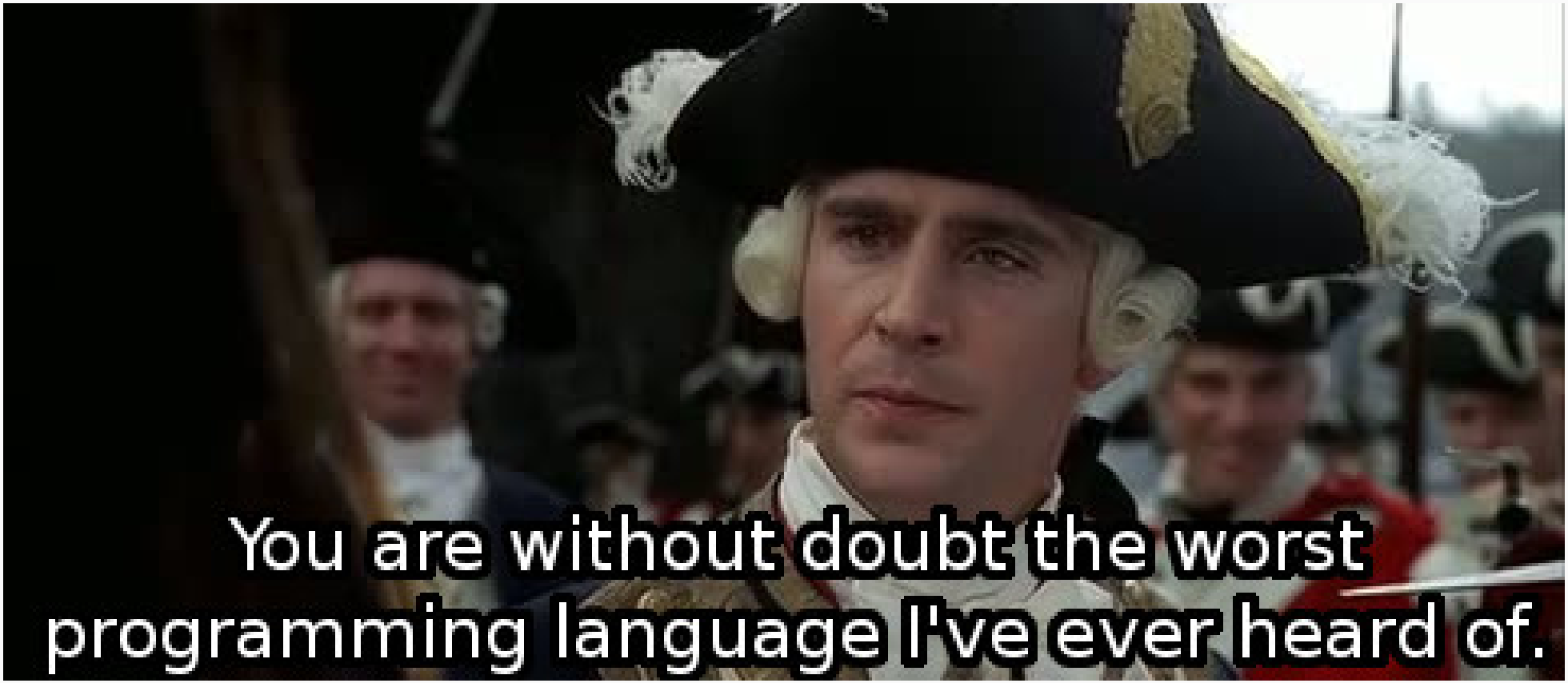
2016

Language Rank	Types	Spectrum Ranking
1. C		100.0
2. Java		98.1
3. Python		98.0
4. C++		95.9
5. R		87.9
6. C#		86.7
7. PHP		82.8
8. JavaScript		82.2
9. Ruby		74.5
10. Go		71.9

Scholarly Impact



From http://r4stats.com/articles/popularity/


You are without doubt the worst
programming language I've ever heard of.


But you HAVE heard of me!

R Resources

- Books
  - Advanced R http://adv-r.had.co.nz/
  - The Art of R Programming http://nostarch.com/artofr.htm
  - An Introduction to R http://cran.r-project.org/doc/manuals/R-intro.pdf
  - The R Inferno http://www.burns-stat.com/pages/Tutor/R_inferno.pdf
- Useful websites
  - Task Views http://cran.at.r-project.org/web/views
  - Mathesaurus: http://mathesaurus.sourceforge.net
  - R language for programmers http://www.johndcook.com/R_language_for_programmers.html
  - aRrgh: a newcomer's (angry) guide to R http://tim-smith.us/arrgh/
- Advanced resources
  - R Installation and Administration http://cran.r-project.org/doc/manuals/R-admin.html
  - Writing R Extensions http://cran.r-project.org/doc/manuals/R-exts.html
  - Mailing list archives: http://tolstoy.newcastle.edu.au/R/
- Getting help
  - The `R` stackoverflow tag
  - The `#rstats` tag on Twitter

Getting Started with R

Interfaces

- Run in the console via `R`
- Windows installs come with RGui, Mac with R.app.
- RStudio
- But more on these later...

Getting Started with R

```
1+1
```

```
## [1] 2
```

```
0:4 + 1
```

```
## [1] 1 2 3 4 5
```

```
runif(5)
```

```
## [1] 0.003761898 0.931115920 0.837614831 0.454063005 0.534433142
```

```
rnorm(5)
```

```
## [1]  0.13901484 -0.60209108  1.21671180 -1.57594543 -0.06197957
```

Getting Started with R

```
example(lm)
```

```
##
## lm> require(graphics)
##
## lm> ## Annette Dobson (1990) "An Introduction to Generalized Linear Models".
## lm> ## Page 9: Plant Weight Data.
## lm> ctl <- c(4.17,5.58,5.18,6.11,4.50,4.61,5.17,4.53,5.33,5.14)
##
## lm> trt <- c(4.81,4.17,4.41,3.59,5.87,3.83,6.03,4.89,4.32,4.69)
##
## lm> group <- gl(2, 10, 20, labels = c("Ctl","Trt"))
##
## lm> weight <- c(ctl, trt)
##
## lm> lm.D9 <- lm(weight ~ group)
##
## lm> lm.D90 <- lm(weight ~ group - 1) # omitting intercept
##
## lm> ## No test:
## lm> ##D anova(lm.D9)
## lm> ##D summary(lm.D90)
## lm> ## End(No test)
## lm> opar <- par(mfrow = c(2,2), oma = c(0, 0, 1.1, 0))
##
```

Getting Started with R

```r
nnet::multinom(Species ~ Sepal.Length + Sepal.Width, data=iris, trace=FALSE)
```

```
## Call:
## nnet::multinom(formula = Species ~ Sepal.Length + Sepal.Width,
##     data = iris, trace = FALSE)
##
## Coefficients:
##            (Intercept) Sepal.Length Sepal.Width
## versicolor   -92.09924     40.40326   -40.58755
## virginica   -105.10096     42.30094   -40.18799
##
## Residual Deviance: 110.425
## AIC: 122.425
```

The CRAN

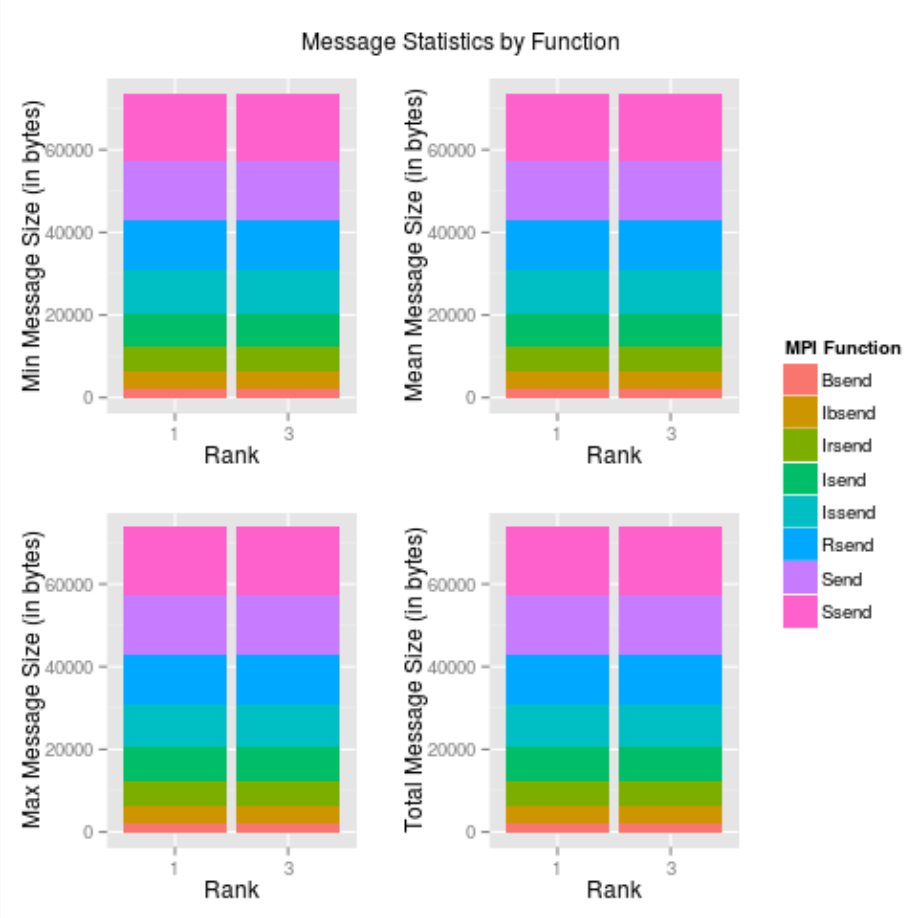
- Comprehensive R Archive Network
- The only good programming language packaging/distribution system.
- Install packages via `install.packages()`:
  - `install.packages("remotes")`
  - `remotes::install_github("wrathematics/openblasctl")`

Performance

"But why should we care about performance???"

Profiling

- Basic profiling
  - `system.time()`: timing blocks of code
  - `Rprof()`: timing all function executions
  - `Rprofmem()`: measuring memory allocations
  - `tracemem()`: tracking data copies
- Other profilers (packages on CRAN/Github)
  - pbdPROF (fpmpi, mpiP)
  - pbdPAPI
  - rbenchmark
  - microbenchmark
  - lineprof



Profiling

```
x <- matrix(rnorm(20000*750), nrow=20000, ncol=750)
str(x)
```

```
##  num [1:20000, 1:750] -0.0543 -0.2879 0.8614 -0.3773 0.5404 ...
```

```
system.time(t(x) %*% x)
```

```
##    user  system elapsed
##   8.176   0.052   8.271
```

```
system.time(crossprod(x))
```

```
##    user  system elapsed
##   6.611   0.020   6.653
```

```
system.time(cov(x))
```

```
##    user  system elapsed
##   6.756   0.039   6.845
```

Profiling

```
system.time({
  y <- x+1
  z <- y*2
})
```

```
##    user  system elapsed
##   0.040   0.023   0.063
```

Profiling

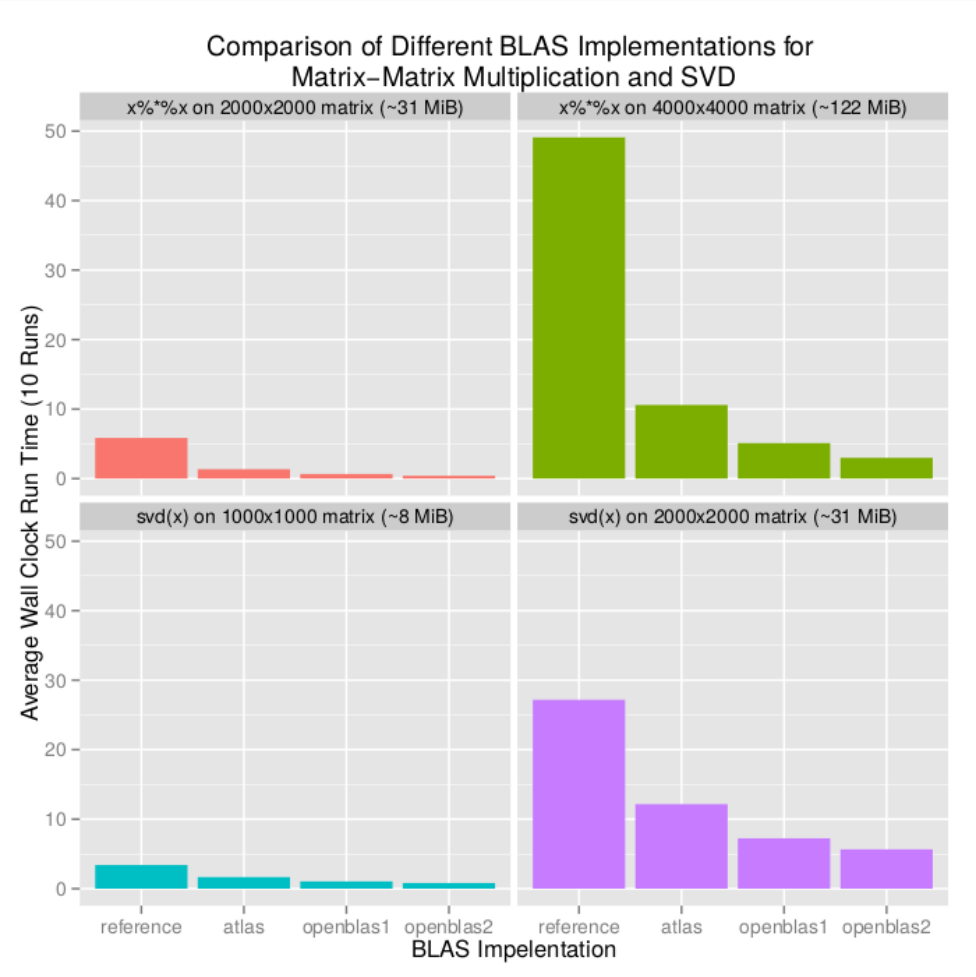
```r
Rprof()
invisible(prcomp(x))
Rprof(NULL)

summaryRprof()
```

```
## $by.self
##                   self.time self.pct total.time total.pct
## "La.svd"              72.88    73.39      73.04     73.55
## "%*%"                 25.82    26.00      25.82     26.00
## "aperm.default"        0.22     0.22       0.22      0.22
## "is.finite"            0.14     0.14       0.14      0.14
## "array"                0.08     0.08       0.08      0.08
## "any"                  0.04     0.04       0.04      0.04
## "matrix"               0.04     0.04       0.04      0.04
## "prcomp.default"       0.02     0.02      99.28     99.98
## "svd"                  0.02     0.02      73.12     73.64
## "sweep"                0.02     0.02       0.32      0.32
## ".External2"           0.02     0.02       0.02      0.02
##
## $by.total
##                       total.time total.pct self.time self.pct
## "block_exec"               99.30    100.00      0.00     0.00
## "call_block"               99.30    100.00      0.00     0.00
## "evaluate_call"            99.30    100.00      0.00     0.00
## "evaluate::evaluate"       99.30    100.00      0.00     0.00
```

Improving Performance

- All the usual HLL stuff
  - Vectorize
  - Write C/C++/Fortran kernels
- All the usual HPC stuff
  - Build with a better compiler
  - Use optimized BLAS/LAPACK
  - Go parallel
- Use the bytecode compiler

High Performance BLAS



Basic Parallelism

```
unlist(lapply(1:5, sqrt))
```

```
## [1] 1.000000 1.414214 1.732051 2.000000 2.236068
```

```
n <- 1:1e6
system.time(lapply(n, sqrt))
```

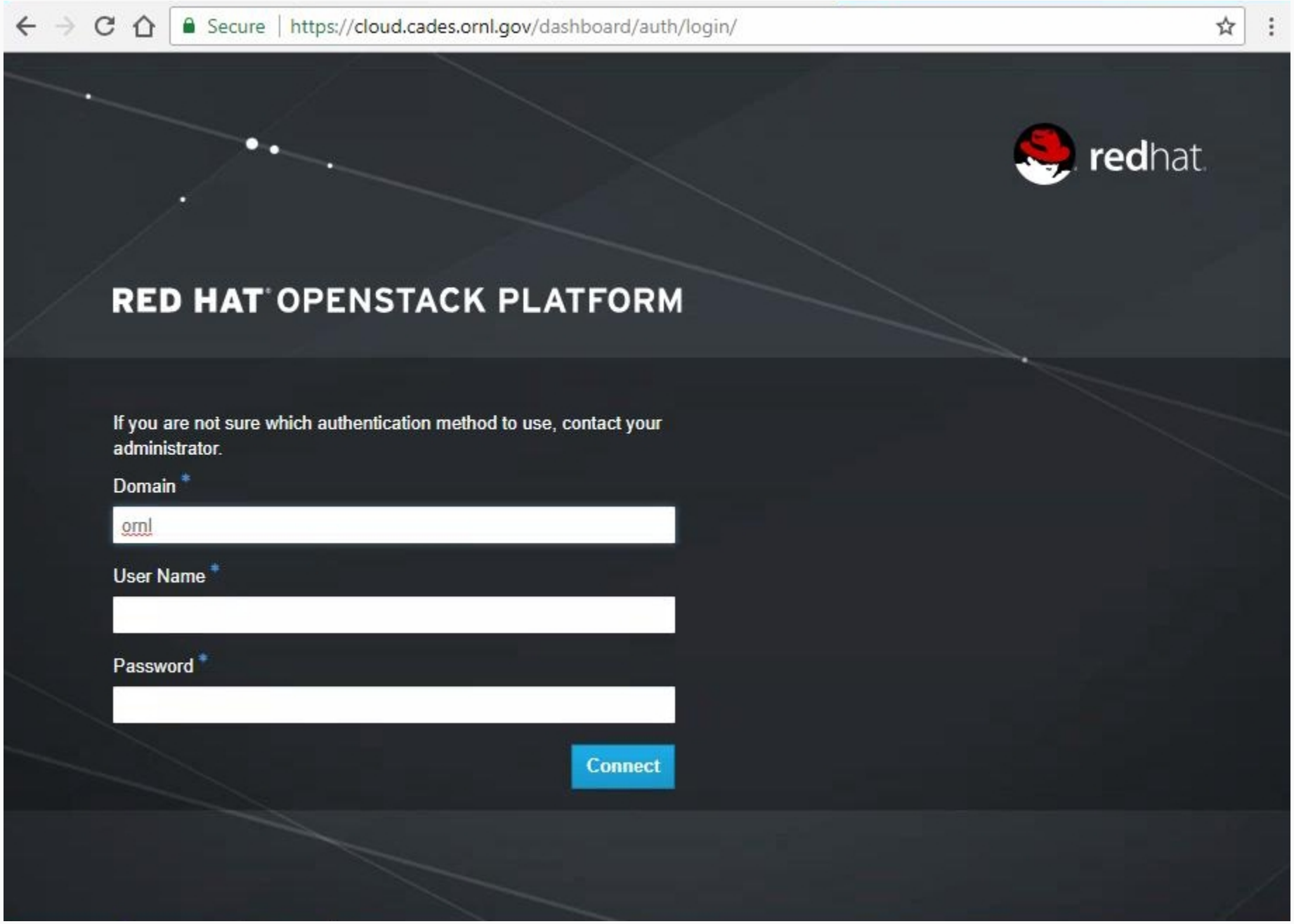
```
##    user  system elapsed
##   0.467   0.028   0.497
```

```
system.time(parallel::mclapply(n, sqrt))
```

```
##    user  system elapsed
##   0.542   0.204   0.452
```

Running R Services in Openstack

Openstack


Secure
https://cloud.cades.ornl.gov/dashboard/auth/login/
redhat
RED HAT OPENSTACK PLATFORM
If you are not sure which authentication method to use, contact your administrator.
Domain *
ornl
User Name *
Password *
Connect

Ways to Interface with Your VM

- ssh
- remoter
- RStudio server
- Dashboards/webapps (shiny)

ssh

Pros

- Ubiquitous
- Good for running things in batch

Cons

- CLI only
- Have to be comfortable with *nix

```
Unauthorized or improper use of this system may result in administrative
disciplinary action and civil and criminal penalties.  By continuing to use
this system you indicate your awareness of and consent to these terms and
conditions of use.  LOG OFF IMMEDIATELY if you do not agree to the
conditions stated in this warning.
******************************************************************************

******************************************************************************
*  Please send questions or comments to the NCCS User Assistance Center
*    help@olcf.ornl.gov
*    http://www.olcf.ornl.gov/support
*
******************************************************************************

va8@titan-ext3:~$ module load r
Swapping PrgEnv-pgi for PrgEnv-gnu
R version 5.2.82
Parallel Batch Use (see r-pbd.org) via mpirun Rscript.
Example: aprun -n 2 Rscript myscript.r
OMP_NUM_THREADS set to 1. Change as needed to use Cray SciLib.
va8@titan-ext3:~$ R
> 1+1
[1] 2
>
```

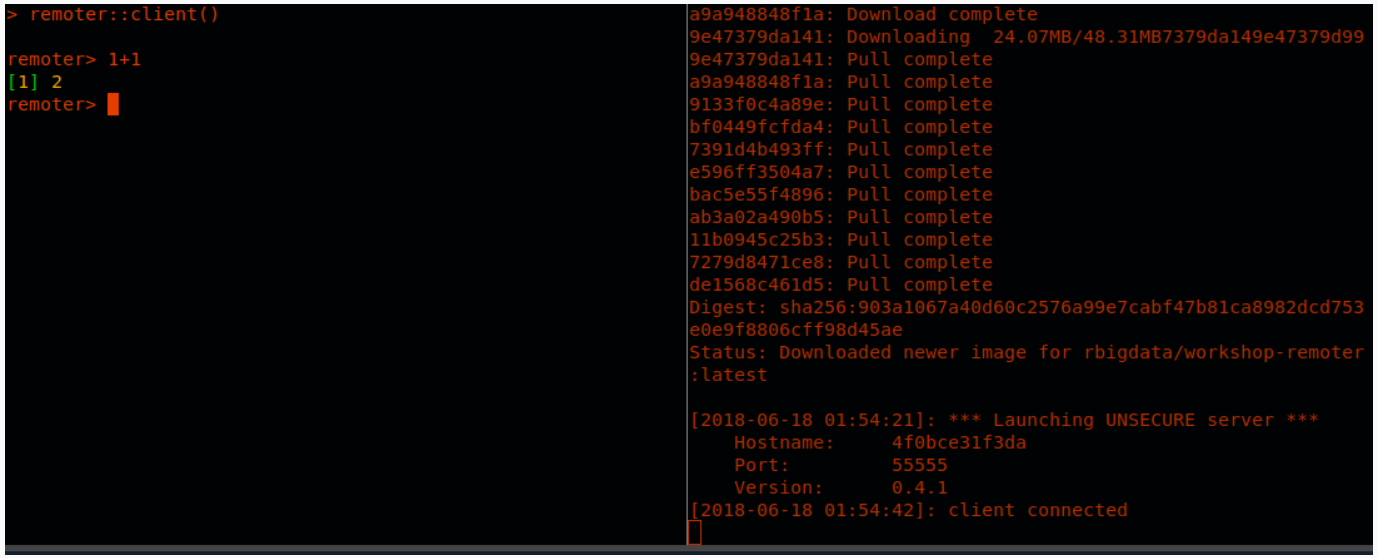
remoter

Pros

- Can use from any local R interface (terminal, R.app, RStudio, ...)
- Can avoid need to use ssh

Cons

- Setting up the server is somewhat DIY
- Lots of ssh tunneling depending on firewall



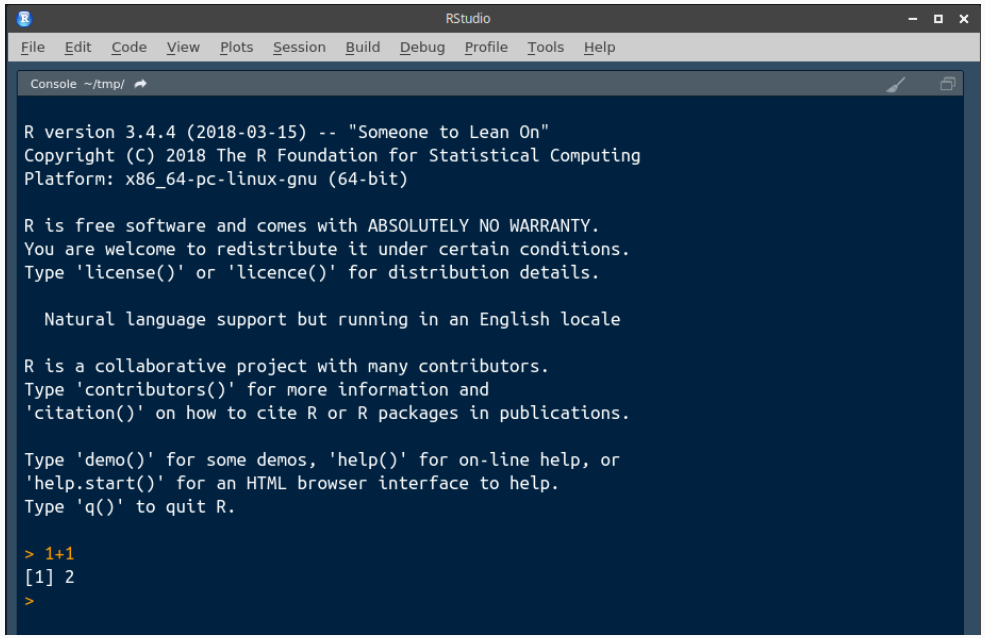
RStudio

Pros

- Ubiquitous among R users
- Well-supported

Cons

- Ubiquitous among R users
- Sever variant has same ssh tunnel issue



Docker

For ease of distributing things, we'll be using Docker.

- Container platform for Linux
- ***NOT A VM***
- ...except on Windows and Mac
- rocker project maintains helpful R distributions:
  - rocker/r-base
  - rocker/rstudio
  - rocker/shiny
  - rocker/tidyverse

Installing Docker on Your Laptop

Windows

- Windows 10 or later
- Install the Docker Community Edition for Windows

Mac

- OS X El Capitan 10.11 or later
- Install the Docker Community Edition for Mac.

Linux

- deb (Debian, Ubuntu): `apt-get install docker.io`
- rpm (Fedora, Centos): `yum install docker-io`

Openstack and Docker Resources

- Request birthright cloud access
- Birthright cloud login (domain: ornl)
- R Docker tutorial

Tunneling

- If running a docker service in openstack, you need to tunnel.
- If you are on the ORNL network, you need 1 tunnel:
  - If your VM's IP is `1.2.3.4`:
  - `ssh -L 8787:localhost:8787 -N cades@1.2.3.4`
- If you're off the ORNL network, you need 2 tunnels:
  - If your XCAMS/UCAMS ID is `abc`:
  - `ssh -L 8787:localhost:8787 abc@cades-extlogin01.ornl.gov ssh -L 8787:localhost:8787 -N cades@1.2.3.4`

remoter

```
sudo docker run -i -t -p 55555:55555 rbigdata/workshop-remoter
```

RStudio

File Edit Code View Plots Session Build Debug Profile Tools Help

Console ~/tmp/

```
R version 3.4.4 (2018-03-15) -- "Someone to Lean On"
Copyright (C) 2018 The R Foundation for Statistical Computing
Platform: x86_64-pc-linux-gnu (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.

  Natural language support but running in an English locale

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.

> remoter::client()

remoter> 1+1
[1] 2
remoter> exit()
>
```

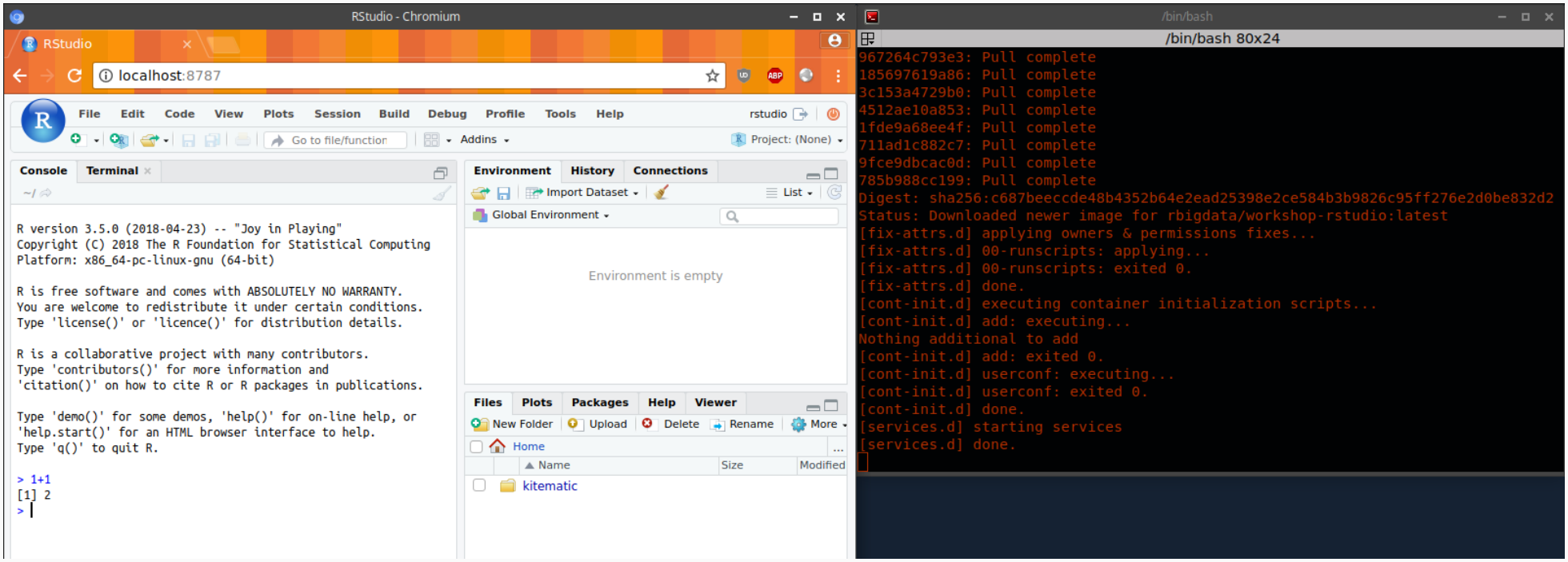
/bin/bash

/bin/bash 80x28

```
Deleted: sha256:9d6f4ac281c18c8285859b32c00067a54c267493a56386ab856166bd40a0ce86
Deleted: sha256:8382b2990f71dc0fd96fbdc1d95c80fef510ee01d32257fbc376c38e1591fe70
Deleted: sha256:0f3a12fef684003e8dc0dfdcea32789db2179c6f9ad1e1e89bc05754ac44c6c5
mschmid3@wootabega-laptop:~$ sudo docker run -i -t -p 55555:55555 rbigdata/works
hop-remoter
Unable to find image 'rbigdata/workshop-remoter:latest' locally
latest: Pulling from rbigdata/workshop-remoter
9e47379da141: Pull complete
a9a948848f1a: Pull complete
9133f0c4a89e: Pull complete
bf0449fcfda4: Pull complete
7391d4b493ff: Pull complete
e596ff3504a7: Pull complete
bac5e55f4896: Pull complete
ab3a02a490b5: Pull complete
11b0945c25b3: Pull complete
7279d8471ce8: Pull complete
de1568c461d5: Pull complete
Digest: sha256:903a1067a40d60c2576a99e7cabf47b81ca8982dcd753e0e9f8806cff98d45ae
Status: Downloaded newer image for rbigdata/workshop-remoter:latest

[2018-06-17 21:52:12]: *** Launching UNSECURE server ***
    Hostname:     a48404b1cd6c
    Port:         55555
    Version:      0.4.1
[2018-06-17 21:52:17]: client connected
[2018-06-17 21:52:20]: client disconnected with call to exit()
```

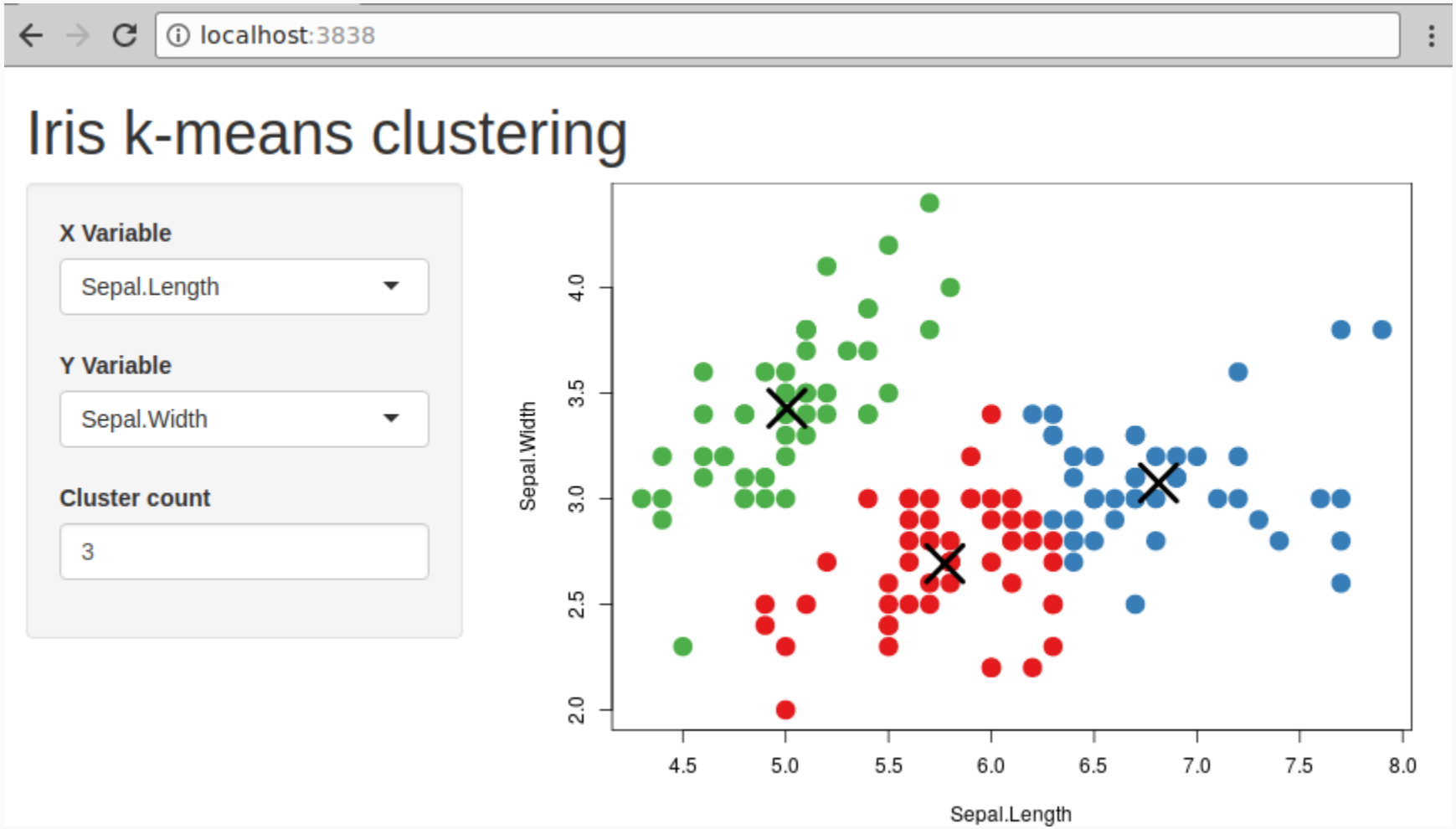
rstudio

```
sudo docker run -i -t -p 8787:8787 rbigdata/workshop-rstudio
```



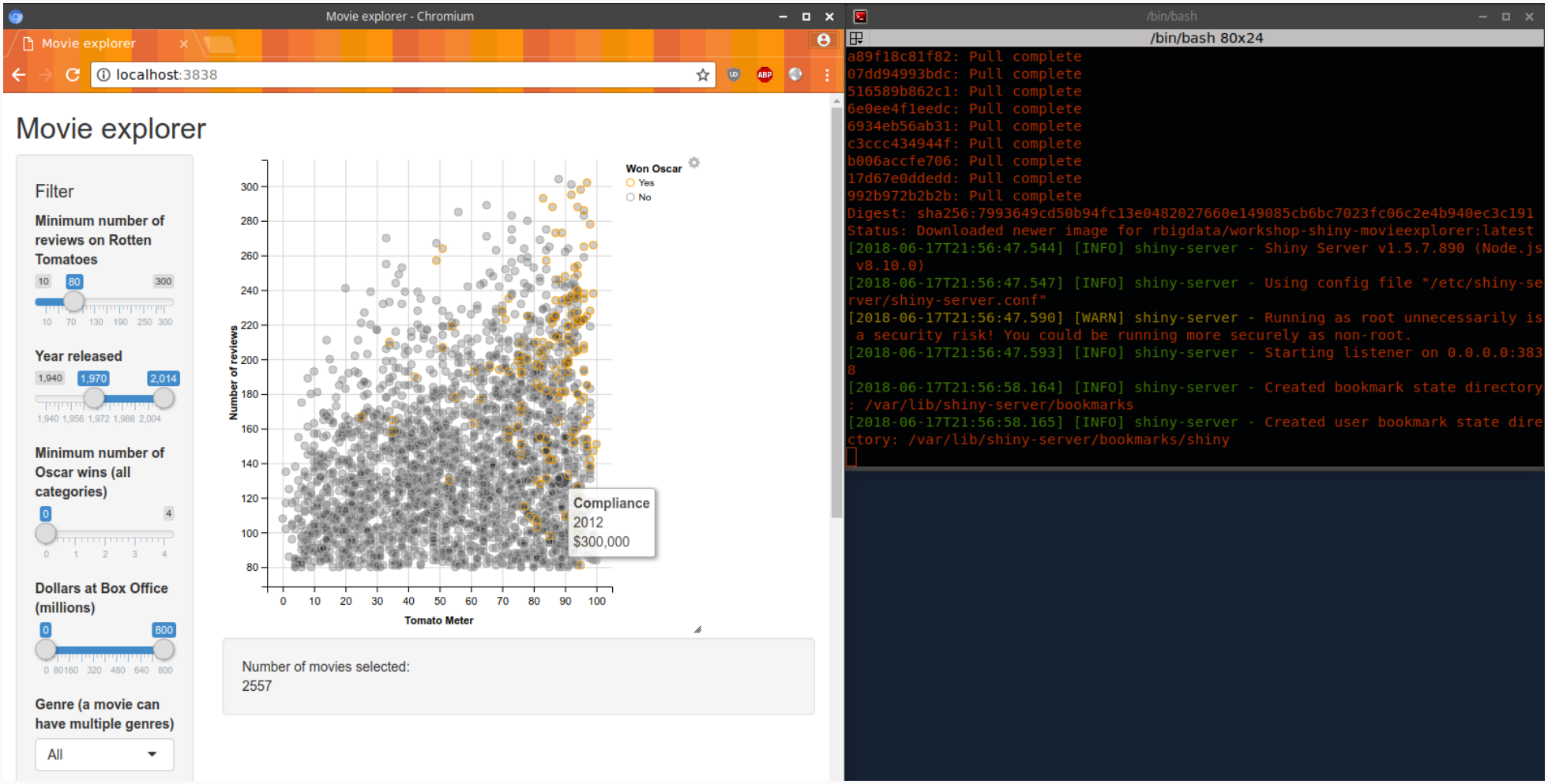
Shiny

```
sudo docker run -i -t -p 3838:3838 rbigdata/workshop-shiny-kmeans
```



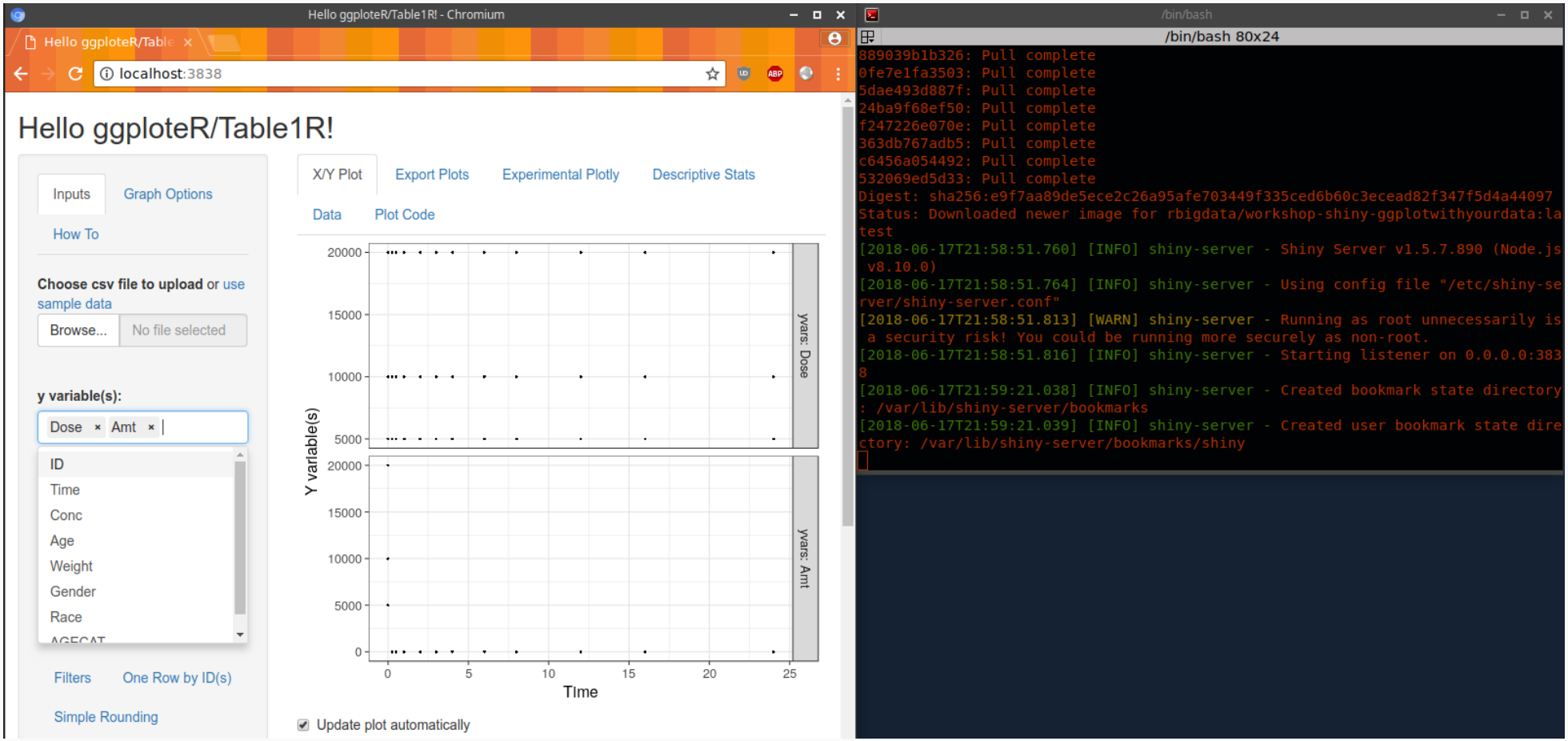
Shiny

```
sudo docker run -i -t -p 3838:3838 rbigdata/workshop-shiny-movieexplorer
```



Shiny

```
sudo docker run -i -t -p 3838:3838 rbigdata/workshop-shiny-ggplotwithyourdata
```



Thanks!