Parallel and high performance processing with R

An introduction to the high performance computing environment at SHARCNET

Ge Baolai SHARCNET <u>Western University</u>

- Running R on SHARCNET
- Running R many simulations at once
- Parallel processing with R
- Other aspects of HPC with R

General Interest Seminar Series Teaching the lab skills for SCIENTIFIC COMPUTING

THE ART OF R PROGRAMMING

A TOUR OF STATISTICAL SOFTWARE DESIGN

NORMAN MATLOFF

Use R!

Christian P. Robert George Casella

Introducing Monte Carlo Methods with R

Deringer

Running R on SHARCNET

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On clusters

\$ module unload intel

Online

http://rstudio.sharcnet.ca/

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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.	cols chr [1:2] "red" "green" labels chr [1:2] "Used" "Free" slices num [1:2] 0.5 100					
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.	tagpos num [1:2] 1 1 tags chr [1:2] "Used: 0.5 GB(0%)" "Unus y 2.71828182845905					
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<pre>> library("ggplot2", lib.loc="/usr/lib64/R/library")</pre>	manipulate Interactive Plots for RStudio 0.98.10 S					
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<pre>> log(exp(1),base=2)</pre>	class Functions for Classification 7.3-13					
<pre>[1] 1.442695 > install.packages("Rmpi") Installing package into '/home/bge/R/x86_64-redhat-linux-gnu-li </pre>	Cluster "Finding Groups in Data": Cluster 2.0.3 Analysis Extended Rousseeuw et al.					
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gz' Content type 'application/x-gzip' length 102182 bytes (00 Kb)	compiler The R Compiler Package 3.2.2 😒					
opened URL	datasets The R Datasets Package 3.2.2 😒					
downloaded 99 Kb	dichromat Color Schemes for Dichromats 2.0-0 😒					
	- digest Create cryptographic hash digests 0.6.4 🔿 🔻					

Running many simulations at once



Example: I am to run 10 simulations, each can go independently. I'd like to run them on SHARCNET systems as 10 independent jobs, by typing the command time times:

\$ sqsub -r 3d -o sim1.log **R CMD BATCH** –no-save --args param1.csv sim.R \$ sqsub -r 3d -o sim2.log **R CMD BATCH** –no-save --args param1.csv sim.R \$ sqsub -r 3d -o sim3.log **R CMD BATCH** –no-save --args param3.csv sim.R \$ sqsub -r 3d -o sim4.log **R CMD BATCH** –no-save --args param4.csv sim.R \$ sqsub -r 3d -o sim5.log **R CMD BATCH** –no-save --args param5.csv sim.R \$ sqsub -r 3d -o sim6.log **R CMD BATCH** –no-save --args param6.csv sim.R \$ sqsub -r 3d -o sim7 log **R CMD BATCH** –no-save --args param7.csv sim.R \$ sqsub -r 3d -o sim8.log **R CMD BATCH** –no-save --args param8.csv sim.R \$ sqsub -r 3d -o sim9.log **R CMD BATCH** –no-save --args param9.csv sim.R \$ sqsub -r 3d -o sim10.log **R CMD BATCH** –no-save --args param10.csv sim.R \$ sqjobs

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Running many simulations at once



But if I need to run 300 simulations, then typing commands 300 times becomes impractical. Instead I'd write a BASH script, say, "run_sims.sh" to automate that:

```
#!/bin/bash
num_sims=300
for ((i=1;i<$num_sims;i++)); do
    sqsub -r 3d -o sim$i.log R CMD BATCH -no-save -args param$i.csv sim.R
done</pre>
```

Then I run the script

\$./run_sims

\$ sqjobs

The 300 jobs are now in the queue. The scheduler will find free cores and place the jobs on them at a later time.

Running many simulations at once



Example (cont'd): Suppose I have 80 simulations, each uses an input file with irregular name, e.g. patient name, SmithKW.csv, JohnFK.csv, WarrenB.csv, how do I automate the submissions?

#!/bin/bash

for f in *.csv; do

sqsub -r 3d -o \$f.log **R CMD BATCH** –no-save –args \$f sim.R

done



Running R on multicores

sqsub -q threaded -n 8 -mpp=4g -o myprog.log R CMD BATCH -no-save myprog.R

Running R across nodes (via MPI)

sqsub -q mpi -n 32 -mpp=4g -o myprog.log R CMD BATCH -no-save myprog.R

We won't talk much about R+MPI (Rmpi) here. Bottom line: tell the scheduler how many MPI process you want to run, and never spawn dynamic MPI processes from within your code without telling the scheduler at the time of submission.

Simulation of diffusion process

- Substance of particles at the centre at the beginning.
- To simulate the distribution of the particles over time.

Assumptions:

- Each particle the walker walks randomly independent of other.
- Each one walks a small distance over a small, unit time step.
- At each point, the probability of a walker arriving at this location depends only on the equal probability of it having reached the neighboring points.

2D











• On a single core – Use **for** loop to iterate through walkers.





• On multicores – Use **foreach**, each core follows a subset of walkers.



Parallel packages

There are many parallel packages:-(that enable one to perform parallel processing from least to advanced levels, including, e.g.

- multicore enables the use of all cores on a single computer. It uses fork(), a Unix mechanism, to spawn multiple instances, not for Windows.
- snow Simple Network Of Workstations, can run on a single computer and a cluster of computers (nodes), works for both Windows and Linux.
- parallel built on top of multicore and snow, now part of R base package.
- **foreach** a package that enables one to perform parallel for loops.
- Rmpi, Rdsn, pbdR, etc.



Exercise: Simulation of 1D diffusion process

Assumptions:

- All particles start at the origin.
- Each particle the walker walks randomly, either leftward or rightward, with equal probability, independent of other.
- Each one walks a distance Δx over a small, unit time step Δt .
- At each point, the probability of a walker arriving at this location depends only on the equal probability of it having reached the neighboring points, that is

$$p(x,t+\Delta t) = \frac{1}{2}p(x-\Delta x,t) + \frac{1}{2}p(x+\Delta x,t).$$



```
# Implementation 1 (inefficient, never do this)
num_walkers = 100000
num_paths = 200
```

```
x = matrix(0,num_paths,num_walkers)
x2 = rep(0,num_paths)
```

```
# Launch random walkers, all starting from x = 0
set.seed(47)
```

```
ts <- proc.time()
```

```
for (i in 1:num_walkers)
```

```
{
```

```
# A walker completes its walk
for (k in 2:num_paths)
{
    #x[k,i] = x[k-1,i] + sample(c(-1,1))[1]
    x[k,i] = x[k-1,i] + rnorm(1,0,1)
}
proc.time() - ts
```

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Use two arrays:

- x paths, in column.
- x2 variance of displacements.
- Note, R stores arrays column major.
 So data access should be by column too.



Implementation 1 (inefficient, never do this)
num_walkers = 100000
num_paths = 200

```
x = matrix(0,num_paths,num_walkers)
x2 = rep(0,num_paths)
```

```
# Launch random walkers, all starting from x = 0
set.seed(47)
ts <- proc.time()
for (i in 1:num_walkers)
{
    # A walker completes its walk</pre>
```

for (k in 2:num_paths)

```
{
#x[k,i] = x[k-1,i] + sample(c(-1,1))[1]
x[k,i] = x[k-1,i] + rnorm(1,0,1)
```

```
proc.time() - ts
```

```
# Compute the variance
for (k in 1:num_paths)
```

ł

x2[k] = sum(x[k,]*x[k,])/num_walkers

```
# Plot a path
plot(x[,1],type='l',xlab='Steps',ylab='Displacement')
```

Plot the variance
plot(1:num_paths,x2,xlab='Displacement',ylab='Variance');

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Plot the distribution of displacements at last step hist(x[num_paths,],freq=TRUE)

save(x,x2,file="vars.RData")

Implementation 2 – using foreach + parallel packages
library(foreach)
library(doParallel) # parallel and iterator loaded implicitly

```
num_walkers = 100000
```

```
num_paths = 200
x2 = rep(0,num paths)
```

Launch random walkers, all starting from x = 0

set.seed(47)

```
See L'Ecuyer generator (1999)
```

```
ts <- proc.time()
```

```
registerDoParallel(4)
```

```
result <- foreach (i=1:num_walkers) %dopar%
```

```
{
```

```
for (k in 2:num_paths) # A walker completes its walk
{
```

```
x2[k] = x2[k-1] + rnorm(1,0,1)
```

```
return(x2)
```

}

}

stopImplicitCluster()

```
proc.time() - ts
```

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Assemble the result to path matrix
x <- matrix(unlist(result),num_paths,num_walkers)</pre>

```
# Compute the variance
for (k in 1:num_paths)
{
    x2[k] = sum(x[k,]*x[k,])/num_walkers
```

}

```
# Plot a path
plot(x[,1],type='l',xlab='Steps',ylab='Displacement')
```

Plot the variance plot(1:num_paths,x2,xlab='Displacement',ylab='Variance');

Plot the distribution of displacements at last step hist(x[num_paths,],freq=TRUE)

```
save(x,x2,file="vars.RData")
```

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Implementation 3 – no parallelism, just using R functions

num_walkers = 100000 num_paths = 200

```
x = matrix(0,num_paths,num_walkers)
x2 = rep(0,num_paths)
```

```
# Launch random walkers, all starting from x = 0
set.seed(47)
ts <- proc.time()
for (i in 1:pum_walkers)</pre>
```

```
for (i in 1:num_walkers)
```

```
{
```

```
disp = rnorm(num_paths,mean=0,1)
```

```
x[,i] = cumsum(disp)
```

```
}
```

```
proc.time() - ts
```

Compute the variance and generate plots.

Vectorization

Notice for each walker, the displacements from the origin are

 $x_{i+1} = x_i + \Delta x_i.$

This cumulative sum can be completed efficiently by one shot using R's function cumsum(). Compare with for (i in 1:num_walkers) { for (k in 2:num_paths) { x[k,i] = x[k-1,i] + rnorm(1,0,1) } }

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Exercise (cont'd): Performance comparison

num_walkers	for loop (sec)	foreach (sec) on 4 cores	for loop + cumsum() (sec)
1,000	2.011	0.630	0.068
10,000	19.327	4.567	0.722
100,000	195.000	50.895	6.740



Using Rmpi – Explicit parallel programming with MPI

- Developed by Prof. Yu Hao from Western University.
- To gain the fine grained control, use direct message passing send/receive calls featured by the message passing interface MPI.
- Offers greater flexibility for implementing complex algorithms, than many other parallel packages.
- There is a learning curve, if not already knowing MPI.
- Requires system installation of MPI.
- Not so straightforward to setup compared to other packages.

Using Rmpi on SHARCNET

- Load gcc and gcc compiled
 OpenMPI module
- Load R module
- Set environment R_LIBS, e.g. to \$HOME/lib/R
- Install Rmpi from withing R
- Copy R to \$HOME/bin/R, add the following lines (red) at line 4

#!/bin/sh

Shell wrapper for R executable.

PATH=\$MPI_ROOT/bin:\$PATH; export PATH LD_LIBRARY_PATH=\$MPI_ROOT/lib/:\$LD_LIBRARY_PATH export R_PROFILE=\$R_LIBS/Rmpi/Rprofile

• • • • • • •

Example

module unload intel openmpi

module load r

module load gcc/5.1.0 openmpi/gcc-5.1.0/std/1.8.7

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sqsub -q mpi -n 8 -r 10m -o yu.log $\$

\$HOME/bin/R CMD BATCH -no-save yu.R

library(Rmpi)

#setup parallel random number generator mpi.setup.rngstream() #create your own function(s) myfun=function(n) mean(rnorm(n)) #transfer your function(s) to all slaves mpi.bcast.Robj2slave(myfun) #run the parallel job output <- mpi.parReplicate(1000,myfun(1000000)) output[1:10]#can save output to a file #must close all slaves mpi.close.Rslaves() mpi.quit()

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Vectorization

Using R functions **xapply()** to performance operations on a list of things at once can make computations really fast.

- Iapply(x, fun, ...) apply a function to each element of a list/vector
- sapply(x, fun, ...) apply a function to each element of a list/vector and simplify to return a vector or array.
- vapply(x, fun, fun_value, ...) Tips: same as sapply, but returns a vector of type matching fun_value (safe); if the length of fun_value==1, then it returns a vector of the same length of x. This will be faster (don't know exactly why).
- **tapply** apply a function to a slice of list, vector, easier for data frames.
- mapply a multivariate version of apply().
- apply(x, margin, fun, ...) apply a function to a row, column or elements of an array, with margin==1 being rows and 2 being columns.



lapply/sapply(x, fun, ...) – passing one argument

```
# Pass ONE argument to the function
> n <- c(2,3,5)
> x <- lapply(n,rnorm)</pre>
> x
[[1]]
[1] 0.6766938 -1.3893758
[[2]]
[1] -1.7145366 -2.4362372 0.2003453
[[3]]
[1] -1.7807025 -0.1330609 -0.2210980 -0.1071721 -0.2836180
> y <- sapply(x,mean)</pre>
> y
[1] -0.3563410 -1.3168095 -0.5051303
```



lapply/sapply(x, fun, ...) cont'd – passing multiple arguments

```
# Pass ONE argument to the function
```

```
ns = c(2,3,5)
```

```
x = lappy(ns,rnorm)
```

y = sapply(x, mean)

Pass TWO or more arguments to the function?

This doesn't work

path < - function(n, x0=0, dev=1) { ds = rnorm(n,mean=x0,sd=dev); return(cumsum(c(x0,ds[1:n-1])); }
y = sapply(1:5, path(n=5,x0=1,dev=1))</pre>

This works, but not so obvious

path < - function(i,n, x0=0, dev=1) { ds = rnorm(n,mean=x0,sd=dev); return(cumsum(c(x0,ds[1:n-1])); }
y = sapply(1:5, path, n=5,x0=1,dev=1)</pre>

This works too, at least consistent to the function definition

path < - function(n, x0=0, dev=1) { ds = rnorm(n,mean=x0,sd=dev); return(cumsum(c(x0,ds[1:n-1])); }
y = sapply(1:5, function(n,x0,dev) path(n=5,x0=1,dev=1))</pre>

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Exercise: Simulating stock prices

- To simulate the closing price at the end of **180 days**.
- Assume the stock price follows the normal distribution (??) on a daily basis.
- Assume an average of 0.1% of gain of its opening price (e.g. \$25), and a volatility of 0.001.
- To generate 100,000 scenarios (paths) of movements and examine the results at the end of 180 days.



Exercise: Simulation of stock prices

```
# Stock price simulation - serial version
stock_prices <- function(price,ndays,gain=0,sigma=0)</pre>
```

```
ds = 1+rnorm(ndays-1,mean=gain,sd=sigma)
return(cumprod(c(price,ds)))
```

```
}
```

{

```
set.seed(47)
system.time(prices <- replicate(100000,
    stock_prices(price=25,
    ndays=180,
    gain=0.001,
    sigma=0.01)))</pre>
```

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Vectorization

Assume the stock price follows a normal distribution (well, not really).

Let q_t be the change rate in stock price, the new price is given by

$$S_{t+1} = q_t S_t, \ t = 1, \dots, N$$

We use R function **rnorm()** to generate a vector of change rates and **cumprod()** to generate a vector of prices over time in one shot.

Then we use function **replicate()** to repeat the process 100,000 times to generate 100,000 paths.

Vectorization is fast!

```
# Stock price simulation - parallel version
library(parallel)
stock prices <- function(price,ndays,gain=0,sigma=0)</pre>
{
  s <- .Random.seed
  nextRNGStream(s)
  set.seed(s)
  ds = rnorm(ndays-1,mean=1+gain,sd=sigma)
  return(cumprod(c(price,ds)))
}
                       See L'Ecuyer generator (1999)
RNGkind("L'Ecuyer-CMRG")
set.seed(47)
system.time(prices <- mclapply(1:100000,
  function(price,ndays,gain,sigma)
  stock_prices(price=25,
  ndays=180,
  gain=0.001,
  sigma=0.01),mc.cores=4))
```

```
paths=matrix(unlist(prices),nrow=180,ncol=100000)
```

Stock price simulation - serial version

stock_prices <- function(price,ndays,gain=0,sigma=0)</pre>

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```
ds = rnorm(ndays-1,mean=1+gain,sd=sigma)
return(cumprod(c(price,ds)))
```

```
}
```

{

```
set.seed(47)
system.time(prices <- replicate(100000,
    stock_prices(price=25,
    ndays=180,
    gain=0.001,
    sigma=0.01)))</pre>
```

paths=matrix(unlist(prices),nrow=180,ncol=100000)



Implicit parallelization

Featured by the underlying libraries, no work needed, free.

```
# In "mm.R"
n = 4*1024
n2 = n*n
A = matrix(rnorm(n2),nrow=n,ncol=n)
B = matrix(rnorm(n2),nrow=n,ncol=n)
system.time(C < - A %*% B)</pre>
```

Set the environment variable **OMP_NUM_THREADS** to different values and run the script, see the execution time difference.

```
$ export OMP_NUM_THREADS=1
```

\$ R –no-save < mm.R

\$ export OMP_NUM_THREADS=2

\$ R --no-save < mm.R

```
$ export OMP_NUM_THREADS=4
$ R -no-save < mm.R</pre>
```

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When things can bite...

Unexpected behavior may occur when using parallel packages



This code is correct, but troublesome. It may suffer from that

- The code does not scale at all
- The code hangs

Why?



Large datasets and linear models

Look for alternatives



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Loading large CSV files

I have a large CSV file containing data extracted from a database, 350MB of size, 1.7 millions of records, 28 columns each. The job data file contains the following

- Number of cores used
- Arrival, start time and end time, etc.

```
> system.time(j <- read.csv("jobs orca.csv",header=T,sep=','))</pre>
   user
         system elapsed
318.522
          1.778 325.615
> j[sample.int(120000,6),c("ncpus","t in","t start")]
       ncpus
                                                    t start
                                t in
          1 2014-12-12 05:25:35-05 2014-12-12 05:27:36-05
90163
94375
          1 2014-12-12 12:38:51-05 2014-12-12 17:13:46-05
13681
        16 2014-11-20 20:07:26-05 2014-11-20 20:11:28-05
37321
          1 2014-11-27 01:02:35-05
                                                                   ← Missing data
          1 2014-12-12 02:52:07-05 2014-12-12 02:53:58-05
89417
          1 2014-11-28 16:27:02-05 2014-11-28 16:27:59-05
48207
```

Using R function **read.csv()** takes nearly 6 minutes to lead the data on my laptop running Windows 7. So, how to improve this?

Certification @





TOP 3 POSTS FROM THE PAST 2 DAYS



Loading large CSV files (cont'd)

I use package data.table, it loads data much faster!

```
> library(data.table)
> system.time(d <- fread("jobs_orca.csv"))
Read 1635034 rows and 28 (of 28) columns from 0.323 GB file in 00:00:22
    user system elapsed
    14.24    0.34    21.65</pre>
```

Next, how should I do to get the following?

- Sorted by number of cores used
- The min, max, mean and median wait time, etc grouped by number of cores.

People used to *procedural programming languages* may get lost. R is better at this sort of things.



Using aggregate functions

I use package data.table, it loads data much faster!

```
> library(data.table)
> system.time(d <- fread("jobs orca.csv"))</pre>
Read 1635034 rows and 28 (of 28) columns from 0.323 GB file in 00:00:22
   user system elapsed
       0.34
  14.24
                  21.65
> names(d)
                      "host"
                                                       "job type"
    "jobid"
 [1]
                                       "state"
                                      "t end"
                                                       "utime"
 [5] "t in"
                      "t start"
     "stime"
                                      "ncpus"
 [9]
                      "atime"
                                                       "nnodes"
                                      "pfaults"
[13]
     "exitstatus"
                      "memory"
                                                       "flags"
     "nodes"
                      "institution"
                                      "user"
                                                       "est runtime"
[17]
                                      "queue_type_id" "pvmem req"
[21]
    "pi user"
                      "exit info"
                                      "apus"
                                                       "backfilled"
[25]
     "vmem"
                      "vmem req"
```

Next, how should I do to get the following?

- Sorted by number of cores used
- The min, max, mean and median wait time, etc grouped by number of cores.

People used to *procedural programming languages* may get lost. R is better at this sort of things.



Using aggregate functions (cont'd)

```
> library(data.table)
> system.time(d <- fread("jobs orca.csv"))</pre>
Read 1635034 rows and 28 (of 28) columns from 0.323 GB file in 00:00:22
   user system elapsed
           0.34
  14.24
                  21.65
> ds <- subset(d,select=c(as.numeric(ncpus),t in,t start,t end))</pre>
> d cpus <- aggregate(ds$ncpus,by=list(ds$ncpus),FUN =length)</pre>
> names(d cpus) < - c("ncpus", "jobs")</pre>
> d cpus[order(as.numeric(d cpus$ncpus)),]
   ncpus
            jobs
1
       1 1351160
       2 45262
31
55
       4 52676
80
       8
          88775
22
      16
          41459
39
      24
          2990
          20180
      32
51
          1361
54
      36
63
      48
           1171
71
      64
           17101
13
     128
             603
. . .
             189
45
     256
```

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Large data and out of core operations

I have a 1.45GB job data (a subset of 5 year's data), 34 million records, that can't *easily* fit in the memory.

```
> library(data.table)
> > system.time(d <- fread('jobs.csv'))</pre>
Read 31629152 rows and 6 (of 6) columns from 1.350 GB file in 00:00:42
  user system elapsed
 21.45 2.48 42.07
> qc()
         used (Mb) gc trigger (Mb) max used (Mb)
Ncells 552184 29.5 940480 50.3 940480 50.3
> names(d)
[1] "jobid" "sysid" "ncpus" "t in" "t start" "t end"
> system.time(wt <- d$t start-d$t in)</pre>
  user system elapsed
      0.06
  0.20
             0.28
> system.time(quantile(wt,probs=0.75))
  user system elapsed
  0.56 0.03 0.64
```

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Large data and out of core operations (cont'd)

I have a 1.45GB job data (a subset of 5 year's data), 34 million records, that can't *easily* fit in the memory. I use *bigmemory* package.

```
> library(bigmemory)
> gc(reset=TRUE)
       used (Mb) gc trigger (Mb) max used (Mb)
Ncells 527579 28.2 940480 50.3 527579 28.2
vcells 886272 6.8 1650153 12.6 886272 6.8 ← Before
>
> system.time(j <-
read.big.matrix('jobs.csv',header=T,backingfile='jobs.bin',descriptorfile='jobs.desc'))
  user system elapsed
239.68
      40.54 291.08
Warning message:
In read.big.matrix("jobs.csv", header = T, backingfile = "jobs.bin", :
 Because type was not specified, we chose integer based on the first line of data.
> qc()
       used (Mb) gc trigger (Mb) max used (Mb)
Ncells 534454 28.6 940480 50.3 557062 29.8
```



Large data and out of core operations (cont'd)

Creating file-backed big matrix off disk is slow, but saves a lot memory. Operations on the data are pretty fast.

```
> library(bigmemory)
> system.time(d <-
read.big.matrix('ts.csv', header=T, backingfile='ts.bin', descriptorfile='ts.desc'))
   user system elapsed
 239.68
        40.54 291.08
> dd <- dget('ts.desc')</pre>
> d <- attach.big.matrix(dd)</pre>
> system.time(wt <- d[,"t start"] - d[,"t in"])</pre>
   user system elapsed
   0.31 0.08
                 0.39
> system.time(quantile(wt,probs=0.75))
   user system elapsed
   0.53
        0.04 0.56
> system.time(wt min <- min(wt))</pre>
   user system elapsed
   0.06
           0.00
                   0.05
```



More workshops

- Introduction to Unix shell (software carpentry)
- Revision control with Git (software carpentry)
- Programming with Python (software carpentry)
- Introduction to R (software carpentry)
- Parallel programming with R (software carpentry)
- Introduction of SQL database (software carpentry)
- Introduction to parallel computing with MATLAB
- Introduction to parallel computing with modern Fortran
- Bi-weekly online seminars: https://www.sharcnet.ca/my/news/calendar
- Summer school on high performance and scientific computing

Slides

http://www.sharcnet.ca/~bge/seminars/parallel-R/parallel-hpc-R.pdf

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Find where we are

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