# Parallel Computing in R

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# Why Parallel Computing?

- Data
  - Large amount of data
  - Large amount of computation
- Computer
  - Multicore processor
  - Many multicore processors
- Many data analysis procedures are embarrassingly parallel

# Different Scales

- Multi-core computer
- Simple network of several computers
- Linux cluster with many computers

# Different Scales in R

- Multi-core computer
  - multicore
- Simple network of several computers
  - snow
- Linux cluster with many computers
  - RMpi, snow

(http://trg.apbionet.org/euasiagrid/docs/parallelR.notes.pdf)

# Example

- Find palindrome regions in C. elegans chromosomes
- "Super" C. elegans with 10X larger genome

# Install

```
# multicore package
install.packages(“multicore”)

# example data
source(“http://bioconductor.org/biocLite.R”)
biocLite(“BSgenome.Celegans.UCSC.ce2”)
```

Requirements for this workshop:
Linux or Mac,
(multicore) laptop or server,
no Windows

# Create Super Celegans

```
# load C elegans genome
library(BSgenome.Celegans.UCSC.ce2)

# overview of the genome
Celegans

# chromosomes in celegans
seqnames(Celegans)

# creating the super bug, with 10X larger genome
chrs <- rep(seqnames(Celegans), 10)
chrs
elegan <- getSeq(Celegans, chrs, as.character = F)
elegan

# convert to a list of chromosomes
elegan <- as.list(elegan)
elegan

# individual chromosomes
elegan[[1]]
elegan[[2]]
elegan[[10]]
```

# Find Palindromes

```
findPalindromes(elegan[[1]])
findPalindromes(elegan[[2]])
findPalindromes(elegan[[3]])
# a “for” loop ???
```

# the R way: lapply

```
> mylist <- list(1:5, 1:10)

> mylist[[1]]
[1] 1 2 3 4 5

> mylist
[[1]]
[1] 1 2 3 4 5

[[2]]
[1]  1  2  3  4  5  6  7  8  9 10
```

```
> mean(mylist[[1]])
[1] 3
> mean(mylist[[2]])
[1] 5.5

> lapply(mylist, mean)
[[1]]
[1] 3

[[2]]
[1] 5.5
```

- lapply(list, FUN)
- apply the function FUN to each element of the list

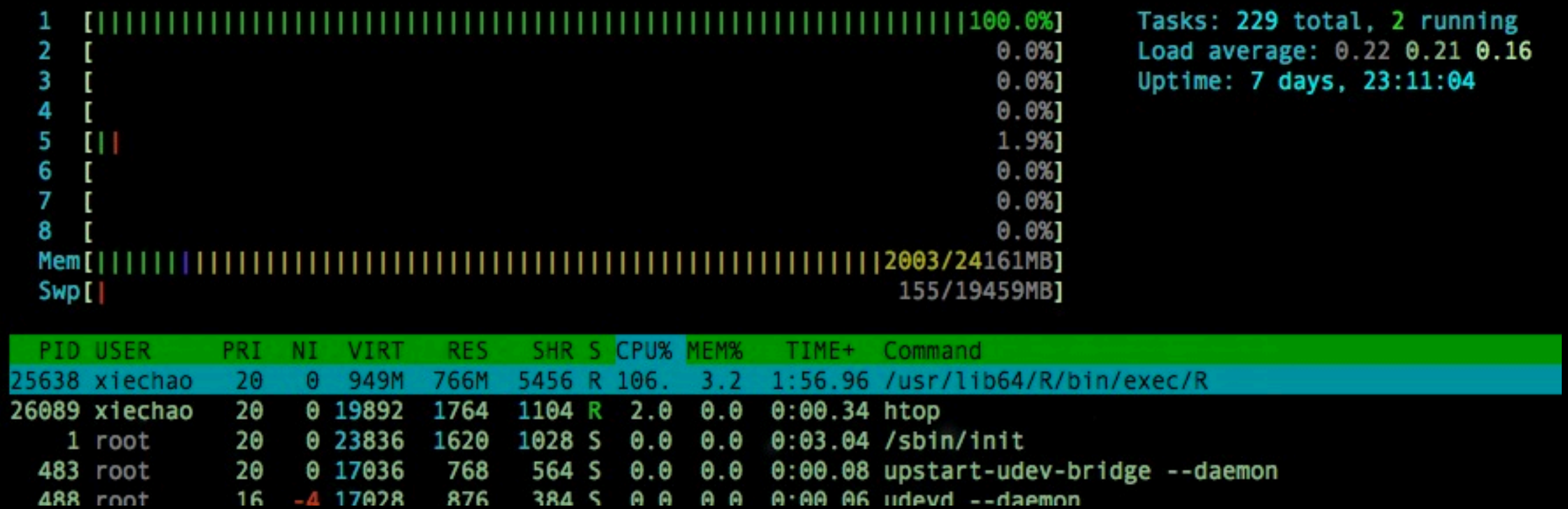
# serial computing

```
> system.time(pld2 <- findPalindromes(elegan[[2]]))
   user  system elapsed
  0.960   0.010   0.971
> pld2

> system.time(pld20 <- findPalindromes(elegan[[20]]))
   user  system elapsed
  1.130   0.030   1.153
> pld20

> system.time(plds <- lapply(elegan, findPalindromes))
   user  system elapsed
 86.290   0.190  86.696
> plds[[2]]
> plds[[20]]
```

# htop




But only one core is utilized

# Multicore Computing

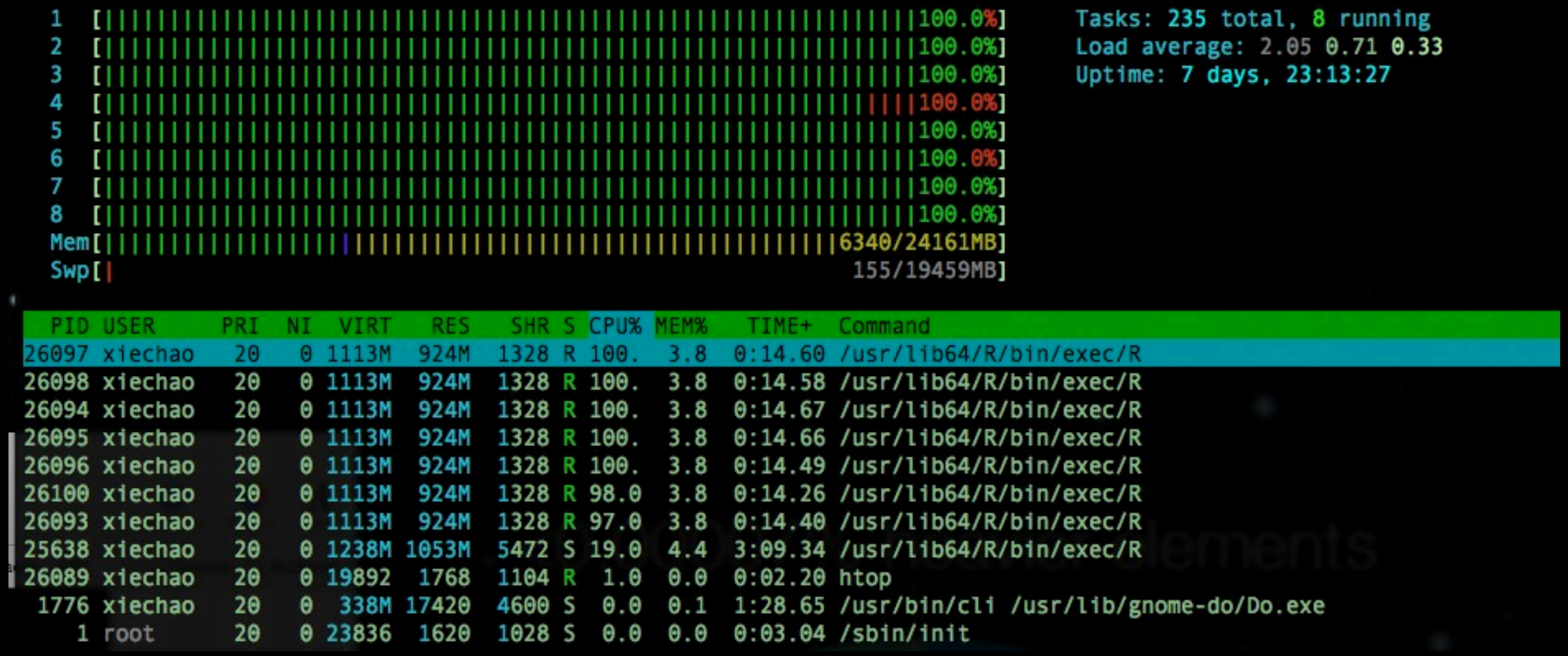
- multicore package by Simon Urbanek
- Linux and Mac OS

# multicore computing

```
> system.time(plds <- lapply(elegan, findPalindromes))
   user  system elapsed
 86.290   0.190  86.696
> plds[[2]]
> plds[[20]]

> library(multicore)
> system.time(pldmc <- mclapply(elegan, findPalindromes))
   user  system elapsed
 85.160   4.140  20.902
> pldmc[[2]]
> pldmc[[20]]
```

in case you have too many processor cores for your RAM:
option(cores = 2)




# All cores are being utilized

(note: I have only 4 cores, not 8)

# one more example

```
> system.time(di.a <- lapply(elegan, dinucleotideFrequency))
   user  system elapsed
  5.660   0.000   5.684
> di.a[[2]]
> di.a[[20]]

> library(multicore)
> system.time(di.b <- mclapply(elegan, dinucleotideFrequency))
   user  system elapsed
 65.120   2.610   1.824
> di.b[[2]]
> di.b[[20]]
```

# Changing parameters...

```
Usage:

     findPalindromes(subject, min.armlength=4, max.looplength=1, min.loop
     palindromeArmLength(x, max.mismatch=0, ...)
     palindromeLeftArm(x, max.mismatch=0, ...)
     palindromeRightArm(x, max.mismatch=0, ...)

     findComplementedPalindromes(subject, min.armlength=4, max.looplengt
     complementedPalindromeArmLength(x, max.mismatch=0, ...)
     complementedPalindromeLeftArm(x, max.mismatch=0, ...)
     complementedPalindromeRightArm(x, max.mismatch=0, ...)

Arguments:

  subject: An XString object containing the subject string, or an
           XStringViews object.

min.armlength: An integer giving the minimum length of the arms of the
           palindromes (or complemented palindromes) to search for.

max.looplength: An integer giving the maximum length of "the loop" (i.e
           the sequence separating the 2 arms) of the palindromes (or
           complemented palindromes) to search for.  Note that by
           default (‘max.looplength=1’), ‘findPalindromes’ will search
           for strict palindromes (or complemented palindromes) only.
```

```
> ?findPalindromes
> findPalindromes(elegan[[2]], min.armlength = 6, max.looplength = 5)
```

# with non-default parameters

```
> system.time(plds <- lapply(elegan, findPalindromes,
min.armlength = 6, max.looplength = 5))
   user  system elapsed
 67.070   0.300  67.541
> plds[[2]]
> plds[[20]]

> library(multicore)
> system.time(pldmc <- mclapply(elegan, findPalindromes,
min.armlength = 6, max.looplength = 5))
   user  system elapsed
132.930   6.570  16.283
> pldmc[[2]]
> pldmc[[20]]
```

# Longest palindrome region?

```
# define our own function
> longest.palindrome <- function(s) {
        pld <- findPalindromes(s);
        pld.width <- width(pld);
        longest <- which.max(pld.width);
        pld[longest]
}

> system.time(pldmc <- mclapply(elegan, longest.palindrome))
   user  system elapsed
135.000   7.360  19.827

> pldmc
```

```
> pldmc
[[1]]
  Views on a 15080483-letter DNAString subject
subject: GCCTAAGCCTAAGCCTAAGCCTAAGCCTAAGCCT...AGGCTTAGGCTTAGGCTTAGGTTTAGGCTTAGGC
views:
      start     end width
[1] 9391035 9391223   189 [GTGTGTGTGTGTGTGTGTGTGTGTG...TGTGTGTGTGTGTGTGTGTGTG]

[[2]]
  Views on a 15279308-letter DNAString subject
subject: CCTAAGCCTAAGCCTAAGCCTAAGCCTAAGCCTA...TAGGCTGAGACTTAGGCTTAGGCTTAGGCTTAGT
views:
     start    end width
[1] 503958 504632   675 [ATATATATATATATATATATATATATAT...ATATATATATATATATATATATATATA]

[[3]]
  Views on a 13783313-letter DNAString subject
subject: CCTAAGCCTAAGCCTAAGCCTAAGCCTAAGCCTA...TAGGCTTAGGCTTAGGCTTAGGCTTAGGCTTAGG
views:
      start     end width
[1] 3334130 3334302   173 [AAAAATAAAAATAAAAATAAAAATA...TAAAAATAAAAATAAAAATAAAAA]

[[4]]
  Views on a 17493791-letter DNAString subject
subject: CCTAAGCCTAAGCCTAAGCCTAAGCCTAAGCCTA...TAGGCTTAGGCTTAGGCTTAGGCTTAGGCTTAGG
views:
```

```
> data.frame(
    chr = chrs,
    start = sapply(pldmc, start),
    end = sapply(pldmc, end),
    width = sapply(pldmc, width)
  )
      chr    start      end width
1    chrI  9391035  9391223   189
2   chrII   503958   504632   675
3  chrIII  3334130  3334302   173
4   chrIV 13116111 13116283   173
5    chrV  6946625  6947010   386
6    chrX  2011047  2011239   193
7    chrM    13362    13400    39
8    chrI  9391035  9391223   189
9   chrII   503958   504632   675
10 chrIII  3334130  3334302   173
11  chrIV 13116111 13116283   173
12   chrV  6946625  6947010   386
13   chrX  2011047  2011239   193
```

# Beyond Multicore...

# Example

- geneData: 500 genes x 26 samples
- Correlation between every pair of genes with bootstrapping

# Data & Compute

```
# the data

library(Biobase)          # load package
data(geneData)            # load data
fakeData <- cbind(geneData, geneData, geneData, geneData)

# the compute

library(boot)
geneCor2 <- function(x, gene = fakeData) {
    mydata <- cbind(gene[x[1], ], gene[x[2], ])
    mycor <- function(x, i) cor(x[i,1], x[i,2])
    boot.out <- boot(mydata, mycor, 1000)
    boot.ci(boot.out, type = 'bca')$bca[4:5]
}
pair <- combn(1:nrow(geneData), 2, simplify = F)
pair2 <- sample(pair, 300)   # let's do 300 pairs
```

# Serial vs Multicore

```
# serial

> system.time(out <- lapply(pair2, geneCor2))
   user  system elapsed
 71.450   0.290  71.997

# multicore

> system.time(out <- mclapply(pair2, geneCor2))
   user  system elapsed
108.650   1.060  15.969
```

# Multiple Machines

- Simple Network Of Workstations (snow)
- snow package by Luke Tierney, A. J. Rossini, Na Li, H. Sevcikova
- Requirement:
  - SSH access to worker nodes
  - Enable password-less login (public key)
  - R package snow installed on all nodes

# parallel computing with snow

```
> library(snow)

> hosts <- c(“localhost”, “137.132.x.x”, “137.132.y.y”)
> cl <- makeCluster(rep(hosts, 2))
                    # two worker per machine

> clusterExport(cl, “fakeData”)
                    # export data to workers
> clusterEvalQ(cl, library(boot))
                    # load package on workers

> system.time(out <- clusterApply(cl, pair2, geneCor2))

> stopCluster(cl)
```

# Cluster

- multicore and multi-machine snow are too slow for you
- Large cluster with MPI support
  - NUS HPC cluster
  - 32 processor-cores per job

# 1 Master + 31 Workers

```
( submit job through MPI environment )

> cl <- makeCluster()
> clusterExport(cl, 'fakeData')
> clusterEvalQ(cl, library(boot))
> system.time(out2 <- clusterApply(cl, pair2, geneCor2))
   user  system elapsed
  2.373   0.001   2.374
```

```
single-core: 72
quad-core:   16
```

# Problem

- How to maintain your code for
  - single core
  - multicore
  - snow
  - cluster with MPI support

# *"one ring to rule them all"*

- The foreach framework
  - by Revolution Analytics
  - open source
- Unified interface for packages:
  - multicore => doMC
  - snow => doSNOW
  - Rmpi => doMPI

# The Serial Code

```
#!/usr/bin/env Rscript
library(foreach)

data(geneData, package = 'Biobase')
pair <- combn(1:nrow(geneData), 2, simplify = F)
fakeData <- cbind(geneData, geneData, geneData, geneData)
pair2 <- sample(pair, 300)

print(system.time(
    out <- foreach(p = pair2, .packages = 'boot', .combine = 'rbind') %dopar%
    {
        mydata <- cbind(fakeData[p[1],], fakeData[p[2], ])
        mycor <- function(x, i) cor(x[i,1], x[i,2])
        boot.out <- boot(mydata, mycor, 1000)
        ci <- boot.ci(boot.out, type = 'bca')$bca[4:5]
        c(p, ci)
    }
))
print(head(out))
```

Save as “base.r”
chmod 700 base.r

# Run The Base Code

```
$ ./base.r

   user  system elapsed
 65.920   0.440  66.355

          [,1] [,2]       [,3]       [,4]
result.1  288  422 -0.3357138 -0.1266808
result.2  243  303 -0.1529784  0.1017721
result.3  234  386 -0.1561772  0.2161708
result.4    5  183  0.2505966  0.4794503
result.5  275  440  0.2420215  0.5738407
result.6   62  457  0.1558987  0.4712927
```

# Multicore with doMC

```
#!/usr/bin/env Rscript

library(doMC)
registerDoMC()

source("base.r")  # or paste content
```

Save as “domc.r”
`chmod 700 domc.r`

# run domc.r

```
$ ./domc.r

   user  system elapsed
 56.410  56.290  19.114

          [,1] [,2]       [,3]        [,4]
result.1  164  172 -0.2668234  0.14122971
result.2   31   67  0.6607894  0.78171239
result.3   62  282 -0.3225335 -0.03370322
result.4   37  293  0.1073143  0.31629694
result.5   38  271 -0.1041704  0.28953027
result.6  211  287 -0.3495002  0.00608487
```

# snow with doSNOW

```
#!/usr/bin/env Rscript

library(doSNOW)
hosts <- c(
   'localhost', 'localhost', 'localhost', 'localhost',
   'variome', 'variome',
   'lams', 'lams',
   'bug'
)
cl <- makeCluster(hosts)
registerDoSNOW(cl)

source("base.r")    # or paste content

stopCluster(cl)
```

change to your own hosts

Save as “dosnow.r”
`chmod 700 dosnow.r`

# run dosnow.r

```
$ ./dosnow.r

   user  system elapsed
  0.130   0.020  12.335

          [,1] [,2]       [,3]        [,4]
result.1   217  332  0.1224703  0.44764756
result.2    19  179 -0.6041616 -0.36109986
result.3   192  426  0.4824728  0.68836742
result.4    46  228 -0.2883579 -0.01718258
result.5   407  426  0.1998271  0.45557312
result.6   165  386 -0.6302590 -0.15638907
```

# MPI cluster with doMPI

```
#!/usr/bin/env Rscript


library(doMPI)
cl <- startMPIcluster()
registerDoMPI(cl)

source("base.r")   # or paste content

closeCluster(cl)
```

Save as “dompi.r”
chmod 700 dompi.r

# run dompi.r

```
$ bsub -q atlas5_parallel -a openmpi -n 32
mpirun.lsf ./dompi.r

   user  system elapsed
  2.742   0.243   3.015

          [,1] [,2]        [,3]       [,4]
result.1  202  231  0.003461775  0.3608233
result.2  174  372  0.009071919  0.3583579
result.3  118  186  0.601903906  0.7885814
result.4  186  362 -0.336281370 -0.1353606
result.5  270  485 -0.491912888 -0.1121098
result.6  168  413 -0.147680243  0.1079481
```

# Summary

- Parallel computing in R is easy
  - for embarrassingly parallel problems
- Different scales of parallel computing
  - multicore
  - snow
  - Rmpi
  - foreach + doMC / doSNOW / doMPI

# More Information

http://cran.r-project.org/web/views/HighPerformanceComputing.html