High Performance Computing, Cloud Computing

JSC 370: Data Science II

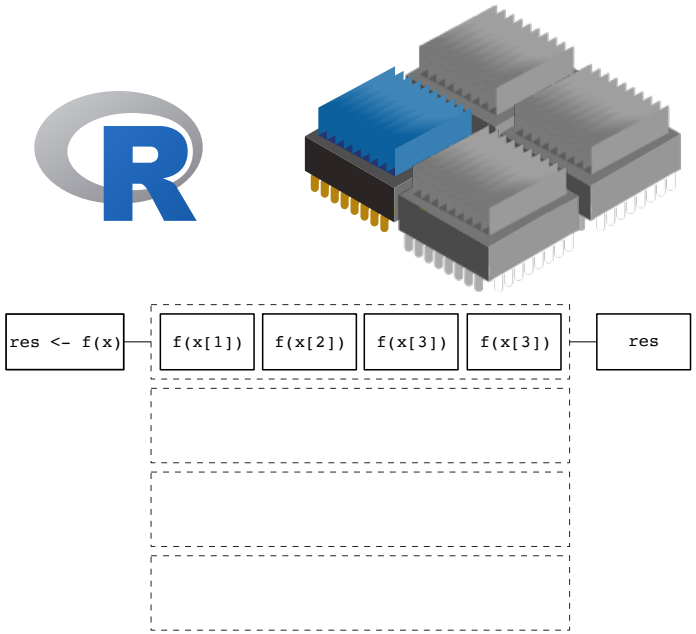
What is HPC

High Performance Computing (HPC) can relate to any of the following:

- **Parallel computing**, i.e. using multiple resources (could be threads, cores, nodes, etc.) simultaneously to complete a task.
- **Big data** working with large datasets (in/out-of-memory).

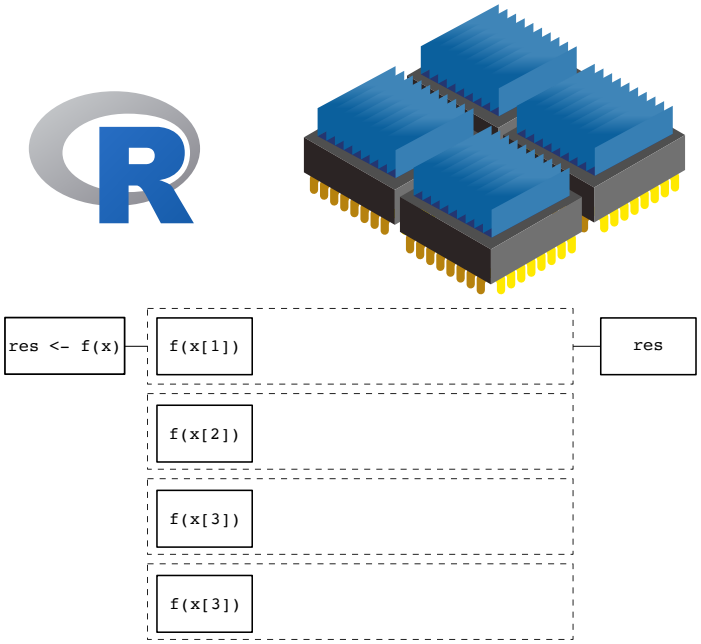
We will mostly focus on parallel computing.

Serial computation



Here we are using a single core. The function is applied one element at a time, leaving the other 3 cores without usage.

Parallel computation



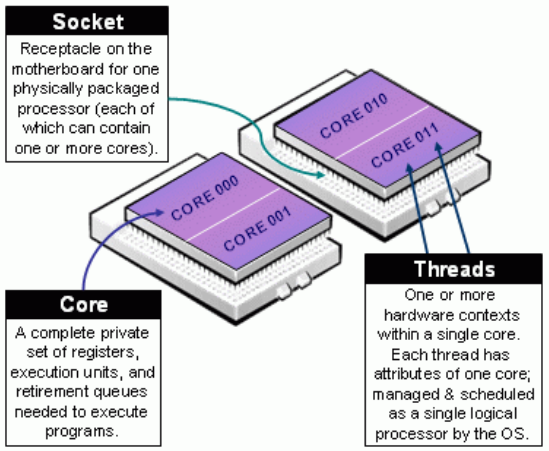
In this more intelligent way of computation, we are taking full advantage of our computer by using all 4 cores at the same time. This will translate in a reduced computation time which, in the case of complicated/long calculations, can be an important speed gain.

Parallel computing: Hardware

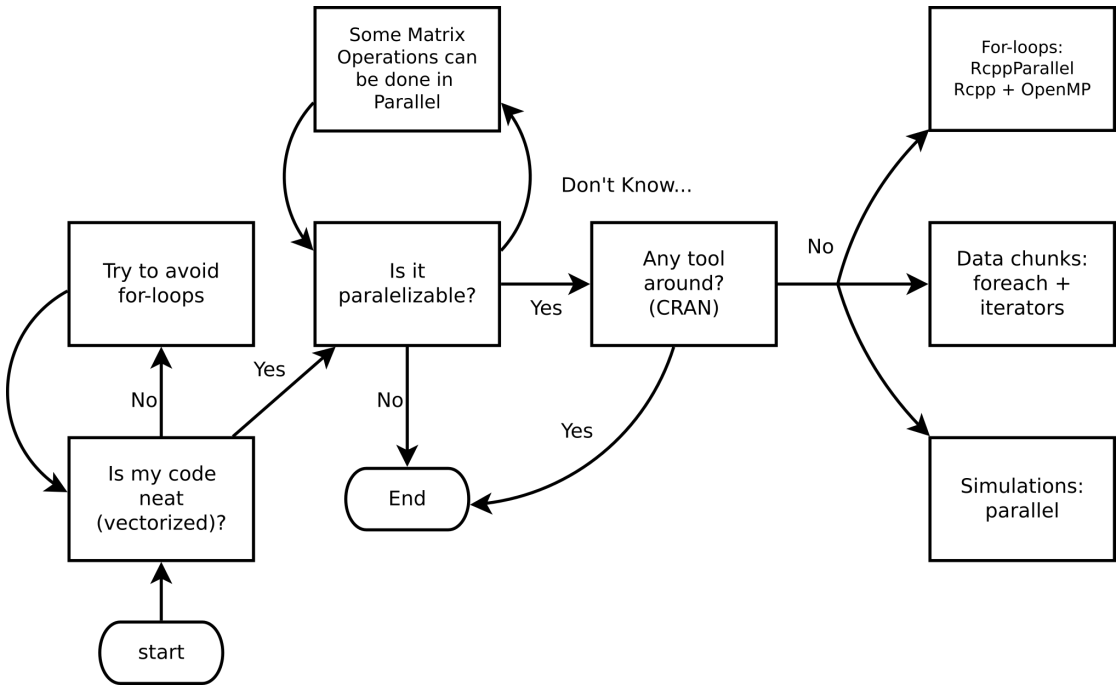
When it comes to parallel computing, there are several ways (levels) in which we can speed up our analysis. From the bottom up:

- **Thread level SIMD instructions**: In most modern processors support some level of what is called vectorization, this is, applying a single (same) instruction to streams of data, for example: adding vector `A` and `B`.
- **Hyper-Threading Technology** (HTT): Intel's hyper-threading generates a virtual partition of a single core (processor) which, while not equivalent to having multiple physical threads, does speedup things.
- **Multi-core processor**: Most modern CPUs (Central Processing Unit) have two or more physical cores. A typical laptop computer has about 8 cores.
- **General-Purpose Computing on Graphics Processing Unit** (GP-GPU): While modern CPUs have a couple of dozens of cores, GPUs can hold thousands of those. Designed for image processing, there's an increasing use of GPUs as an alternative of CPUs for scientific computing.
- **High-Performance Computing Cluster** (HPC): A collection of computing nodes that are interconnected using a fast Ethernet network.
- **Grid Computing**: A collection of loosely interconnected machines that may or may not be in the same physical place, for example: HTCondor clusters.

Parallel computing: CPU components



Taxonomy of CPUs (Downloaded from https://slurm.schedmd.com/mc_support.html)



Ask yourself these questions before jumping into HPC!

Parallel computing in R

While there are several ways to do parallel computing in R (just take a look at the High-Performance Computing Task View), we'll focus on the following R-packages for **explicit parallelism**

Some examples:

- **parallel**: R package that provides '[s]upport for parallel computation, including random-number generation'.
- **foreach**: R package for 'general iteration over elements' in parallel fashion.
- **future**: '[A] lightweight and unified Future API for sequential and parallel processing of R expression via futures.' (won't cover here)

Implicit parallelism, on the other hand, are out-of-the-box tools that allow the programmer not to worry about parallelization, e.g. such as **gpuR** for Matrix manipulation using GPU, **tensorflow**

And there's also a more advanced set of options

- **Rcpp** + OpenMP: Rcpp is an R package for integrating R with C++, and OpenMP is a library for high-level parallelism for C/C++ and Fortran.
- A ton of other type of resources, notably the tools for working with batch schedulers such as Slurm, HTCondor, etc.

Embarrasingly Parallel

Many problems can be executed in an “embarrassingly parallel” way, whereby multiple independent pieces of a problem are executed simultaneously because the different pieces of the problem never really have to communicate with each other (except perhaps at the end when all the results are assembled).

The basic mode of an embarrassingly parallel operation can be seen with `lapply()`. Recall that the `lapply()` function has two arguments:

- a list, or an object that can be coerced to a list.
- a function to be applied to each element of the list.

The `lapply()` function works much like a loop–it cycles through each element of the list and applies the supplied function to that element.

NOTE: we can also relate this to the `apply()` function, which takes a matrix rather than a list.

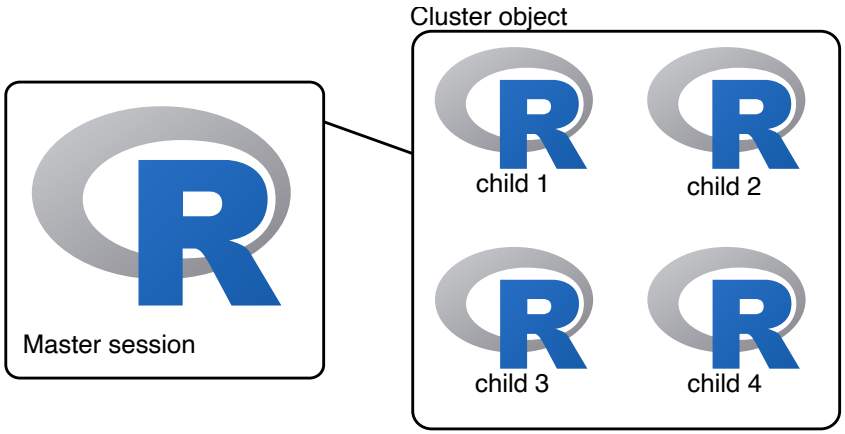
Parallelization

Conceptually, the steps in the parallel procedure are:

1. Split list X across multiple cores
2. Copy the supplied function (and associated environment) to each of the cores
3. Apply the supplied function to each subset of the list X on each of the cores in parallel
4. Assemble the results of all the function evaluations into a single list and return

The parallel package

- Based on the `snow` and `multicore` R Packages.
- Explicit parallelism.
- Simple yet powerful idea: Parallel computing as multiple R sessions.
- Clusters can be made of both local and remote sessions
- Multiple types of cluster: `PSOCK`, `Fork`, `MPI`, etc.



Parallel workflow

(Usually) We do the following:

1. Create a `PSOCK/FORK` (or other) cluster using `makePSOCKCluster`/`makeForkCluster` (or `makeCluster`)
2. Copy/prepare each R session (if you are using a `PSOCK` cluster):

   a. Copy objects with `clusterExport`

   b. Pass expressions with `clusterEvalQ`

   c. Set a seed
3. Do your call: `parApply`, `parLapply`, `mclapply`.
4. Stop the cluster with `clusterStop`

The parallel package

- The `mclapply()` function essentially parallelizes calls to `lapply()`.
- The first two arguments to `mclapply()` are exactly the same as they are for `lapply()`.
- `mclapply()` has further arguments (that must be named), the most important of which is the mc.cores argument which you can use to specify the number of processors/cores you want to split the computation across.
- For example, if your machine has 4 cores on it, you might specify mc.cores = 4 to break your parallelize your operation across 4 cores (although this may not be the best idea if you are running other operations in the background besides R).
- check for the number of cores you have with:

```
library(parallel)
detectCores()
```

```
## [1] 8
```

Ex 1: Hello world!

```r
# 1. CREATING A CLUSTER
library(parallel)
cl <- makePSOCKcluster(4)
x  <- 20

# 2. PREPARING THE CLUSTER
clusterSetRNGStream(cl, 123) # Equivalent to `set.seed(123)`
clusterExport(cl, "x")

# 3. DO YOUR CALL
clusterEvalQ(cl, {
  paste0("Hello from process #", Sys.getpid(), ". I see x and it is equal to ", x)
})
```

```
## [[1]]
## [1] "Hello from process #38185. I see x and it is equal to 20"
##
## [[2]]
## [1] "Hello from process #38187. I see x and it is equal to 20"
##
## [[3]]
## [1] "Hello from process #38186. I see x and it is equal to 20"
##
## [[4]]
## [1] "Hello from process #38184. I see x and it is equal to 20"
```

```r
# 4. STOP THE CLUSTER
stopCluster(cl)
```

Ex 2: Parallel regressions

Problem: Run multiple regressions on a very wide dataset. We need to fit the following model:

$$y = X_i\beta_i + \varepsilon, \quad \varepsilon \sim N(0, \sigma_i^2), \quad \forall i$$

```
dim(X)
```

```
## [1] 500 999
```

```
X[1:6, 1:5]
```

```
##          x001        x002       x003       x004      x005
## 1  0.61827227  1.72847041 -1.4810695 -0.2471871 1.4776281
## 2  0.96777456 -0.19358426 -0.8176465  0.6356714 0.7292221
## 3 -0.04303734 -0.06692844  0.9048826 -1.9277964 2.2947675
## 4  0.84237608 -1.13685605 -1.8559158  0.4687967 0.9881953
## 5 -1.91921443  1.83865873  0.5937039 -0.1410556 0.6507415
## 6  0.59146153  0.81743419  0.3348553 -1.8771819 0.8181764
```

```
str(y)
```

```
##  num [1:500] -0.8188 -0.5438 1.0209 0.0467 -0.4501 ...
```

Ex 2: Parallel regressions (cont'd 1)

Serial solution: Use `apply` (forloop) to solve it

```
#
#
#
ans <- apply(

  X      = X,
  MARGIN = 2,
  FUN    = function(x) coef(lm(y ~ x))
  )

ans[,1:5]
```

```
##                     x001        x002        x003        x004        x005
## (Intercept) -0.03449819 -0.03339681 -0.03728140 -0.03644192 -0.03717344
## x           -0.06082548  0.02748265 -0.01327855 -0.08012361 -0.04067826
```

Ex 2: Parallel regressions (cont'd 2)

Parallel solution: Use `parApply`

```
library(parallel)
cl <- makePSOCKcluster(4)
clusterExport(cl, "y")
ans <- parApply(
  cl     = cl,
  X      = X,
  MARGIN = 2,
  FUN    = function(x) coef(lm(y ~ x))
  )

ans[,1:5]
```

```
##                    x001        x002        x003        x004        x005
## (Intercept) -0.03449819 -0.03339681 -0.03728140 -0.03644192 -0.03717344
## x           -0.06082548  0.02748265 -0.01327855 -0.08012361 -0.04067826
```

Are we going any faster?

```
microbenchmark::microbenchmark(
  parallel = parApply(
    cl  = cl,
    X   = X, MARGIN = 2,
    FUN = function(x) coef(lm(y ~ x))
    ),
  serial = apply(
    X   = X, MARGIN = 2,
    FUN = function(x) coef(lm(y ~ x))
    ), unit="ms"
)
```

```
## Unit: milliseconds
##       expr      min       lq     mean   median       uq      max neval
##  parallel 189.3619 211.8326 226.1504 221.3169 230.7429 345.5169   100
##    serial 553.7184 586.4854 604.3711 598.8101 609.3490 776.1760   100
```

Extended Example: SARS-CoV2 simulation

An altered version of Conway's game of life

1. People live in torus, each individual having 8 neighbors.
2. A healthy individual interacting with a sick neighbor has the following probabilities of contracting the disease:

    a. 100% if neither wears a face-mask.

    b. 50% if only he wears the face-mask.

    c. 20% if only his neighbor wears the mask.

    d. 5% if both wear the face-mask.
3. Infected individuals may die with probability 10%.

We want to illustrate the importance of wearing face masks. We need to simulate a system with 2,500 (50 x 50) individuals, 1,000 times so we can analyze: (a) contagion curve, (b) death curve.

More models like this: The SIRD model (Susceptible-Infected-Recovered-Deceased)

Conway's Game of Masks

Download the program here.

```
source("sars-cov2.R", echo=FALSE)

# Looking at some constants
probs_sick # Sick individual's probabilities
```

```
##  deceased  infected recovered
##       0.1       0.4       0.5
```

```
probs_susc # Probabilities of i getting the disease
```

```
##                 j doesn't wear j wears
## i doesn't wear             0.9    0.20
## i wears                    0.5    0.05
```

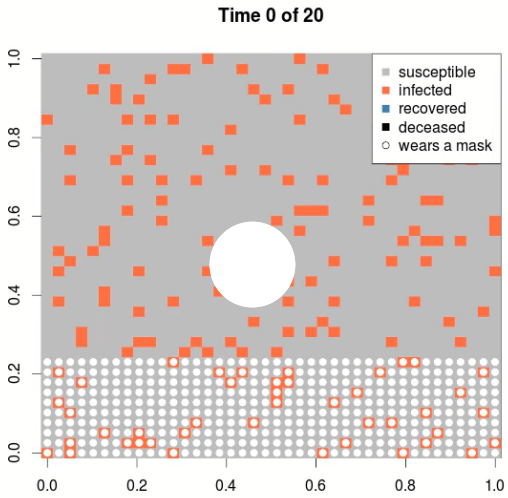
First look: How does the simulation looks like?

```
set.seed(7123)
one <- simulate_covid(
    pop_size    = 1600,
    nsick       = 160,
    nwears_mask = 1:400,
    nsteps      = 20,
    store       = TRUE
    )

one$statistics[c(1:5, 16:20),]
```

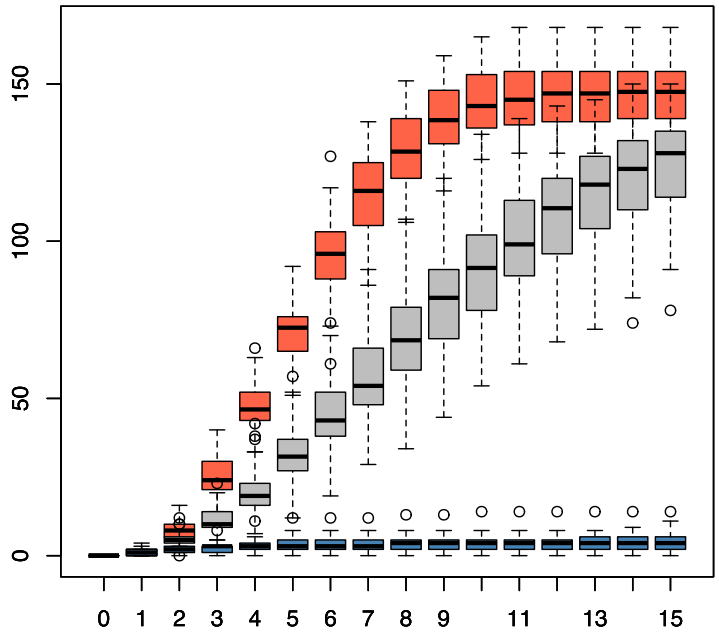
```
##    susceptible infected recovered deceased
## 0         1440      160         0        0
## 1         1265      234        85       16
## 2         1064      307       190       39
## 3          876      321       334       69
## 4          717      287       499       97
## 15         430        1       990      179
## 16         429        2       990      179
## 17         429        0       992      179
## 18         429        0       992      179
## 19         429        0       992      179
```

First look: How does the simulation looks like? (contd')

```
# Location of who wears the facemask. This step is only for plotting
wears <- which(one$wears, arr.ind = TRUE) - 1
wears <- wears/(one$nr) * (1 + 1/one$nr)

# Initializing the animation
fig   <- magick::image_device(600, 600, res = 96/2, pointsize = 24)
for (i in 1:one$current_step) {

  # Plot
  image(
    one$temporal[,,i], col=c("gray", "tomato", "steelblue","black"),
    main = paste("Time", i - 1L, "of", one$nsteps),
    zlim = c(1,4)
    )
  points(wears, col="white", pch=20, cex=1.5)
  legend(
    "topright",
    col    = c("gray", "tomato", "steelblue","black", "black"),
    legend = c(names(codes), "wears a mask"),
    pch    = c(rep(15, 4), 21)
  )
}

# Finalizing plot and writing the animation
dev.off()
animation <- magick::image_animate(fig, fps = 2)
magick::image_write(animation, "covid1.gif")
```


Time 0 of 20
susceptible
infected
recovered
deceased
wears a mask
0.0
0.2
0.4
0.6
0.8
1.0

```
set.seed(123355)
stats_nobody_wears_masks <- replicate(50, {
  simulate_covid(
    pop_size    = 900,
    nsick       = 10,
    nwears_mask = 0,
    nsteps      = 15)$statistics[,"deceased"]
  }, simplify = FALSE
  )

set.seed(123355)
stats_half_wears_masks <- replicate(50, {
  simulate_covid(
    pop_size    = 900,
    nsick       = 10,
    nwears_mask = 450,
    nsteps      = 15)$statistics[,"deceased"]
  }, simplify = FALSE
  )

set.seed(123355)
stats_all_wears_masks <- replicate(50, {
  simulate_covid(
    pop_size    = 900,
    nsick       = 10,
    nwears_mask = 900,
    nsteps      = 15)$statistics[,"deceased"]
  }, simplify = FALSE
  )
```



Cumulative number of deceased as a function of whether none, half, or all individuals wear a face mask.

Speed things up: Timing under the serial implementation

We will use the function `system.time` to measure how much time it takes to complete 20 simulations in serial versus paralle fashion using 4 cores

```
time_serial <- system.time({
  ans_serial <- replicate(50, {
    simulate_covid(
      pop_size    = 900,
      nsick       = 10,
      nwears_mask = 900,
      nsteps      = 20)$statistics[,"deceased"]
    },
    simplify = FALSE
    )
})
```

Speed things up: Parallel a Forking Cluster

Alternative 1: If you are using Unix-like system (Ubuntu, OSX, etc.), you can take advantage of process forking, and thus, parallel's `mclapply` function:

```
set.seed(1231)
time_parallel_fork <- system.time({
  ans_parallel <- parallel::mclapply(1:50, function(i) {
    simulate_covid(
      pop_size    = 900,
      nsick       = 10,
      nwears_mask = 900,
      nsteps      = 20)$statistics[,"deceased"]
    }, mc.cores = 4
  )
})
```

Speed things up: Parallel with a Socket Cluster

Alternative 2: Regardless of the operating system, we can use a Socket cluster, which is simply a group of fresh R sessions that listen to the parent/main/mother session.

```
# Step 1: Make the cluster
cl <- parallel::makePSOCKcluster(2)
```

```
# Step 2: Prepare the cluster
# We could either export all the needed variables
parallel::clusterExport(
  cl,
  c("calc_stats", "codes", "dat", "get_neighbors", "init", "probs_sick",
    "probs_susc", "simulate_covid", "update_status", "update_status_all"
    )
  )
```

Or simply running the simulation script in the other sessions

```
# Step 2 (alt): Prepare the cluster
parallel::clusterEvalQ(cl, source("sars-cov2.R"))
parallel::clusterSetRNGStream(cl, 123) # Make sure it is reproducible!
```

```
(pids <- c(
  master    = Sys.getpid(),
  offspring = unlist(parallel::clusterEvalQ(cl, Sys.getpid()))
  ))
#      master offspring1 offspring2
#     14810      15998      16012
```

If you are using Unix, you can see more details:

```
UID        PID  PPID  C STIME TTY          TIME CMD
george   14810 10376  0 12:31 ?        00:00:09 /usr/lib/
george   15998     1  0 12:56 ?        00:00:00 /usr/lib/
george   16012     1  0 12:56 ?        00:00:00 /usr/lib/
```

Speed things up: Parallel with a Socket Cluster (cont'd)

```
# Step 3: Do your call
time_parallel_sock <- system.time({
  ans_parallel <- parallel::parLapply(cl, 1:50, function(i) {
    simulate_covid(
      pop_size    = 900,
      nsick       = 10,
      nwears_mask = 900,
      nsteps      = 20)$statistics[,"deceased"]
    }
  )
})

# Step 4: Stop
parallel::stopCluster(cl)
```

Using two threads/processes, you can obtain the following speedup

```
time_serial;time_parallel_sock;time_parallel_fork
```

```
##    user  system elapsed
##  20.514   0.238  21.166

##    user  system elapsed
##   0.001   0.000  11.585

##    user  system elapsed
##  15.876   0.401   5.826
```

Cloud Computing (a.k.a. on-demand computing)

HPC clusters, super-computers, etc. need not to be bought... you can rent:

- Amazon Web Services (AWS)
- Google Cloud Computing
- Microsoft Azure

These services provide more than just computing (storage, data analysis, etc.). But for computing and storage, there are other free resources, e.g.:

- The Extreme Science and Engineering Discovery Environment (XSEDE)

There are many ways to run R in the cloud

At USC:

- Center for Advanced Research Computing (CARC). USC users can request hundreds of cores (literally). Take a look at the slurmR package

Running R in:

- Google Cloud: https://cloud.google.com/solutions/running-r-at-scale
- Amazon Web Services: https://aws.amazon.com/blogs/big-data/running-r-on-aws/
- Microsoft Azure: https://docs.microsoft.com/en-us/azure/architecture/data-guide/technology-choices/r-developers-guide

Submitting jobs

- A key feature of cloud services > interact via command line.
- You will need to familiarize with `Rscript` and `R CMD BATCH`.
- Which is better? It depends on the application.

Submitting jobs (examples)

Imagine we have the following R script (download here):

```
library(data.table)
set.seed(1231)
dat <- data.table(y = rnorm(1e3), x = sample.int(5, 1e3, TRUE))
dat[,mean(y), by = x]
```

R CMD BATCH

This will run a non-interactive R session and put all the output (stdout and stderr) to the file `dummy.Rout`.

```
R CMD BATCH --vanilla dummy.R dummy.Rout &
```

Rscript

This will also execute R in the background, with the difference that the output `dummy.Rout` will not capture `stderr` (messages, warnings and errors from R).

```
Rscript --vanilla dummy.R > dummy.Rout &
```

The `&` at the end makes sure the job is submitted and does not wait for it to end. Try it yourself (5 mins)!

Rscript

The R script can be executed as program directly, if you specify where the `Rscript` program lives.

The following example works in Unix. This is an R script named `since_born.R` (download here)

```
#!/usr/bin/Rscript
args <- tail(commandArgs(), 0)
message(Sys.Date() - as.Date(args), " days since you were born.")
```

This R script, can be executed in various ways...

Rscript as a program

For this we would need to change it to an executable. In unix you can use the chmod command: `chmod +x since_born.R`. This allows to:

```
./since_born.R 1988-03-02
```

Rscript in a bash script (most common)

In the case of running jobs in a cluster or something similar, we usually need to have a bash script, In our case, here we have a file named `since_born_bash.sh` that calls `Rscript` (download here)

```
#!/bin/bash
Rscript since_born.R 1988-03-02
```

Which we would execute something like this

```
sh since_born_bash.sh
```

```
## 12424 days since you were born.
```

Summary

- Parallel computing can speed up things.
- Not always needed... need to make sure that you are taking advantage of vectorization.
- Most of the time we look at "Embarrassingly parallel computing."
- In R, explicit parallelism can be achieved using the **parallel** package:
    1. Load the package and create a cluster **parallel::makeCluster()**
    2. Setup the environment **parallel::clusterEvalQ()**, **parallel::clusterExport()**, and **parallel::clusterSetRNGStream()**
    3. Make the call, e.g., **parallel::parLapply()**
    4. Stop the cluster **parallel::stopCluster()**
- Regardless of the Cloud computing service we are using, we will be using either `R CMD BATCH` or `Rscript` to submit jobs.

Session info

```
## R version 4.1.2 (2021-11-01)
## Platform: x86_64-apple-darwin17.0 (64-bit)
## Running under: macOS Big Sur 10.16
##
## Matrix products: default
## BLAS:   /Library/Frameworks/R.framework/Versions/4.1/Resources/lib/libRblas.0.dylib
## LAPACK: /Library/Frameworks/R.framework/Versions/4.1/Resources/lib/libRlapack.dylib
##
## locale:
## [1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
##
## attached base packages:
## [1] parallel  stats     graphics  grDevices utils     datasets  methods
## [8] base
##
## loaded via a namespace (and not attached):
##  [1] digest_0.6.29   R6_2.5.1        jsonlite_1.7.2  magrittr_2.0.2
##  [5] evaluate_0.14   highr_0.9       xaringan_0.22   stringi_1.7.6
##  [9] rlang_1.0.0     cli_3.1.1       rstudioapi_0.13 jquerylib_0.1.4
## [13] bslib_0.3.1     rmarkdown_2.11  tools_4.1.2     stringr_1.4.0
## [17] xfun_0.29       yaml_2.2.1      fastmap_1.1.0   compiler_4.1.2
## [21] htmltools_0.5.2 knitr_1.37      sass_0.4.0
```

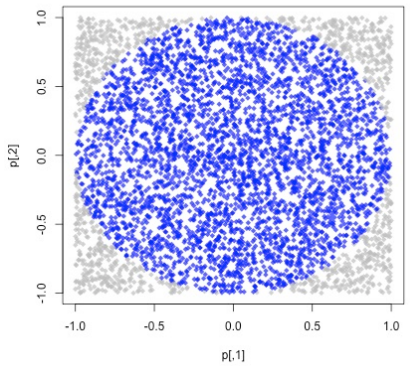
Resources

- Package parallel
- Using the iterators package
- Using the foreach package
- 32 OpenMP traps for C++ developers
- The OpenMP API specification for parallel programming
- 'openmp' tag in Rcpp gallery
- OpenMP tutorials and articles

For more, checkout the CRAN Task View on HPC{target="_blank"}

Simulating π

- We know that $\pi = \frac{A}{r^2}$. We approximate it by randomly adding points x to a square of size 2 centered at the origin.
- So, we approximate π as $\Pr\{\|x\| \leq 1\} \times 2^2$



The R code to do this

```
pisim <- function(i, nsim) {  # Notice we don't use the -i-
  # Random points
  ans  <- matrix(runif(nsim*2), ncol=2)

  # Distance to the origin
  ans  <- sqrt(rowSums(ans^2))

  # Estimated pi
  (sum(ans <= 1)*4)/nsim
}
```

```r
library(parallel)
# Setup
cl <- makePSOCKcluster(4L)
clusterSetRNGStream(cl, 123)

# Number of simulations we want each time to run
nsim <- 1e5

# We need to make -nsim- and -pisim- available to the
# cluster
clusterExport(cl, c("nsim", "pisim"))

# Benchmarking: parSapply and sapply will run this simulation
# a hundred times each, so at the end we have 1e5*100 points
# to approximate pi
microbenchmark::microbenchmark(
  parallel = parSapply(cl, 1:100, pisim, nsim=nsim),
  serial   = sapply(1:100, pisim, nsim=nsim), times = 1, unit="ms"
)
```

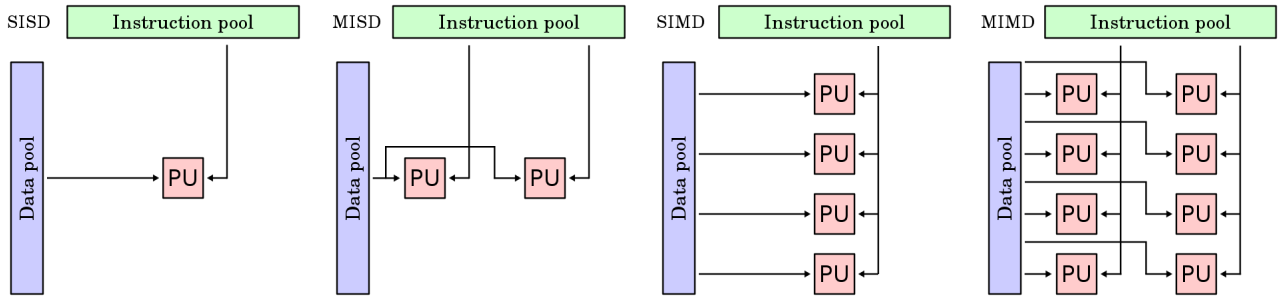
```
## Unit: milliseconds
##       expr      min       lq     mean   median       uq      max neval
##  parallel 320.6614 320.6614 320.6614 320.6614 320.6614 320.6614     1
##    serial 861.9523 861.9523 861.9523 861.9523 861.9523 861.9523     1
```

(Bonus) Overview of HPC

Using Flynn's classical taxonomy, we can classify parallel computing according to the following two dimmensions:

a. Type of instruction: Single vs Multiple

b. Data stream: Single vs Multiple



Michael Flynn's Taxonomy (wiki)

(Bonus) Parallel computing: Software

Implicit parallelization:

- tensorflow: Machine learning framework
- pqR: Branched version of R.
- Microsoft R: Microsoft's R private version (based on Revolution Analytics' R version).
- data.table (R package): Data wrangling using multiple cores.
- caret (R package): A meta package, has various implementations using parallel computing.

Explicit parallelization (DIY):

- CUDA (C/C++ library): Programming with GP-GPUs.
- Open MP (C/C++ library): Multi-core programming (CPUs).
- Open MPI (C/C++ library): Large scale programming with multi-node systems.
- Threading Building Blocks (C/C++ library): Intel's parallel computing library.
- Kokkos (C++ library): A hardware-agnostic programming framework for HPC applications.
- parallel (R package): R's built-in parallel computing package
- future (R package): Framework for parallelzing R.
- RcppParallel (R C++ API wrapper): Header and templates for building Rcpp+multi-threaded programs.
- julia (programming language): High-performing, has a framework for parallel computing as well.