CBS COPENHAGEN BUSINESS SCHOOL
HANDELSHØJSKOLEN

HPC & PARALLEL PROGRAMMING IN R

New cloud computing possibilities for researchers & students

Kristoffer Gulmark Poulsen & Lars Nondal
CBS

Program Today

- Basic theory of parallel programming
- Parallel programming basics within R.
- Parallelization of a ML models within the Tidymodels framework.
- Distributed parallelization on a SLURM Cluster.

- https://cbs-hpc.github.io/

What is High Performance Computing (supercomputer)?

- Network of processors, hard drives & other hardware

Hardware

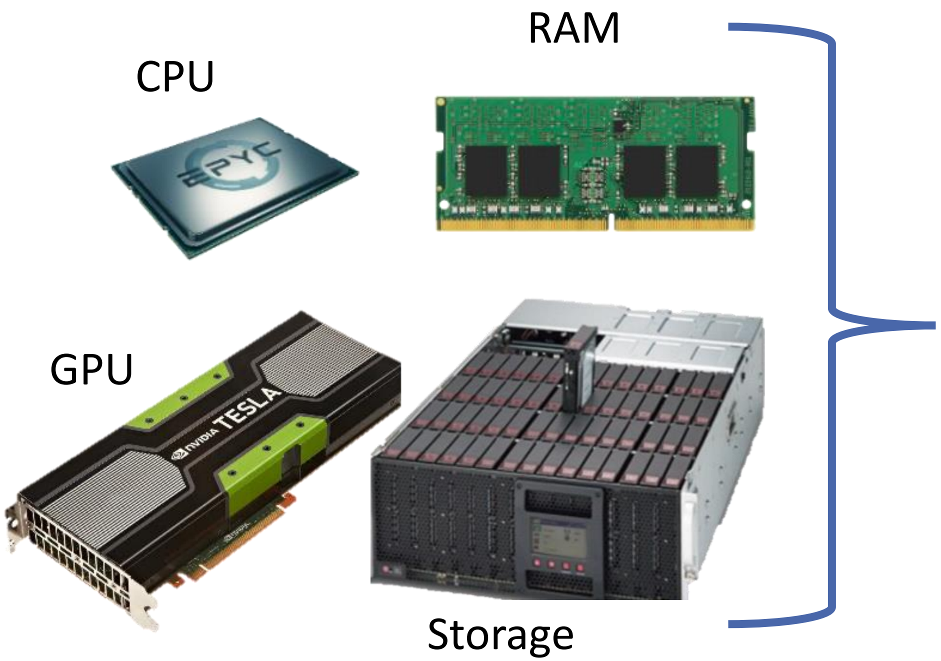
- **Core**: Processing unit on a single machine.
- **Node**: A single machine.
- **Cluster**: Network of multiple nodes.

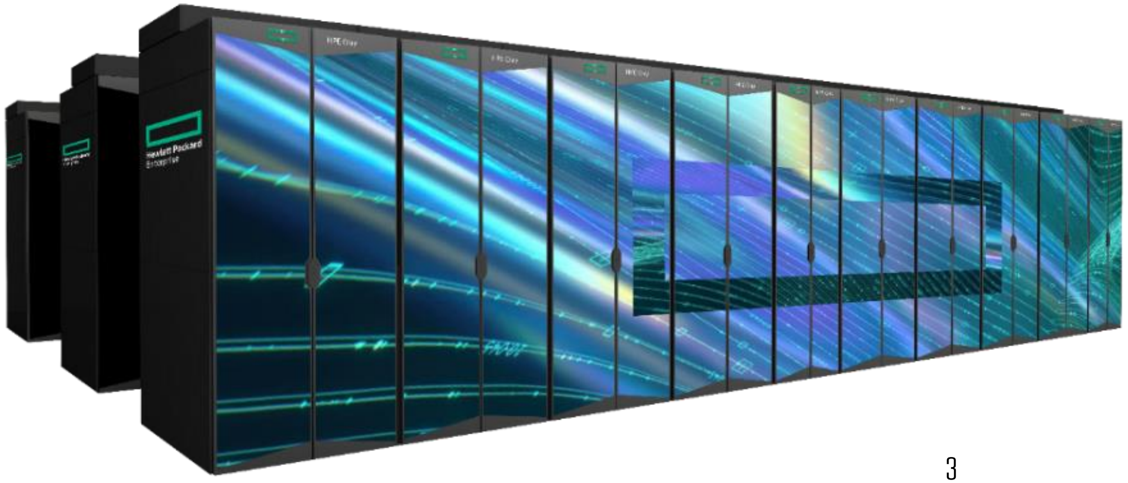
Message Passing Interface (MPI)

- A standard protocol for passing data and other messages between **nodes** in a **cluster**.

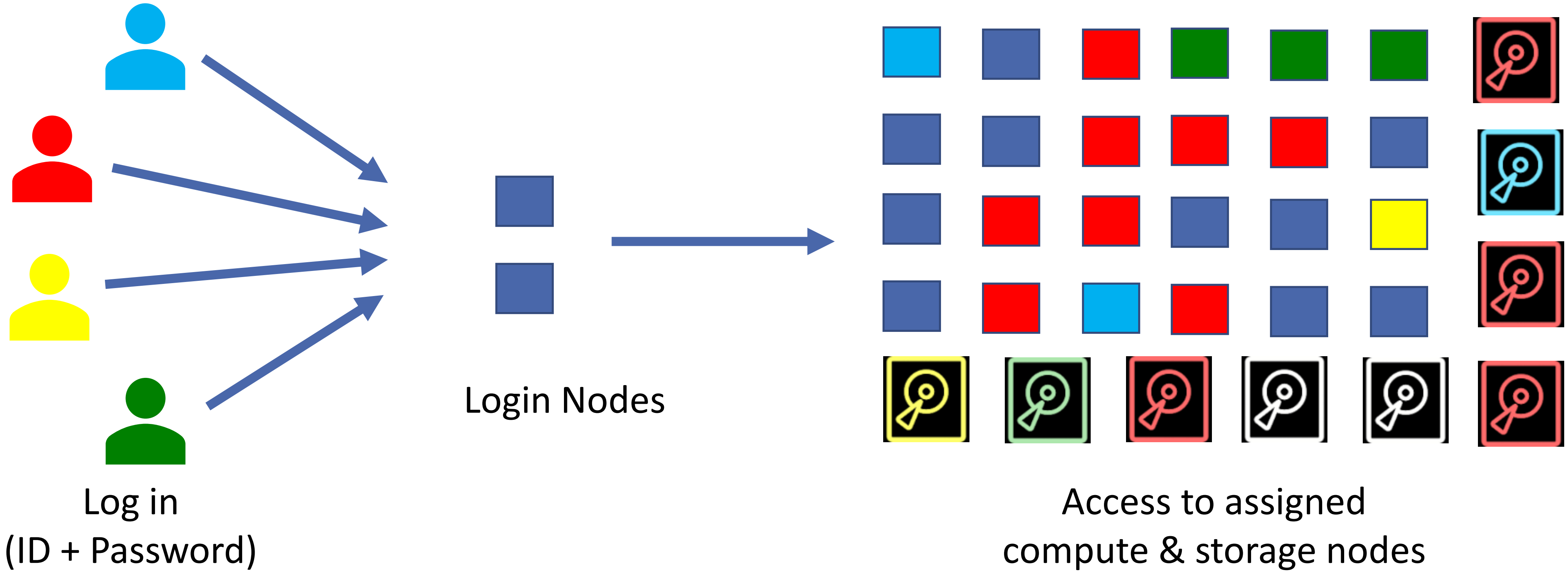
Simple Linux Utility for Resource Management (SLURM)

- A free MPI framework for Linux and Unix-like kernels.



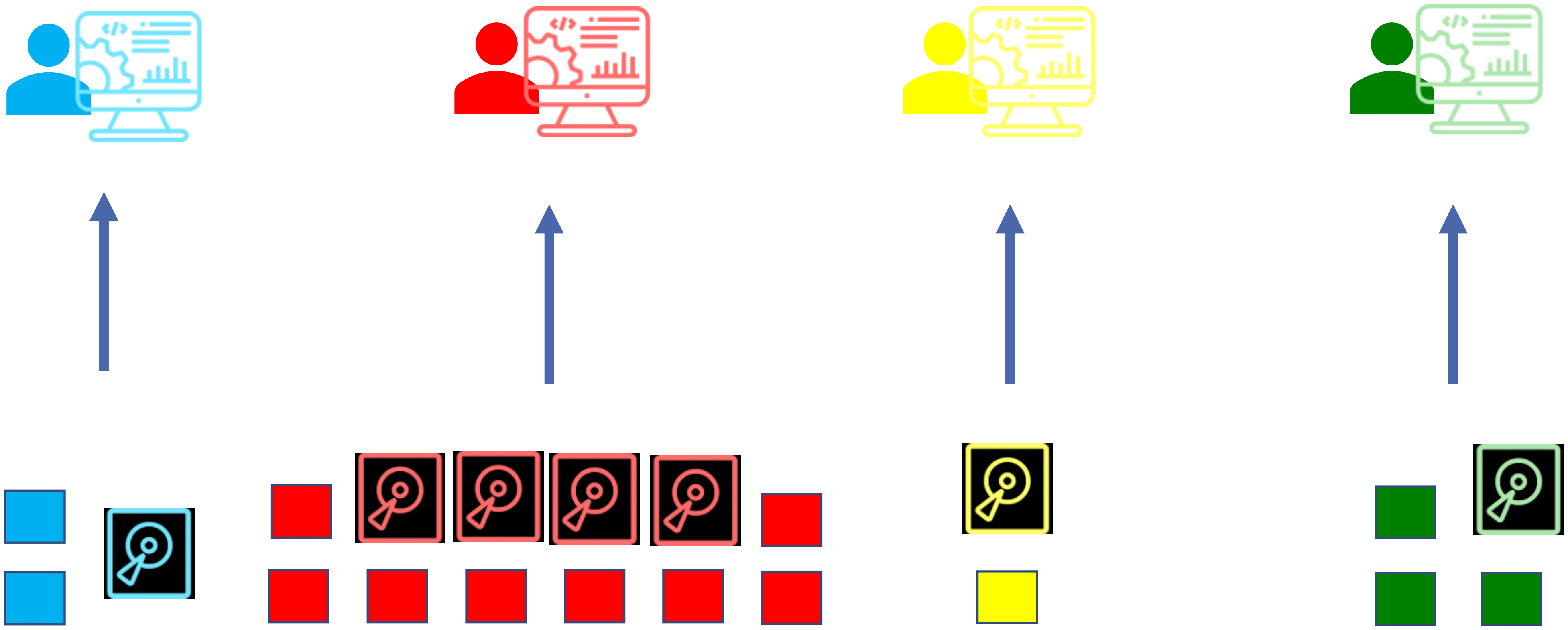


Accessing an HPC...



Accessing an HPC…

- Your assigned resources (HW + SW) can be used from your PC



When HPC might be for you

- Applying ML/AI
- Running simulation and resampling techniques
- Working with large datasets
- My laptop runs out of memory
- My workflow is running very slow

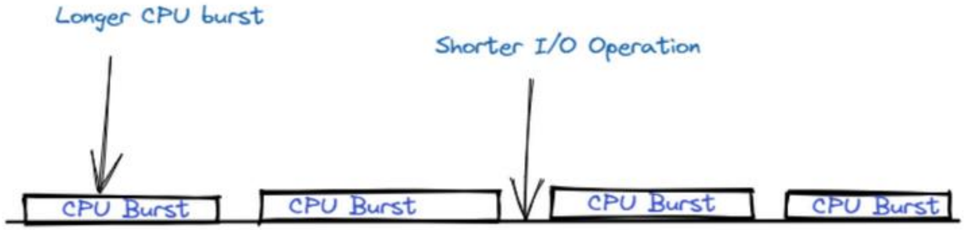
Why is it taking so long?

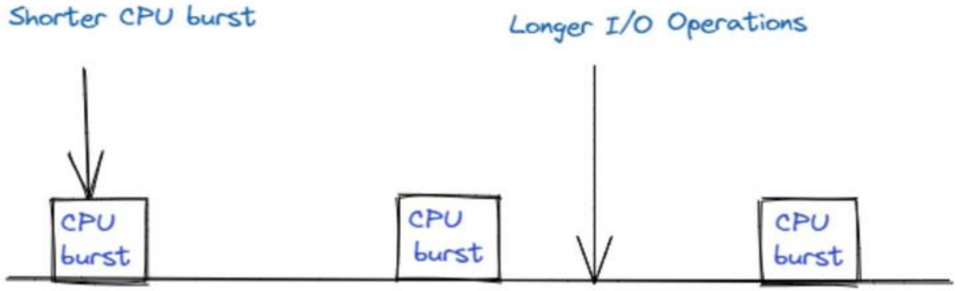
Computation can be slow for one of three reasons:

CPU bound when computational time is restricted by processor.

I/O bound when reading **from** and **to disk/database** is limiting factor.

Memory bound when limited by the memory required to hold the working data.

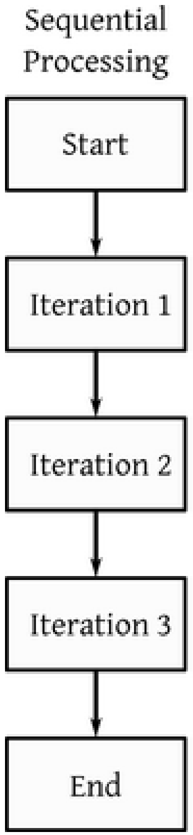




Parallel Programming

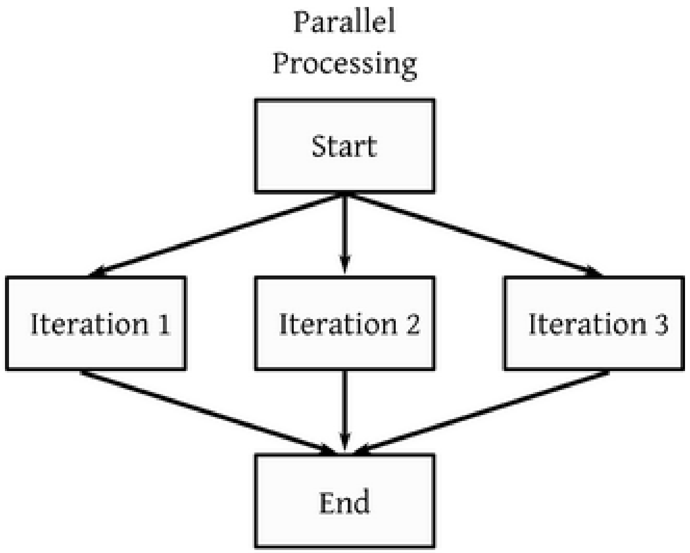
Sequential Computing

- Single core processor
- Multiple tasks which runs overlapping but **not** at same time
- Synchronous tasks



Parallel Computing

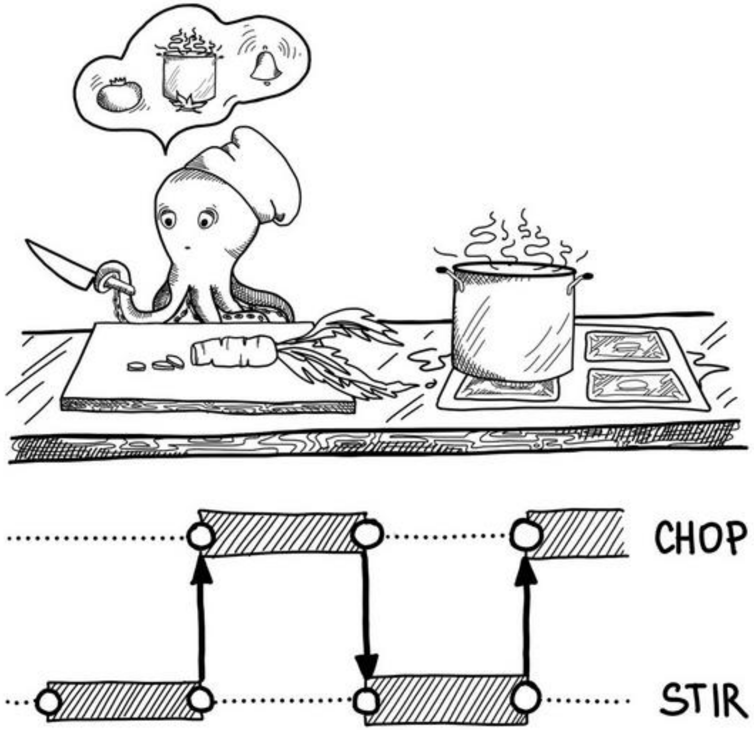
- Multi-core processor
- Multiple tasks which runs overlapping.
- Synchronous/Asynchronous



Parallel Programming

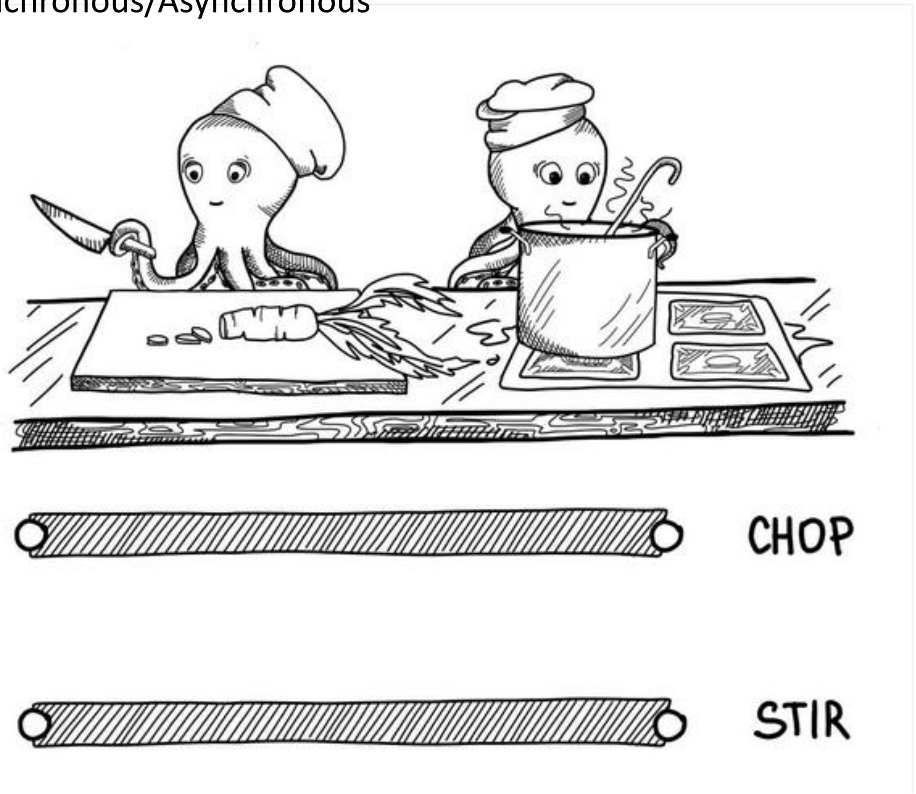
Sequential Computing

- Single core processor
- Multiple tasks which runs overlapping but **not** at same time.
- Synchronous tasks



Parallel Computing

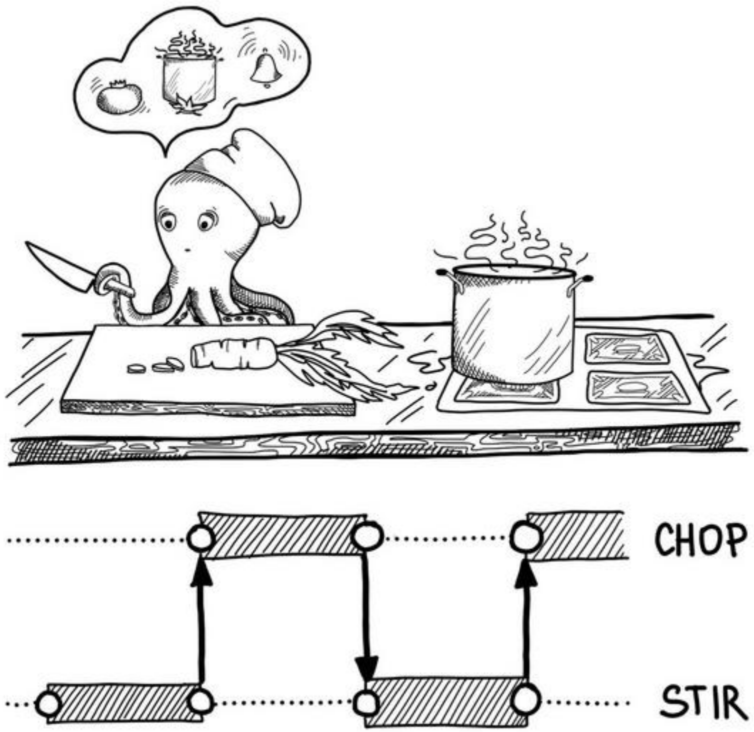
- Multi-core processor
- Multiple tasks which runs overlapping.
- Synchronous/Asynchronous



Parallel Programming

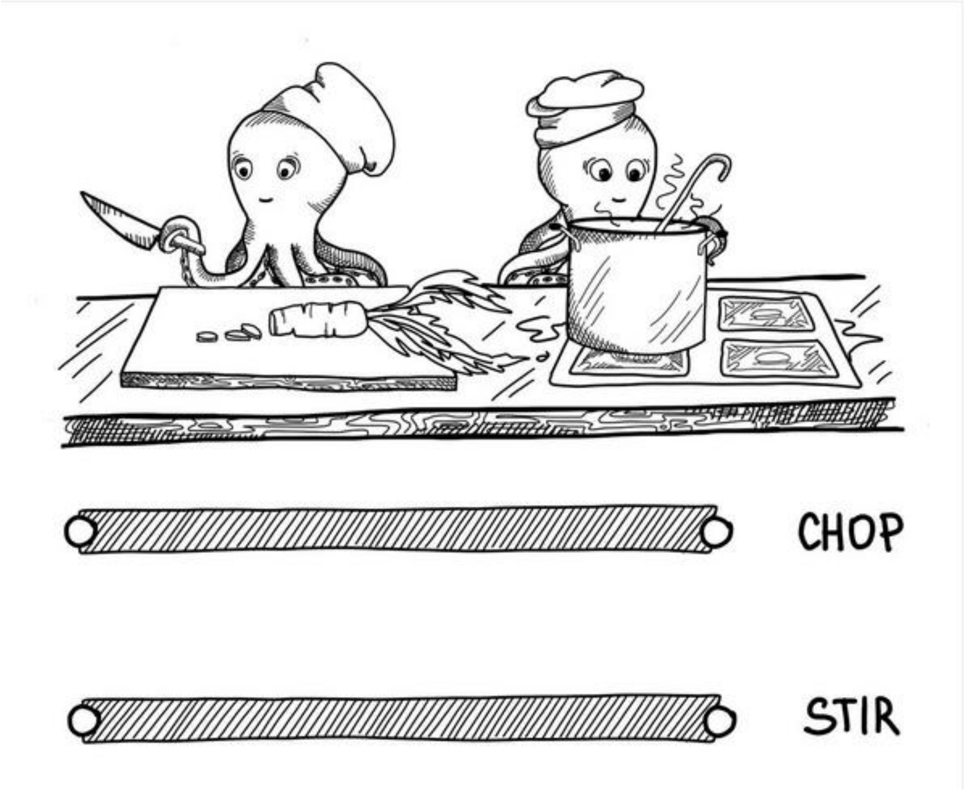
Concurrency

- Executing multiple tasks at the same time but not necessarily simultaneously.



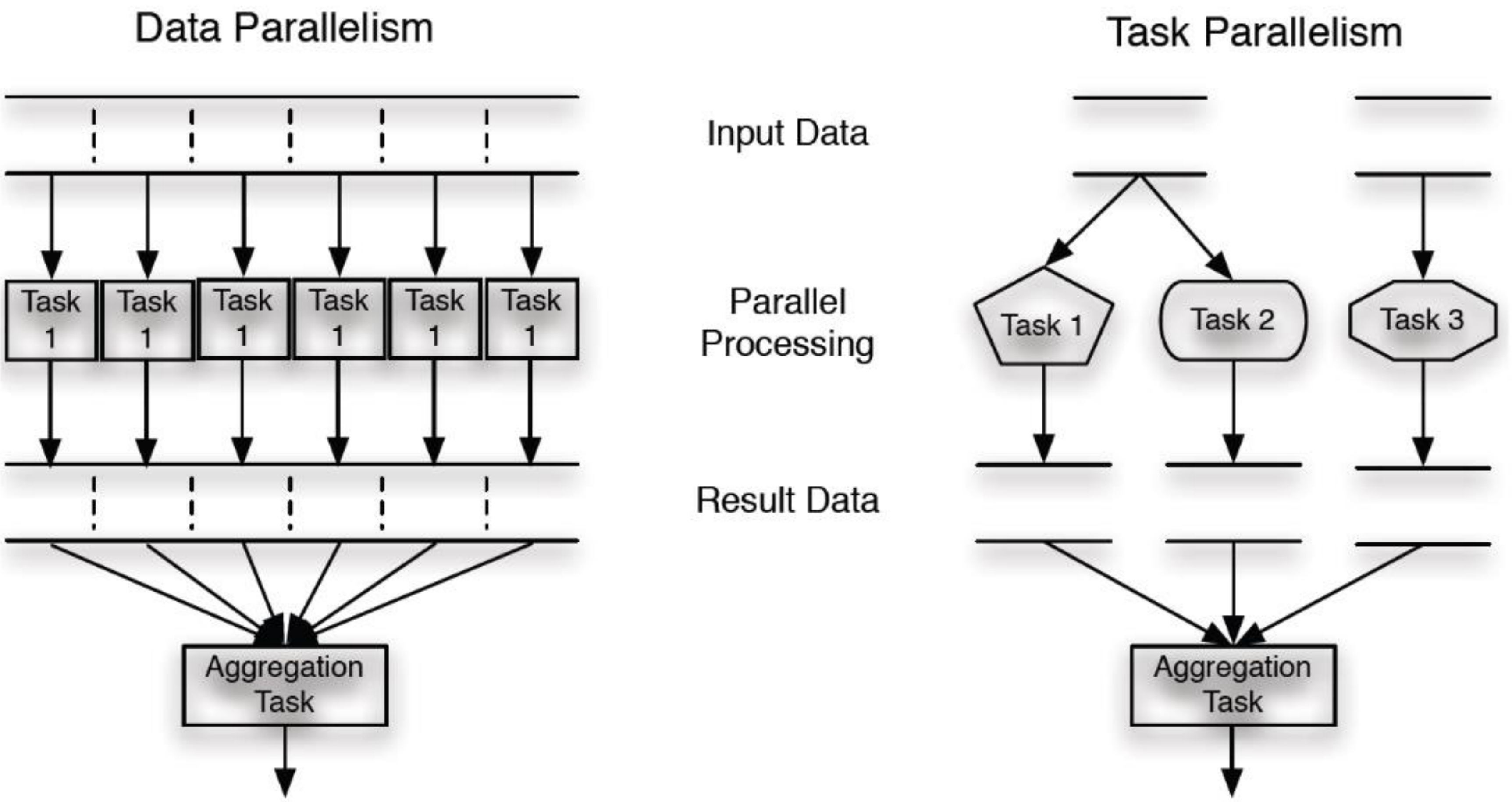
Parallelism

- One task is split into subtasks and run in parallel at the exact same time.
- Run multiple tasks in in parallel on multiple CPUs at the exact same time



CBS

Parallel Programming



Models for Parallel Programming

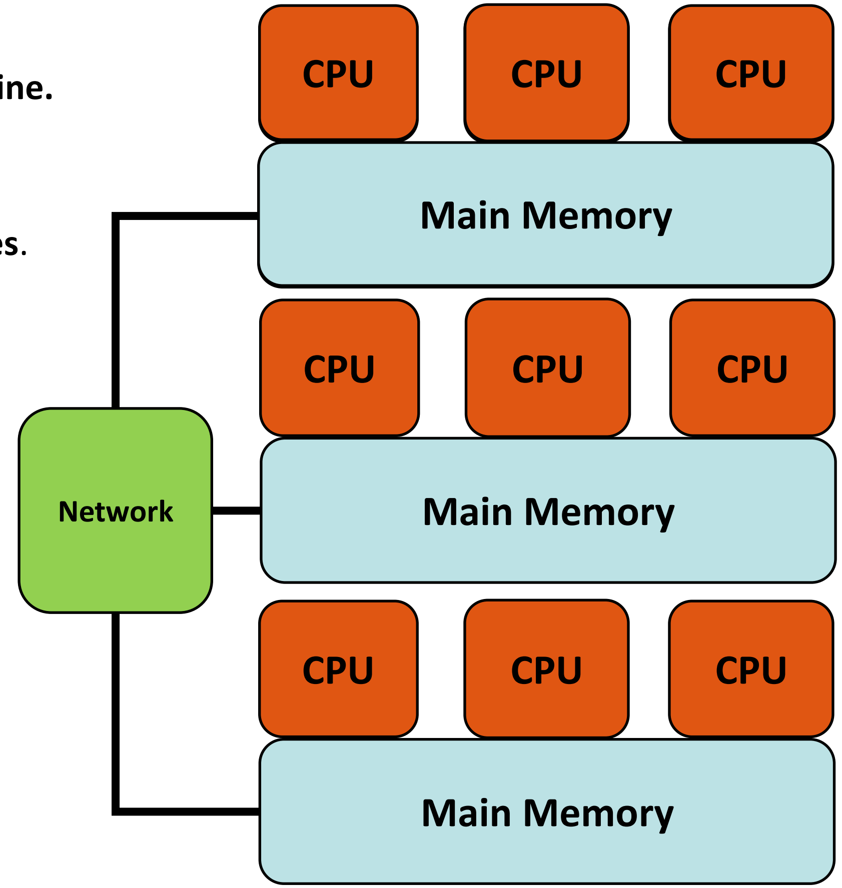
Shared Memory Parallelism (SMP) work is divided between **multiple cores** running on a **single machine.**

Distributed Memory Parallelism (Distributed Computing) work is divided between **multiple machines**.

Embarrassing/ Perfectly Parallel - the tasks can be run independently, and they don’t need to communicate.

Implicit/Hidden Parallelism - is implemented automatically by the Compiler, Interpreter or Library.

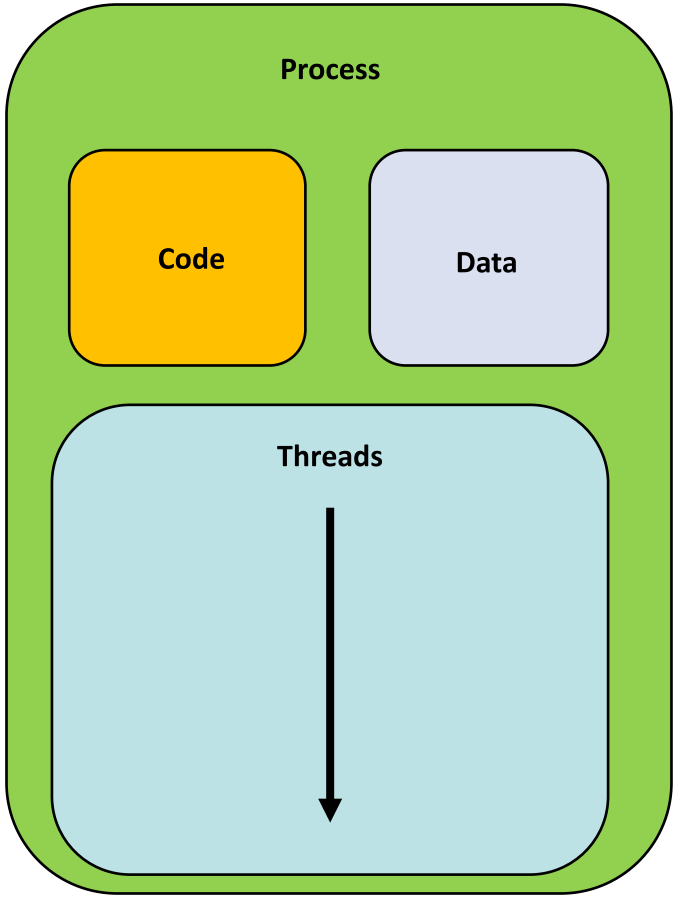
Explicit Parallelism - is written into the source code by the Programmer.



Terminology

- **Process**: Execution of a program . A given executable (e.g., Python or R) may start up multiple processes.

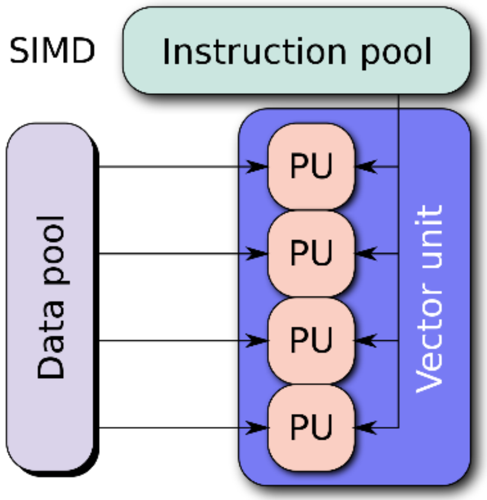
- **Thread**: Path of execution within a single process.



SIMD & Multi-Threading

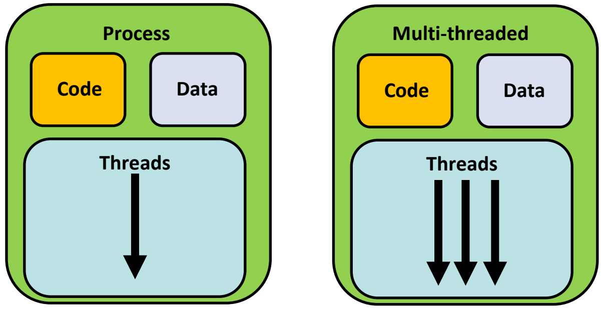
Single Instruction, Multiple Data (SIMD)

- single thread/processor where each processing unit (PU) performs the same instruction on different data.
- **Vectorization**.



Multi-Threading

- **Threads** are multiple paths of execution within a single process.
- Appears as a single process.



Single instruction, multiple threads (SIMT)

<u>**Python** and **R** are examples of single-threaded programming languages.</u>

```
top - 15:12:02 up 2 days, 54 min,  0 users,  load average: 6.42, 6.45, 6.45
Tasks:  10 total,   1 running,   9 sleeping,   0 stopped,   0 zombie
%Cpu(s): 11.0 us,  0.3 sy,  0.0 ni, 88.7 id,  0.0 wa,  0.0 hi,  0.0 si,  0.0 st
MiB Mem : 385583.7 total, 193583.0 free, 102124.0 used,  89876.6 buff/cache
MiB Swap:   8192.0 total,   4461.5 free,   3730.5 used. 280235.0 avail Mem

  PID USER      PR  NI    VIRT    RES    SHR   %CPU  MEM     TIME+ COMMAND
  243 ucloud    20   0 3970780 962704  74288   278.1  0.2   0:44.50 rsession
  202 rstudio+  20   0  182200  18268  14724          0.0   0:01.00 rserver
    1 ucloud    20   0    6896   3428   3196 S  0.0   0.0   0:00.05 start-rstu+
    7 root      20   0   10420   4920   4376 S  0.0   0.0   0:00.00 sudo
    8 root      20   0     200      4      0 S  0.0   0.0   0:00.01 s6-svscan
   37 root      20   0     200      4      0 S  0.0   0.0   0:00.00 s6-supervi+
  198 root      20   0     200      4      0 S  0.0   0.0   0:00.00 s6-supervi+
  265 ucloud    20   0    2492    580    512 S  0.0   0.0   0:00.01 sh
  271 ucloud    20   0    8168   4904   3408 S  0.0   0.0   0:00.01 bash
  273 ucloud    20   0   10032   3824   3316 R  0.0   0.0   0:00.12 top
```

CBS

SIMD & Multi-Threading in Python and R

SIMT is achieved in several ways:

Through external libraries

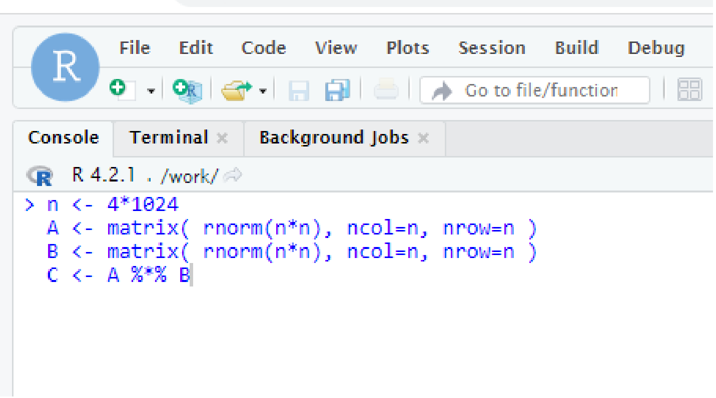
- Written in other languages (e.g. C, C++, Fortran) that run multi-threaded.
- Linear algebra routines (BLAS & LAPACK) implemented in libraries such as MKL, OpenBLAS or BLIS.
- NumPy, SciPy and Pandas
- built-in R functions

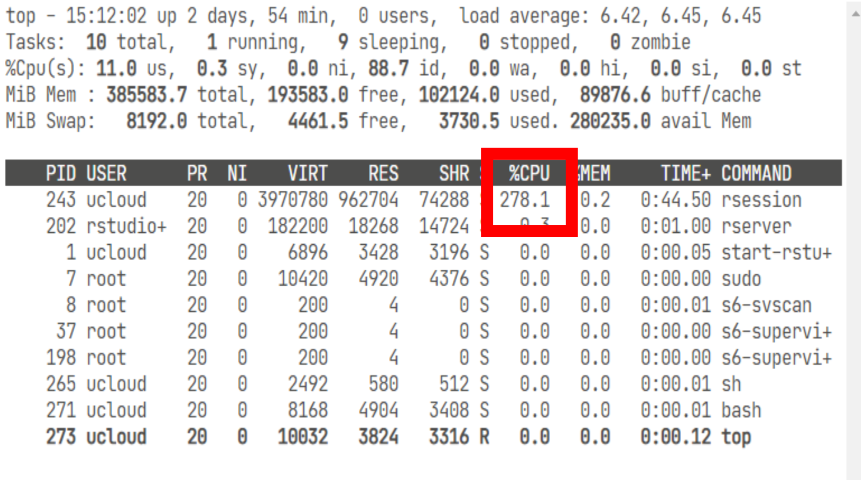
"Static Compilers"

- OpenMP/GCC (GNU Compiler Collection)
- Rcpp
- Cython

Dynamic/JIT Compilers:

- Numba
- JITR

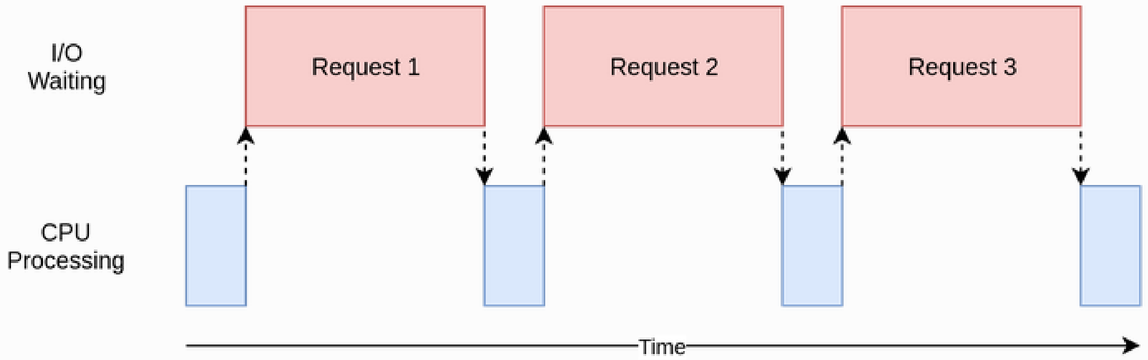




CBS

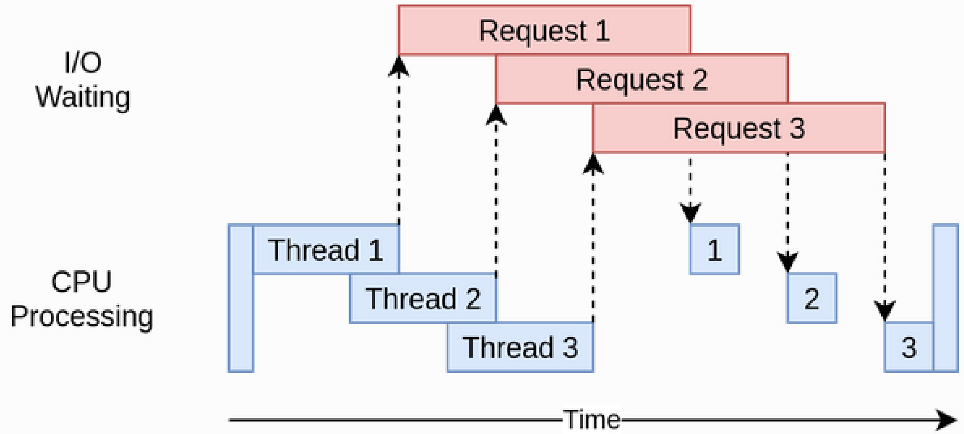
Multi-Threading I/O

This is how an I/O-bound application might look:



From https://realpython.com/, distributed via a Creative Commons Attribution-NonCommercial-ShareAlike 3.0 Unported licence

The speedup gained from multithreading I/O bound problems can be understood from the following image.



From https://realpython.com/, distributed via a Creative Commons Attribution-NonCommercial-ShareAlike 3.0 Unported licence

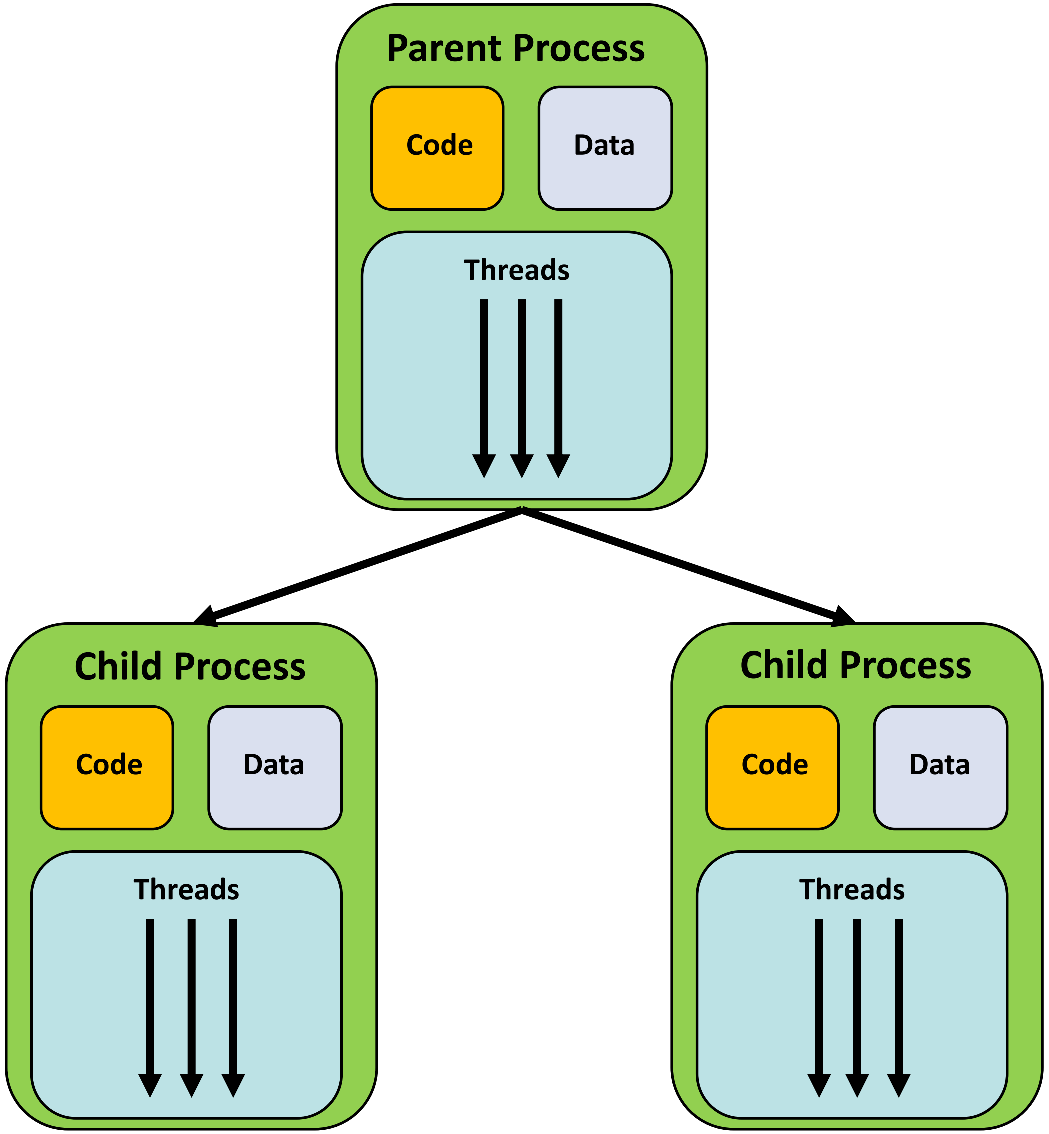
Multi-Processing

Fork

- Only available on UNIX machines (Linux, Mac, and the likes).
- The **child process** is an identical “cloned” of the **parent process**.
- Single machine

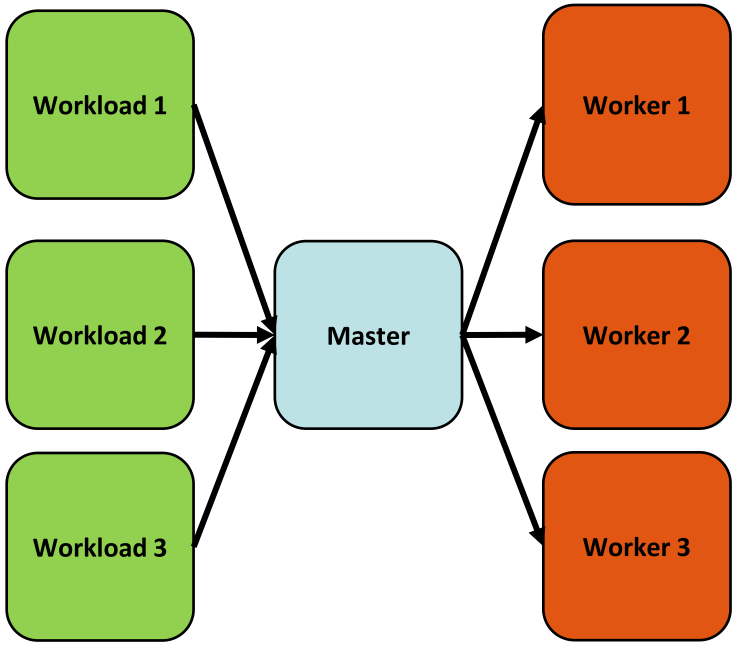
Spawn/Socket (PSOCK)

- Available on Unix and Windows.
- The **parent process** starts a fresh/empty process.
- Code & data needs to copied onto the new **child process**
- Can be scaled to multiple machines/cluster.



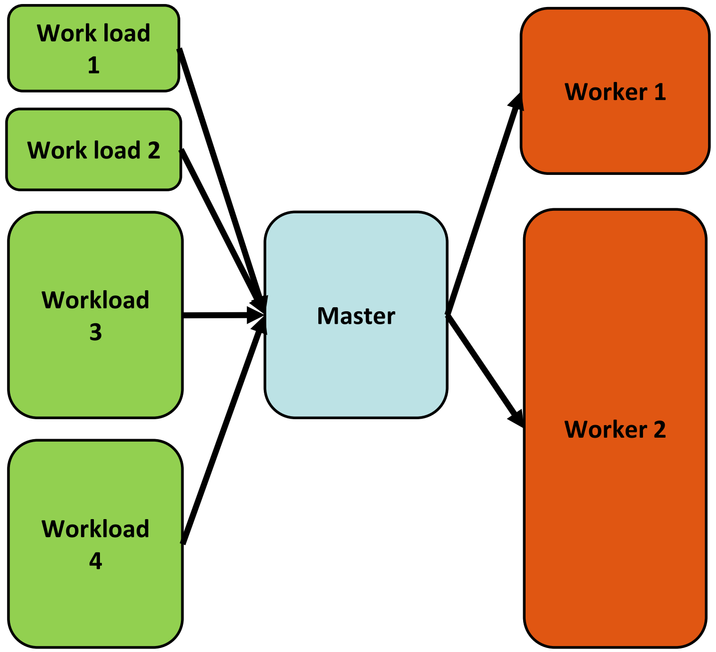
Multi-Processing – Load Balancing

Master/Worker Approach



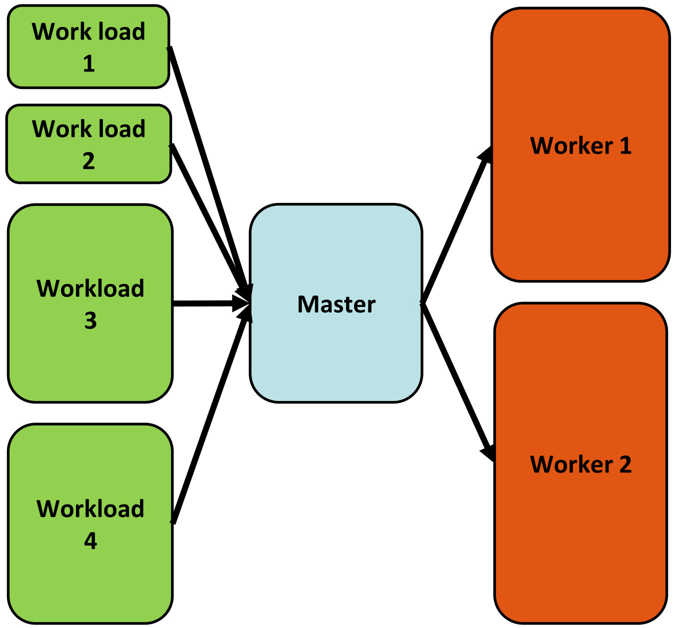
No distribution

- Low Overhead
- Bad ***load balance***.



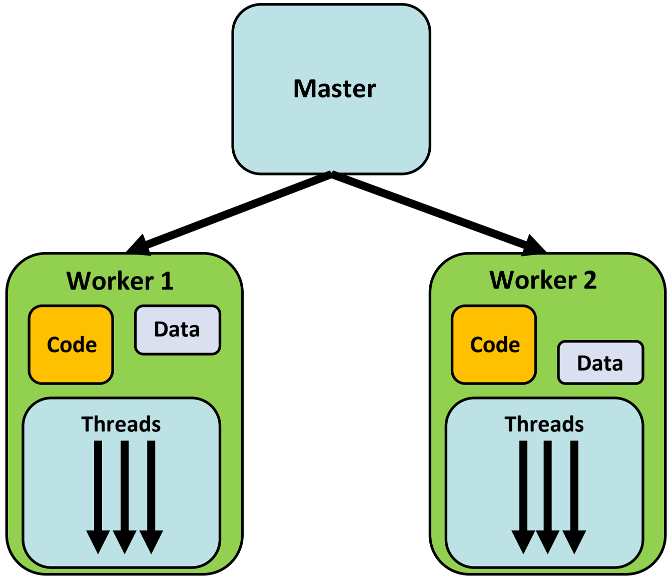
Dynamic balancer/scheduler

- Better work distribution
- More overhead



Multi-Processing – Splitting Data

Passing only data "chucks" to each worker



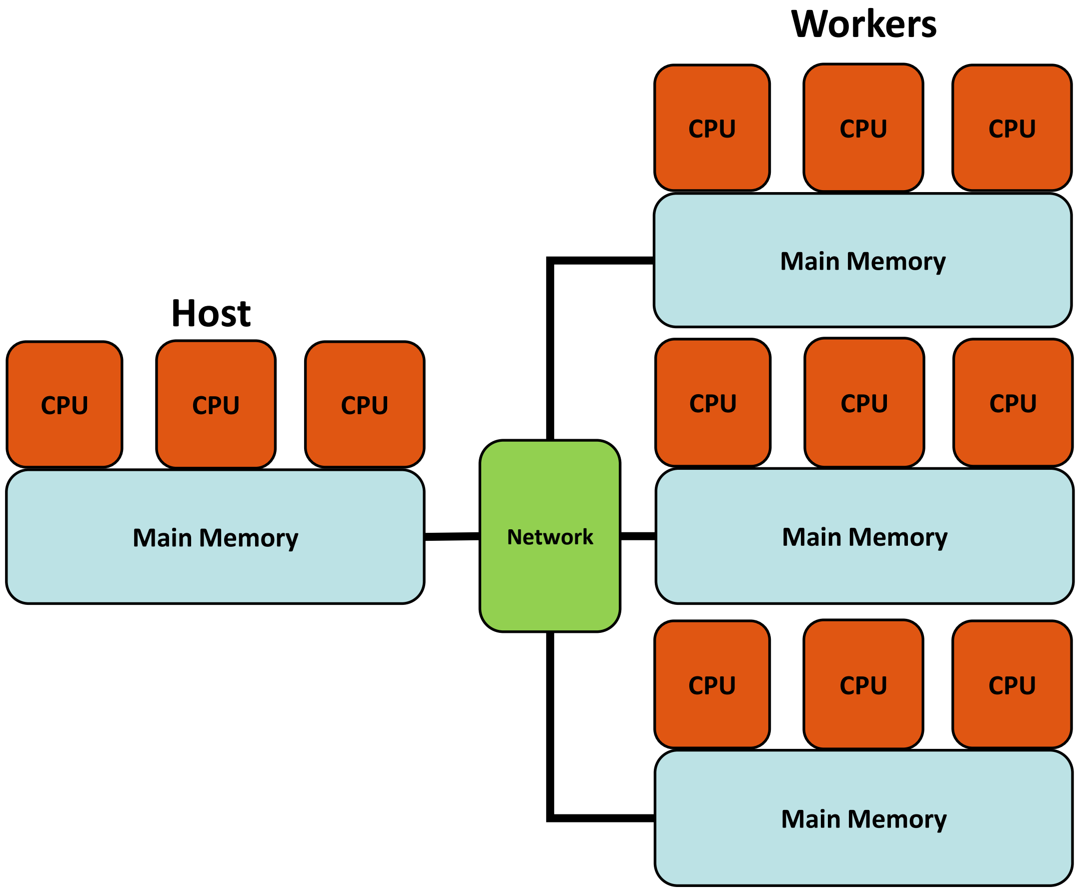
Big chunks are generally better than little chunks

```
for (i in 1:10) {
  for (j in 1:1000000) {

    # Execution of code

    }
  }
```

Distributed Computing on HPC

Distributed Memory Parallelism (Distributed Computing)

- **Multiple machines** with its own **private memory**.
- **Message Passing Interface (MPI)**
- **Host** schedules the work across the **workers**



HPC Job Schedulers:

- Portable Batch System (PBS)
- **Simple Linux Utility for Resource Management (SLURM)**
- IBM Spectrum LSF
- Sun Grid Engine (SGE)

CBS

CBS COPENHAGEN BUSINESS SCHOOL
HANDELSHØJSKOLEN

PARALLEL PROGRAMMING IN R

Kristoffer Gulmark Poulsen & Lars Nondal
CBS

EQUIS ACCREDITED AACSB ACCREDITED ASSOCIATION OF MBAS ACCREDITED CEMS PIM

R Packages - Overview

Compilers (Not covered)

- ***Rcpp***
- ***JIT***

parallel package

- ***multicore***
- ***Snow***

foreach loop adaptation of ***parallel***

- ***doParallel, doSnow, doMC & doMPI…***

Tidymodels framework

- Examples of parallel computing

Scalable Frameworks(Not covered)

- ***future***
- ***SparkR***

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

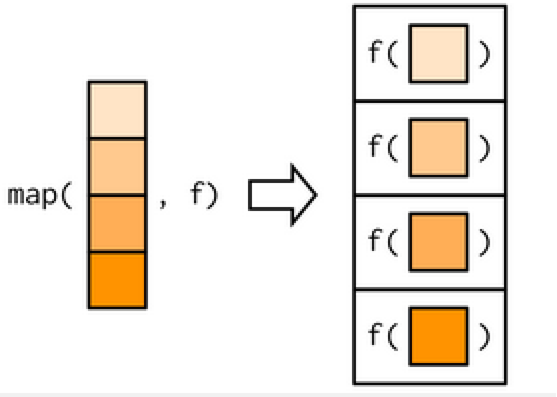
Iterations

There are two styles of iterations

```r
for (i in 1:3) print(sqrt(i))
```

for and *while* loops

- It is often the most intuitive way to begin.
- **Imperative programming .**



functional programming

- Readability & code redundancy
- **Functionals** are a functions that takes a function as an input and returns a vector as output.
- E.g. **apply()** or **map()**

R Packages- *Parallel*

- ***multicore***: Multi-processing on **single machine** through **forking** (Not Covered Today).
- ***Snow (Simple Network of Workstations)***: Can **fork/spawning** on multiple machines/clusters.
- ***paralellel*** serve as ***"parallel backend"*** to many/most packages, so worth understanding.
- It is all based on ***apply*** form of R iteration:

Base R	snow
lapply	parLapply
sapply	parSapply
vapply	-
apply(rowwise)	parRapply, parApply(,1)
apply(columnwise)	parCapply, parApply(,2)

CBS

R Packages- *Parallel /snow*

Snow (Simple Network of Workstations): Can **fork/spawning** on multiple machines/clusters.

Functions:

- ***cl<- makeCluster(n,type ="PSOCK")*** - (Default)
- ***cl<- makeCluster(n,type ="FORK")***
- ***stopCluster(cl)*** – stops clusters
- ***clusterExport(cl,data)*** - Copies data to processes
- ***clusterApply(cl,data,func)*** – Runs analysis in parallel
- ***clusterApplyLB()*** – dynamic load balancing
- ***clusterEvalQ(cl, expr)*** – Evaluating an expression
- ***clusterSplit(cl,data)*** – data splitting

ClusterApply

```
cl <- makeCluster(4)
clusterExport(cl, "jan2010")


cares <- clusterApply(cl, rep(5,4), do.n.kmeans)
```

CBS

R Packages- *foreach* loop adaptation of *parallel*

Parallelization using the “**for loop”** iteration through the ***foreach*** package.

```
for (i in 1:3) print(sqrt(i))
```

```
library(foreach)
foreach (i=1:3) %do% sqrt(i)
```

```
library(doParallel)
registerDoParallel(3)  # use multicore-style forking
foreach (i=1:3) %dopar% sqrt(i)
```

```
cl <- makePSOCKcluster(3)
registerDoParallel(cl)  # use the just-made PSOCK cluster
foreach (i=1:3) %dopar% sqrt(i)
```

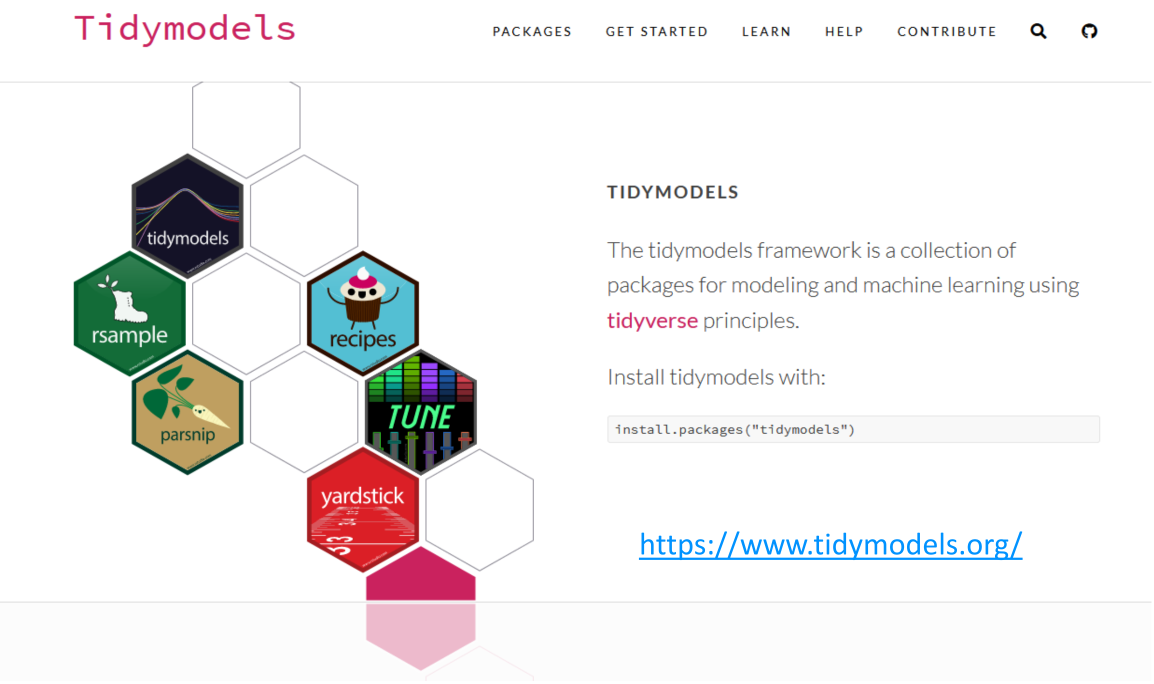
Many different backends:

- ***doParallel*** - https://cran.r-project.org/web/packages/doParallel/index.html
- ***doSnow*** - https://cran.r-project.org/web/packages/doSNOW/index.html
- ***doMC*** - https://cran.r-project.org/web/packages/doMC/index.html
- ***doMPI*** - https://cran.r-project.org/web/packages/doMPI/index.html

Tidymodels

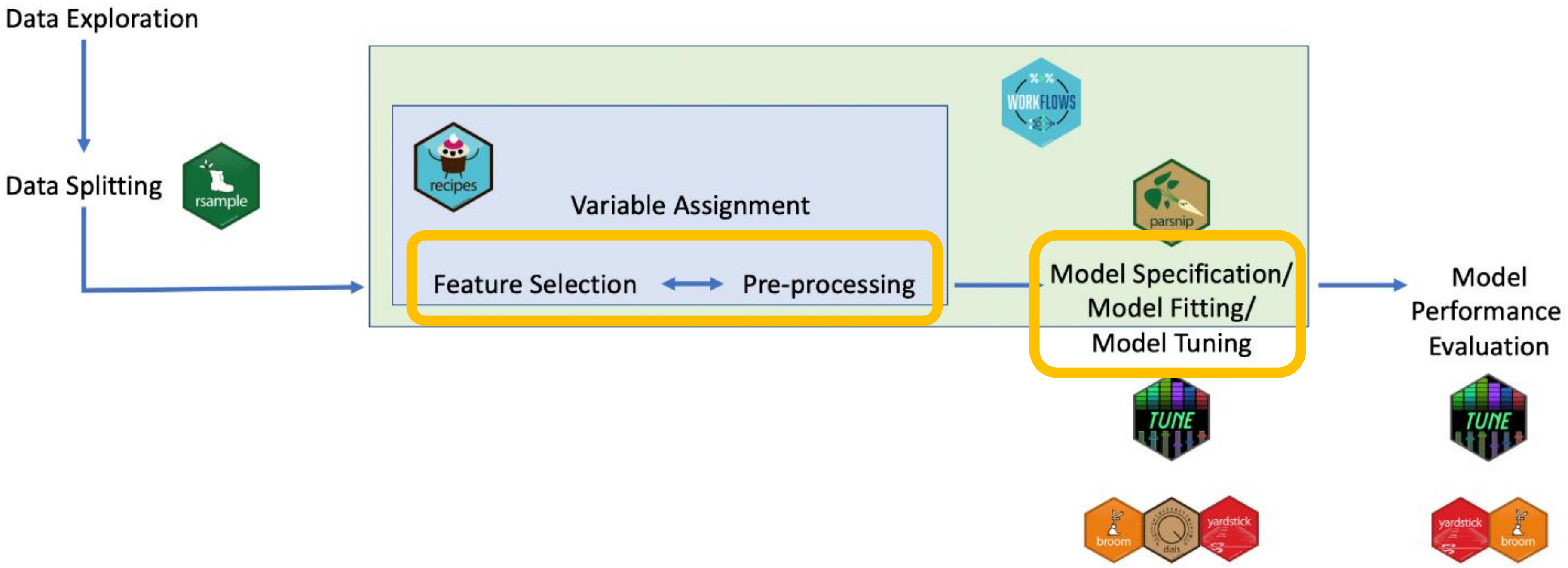
Tidyverse/Tidymodels

- The **tidyverse** is a language for solving data science challenges with R code.
- Both **tidymodels** is built on the **tidyverse** principles**:**
  - Should be intuitive
  - Consistence syntax: function naming, arguments.



https://www.tidymodels.org/

Tidymodels - Workflow

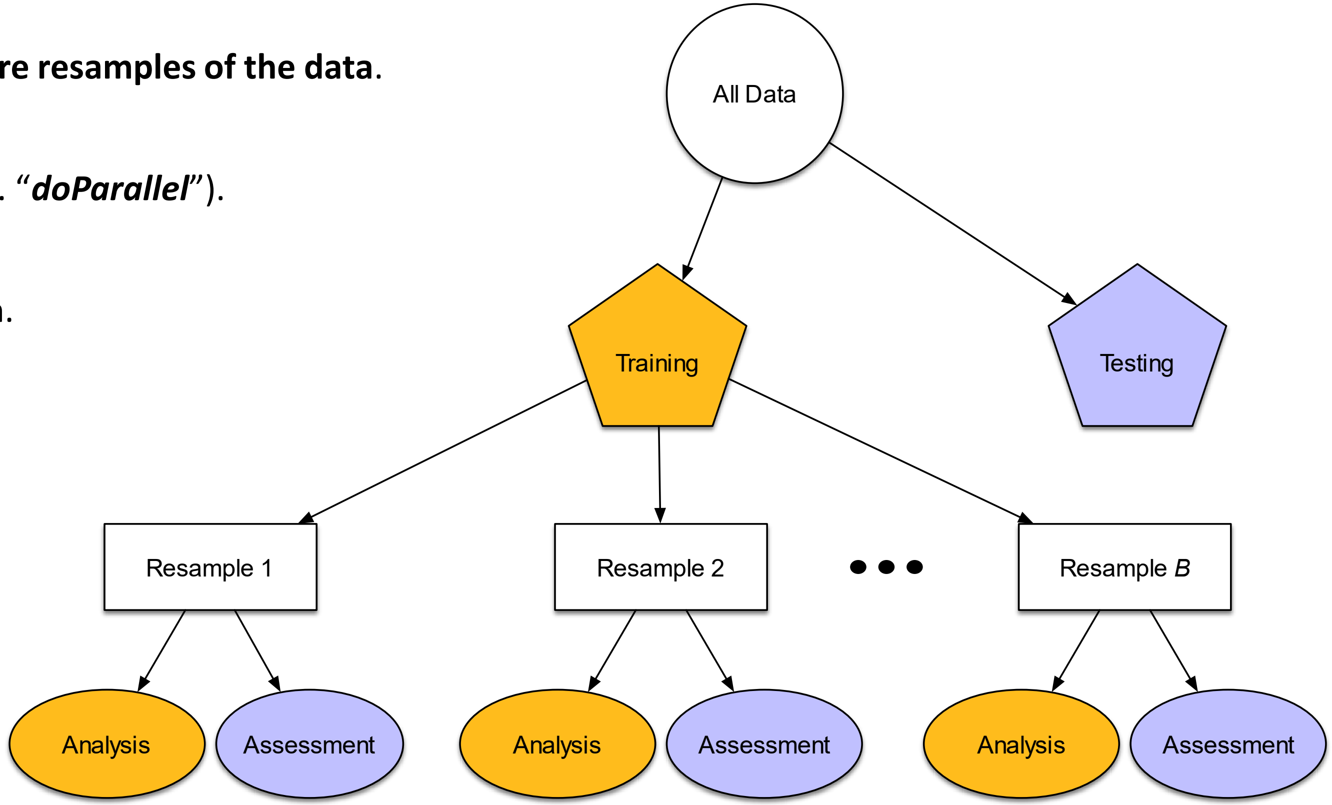


https://jhudatascience.org/tidyversecourse/model.html

Tidymodels - Model Fitting and Tuning

Model **performance** and **optimization** is based on **resampling methods** which are just **embarrassing parallel!!**

- **fit_resamples()** computes a set of performance metrics across **one** or **more resamples**.
- **tune_grid()** of performance for **tuning parameters** across **one** or **more resamples of the data**.
- ***foreach*** package is used in combination with a backend package (e.g. "***doParallel***").
- Many ML/AI packages within Tidymodels have built-in parallelisation.



CBS

Tidymodels - Model Fitting and Tuning

```
nnet_tune <-
  nnet_workflow  %>%
  tune_grid(hotel_validation,
        grid = nGrid,
        control = control_grid(save_pred = TRUE,parallel_over = "everything"),
        metrics = metric_set(roc_auc))
```

"resamples"

- then tuning will be performed in parallel over **resamples alone.**
- Within each resample, the **preprocessor (i.e. recipe or formula)** is reused across all models.

"everything"

- An outer parallel loop will iterate over **resamples**.
- An inner parallel loop will iterate over all **unique combinations of preprocessor** and **model tuning parameters** for that specific resample.
- This will result in the preprocessor being re-processed multiple times
- Pre-processing depended.

CBS

Tidymodels - Case

- Hotel bookings data from [Antonio, Almeida, and Nunes (2019)]
- **Aim:** to predict which hotels are preferred by families with children.
- Data frame: 50.000 entries and 23 variables

Data Splitting

```
set.seed(123)

# Split into Training and Testing set
splits  <- initial_split(hotels, strata = children)
hotel_train <- training(splits)
hotel_test  <- testing(splits)

# Split Validation set from Training set (Alternative to Cross Validation)
set.seed(234)
hotel_validation <- validation_split(hotel_train,
                        strata = children,
                        prop = 0.80)
```

Methodology used: Classification

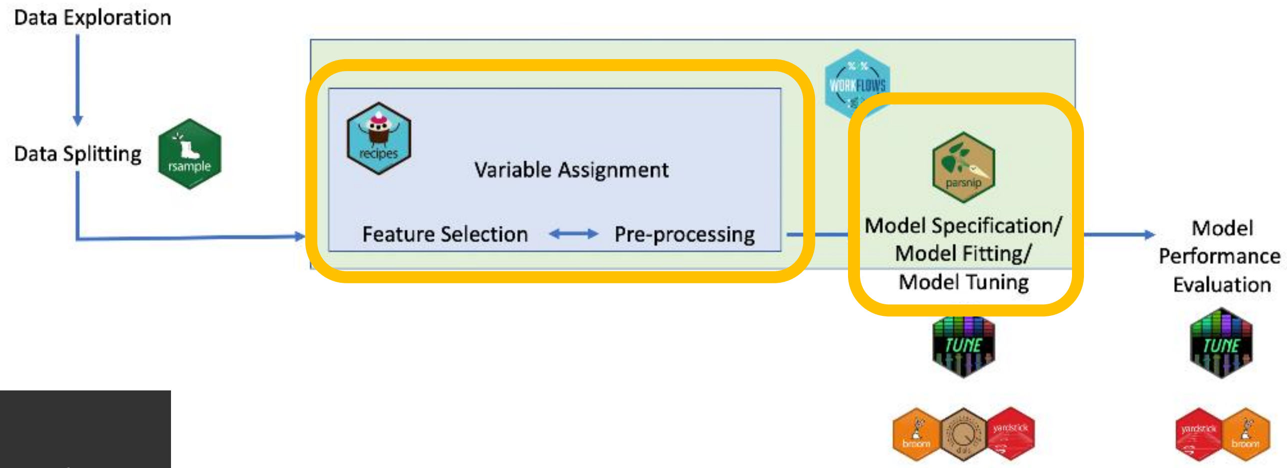
- Random Forrest - ***ranger::ranger()***
- Neural Network - ***nnet::nnet()***

	x
1	hotel
2	lead_time
3	stays_in_weekend_nights
4	stays_in_week_nights
5	adults
6	children
7	meal
8	country
9	market_segment
10	distribution_channel
11	is_repeated_guest
12	previous_cancellations
13	previous_bookings_not_canceled
14	reserved_room_type
15	assigned_room_type
16	booking_changes
17	deposit_type
18	days_in_waiting_list
19	customer_type
20	average_daily_rate
21	required_car_parking_spaces
22	total_of_special_requests
23	arrival_date

CBS

https://www.tidymodels.org/start/case-study/

Tidymodels - Model Tuning



https://jhudatascience.org/tidyversecourse/model.html

Random Forrest - ***ranger::ranger()***

Pre-processing with recipes

```
rf_recipe <-
  recipe(children ~ ., data = hotel_train) %>%
  step_date(arrival_date) %>%  # creates predictors for the year, month, and day of the week.
  step_holiday(arrival_date) %>% # generates a set of indicator variables for specific holidays.
  step_rm(arrival_date) #removes variables;
```

Model Specifications

```
Cores = parallel::detectCores()
set.seed(345)
# Define Model
rf_model <-
  rand_forest(mtry = tune(), min_n = tune(), trees = 1000) %>%
  set_engine("ranger", num.threads = Cores) %>%
  set_mode("classification")

# Define Workflow
rf_workflow <-
  workflow() %>%
  add_model(rf_model) %>%
  add_recipe(rf_recipe)
```

Grid Tuning – In Parallel

```
# Grid-Tune with 8(4) Cores
tic()
rf_tune <-
  rf_workflow %>%
  tune_grid(hotel_validation,
        grid = nGrid,
        control = control_grid(save_pred = TRUE),
        metrics = metric_set(roc_auc))
toc()

47.3 sec elapsed
```

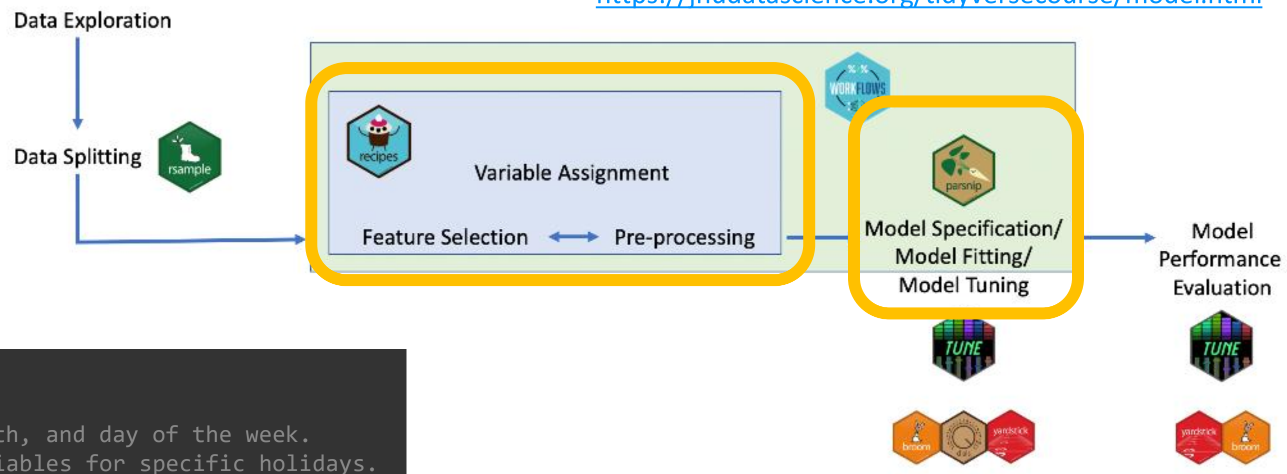
Grid Tuning – Not in Parallel

```
# Grid-Tune with 1 Core
tic()
rf_tune <-
  rf_workflow %>%
  tune_grid(hotel_validation,
        grid = nGrid,
        control = control_grid(save_pred = TRUE),
        metrics = metric_set(roc_auc))
toc()

208.8 sec elapsed
```

CBS

https://jhudatascience.org/tidyversecourse/model.html

Tidymodels - Model Tuning



Neural Network - ***nnet::nnet()***

Pre-processing with recipes

```
nnet_recipe <-
  recipe(children ~ ., data = hotel_train) %>%
  step_date(arrival_date) %>%                        # creates predictors for the year, month, and day of the week.
  step_holiday(arrival_date, holidays = holidays) %>%   # generates a set of indicator variables for specific holidays.
  step_rm(arrival_date) %>%                          # removes orginal variables;
  step_dummy(all_nominal_predictors()) %>%           # Converts characters or factors dummy variables.
  step_zv(all_predictors()) %>%                      # removes orginal variables;
  step_normalize(all_predictors())
```

Model Specifications

```
# Define Model
nnet_model <-
  mlp(hidden_units = tune(), penalty = tune(),
epochs = tune()) %>%
  set_engine("nnet", trace = 0,MaxNWts = 10000) %>%
  set_mode("classification")


# Define Workflow
nnet_workflow <-
  workflow() %>%
  add_model(nnet_model) %>%
  add_recipe(nnet_recipe)
```

Grid Tuning – In Parallel

```
# Grid-Tune with Multiple Cores
library(doParallel)
library(foreach)
cl <- makePSOCKcluster(parallel::detectCores())
registerDoParallel(cl)


tic()
nnet_tune <-
  nnet_workflow  %>%
  tune_grid(hotel_validation,
        grid = 5,
        control = control_grid(save_pred = TRUE,parallel_over = "everything"),
        metrics = metric_set(roc_auc))
toc()
stopCluster(cl)

293.41 sec elapsed
```

Grid Tuning – Not in Parallel

```
# Grid-Tune with Multiple Cores
library(doParallel)
library(foreach)
cl <- makePSOCKcluster(parallel::detectCores())
registerDoParallel(cl)


tic()
nnet_tune <-
  nnet_workflow  %>%
  tune_grid(hotel_validation,
        grid = 5,
        control = control_grid(save_pred = TRUE,parallel_over = "resamples"),
        metrics = metric_set(roc_auc))
toc()
stopCluster(cl)

600.77 sec elapsed
```

```
# Grid-Tune with No Parallelisation
tic()
nnet_tune <-
  nnet_workflow  %>%
  tune_grid(hotel_validation,
        grid = 5,
        control = control_grid(save_pred = TRUE,parallel_over = "everything"),
        metrics = metric_set(roc_auc))
toc()

676.7 sec elapsed
```

Distributed Computing on UCloud (SLURM cluster)

Neural Network - ***nnet::nnet()***

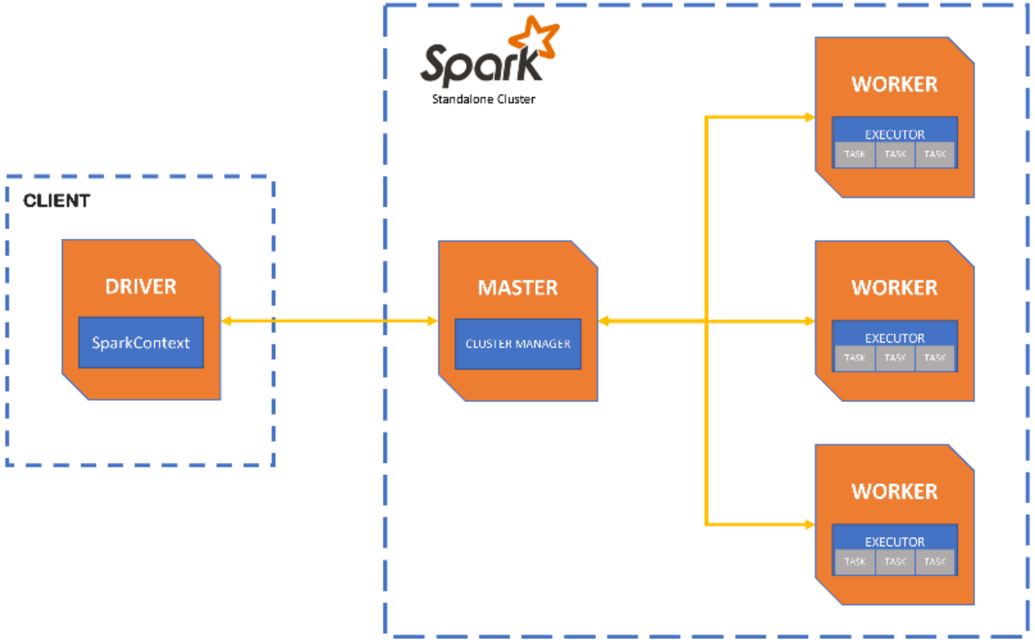
```
# Get Input arguments
args = commandArgs(trailingOnly=TRUE)
nproces = as.numeric(args[1])


# Get Cluster Info
hostlist <- paste(unlist(read.delim(file="hostnames.txt", header=F, sep =" ")))
for (i in 0:length(hostlist)){
  if (i == 0){
hosts <- rep(hostlist[i],nproces)
  } else {
hosts <-c(hosts, rep(hostlist[i],nproces))
  }
}


tic()
# Starting Up Cluster
cl <- makePSOCKcluster(names=hosts)
#cl <- makePSOCKcluster(parallel::detectCores())

registerDoParallel(cl)

# Grid-Tune
nnet_tune <-
  nnet_workflow  %>%
  tune_grid(hotel_validation,
        grid = nGrid,
        control = control_grid(save_pred = TRUE,parallel_over = "everything"),
        metrics = metric_set(roc_auc))
toc()
stopCluster(cl)
```

https://cbs-hpc.github.io/Tutorials/SLURM/SLURM/

https://cloud.sdu.dk/app/jobs/properties/792600?app=

```
#run the parallel calculation
x <- iris[which(iris[,5] != "setosa"), c(1,5)]
trials <- 200000
system.time({
r <- foreach(icount(trials), .combine=rbind) %dopar% {
ind <- sample(100, 100, replace=TRUE)
result1 <- glm(x[ind,2]~x[ind,1], family=binomial(logit))
coefficients(result1)
}
})

stopCluster(cl)
```

Apache Spark (RSpark) Cluster on UCloud



https://docs.cloud.sdu.dk/Apps/jupyter-lab.html?highlight=jupyterlab

https://docs.cloud.sdu.dk/Apps/spark-cluster.html?highlight=spark

https://cloud.sdu.dk/app/jobs/create?app=spark-cluster&version=3.4.0

CBS COPENHAGEN BUSINESS SCHOOL
HANDELSHØJSKOLEN

QUESTIONS?

Kristoffer Gulmark Poulsen & Lars Nondal
CBS