Efficient R

Scientific workflows: Tools and Tips 🛠️

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What is this lecture series?

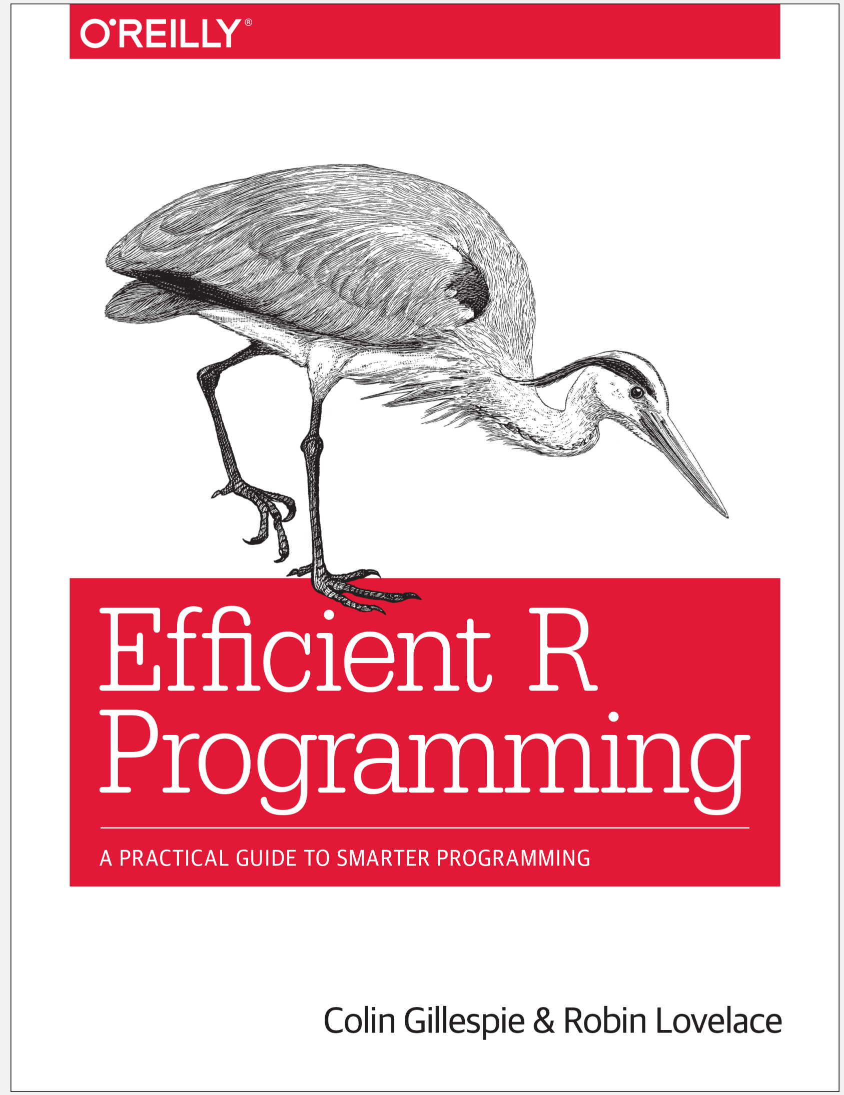
Scientific workflows: Tools and Tips 🛠️

📅 Every 3rd Thursday 🕓 4-5 p.m. 📍 Webex

- One topic from the world of scientific workflows
- Material provided online
- If you don't want to miss a lecture
    - Subscribe to the mailing list

Main reference

Efficient R book by Gillespie and Lovelace, read it here



What is efficiency?

$$\text{efficiency} = \frac{\text{work done}}{\text{unit of effort}}$$

Computational efficiency

💻 Computation time

💾 Memory usage

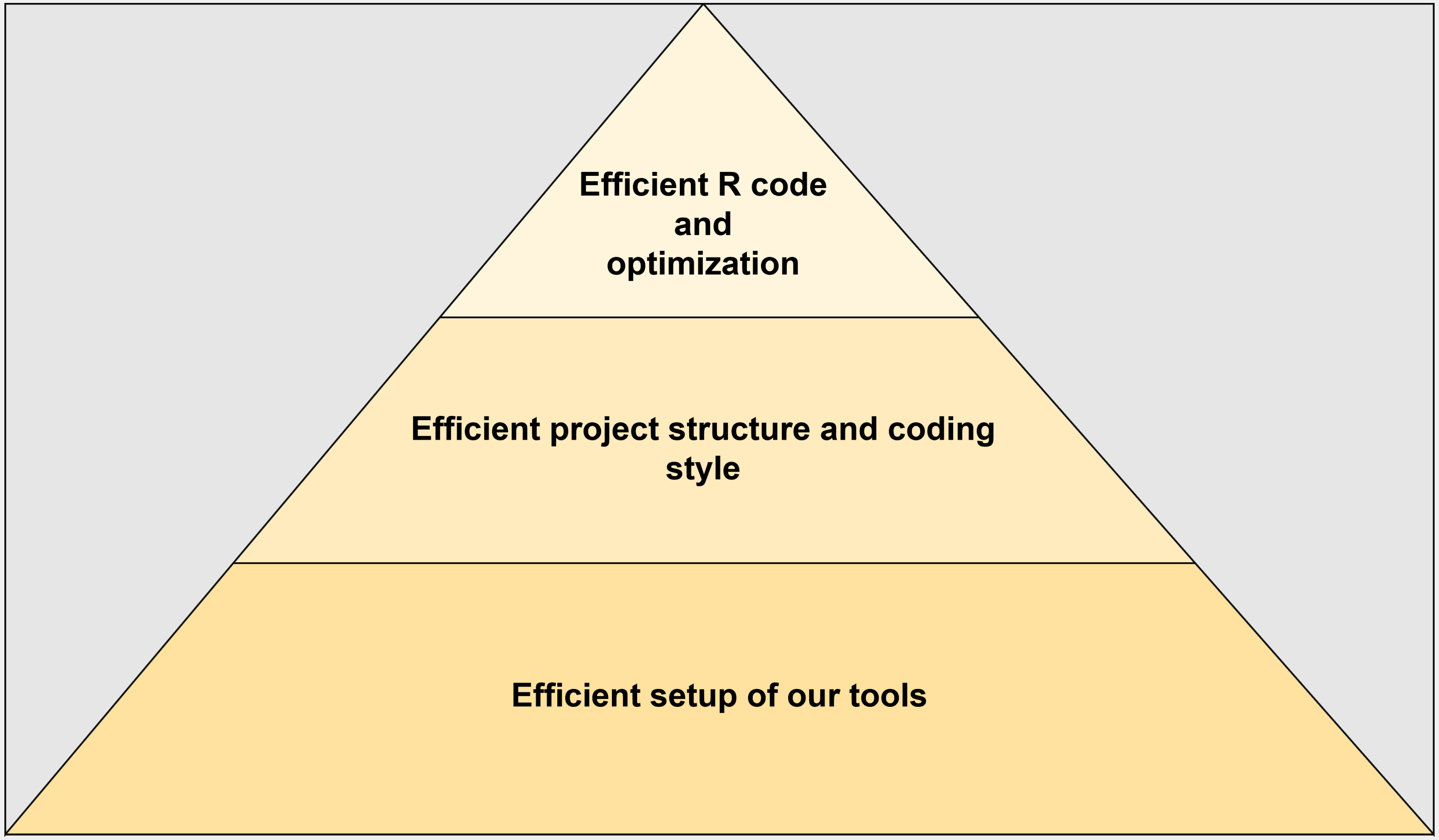
Programmer efficiency

🧍 How long does it take to

- *write* code?
- *maintain* code?
- *read* and *understand* the code?

Tradeoffs and **Synergies** between these types of efficiencies

Today

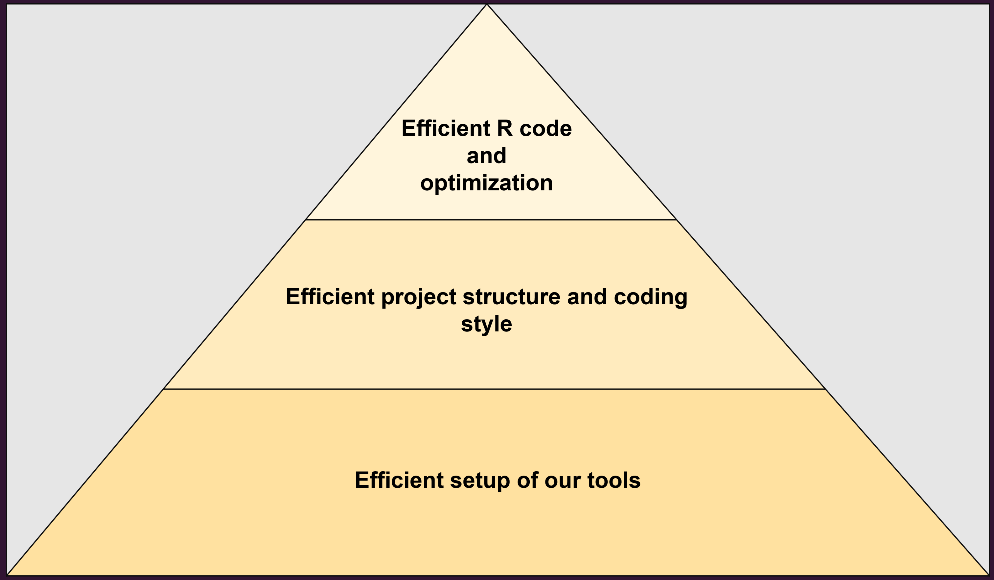


Principles and **tools** to make R programming more effiicent for 💻

Check out my talk "What they forgot to teach you about R" for first two levels

Efficient R code and optimization

> How can I make my R code faster?



Is R slow?

- R is slow compared to other programming languages (e.g. C++).
  - R is designed to make programming easy, not fast
- R is not designed to be memory efficient
- But: R is fast and memory efficient enough for most tasks.

Should I optimize?

> It's easy to get caught up in trying to remove all bottlenecks. Don't! Your time is valuable and is better spent analysing your data, not eliminating possible inefficiencies in your code. **Be pragmatic**: don't spend hours of your time to save seconds of computer time.
> (Hadley Wickham in Advanced R)

Think about

- How much time do I **save** by optimizing?
- **How often** do I run the code?
- How much time do I **spend** optimizing?

Often: Trade-off between **readability** and **efficiency**

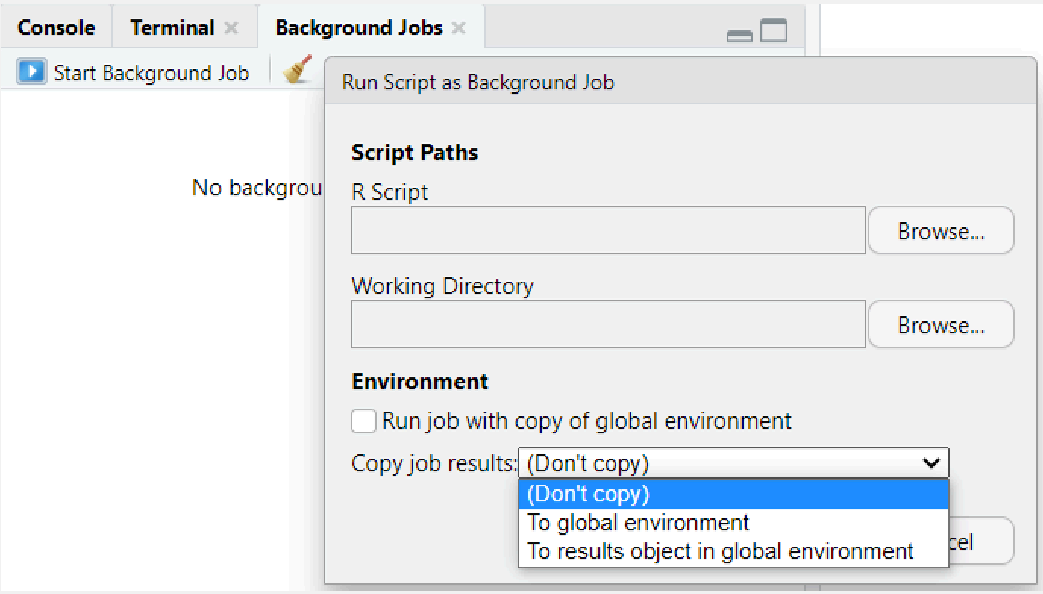
Should I optimize?

If your code is to slow for you, you can go through these steps:

1. If possible, **run the code somewhere else**

Run the code somewhere else

- For this, RStudio has **background jobs**



- Or: run it on a cluster (e.g. FU Curta)

Should I optimize?

If your code is to slow for you, you can go through these steps:

1. If possible, **run the code somewhere else**
2. **Identify the critical** (slow) **parts** of your code
3. Then **optimize only the bottlenecks**

Identify critical parts of your code

> **Profiling** & **Benchmarking** to measure the speed and memory use of your code

Profiling R code

What are the speed & memory bottlenecks in my code?

- Use the `profvis` package

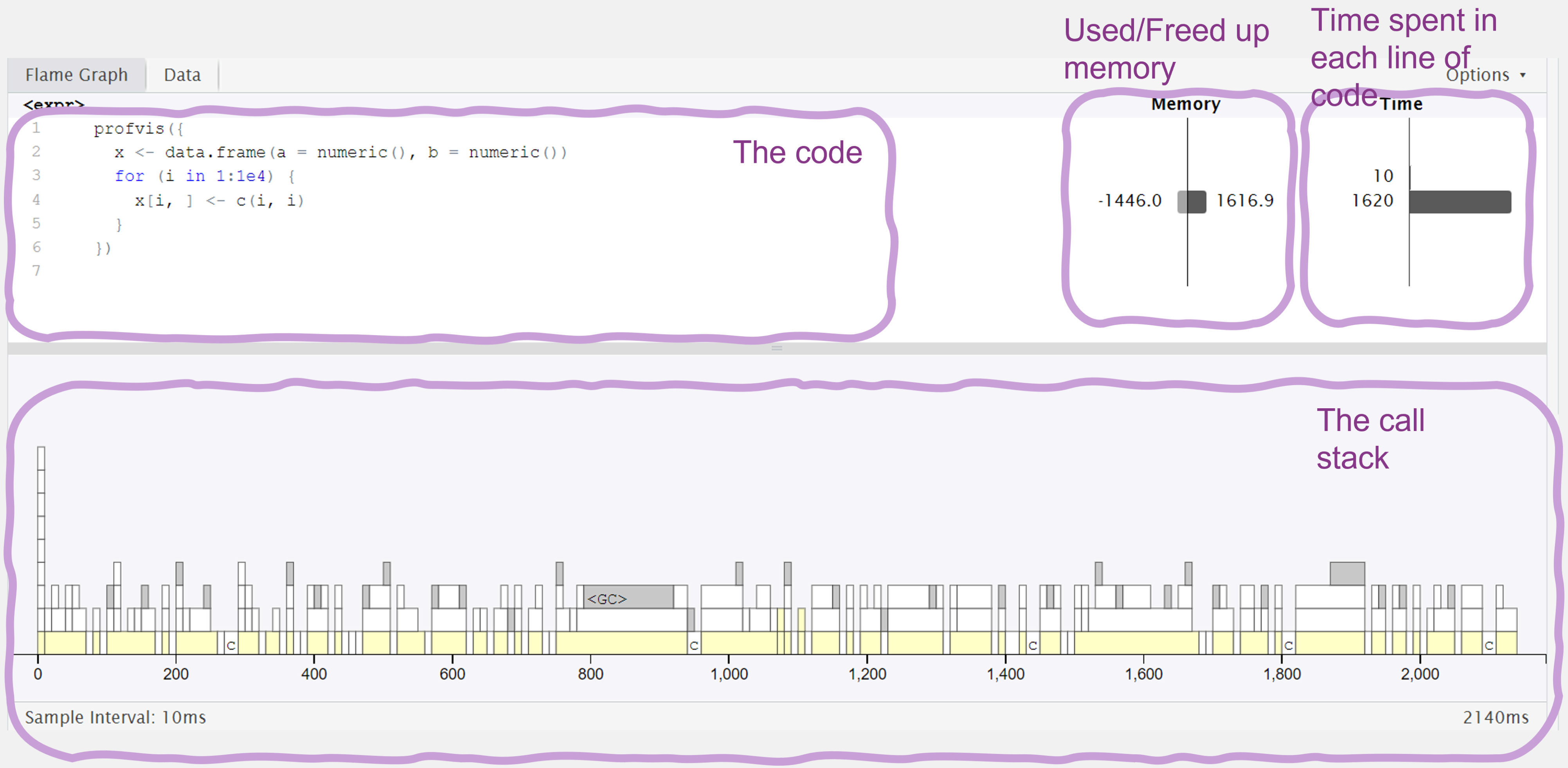
Profiling R code

You can profile a section of code like this:

```
# install.packages("profvis")
library(profvis)

# Create a data frame with 150 columns and 400000 rows
df <- data.frame(matrix(rnorm(150 * 400000), nrow = 400000))

profvis({
  # Calculate mean of each column and put it in a vector
  means <- apply(df, 2, mean)

  # Subtract mean from each value in the table
  for (i in seq_along(means)) {
    df[, i] <- df[, i] - means[i]
  }
})
```

Profiling R code

Profvis flame graph shows time and memory spent in each line of code.



Profiling R code

Profvis data view for details on time spent in each function in the call stack.

Flame Graph | Data | Options ▾

Code	File	Memory (MB)		Time (ms)
▶ [<-.data.frame	<expr>	-1446.0	1547.2	1600
c		-445.2	355.7	360
any		-69.9	83.5	70
length		-78.5	34.4	40
[<-	<expr>	0	34.9	20
▶ compiler:::tryCompile	<expr>	0	0	10
attr		-44.4	0	10
as.character		0	16.7	10
dim		0	17.7	10
all		0	10.9	10

Profiling R code

You can also interactively profile code in RStudio:

- Go to **Profile -> Start profiling**
- Now interactively run the code you want to profile
- Go to **Profile -> Stop profiling** to see the results

Benchmarking R code

Which version of the code is faster?

```
# Fill a data frame in a loop
f1 <- function() {
  x <- data.frame(a = numeric(), b = numeric())
  for (i in 1:1e4) {
    x[i, ] <- c(i, i)
  }
}

# Fill a data frame directly with vectors
f2 <- function() {
  x <- data.frame(a = 1:1e4, b = 1:1e4)
}
```

Benchmarking R code

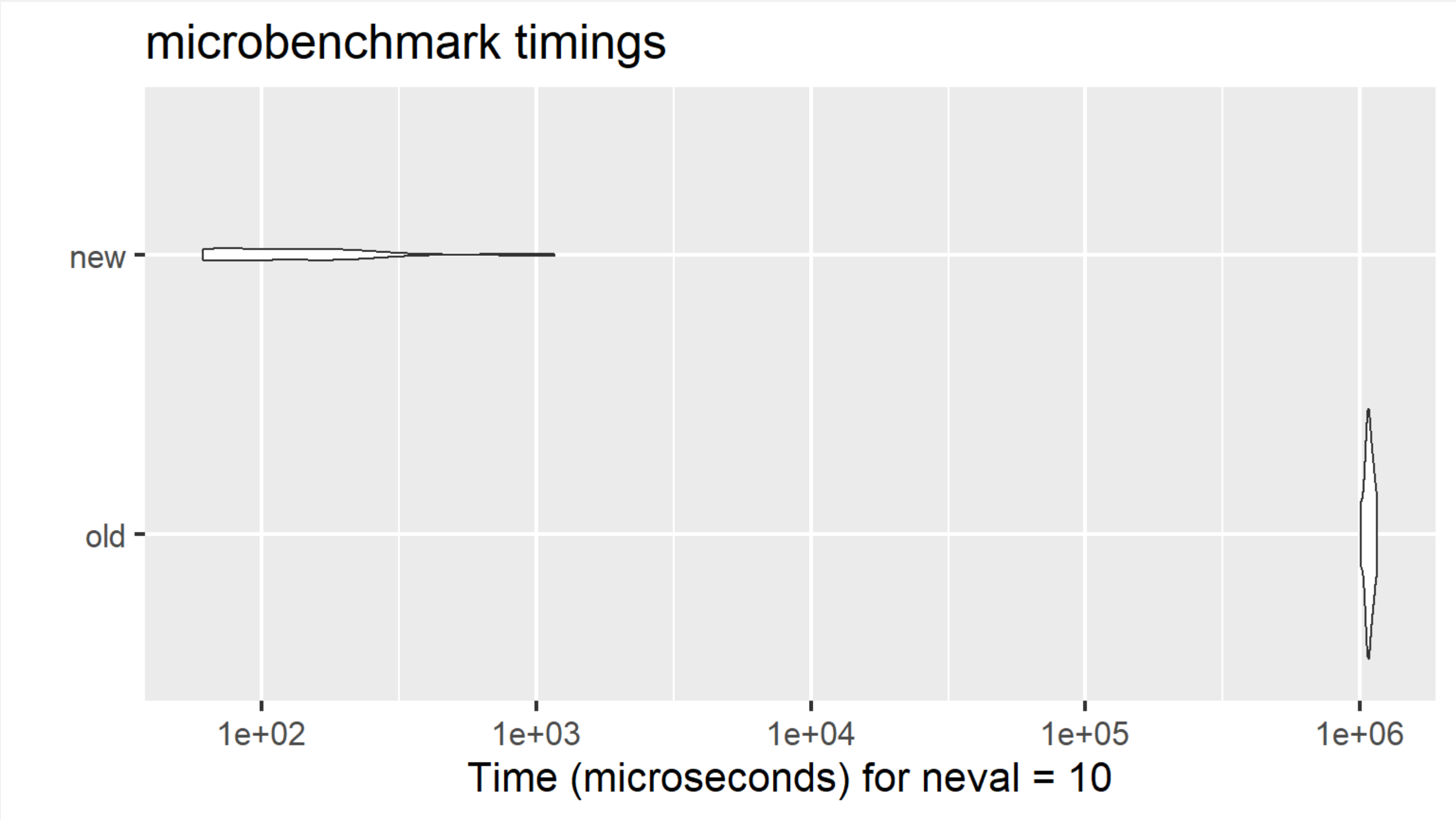
Use the `microbenchmark` package to compare the functions:

```r
# install.packages("microbenchmark")
library(microbenchmark)

compare_functions <- microbenchmark(
  old = f1(),
  new = f2(),
  times = 10 # default is 100
)

compare_functions
#> Unit: microseconds
#>  expr       min        lq       mean     median        uq       max neval cld
#>   old 1002499.6 1060133.0 1079288.02 1076095.05 1114314.0 1154355.1    10  a
#>   new      61.2      75.4     224.95     128.25     188.7    1159.9    10   b
```

We can look at benchmarking results using ggplot

```r
library(ggplot2)
autoplot(compare_functions)
```

Benchmarking R code



Optimize your code

- Basic principles
- Data analysis bottlenecks
- Advanced optimization: Parallelization and C++

Basic principles

Vectorize your code

- Vectors are central to R programming
- R is optimized for vectorized code
  - Implemented directly in C/Fortran
- Vector operations can often replace for-loops in R
- If there is a vectorized version of a function: Use it

Vectorize your code

Example: Calculate the log of every value in a vector and sum up the result

```r
# A vector with 1 million values
x <- 1:1e6

microbenchmark(
  for_loop = {
    log_sum <- 0
    for (i in 1:length(x)) {
      log_sum <- log_sum + log(x[i])
    }
  },
  sum = sum(log(x)),
  times = 10
)
#> Unit: milliseconds
#>      expr     min      lq     mean  median      uq     max neval cld
#>  for_loop 57.4552 57.6585 58.30977 57.8171 58.5632 60.5313    10  a
#>       sum 34.4765 34.5689 35.97568 35.9104 37.1005 37.4713    10   b
```

For-loops in R

- For-loops are **relatively slow** and it is easy to make them even slower with bad design
- Often they are used when vectorized code would be better
- For loops can often be replaced, e.g. by
  - Functions from the apply family (e.g. `apply`, `lapply`, …)
  - Vectorized functions (e.g. `sum`, `colMeans`, …)
  - Vectorized functions from the `purrr` package (e.g. `map`)

But: For loops are not necessarily bad, **sometimes** they are the **best solution** and **more readable** than vectorized code.

Cache variables

If you use a value multiple times, store it in a variable to avoid re-calculation

Example: Calculate column means and normalize them by the standard deviation

```
# A matrix with 1000 columns
x <- matrix(rnorm(10000), ncol = 1000)

microbenchmark(
  no_cache = apply(x, 2, function(i) mean(i) / sd(x)),
  cache = {
    sd_x <- sd(x)
    apply(x, 2, function(i) mean(i) / sd_x)
  }
)
#> Unit: milliseconds
#>      expr     min       lq      mean   median       uq      max neval cld
#>  no_cache 53.2709 55.12830 57.713778 56.75735 58.37760 144.2293   100   a
#>     cache  3.2145  3.34235  3.497462  3.42090  3.53655   5.3185   100   b
```

Efficient data analysis

Efficient workflow

- Prepare the data to be clean and concise for analysis
  - Helps to avoid unnecessary calculations
- Save intermediate results
  - Don’t re-run time consuming steps if not necessary
- Use the right packages and functions

Read data

Example: Read csv data on worldwide emissions of greenhouse gases (~14000 rows, 7 cols).

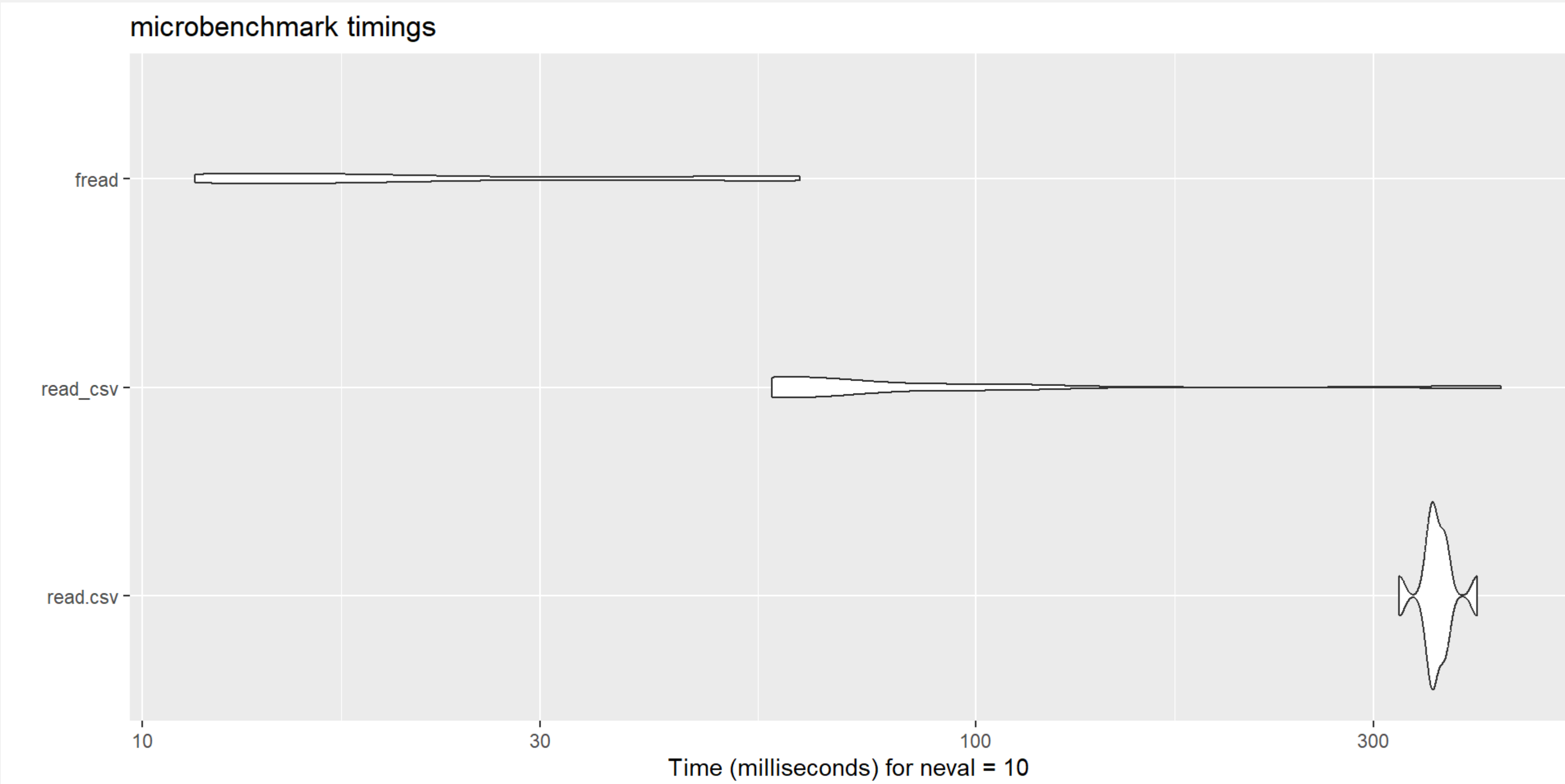
- Base-R functions to read csv files are:
  - `read.table`
  - `read.csv`
- There are many alternatives to read data, e.g.:
  - `read_csv` from the `readr` package (tidyverse)
  - `fread` from the `data.table` package

Read data

Compare some alternative reading functions

```r
file_path_csv <- here::here("slides/data/ghg_ems_large.csv")

compare_input <- microbenchmark::microbenchmark(
  read.csv = read.csv(file_path_csv),
  read_csv = readr::read_csv(file_path_csv, progress = FALSE, show_col_types = FALSE),
  fread = data.table::fread(file_path_csv, showProgress = FALSE),
  times = 10
)

autoplot(compare_input)
```

Read data

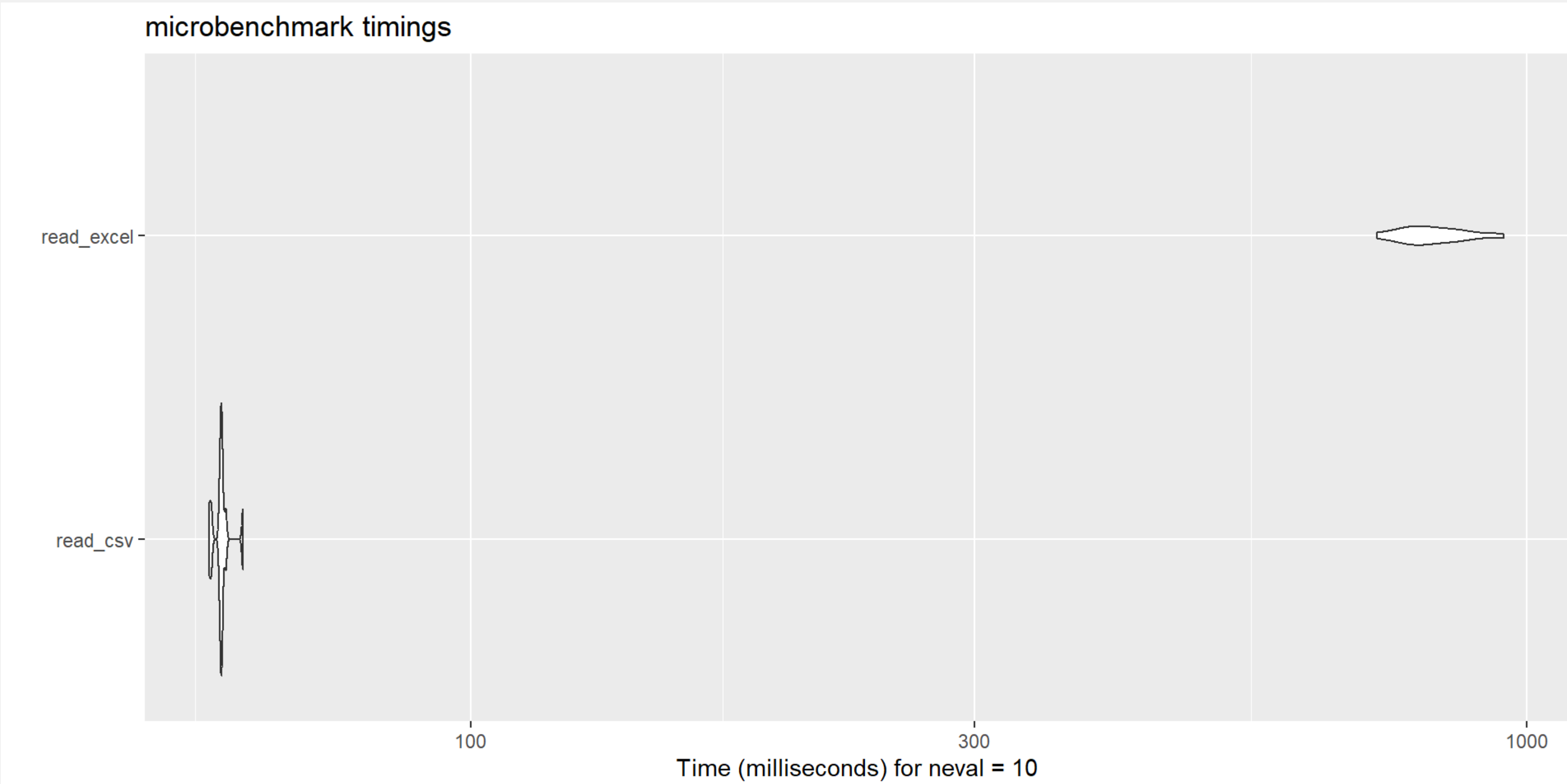

microbenchmark timings
fread
read_csv
read.csv
10
30
100
300
Time (milliseconds) for neval = 10

Use plain text data

Reading plain text is faster than excel files

```r
file_path_xlsx <- here::here("slides/data/ghg_ems_large.xlsx")

compare_excel <- microbenchmark(
  read_csv = readr::read_csv(file_path_csv, progress = FALSE, show_col_types = FALSE),
  read_excel = readxl::read_excel(file_path_xlsx),
  times = 10
)

autoplot(compare_excel)
```

Use plain text data



Write data

- Base-R functions to write files are:
  - `write.table`
  - `write.csv`
- Faster alternatives are:
  - `write_csv` from the `readr` package (tidyverse)
  - `fwrite` from the `data.table` package

Write data

Efficient data manipulation

Different packages offer fast and efficient data manipulation and analysis:

- `dplyr` package has a C++ backend and is often faster than base R
- `data.table` package is fast and memory efficiency
  - Syntax is quite different from base R and `tidyverse`
- `collapse` package is a C++ based and specifically developed for fast data analysis
  - Works together with both `tidyverse` and `data.table` workflows
  - Many functions similar to base R or `dplyr` just with prefix "f" (e.g. `fselect`, `fmean`, …)

Summarize data by group

Example: Summarize mean carbon emissions from Electricity by Country

```
library(data.table)
library(dplyr)
library(collapse)
```

Summarize data by group

Example: Summarize mean carbon emissions from Electricity by Country

```r
# 1. The data table way
# Convert the data to a data.table
setDT(ghg_ems)
summarize_dt <- function(){
  ghg_ems[, mean(Electricity, na.rm = TRUE), by = Country]
}

# 2. The dplyr way
summarize_dplyr <- function(){
  ghg_ems |>
      group_by(Country) |>
      summarize(mean_e = mean(Electricity, na.rm = TRUE))
}

# 3. The collapse way
summarize_collapse <- function(){
  ghg_ems |>
      fgroup_by(Country) |>
      fsummarise(mean_e = fmean(Electricity))
}
```

Summarize data by group

Example: Summarize mean carbon emissions from Electricity by Country

```
# compare the speed of all versions
microbenchmark(
  dplyr = summarize_dplyr(),
  data_table = summarize_dt(),
  collapse = summarize_collapse(),
  times = 10
)
#> Unit: microseconds
#>        expr    min     lq    mean  median     uq    max neval cld
#>       dplyr 2171.6 2247.2 2770.77 2292.95 2385.4 6200.0    10  a
#>  data_table 1117.7 1165.2 1701.59 1336.75 1475.6 4723.7    10  a
#>    collapse  121.0  135.1  317.80  171.60  183.7 1086.3    10   b
```

Select columns

Example: Select columns Country, Year, Electricity, Transportation

```
microbenchmark(
  dplyr = select(ghg_ems, Country, Year, Electricity, Transportation),
  data_table = ghg_ems[, .(Country, Electricity, Transportation)],
  collapse = fselect(ghg_ems, Country, Electricity, Transportation),
  times = 10
)
#> Unit: microseconds
#>        expr   min    lq   mean median    uq    max neval cld
#>       dplyr 578.7 618.2 945.12  668.2 998.4 2777.2    10 a
#>  data_table 345.8 357.8 468.37  398.7 481.7  888.5    10  b
#>    collapse   3.4   3.7  14.47    7.4  12.0   74.9    10   c
```

Advanced optimization

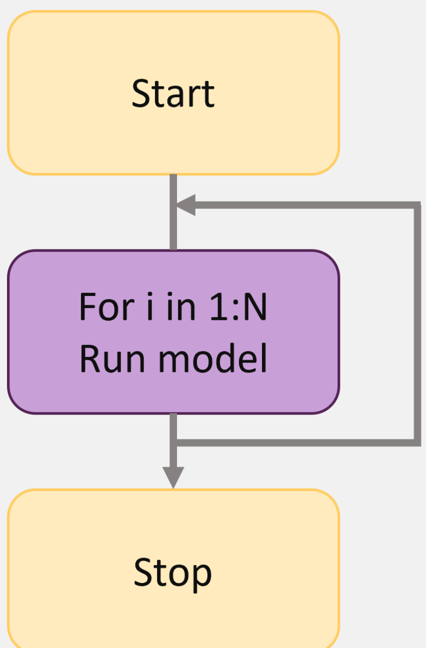
Parallelization and C++

Parallelization

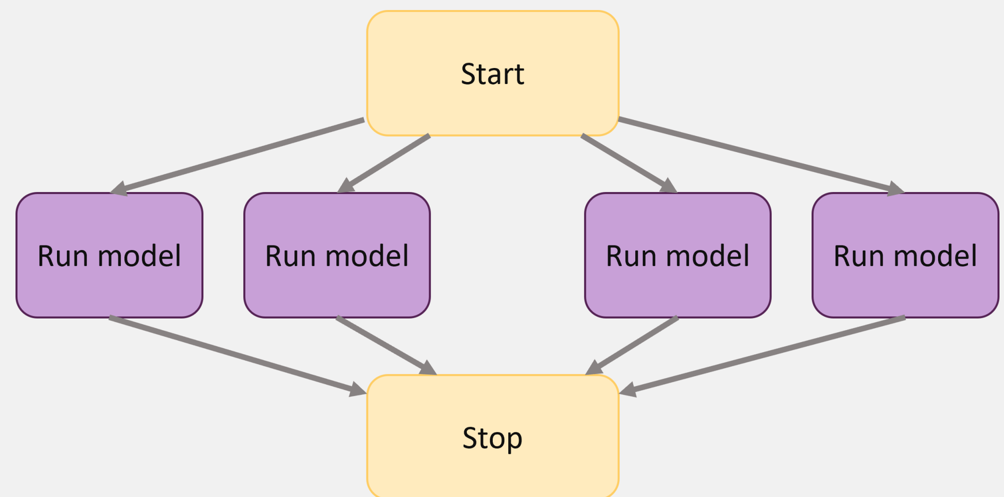
By default, R works on one core but CPUs have multiple cores

```
# Find out how many cores you have with the parallel package
# install.packages("parallel")
parallel::detectCores()
#> [1] 32
```

Sequential



Parallel



Parallelization with the futureverse

- `future` is a framework to help you parallelize existing R code
  - Parallel versions of base R apply family
  - Parallel versions of `purrr` functions
  - Parallel versions of `foreach` loops
- Find more details here
- Find a tutorial for different use cases here

A slow example

Let's create a very slow square root function

```
slow_sqrt <- function(x){
  Sys.sleep(1) # simulate 1 second of computation time
  sqrt(x)
}
```

Before you run anything in parallel, tell R how many cores to use:

```
library(future)
# Plan parallel session with 6 cores
plan(multisession, workers = 6)
```

Parallel apply functions

To run the function on a vector of numbers we could use

The **sequential** version

```
# to measure the runtime
library(tictoc)

# create a vector of 10 numbers
x <- 1:10

tic()
result <- lapply(x, slow_sqrt)
toc()
#> 10.16 sec elapsed
```

The **parallel** version

```
# Load future.apply package
library(future.apply)

tic()
result <- future_lapply(x, slow_sqrt)
toc()
#> 2.38 sec elapsed
```

Parallel apply functions

Selected base R apply functions and their future versions:

base	future.apply
`lapply`	`future_lapply`
`sapply`	`future_sapply`
`vapply`	`future_vapply`
`mapply`	`future_mapply`
`tapply`	`future_tapply`
`apply`	`future_apply`
`Map`	`future_Map`

Parallel for loops

A normal for loop:

```
z <- list()
for (i in 1:10){
  z[i] <- slow_sqrt(i)
}
```

Use `foreach` to write the same loop

```
library(foreach)
z <- foreach(i = 1:10) %do% {
  slow_sqrt(i)
}
```

Parallel for loops

Use `doFuture` and `foreach` package to parallelize for loops

The **sequential** version

```
library(foreach)

tic()
z <- foreach(i = 1:10) %do% {
  slow_sqrt(i)
}
toc()
#> 10.17 sec elapsed
```

The **parallel** version

```
library(doFuture)

tic()
z <- foreach(i = 1:10) %dofuture% {
  slow_sqrt(i)
}
toc()
#> 2.25 sec elapsed
```

Close multisession

When you are done working in parallel, explicitly close your multisession:

```
# close the multisession plan
plan(sequential)
```

Replace slow code with C++

- Use the `Rcpp` package to re-write R functions in C++
- `Rcpp` is also used internally by many R packages to make them faster
- Requirements:
  - C++ compiler installed
  - Some knowledge of C++
- See this book chapter and the online documentation for more info

Rewrite a function in C++

Example: R function to calculate Fibonacci numbers

```r
# A function to calculate Fibonacci numbers
fibonacci_r <- function(n){
  if (n < 2){
    return(n)
  } else {
    return(fibonacci_r(n - 1) + fibonacci_r(n - 2))
  }
}
```

```r
# Calculate the 30th Fibonacci number
fibonacci_r(30)
#> [1] 832040
```

Rewrite a function in C++

Use `cppFunction` to rewrite the function in C++:

```
library(Rcpp)

# Rewrite the fibonacci_r function in C++
fibonacci_cpp <- cppFunction(
  'int fibonacci_cpp(int n){
    if (n < 2){
      return(n);
    } else {
      return(fibonacci_cpp(n - 1) + fibonacci_cpp(n - 2));
    }
  }'
)
```

```
# calculate the 30th Fibonacci number
fibonacci_cpp(30)
#> [1] 832040
```

Rewrite a function in C++

You can also source C++ functions from C++ scripts.

C++ script `fibonacci.cpp`:

```
#include "Rcpp.h"

// [[Rcpp::export]]
int fibonacci_cpp(const int x) {
   if (x < 2) return(x);
   return (fibonacci(x - 1)) + fibonacci(x - 2);
}
```

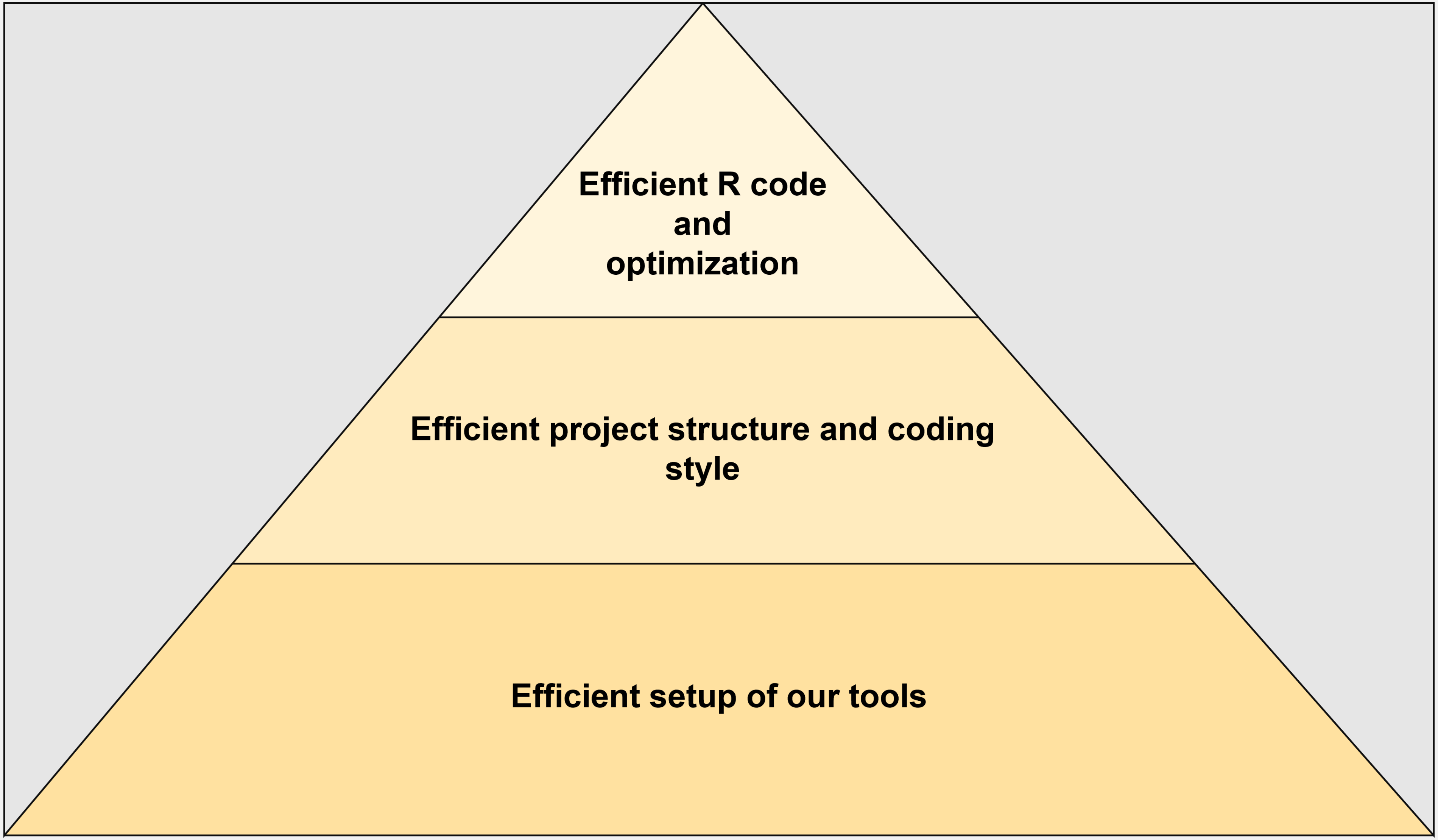
Then source the function in your R script using `sourceCpp`:

```
sourceCpp("fibonacci.cpp")

# Use the function in your R script like you are used to
fibonacci_cpp(30)
```

How much faster is C++?

```
microbenchmark(
  r = fibonacci_r(30),
  rcpp = fibonacci_cpp(30),
  times = 10
)
#> Unit: microseconds
#>  expr      min       lq     mean   median       uq      max neval cld
#>     r 508682.9 509692.8 514182.4 510576.9 521544.7 524277.9    10  a
#>  rcpp    837.4    840.2    920.2    849.8    872.3   1546.9    10   b
```

Summary


Efficient R code and optimization
Efficient project structure and coding style
Efficient setup of our tools

Next lecture

Topic t.b.a.

📆 18th January 🕓 4-5 p.m. 📍 Webex

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Thank you for your attention :)

Questions?