Future: Parallel & Distributed Processing in R for Everyone

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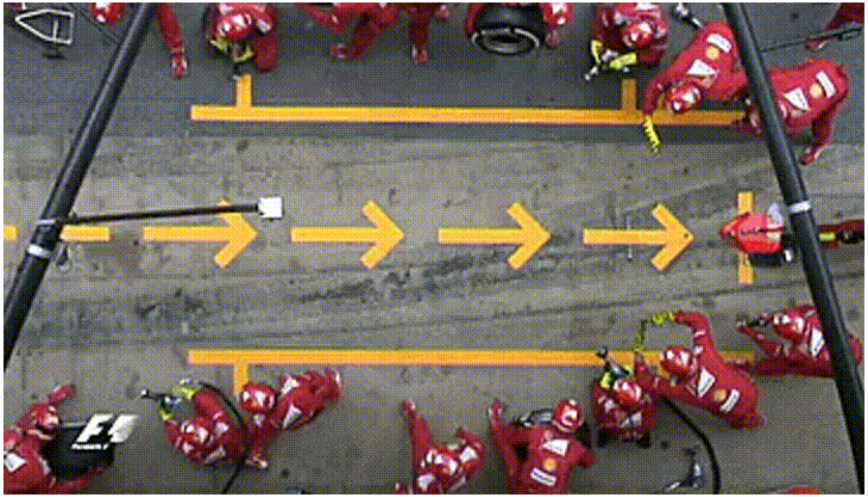


Acknowledgments

- eRum 2018
- R Consortium
- R Core, CRAN, devels & users!

A 20-minute presentation, eRum 2018, Budapest, 2018-05-16

Why do we parallelize software?

Parallel & distributed processing can be used to:

1. **speed up processing** (wall time)
2. **decrease memory footprint** (per machine)
3. **avoid data transfers**

Comment: I'll focuses on the first two in this talk.

Definition: Future

- A **future** is an abstraction for a **value** that will be **available later**
- The value is the **result of an evaluated expression**
- The **state of a future** is **unevaluated** or **evaluated**

Friedman & Wise (1976, 1977), Hibbard (1976), Baker & Hewitt (1977)

Definition: Future

- A **future** is an abstraction for a **value** that will be **available later**
- The value is the **result of an evaluated expression**
- The **state of a future** is **unevaluated** or **evaluated**

Standard R:

```
v <- expr
```

Future API:

```
f <- future(expr)
v <- value(f)
```

Example: Sum of 1:50 and 51:100 in parallel

```
> library(future)
> plan(multiprocess)

> fa <- future( slow_sum( 1:50 ) )
> fb <- future( slow_sum(51:100) )
> 1:3
[1] 1 2 3

> value(fa)
[1] 1275
> value(fb)
[1] 3775

> value(fa) + value(fb)
[1] 5050
```

Definition: Future

Standard R:

```
v <- expr
```

Future API (implicit):

```
v %<-% expr
```

Example: Sum of 1:50 and 51:100 in parallel (implicit API)

```
> library(future)
> plan(multiprocess)

> a %<-% slow_sum( 1:50 )
> b %<-% slow_sum(51:100)
> 1:3
[1] 1 2 3

> a + b
[1] 5050
```

Many ways to resolve futures

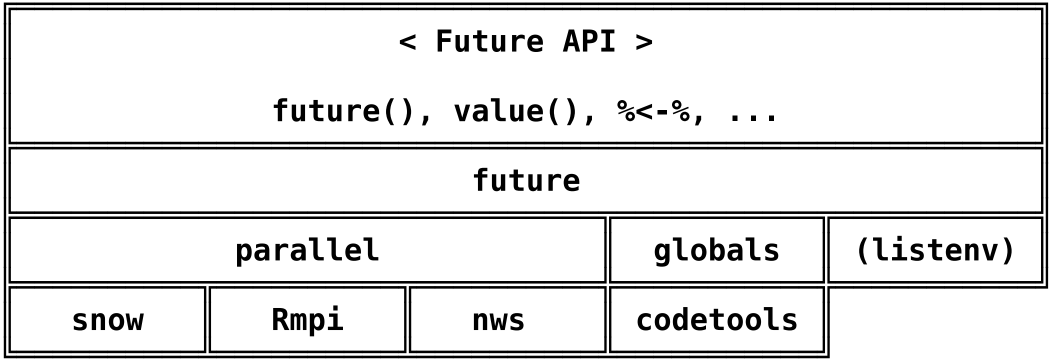
```
plan(sequential)
plan(multiprocess)
plan(cluster, workers = c("n1", "n2", "n3"))
plan(cluster, workers = c("remote1.org", "remote2.org"))
...
```

```
> a %<-% slow_sum( 1:50 )
> b %<-% slow_sum(51:100)
> a + b
[1] 5050
```

R package: future

CRAN 1.8.1 codecov 90%

- "Write once, run anywhere"
- A simple **unified API** ("interface of interfaces")
- **100% cross platform**
- **Easy to install** (~0.4 MiB total)
- **Very well tested, lots of CPU mileage, production ready**



< Future API >

future(), value(), %<-%, ...

future

parallel globals (listenv)

snow Rmpi nws codetools

Why a Future API?

Problem: heterogeneity

- Different parallel backends ⇔ different APIs
- Choosing API/backend, limits user's options

```
x <- list(a = 1:50, b = 51:100)
y <- lapply(x, FUN = slow_sum)
```

```
y <- parallel::mclapply(x, FUN = slow_sum)
```

```
library(parallel)
cluster <- makeCluster(4)
y <- parLapply(cluster, x, fun = slow_sum)
stopCluster(cluster)
```

Why a Future API?

Solution: "interface of interfaces"

- The Future API encapsulates heterogeneity
  - fever decisions for developer to make
  - more power to the end user
- Philosophy:
  - **developer decides what to parallelize - user decides how to**
- Provides **atomic building blocks** for richer parallel constructs, e.g. 'foreach' and 'future.apply'
- Easy to implement new backends, e.g. 'future.batchtools' and 'future.callr'

Why a Future API?

99% Worry Free

- **Globals**: automatically **identified & exported**
- **Packages**: automatically **identified & exported**
- **Static-code inspection** by walking the AST

```
x <- rnorm(n = 100)
y <- future({ slow_sum(x) })
```

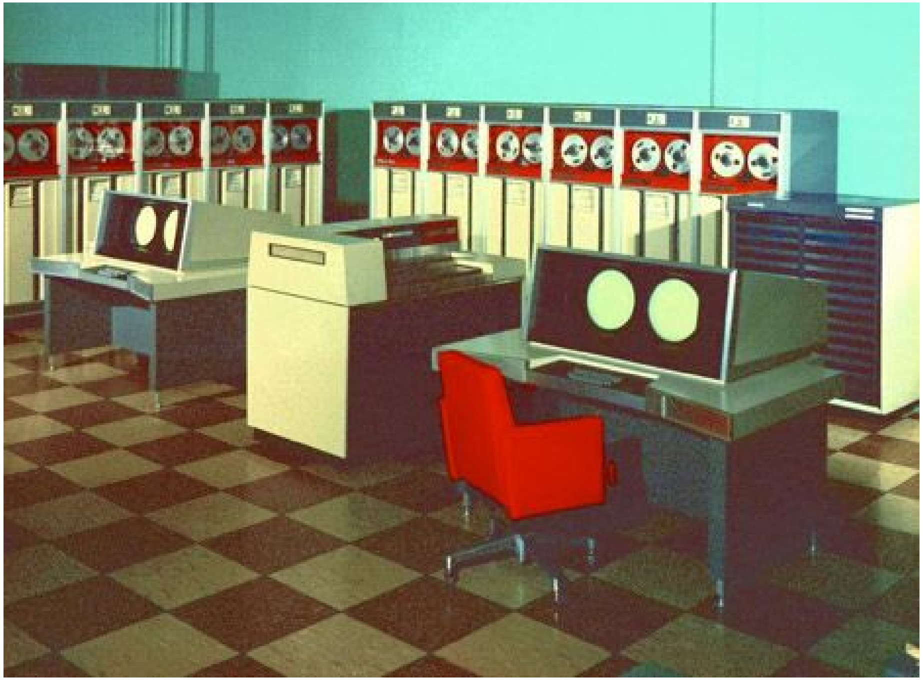
Globals identified and exported:

1. `slow_sum()` - a function (also searched recursively)

2. `x` - a numeric vector of length 100

Globals & packages can be specified manually too

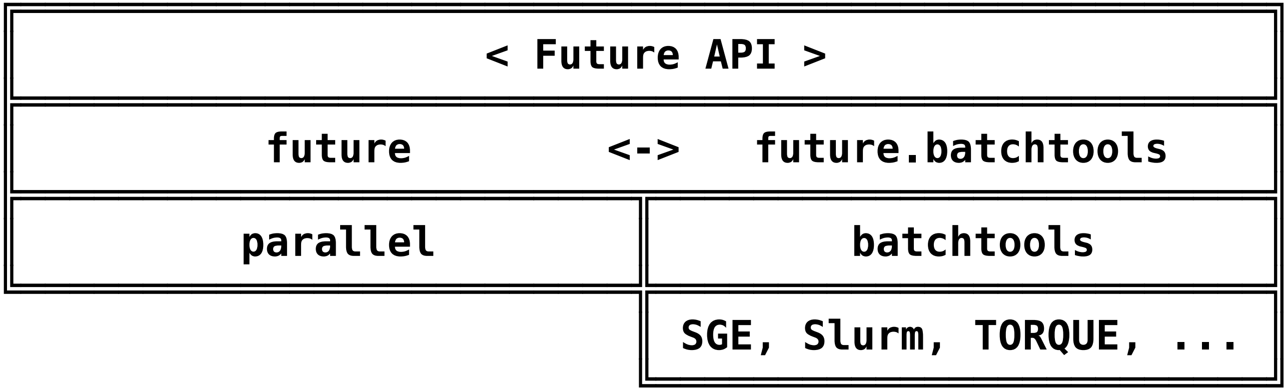
High Performance Compute (HPC) clusters



Backend: future.batchtools

CRAN 0.7.0 codecov 89%

- **batchtools**: Map-Reduce API for **HPC schedulers**,
  e.g. LSF, OpenLava, SGE, Slurm, and TORQUE / PBS
- **future.batchtools**: **Future API** on top of **batchtools**



< Future API >

future <-> future.batchtools

parallel

batchtools

SGE, Slurm, TORQUE, ...

Backend: future.batchtools

CRAN 0.7.0 codecov 89%

```
> library(future.batchtools)
> plan(batchtools_sge)

> a %<-% slow_sum(1:50)
> b %<-% slow_sum(51:100)
> a + b
[1] 5050
```

Real Example: DNA Sequence Analysis

- DNA sequences from 100 cancer patients
- 200 GiB data / patient (~ 10 hours)

```
raw <- dir(pattern = "[.]fq$")
aligned <- listenv()
for (i in seq_along(raw)) {
  aligned[[i]] %<-% DNAseq::align(raw[i])
}
aligned <- as.list(aligned)
```

- `plan(multiprocess)`
- `plan(cluster, workers = c("n1", "n2", "n3"))`
- `plan(batchtools_sge)`

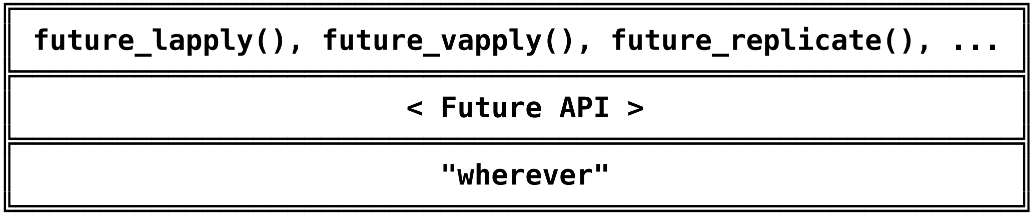
Comment: The use of `listenv` is non-critical and only needed for implicit futures when assigning them by index (instead of by name).

Building on top of Future API

Frontend: future.apply

CRAN 0.2.0 codecov 95%

- Futurized version of base R's **`lapply()`**, **`vapply()`**, **`replicate()`**, ...
- ... on **all future-compatible backends**



future_lapply(), future_vapply(), future_replicate(), ...

< Future API >

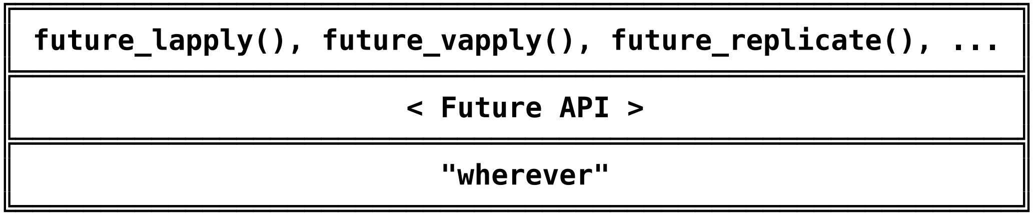
"wherever"

```
aligned <- lapply(raw, DNAseq::align)
```

Frontend: future.apply

CRAN 0.2.0 codecov 95%

- Futurized version of base R's **`lapply()`**, **`vapply()`**, **`replicate()`**, ...
- ... on **all future-compatible backends**



future_lapply(), future_vapply(), future_replicate(), ...

< Future API >

"wherever"

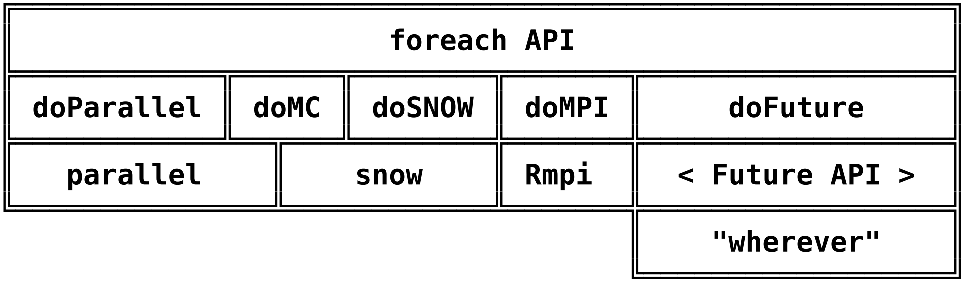
```r
aligned <- future_lapply(raw, DNAseq::align)
```

- **`plan(multiprocess)`**
- **`plan(cluster, workers = c("n1", "n2", "n3"))`**
- **`plan(batchtools_sge)`**

Frontend: doFuture

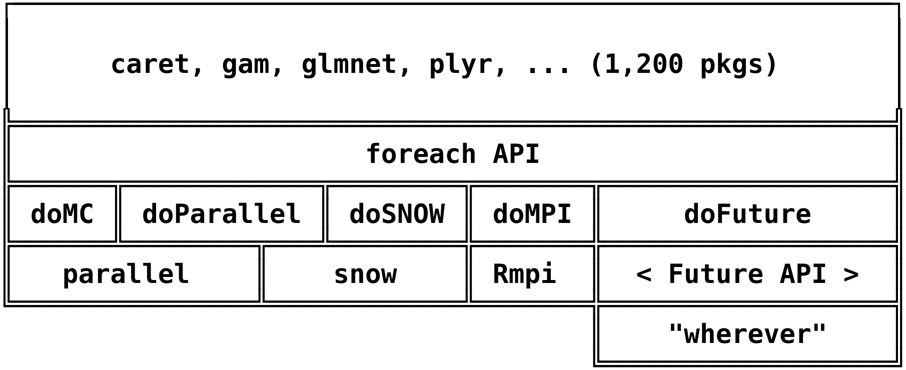
CRAN 0.6.0 codecov 83%

- A **foreach** adapter on top of the Future API
- Foreach on **all future-compatible backends**



```
doFuture::registerDoFuture()
plan(batchtools_sge)
aligned <- foreach(x = raw) %dopar% {
  DNAseq::align(x)
}
```

1,200+ packages can now parallelize on HPC



caret, gam, glmnet, plyr, ... (1,200 pkgs)

foreach API

doMC | doParallel | doSNOW | doMPI | doFuture

parallel | snow | Rmpi | < Future API >

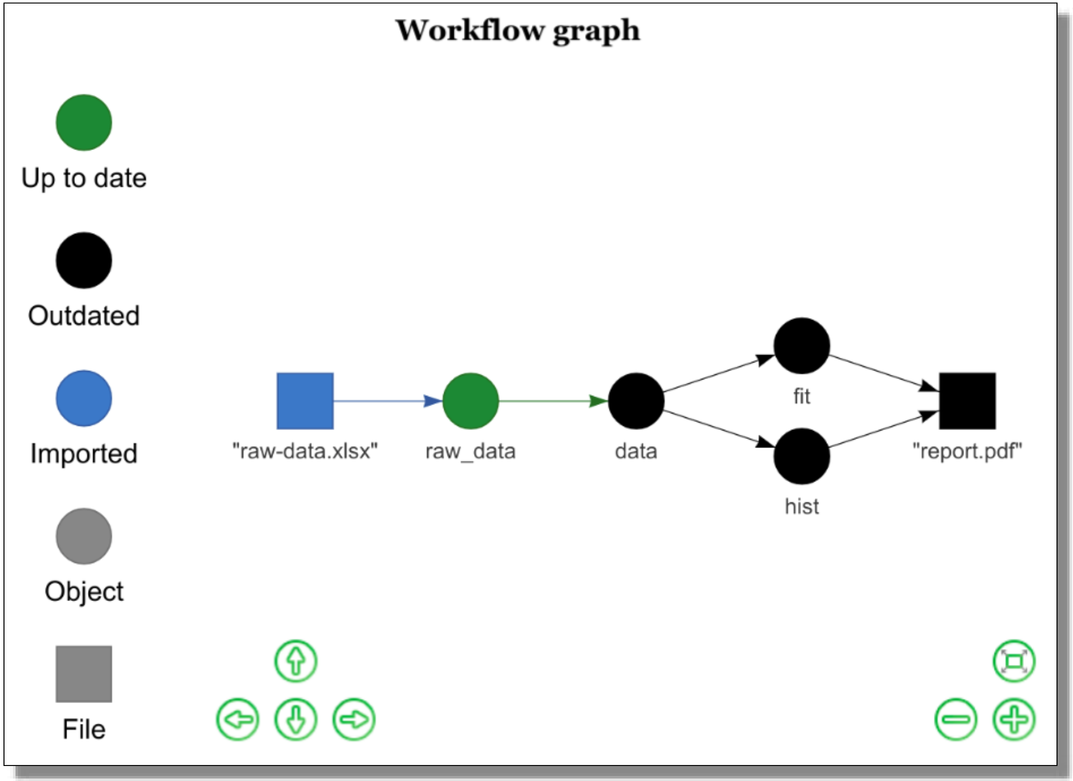
"wherever"

```
doFuture::registerDoFuture()
plan(future.batchtools::batchtools_sge)

library(caret)
model <- train(y ~ ., data = training)
```

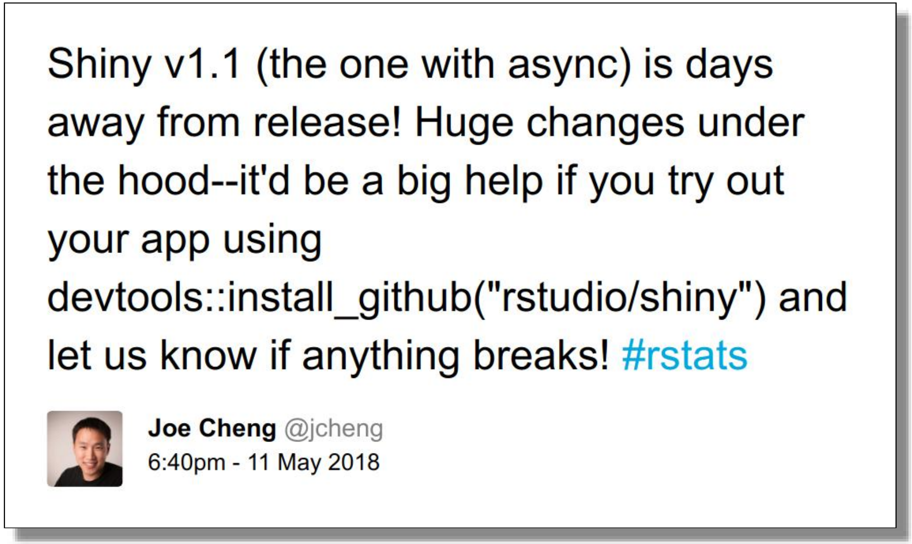
Futures in the Wild

Frontend: *drake* - A Workflow Manager

```
tasks <- drake_plan(
  raw_data = readxl::read_xlsx(file_in("raw-data.xlsx")),

  data = raw_data %>% mutate(Species =
         forcats::fct_inorder(Species)) %>% select(-X__1),

  hist = ggplot(data, aes(x = Petal.Width, fill = Species))
         + geom_histogram(),

  fit = lm(Sepal.Width ~ Petal.Width + Species, data),

  rmarkdown::render(knitr_in("report.Rmd"),
                    output_file = file_out("report.pdf"))
)

future::plan("multiprocess")
make(tasks, parallelism = "future")
```


Workflow graph
Up to date
Outdated
Imported
Object
File
"raw-data.xlsx"
raw_data
data
fit
hist
"report.pdf"

shiny - Now with Asynchronous UI



Shiny v1.1 (the one with async) is days away from release! Huge changes under the hood--it'd be a big help if you try out your app using devtools::install_github("rstudio/shiny") and let us know if anything breaks! #rstats

Joe Cheng @jcheng
6:40pm - 11 May 2018

```
library(shiny)
future::plan("multiprocess")
...
```

Summary of features

- **Unified API**
- **Portable code**
- **Worry-free**
- **Developer decides what to parallelize - user decides how to**
- For beginners as well as advanced users
- Nested parallelism on nested heterogeneous backends
- Protects against recursive parallelism
- Easy to add new backends
- Easy to build new frontends

In the near future ...

- Capturing standard output
- Benchmarking (time and memory)
- Killing futures

Building a better future

I ♥ feedback,
bug reports,
and suggestions

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Thank you!

Appendix (Random Slides)

A1. Features - more details

A1.1 Well Tested

- Large number of unit tests
- System tests
- High code coverage (union of all platform near 100%)
- Cross platform testing
- CI testing
- Testing several R versions (many generations back)
- Reverse package dependency tests
- All backends highly tested
- Large of tests via doFuture across backends on `example()`:s from foreach, NMF, TSP, glmnet, plyr, caret, etc. (example link)

R Consortium Infrastructure Steering Committee (ISC) Support Project

- **Backend Conformance Test Suite** - an effort to formalizing and standardizing the above tests into a unified go-to test environment.

A1.2 Nested futures

```r
raw <- dir(pattern = "[.]fq$")

aligned <- listenv()
for (i in seq_along(raw)) {
  aligned[[i]] %<-% {
    chrs <- listenv()
    for (j in 1:24) {
      chrs[[j]] %<-% DNAseq::align(raw[i], chr = j)
    }
    merge_chromosomes(chrs)
  }
}
```

- **plan(batchtools_sge)**
- **plan(list(batchtools_sge, sequential))**
- **plan(list(batchtools_sge, multiprocess))**

A1.3 Lazy evaluation

By default all futures are resolved using eager evaluation, but the *developer* has the option to use lazy evaluation.

Explicit API:

```
f <- future(..., lazy = TRUE)
v <- value(f)
```

Implicit API:

```
v %<-% { ... } %lazy% TRUE
```

A1.4 False-negative & false-positive globals

Identification of globals from static-code inspection has limitations (but defaults cover a large number of use cases):

- False negatives, e.g. **`my_fcn`** is not found in **`do.call("my_fcn", x)`**. Avoid by using **`do.call(my_fcn, x)`**.
- False positives - non-existing variables, e.g. NSE and variables in formulas. Ignore and leave it to run-time.

```r
x <- "this FP will be exported"

data <- data.frame(x = rnorm(1000), y = rnorm(1000))

fit %<-% lm(x ~ y, data = data)
```

Comment: … so, the above works.

A1.5 Full control of globals (explicit API)

Automatic (default):

```r
x <- rnorm(n = 100)
y <- future({ slow_sum(x) }, globals = TRUE)
```

By names:

```r
y <- future({ slow_sum(x) }, globals = c("slow_sum", "x"))
```

As name-value pairs:

```r
y <- future({ slow_sum(x) }, globals =
                                 list(slow_sum = slow_sum, x = rnorm(n = 100)))
```

Disable:

```r
y <- future({ slow_sum(x) }, globals = FALSE)
```

A1.5 Full control of globals (implicit API)

Automatic (default):

```r
x <- rnorm(n = 100)
y %<-% { slow_sum(x) } %globals% TRUE
```

By names:

```r
y %<-% { slow_sum(x) } %globals% c("slow_sum", "x")
```

As name-value pairs:

```r
y %<-% { slow_sum(x) } %globals% list(slow_sum = slow_sum, x = rnorm(n = 100))
```

Disable:

```r
y %<-% { slow_sum(x) } %globals% FALSE
```

A1.6 Protection: Exporting too large objects

```r
x <- lapply(1:100, FUN = function(i) rnorm(1024 ^ 2))
y <- list()
for (i in seq_along(x)) {
  y[[i]] <- future( mean(x[[i]]) )
}
```

gives error: "The total size of the 2 globals that need to be exported for the future expression ('mean(x[[i]])') is **800.00 MiB. This exceeds the maximum allowed size of 500.00 MiB (option 'future.globals.maxSize')**. There are two globals: 'x' (800.00 MiB of class 'list') and 'i' (48 bytes of class 'numeric')."

```r
for (i in seq_along(x)) {
  x_i <- x[[i]]  ## Fix: subset before creating future
  y[[i]] <- future( mean(x_i) )
}
```

Comment: Interesting research project to automate via code inspection.

A1.7 Free futures are resolved

Implicit futures are always resolved:

```
a %<-% sum(1:10)
b %<-% { 2 * a }
print(b)
## [1] 110
```

Explicit futures require care by developer:

```
fa <- future( sum(1:10) )
a <- value(fa)
fb <- future( 2 * a )
```

For the lazy developer - not recommended (may be expensive):

```
options(future.globals.resolve = TRUE)
fa <- future( sum(1:10) )
fb <- future( 2 * value(fa) )
```

A1.8 What's under the hood?

- **Future class** and corresponding methods:
  - abstract S3 class with common parts implemented,
    e.g. globals and protection
  - new backends extend this class and implement core methods,
    e.g. **`value()`** and **`resolved()`**
  - built-in classes implement backends on top the parallel package

A1.9 Universal union of parallel frameworks

	future	parallel	foreach	batchtools	BiocParallel
	future	**parallel**	**foreach**	**batchtools**	**BiocParallel**
Synchronous	✔	✓	✓	✓	✓
Asynchronous	✔	✓	✓	✓	✓
Uniform API	✔		✓	✓	✓
Extendable API	✔		✓	✓	✓
Globals	✔		(✓)		
Packages	✔				
Map-reduce ("lapply")	✔	✓	`foreach()`	✓	✓
Load balancing	✔	✓	✓	✓	✓
For loops	✔				
While loops	✔				
Nested config	✔				
Recursive protection	✔	mc	mc	mc	mc
RNG stream	✔+	✓	doRNG	(soon)	SNOW
Early stopping	✔				✓
Traceback	✔				✓

A2 Bells & whistles

A2.1 availableCores() & availableWorkers()

- **`availableCores()`** is a "nicer" version of **`parallel::detectCores()`** that returns the number of cores allotted to the process by acknowledging known settings, e.g.
  - **`getOption("mc.cores")`**
  - HPC environment variables, e.g. **`NSLOTS`**, **`PBS_NUM_PPN`**, **`SLURM_CPUS_PER_TASK`**, …
  - **`_R_CHECK_LIMIT_CORES_`**
- **`availableWorkers()`** returns a vector of hostnames based on:
  - HPC environment information, e.g. **`PE_HOSTFILE`**, **`PBS_NODEFILE`**, …
  - Fallback to **`rep("localhost", availableCores())`**

Provide safe defaults to for instance

```
plan(multiprocess)
plan(cluster)
```

A2.2: makeClusterPSOCK()

`makeClusterPSOCK()`:

- Improves upon `parallel::makePSOCKcluster()`
- Simplifies cluster setup, especially remote ones
- Avoids common issues when workers connect back to master:
  - uses SSH reverse tunneling
  - no need for port-forwarding / firewall configuration
  - no need for DNS lookup
- Makes option `-l <user>` optional (such that `~/.ssh/config` is respected)

A2.3 HPC resource parameters

With 'future.batchtools' one can also specify computational resources, e.g. cores per node and memory needs.

```
plan(batchtools_sge, resources = list(mem = "128gb"))
y %<-% { large_memory_method(x) }
```

Specific to scheduler: **`resources`** is passed to the job-script template where the parameters are interpreted and passed to the scheduler.

Each future needs one node with 24 cores and 128 GiB of RAM:

```
resources = list(l = "nodes=1:ppn=24", mem = "128gb")
```

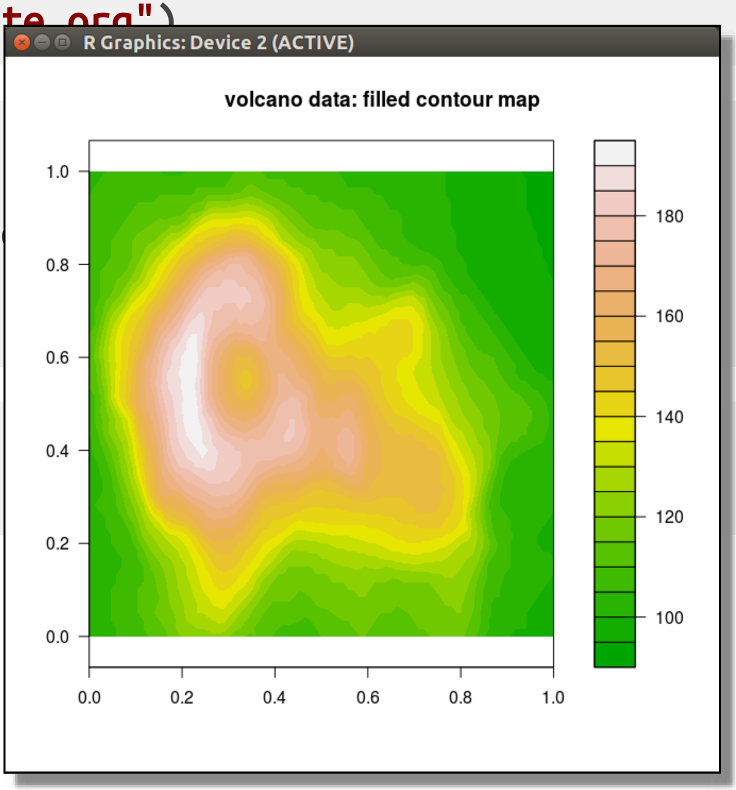
A3. More Examples

A3.1 Plot remotely - display locally

```
> library(future)
> plan(cluster, workers = "remote.org")
```

```
## Plot remotely
> g %<-% R.devices::capturePlot
    filled.contour(volcano, col
    title("volcano data: filled
 })
```

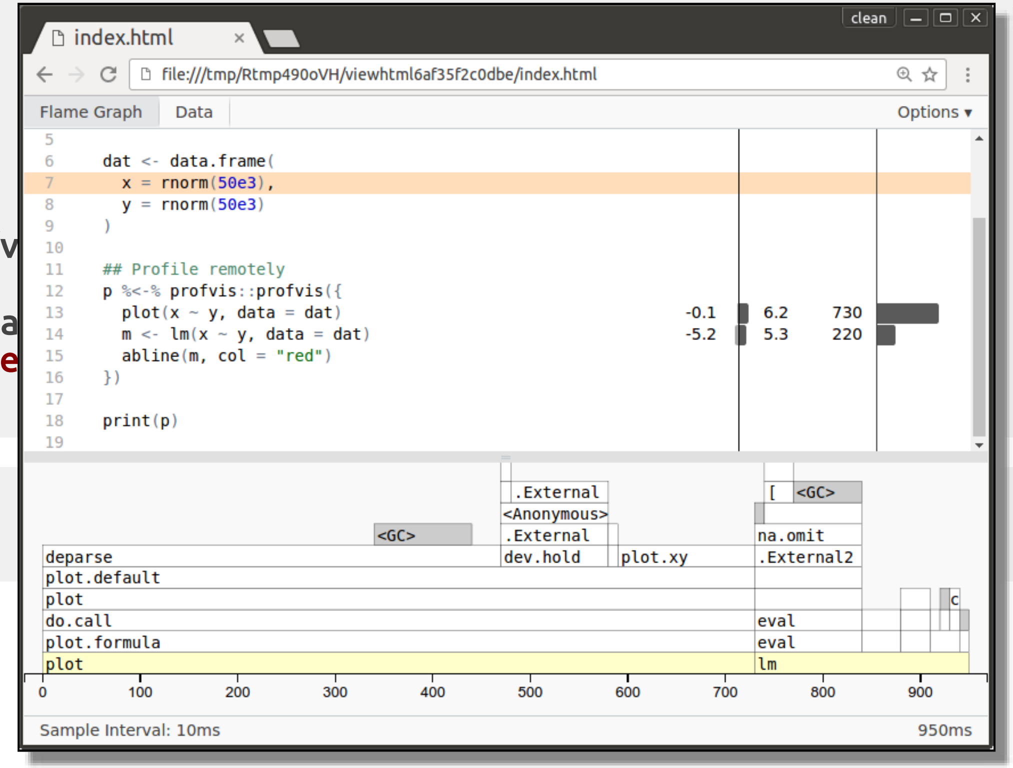
```
## Display locally
> g
```


R Graphics: Device 2 (ACTIVE)
volcano data: filled contour map
1.0
0.8
0.6
0.4
0.2
0.0
0.0
0.2
0.4
0.6
0.8
1.0
180
160
140
120
100

A3.2 Profile code remotely - display locally

```
> plan(cluster, workers = "remote.org")

> dat <- data.frame(
+   x = rnorm(50e3),
+   y = rnorm(50e3)
+ )

## Profile remotely
> p %<-% profvis::profv
+   plot(x ~ y, data =
+   m <- lm(x ~ y, data
+   abline(m, col = "re
+ })
```

```
## Browse locally
> p
```



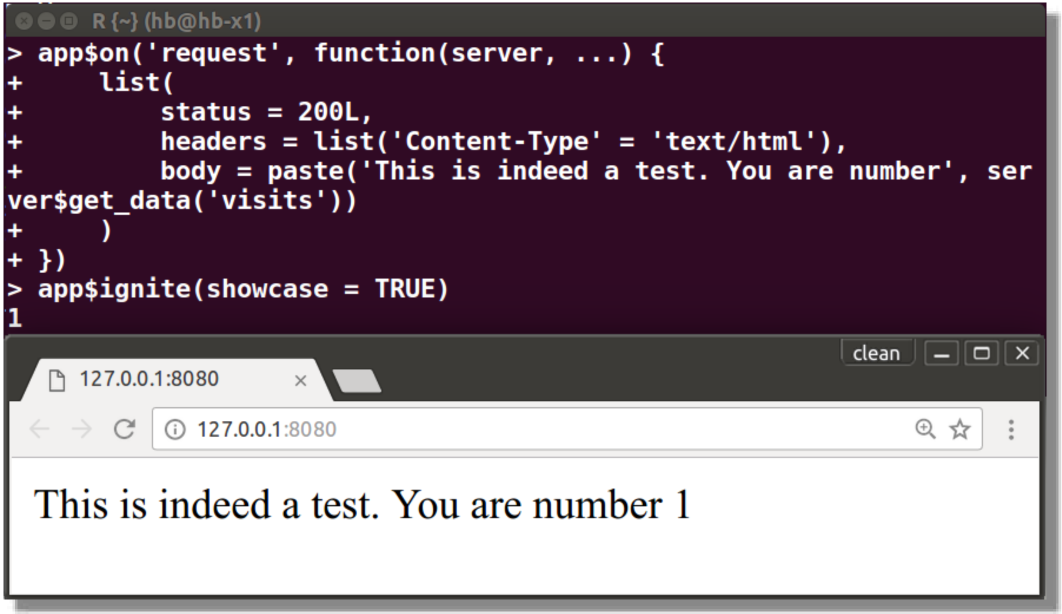
```
dat <- data.frame(
  x = rnorm(50e3),
  y = rnorm(50e3)
)

## Profile remotely
p %<-% profvis::profvis({
  plot(x ~ y, data = dat)                    -0.1   6.2   730
  m <- lm(x ~ y, data = dat)                 -5.2   5.3   220
  abline(m, col = "red")
})

print(p)
```

Sample Interval: 10ms

950ms

A3.3 *fiery* - flexible lightweight web server

"... framework for building web servers in R. ... from serving static content to full-blown dynamic web-apps"



```
> app$on('request', function(server, ...) {
+     list(
+         status = 200L,
+         headers = list('Content-Type' = 'text/html'),
+         body = paste('This is indeed a test. You are number', ser
ver$get_data('visits'))
+     )
+ })
> app$ignite(showcase = TRUE)
1
```

This is indeed a test. You are number 1

A3.4 "It kinda just works" (furrr = future + purrr)

```
plan(multisession)
mtcars %>%
  split(.$cyl) %>%
  map(~ future(lm(mpg ~ wt, data = .x))) %>% values %>%
  map(summary) %>%
  map_dbl("r.squared")
##         4         6         8
## 0.5086326 0.4645102 0.4229655
```

Comment: This approach not do load balancing. I have a few ideas how support for this may be implemented in future framework, which would be beneficial here and elsewhere.

A3.5 Backend: Google Cloud Engine Cluster

```
library(googleComputeEngineR)
vms <- lapply(paste0("node", 1:10),
              FUN = gce_vm, template = "r-base")
cl <- as.cluster(lapply(vms, FUN = gce_ssh_setup),
               docker_image = "henrikbengtsson/r-base-future")

plan(cluster, workers = cl)
```

```
data <- future_lapply(1:100, montecarlo_pi, B = 10e3)
pi_hat <- Reduce(calculate_pi, data)

print(pi_hat)
## 3.1415
```

A4. Future Work

A4.1 Standard resource types(?)

For any type of futures, the develop may wish to control:

- memory requirements, e.g. `future(..., memory = 8e9)`
- local machine only, e.g. `remote = FALSE`
- dependencies, e.g. `dependencies = c("R (>= 3.5.0)", "rio"))`
- file-system availability, e.g. `mounts = "/share/lab/files"`
- data locality, e.g. `vars = c("gene_db", "mtcars")`
- containers, e.g. `container = "docker://rocker/r-base"`
- generic resources, e.g. `tokens = c("a", "b")`
- …?

Risk for bloating the Future API: Which need to be included? Don't want to reinvent the HPC scheduler and Spark.