There is an elephant in the room. . .

Jan Salecker » jsaleck@gwdg.de

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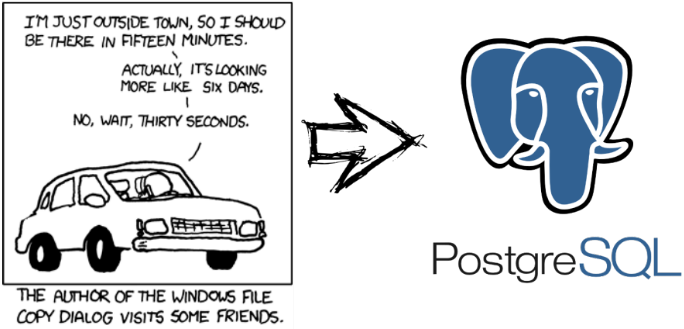

I'M JUST OUTSIDE TOWN, SO I SHOULD BE THERE IN FIFTEEN MINUTES.
ACTUALLY, IT'S LOOKING MORE LIKE SIX DAYS.
NO, WAIT, THIRTY SECONDS.
THE AUTHOR OF THE WINDOWS FILE COPY DIALOG VISITS SOME FRIENDS.
PostgreSQL

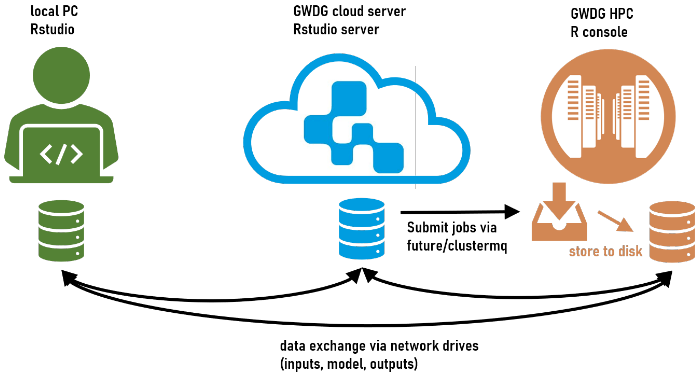
Motivation

Motivation

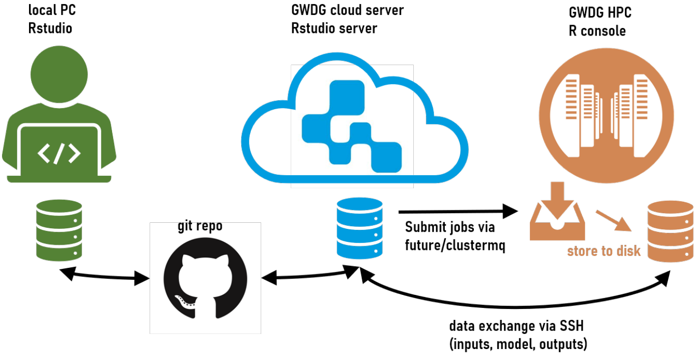
My current R workflow consists of:

- Local desktop/laptop
  - Daily work
  - Development of scripts, analyses
  - Post-processing of simulation results
  - Writing papers (RMarkdown)
- GWDG Cloud server running RStudio Server
  - Conducting heavy load simulation jobs
  - Submitting jobs to the GWDG HPC
- GWDG HPC
  - Only executes simulations sent from the cloud server

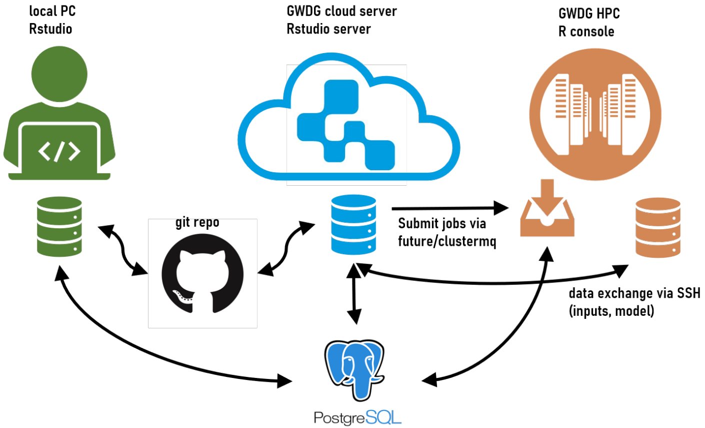
Route to SQL step 1: The Ignorant



Route to SQL step 2: The educated



Route to SQL step 3: The sophisticated



Lessons learned

- manual copying is bad and error-prone
- github enables reliable file transfer between local PC and cloud server
- ssh enables convenient file transfer between cloud server and HPC

But:

- big data cannot be transfered via github or SSH
- handling thousands of *.rds files is cumbersome

SQL database is a great addition to manage file transfer between all three instances of R, especially for big data

SQL

- not as powerful as Apache hadoop but adequate for our purposes
- database based on tables
  - relates well to data.frames / tibbles / data.tables
- R packages allow easy access to SQL databases, even remotely

PostgreSQL

- open-source version of SQL
- easy to setup/access
- unlimited database size & unlimited rows per table
- maximum table size of 32 TB
- maximum cell size og 1 GB

How to setup PostgreSQL

How to setup PostgreSQL

I have installed the PostgreSQL server on my GWDG cloud server because it is available 24/7.

I used this detailed guide on how to install the postgresql server:

https://wiki.ubuntuusers.de/PostgreSQL/

Afterwards some configuration needs to be done. . .

Remote access

Step 1: Open SQL communication port

- Open port 5432 on GWDG cloud server (GWDG services)

Step 2: Edit postgresql.conf file:

- `sudo nano /etc/postgresql/xx/main/postgresql.conf` (exchange xx with version number)
- Change line `listen_addresses='localhost'` to `listen_addresses='*'`

Remote access

Step 3: Edit `hba_file`:

In order to find location of `hba_file` log into postgresql:

- `sudo -u postgres psql`
- then type `SHOW hba_file;` and copy the path (e.g. /etc/postgresql/12/main/pg_hba.conf)
- close postgresql: `\q`
- edit the file: `sudo nano /etc/postgresql/12/main/pg_hba.conf`

Remote access

- Original settings of pg_hba.conf:

```
# local   replication     all
# host    replication     all                 127.0.0.1/32
# host    replication     all                 ::1/128
```

- change `replication` to `all`
- change ip4 host to `0.0.0.0/0`
- change ip6 host to `::0/0`
- Then restart postgresql `sudo /etc/init.d/postgresql restart`

Configure SQL database:

Some important terminal commands:

- stop/restart/start:
  - `sudo /etc/init.d/postgresql restart`
  - `sudo /etc/init.d/postgresql stop`
  - `sudo /etc/init.d/postgresql start`
- Create/remove user:
  - `sudo -u postgres createuser -P -d NUTZERNAME`
  - `sudo -u postgres dropuser NUTZERNAME`

Configure SQL database:

Some important terminal commands:

- Create/remove database (each user can have multiple databases):
    - `sudo -u postgres createdb -O NUTZERNAME DATENBANK`
    - `sudo -u postgres dropdb DATENBANK`
- Connect into database locally from terminal:
    - choose user/database: `psql -d smnws -U NUTZERNAME`
    - as admin user: `sudo -u postgres psql`

How to use PostgreSQL from R

- The R packages `RPostgres` and `DBI` allow to access SQL databases
- Assuming we have setup a user account (`jan`) and a database (`projectXY`) we can setup a connection:

```r
library(RPostgres)
library(DBI)
con <- dbConnect(RPostgres::Postgres(),
                 dbname = 'projectXY',
                 port = 5432,
                 user = 'jan',
                 password = 'xyz')
```

How to use PostgreSQL from R

```
# Print tables in db (each database can have multiple table
dbListTables(con)

# Write tables to db:
dbWriteTable(con, "mtcars", mtcars)

# Read tables from db:
dbReadTable(con, "mtcars")

# Modify tables:
newlines <- data.frame(mpg=99, cyl=99, disp=99, hp=99, drat
dbAppendTable(con, "mtcars", newlines)
dbReadTable(con, "mtcars")

# Delete tables:
dbRemoveTable(con, "mtcars")

# Disconnet:
dbDisconnect(con)
```

Remote access

When remote access is configured correctly (see above) you can enter the remote host in the connection (in my case the IP address of my GWDG cloud server):

```
con <- dbConnect(RPostgres::Postgres(),
                 dbname = 'projectXY',
                 host = "141.5.105.225",
                 port = 5432,
                 user = 'jan',
                 password = 'xyz')
dbListTables(con)
dbDisconnect(con)
```

Write SQL tables in parallel

- I want to fill up an empty table from the HPC in parallel
- To do this, the table need to exist in advance
- Thus, before submitting my jobs I create an empty tibble to initialize the table

```
 results_template <- tibble::tibble(name=character(), value
results_template
```

```
## # A tibble: 0 x 2
## # ... with 2 variables: name <chr>, value <dbl>
```

```
 dbWriteTable(con,
             "tablename",
             results_template,
             overwrite=TRUE)
```

Fill up table in parallel

- We can then use a function that writes directly to that table

```
simfun <- function(x, con, tablename)
{
  # Output (probably another function is called to do some
  out <- tibble::tibble(name=x, value=x)

  # append data
  dbAppendTable(con, "tablename", out)

  # close connection
  dbDisconnect(con)

  # Return nothing
  return()
}
```

Intermission: File tranfser via SSH

File transfer via SSH

```
hpc.upload <- function (from = NA, to = NA, user = NA,
                        host = "transfer.gwdg.de", key = NA
{
  session <- ssh::ssh_connect(paste0(user, "@", host), keyf
  ssh::scp_upload(session, files = from, to = to)
  ssh::ssh_disconnect(session)
}
```

```
hpc.download <- function (from = NA, to = NA, user = NA,
                          host = "transfer.gwdg.de", key =
{
  session <- ssh::ssh_connect(paste0(user, "@", host), keyf
  ssh::scp_download(session, files = from, to = to)
  ssh::ssh_disconnect(session)
}
```

File transfer via SSH

```
hpc.delete <- function (folder = NA, user = NA,
                        host = "transfer.gwdg.de", key = NA
{
  session <- ssh::ssh_connect(paste0(user, "@", host), keyf
  ssh::ssh_exec_wait(session,
                     command = paste0("find ",
                                      folder,
                                      "/ -maxdepth 1 -type
  ssh::ssh_disconnect(session)
}
```

A complete workflow example

Introduction

- I want to use EFForTS-ABM as an example how my workflow looks at the moment
- Lets imagine I start by implementing a new feature into EFForTS-ABM
- Afterwards I want to run some analyses on the HPC

Step 01

- Local PC
    - Implement features in NetLogo
    - Prepare analysis scripts
    - Do some test runs
    - Push everything to the github repo

Step 02

- Cloud server
    - Pull the changes
    - Send model files and inputs to HPC via SSH
    - Prepare empty SQL table (dbwriteTable, overwrite=TRUE)
    - Execute Q function to start HPC jobs
- Log into HPC terminal to inspect job status
    - Once all jobs are finished, proceed

Step 03

- Cloudserver
  - Load results from SQL table (dbreadtable)
  - Attach results tibble to nl object
  - Store complete nl object as *.rds
  - Push to git repo
- Local PC
  - pull git repo
  - continue analysing simulation results, make plots, write paper, ...

Questions?

Jan Salecker jsaleck@gwdg.de