Big jobs/simulations

Tools for Reproducible Research

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Course web: `bit.ly/tools4rr`

But first…

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- Make it an R package
- Write a test or two
- Commit it to a git repository

So what's the big deal?

- You don't want `knitr` running for a year.
- You don't want to re-run things if you don't have to.

Unix basics

```
nice +19 R CMD BATCH input.R output.txt &

fg

ctrl-Z

bg

ps ux

top

kill

kill -9
```

Disk thrashing

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– Wikipedia

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In computer science, thrashing occurs when a computer's virtual memory subsystem is in a constant state of paging, rapidly exchanging data in memory for data on disk, to the exclusion of most application-level processing.

– Wikipedia

Biggish jobs in knitr

- Manual caching
- Built-in `cache=TRUE`
- Split the work and write a `Makefile`

Manual caching

~~~
```{r a_code_chunk}
file <- "cache/myfile.RData"

if(file.exists(file)) {
  load(file)
} else{

  ....

  save(object1, object2, object3, file=file)
}
```
~~~

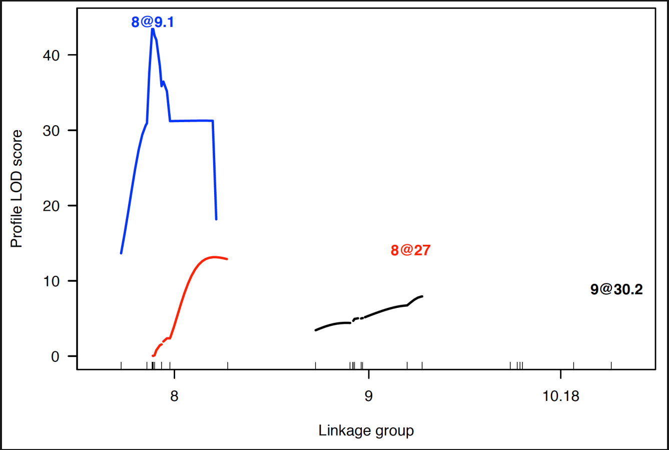
Chunk references

~~~
```{r not_shown, eval=FALSE}
code_here <- 0
```

```{r a_code_chunk, echo=FALSE}
file <- "cache/myfile.RData"

if(file.exists(file)) {
  load(file)
} else{
<<not_shown>>
  save(code_here, file=file)
}
```
~~~

A cache gone bad



Knitr's cache system

~~~
```{r chunk_name, cache=TRUE}
load("a_big_file.RData")
med <- apply(object, 2, median, na.rm=TRUE)
```
~~~

- Chunk is re-run if edited.
- Otherwise, objects from previous run are loaded.
- Don't cache things with side effects

  e.g., `options()`, `par()`

Cache dependencies

Manual dependencies

~~~
```{r chunkA, cache=TRUE}
Sys.sleep(2)
x <- 5
```

```{r chunkB, cache=TRUE, dependson="chunkA"}
Sys.sleep(2)
y <- x + 1
```

```{r chunkC, cache=TRUE, dependson="chunkB"}
Sys.sleep(2)
z <- y + 1
```
~~~

Cache dependencies

Automatic dependencies

~~~
```{r setup, include=FALSE}
opts_chunk$set(autodep = TRUE)
dep_auto()
```
~~~

Parallel computing

If your computer has multiple processors, use `library(parallel)` to make use of them.

- `detectCores()`
- `RNGkind("L'Eucyer-CMRG")` and `mclapply` (Unix/Mac)
- `makeCluster`, `clustersetRNGStream`, `clusterApply`, and `stopCluster` (Windows)

Systems for distributed computing

- HTCondor and the UW-Madison CHTC
- Other condor-like systems
- "By hand"
  - e.g., perl script + template R script

Simulations

- Computer simulations require RNG seeds (`.Random.seed` in R).
- Multiple parallel jobs need different seeds.
- Don't rely on the current seed, or on having it generated from the clock.
- Use something like `set.seed(91820205 + i)`
- An alternative is create a big batch of simulated data sets in advance.

Save everything

- RNG seeds
- input
- output
- version numbers, with `sessionInfo()`
- raw results
- script to combine results
- combined results
- `ReadMe` describing the point

One Makefile to rule them all

- Separate directory for each batch of big computations.
- Makefile that controls the combination of the results (and everything else).
- KnitR-based documents for the analysis/use of those results.

Potential problems

- Forgetting `save()` in your distributed jobs
- A bug in the `save()` command
- `make` clobbers some important results
  - Scripts should refuse to overwrite output files

Summary

- Careful organization and modularization.
- Save everything.
- Document everything.
- Learn the basic skills for distributed computing.