Parallel R and ARCHER2

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archer2

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Reusing this material

Partners

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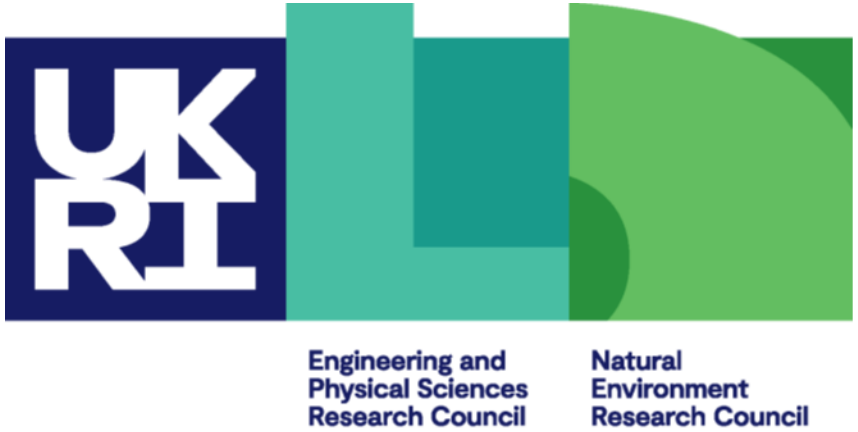

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Parallel R

- Different motivations for parallelising R
  - Too much computational work
    - My program takes too long
  - Too much data to process
    - My program is quick enough, but I've too much data to process
  - Data is too large
    - My data set is too big to fit into memory
- Wide range of options:
  - https://cran.r-project.org/web/views/HighPerformanceComputing.html
  - Implicit parallelism
  - Explicit parallelism
  - Applications
  - Batch system integration, hardware resources, distributed computing integration
  - Native code interfaces
  - Big memory

Parallel options for R

- Shared memory parallelisation
  - Trivially parallel
    - (l)apply
    - Map
  - Loop parallelism
    - foreach
  - Threads
    - Rdsm
- Distributed memory parallelisation
  - parallel
  - snow
  - Rmpi
  - pbdR
  - foreach

Automatic parallelism

- R has some parallelism built in
- BLAS libraries and other underlying functionality already using shared memory parallelism, i.e.:

```
A <- matrix( rnorm(n*n), ncol=n, nrow=n )
B <- matrix( rnorm(n*n), ncol=n, nrow=n )
C <- A %*% B
```

```
> library("data.table")
data.table 1.14.2 using 128 threads (see ?getDTthreads).  Latest news: r-datatable.com
```

- Can control number of workers on ARCHER2 using

```
export OMP_NUM_THREADS=
```

i.e.

```
export OMP_NUM_THREADS=2
…
> library("data.table")
data.table 1.14.2 using 2 threads (see ?getDTthreads).  Latest news: r-datatable.com
```

- By default will use all available workers
  - Can be the wrong thing to do

Trivial trivial parallelism

- Task farms
  - Same code executed independently
  - Different initial conditions or different data sets
  - Slurm array jobs can support this

```
args <- commandArgs(TRUE)
set.seed(args[1])
data <- read.csv('dataset.csv')
result <- kmeans(data, centers=10, nstart=100)
print(result)

Rscript kmeans-trivial.R 1 > 1_output.dat
```

- Requires manual processing of the data
- Requires some care if using random number generators

Trivial parallelism

- Split, Apply, Combine
  - Partition data into groups to be worked on
  - Apply operations to each group
  - Combine results with some form of reduction at the end
- Requires making some workflows more complex to enable parallelisation:

```
data <- read.csv('dataset.csv')
result <- kmeans(data, centers=4, nstart=100)
print(result)
-----------------------------------------------------------
data <- read.csv('dataset.csv')
parallel.function <- function(i) {
    kmeans( data, centers=4, nstart=i )
}
results <- lapply( c(25, 25, 25, 25), FUN=parallel.function )

temp.vector <- sapply( results, function(result) { result$tot.withinss } )
result <- results[[which.min(temp.vector)]]
```

Combining results

- Some of the functionality use can create lists of answers, i.e.:

```
> res <- lapply(1:3, function(i) {
+   sqrt(i)*sqrt(i*2)
+ })
>
> print(res)
[[1]]
[1] 1.414214

[[2]]
[1] 2.828427

[[3]]
[1] 4.242641
```

- Can combine the results to produce a single vector or results, i.e.:

```
> do.call('c', res)
[1] 1.414214 2.828427 4.242641
```

mcapply

```
library(parallel)
data <- read.csv('dataset.csv')
parallel.function <- function(i) {
    kmeans( data, centers=4, nstart=i )
}
results <- mclapply( c(25, 25, 25, 25), FUN=parallel.function )

temp.vector <- sapply( results, function(result) { result$tot.withinss } )
result <- results[[which.min(temp.vector)]]
print(result)
```

- Uses processes rather than threads on ARCHER2.
- Uses `MC_CORES` environment variable to control parallelism (not `OMP_NUM_THREADS`)
  - Default to 2, can change, i.e.:

```
export MC_CORES=16
```

- Uses `mc_cores` argument as well:

```
results <- mclapply( c(25, 25, 25, 25), FUN=parallel.function, mc_cores=16 )
```

- Can modify task scheduling/load balancing etc… with further arguments:

```
results <- mclapply( c(25, 25, 25, 25), FUN=parallel.function, mc_cores=16,
mc.preschedule=FALSE )
```

mcparallel mccollect

```
library(parallel)
p <- mcparallel(1:10)
q <- mcparallel(1:20)
# wait for both jobs to finish and collect all results
res <- mccollect(list(p, q))
```

```
library(parallel, quiet=TRUE)
source("data/airline/read_airline.R")
jan2010 <- read.airline("data/airline/airOT201001.csv.gz")
unique.planes <- mcparallel( length( unique( sort(jan2010$TAIL_NUM) ) ) )
median.elapsed <- mcparallel( median( jan2010$ACTUAL_ELAPSED_TIME, na.rm=TRUE ) )
ans <- mccollect( list(unique.planes, median.elapsed) )
ans
```

foreach

```
library(foreach)
data <- read.csv('dataset.csv')
results <- foreach( i = c(25,25,25,25) ) %do% {
    kmeans( x=data, centers=4, nstart=i )
}
temp.vector <- sapply( results, function(result)
    { result$tot.withinss } )
result <- results[[which.min(temp.vector)]]

print(result)
…
x <- foreach(i=1:4, .combine='cbind') %do%
rnorm(4)
```

foreach parallel

```
library(foreach)
library(doMC)
data <- read.csv('dataset.csv')

registerDoMC(4)
results <- foreach( i = c(25,25,25,25) ) %dopar% {
    kmeans( x=data, centers=4, nstart=i )
}

temp.vector <- sapply( results, function(result)
    { result$tot.withinss } )
result <- results[[which.min(temp.vector)]]

print(result)
```

parLapply

```
library(snow)
data <- read.csv( 'dataset.csv' )
parallel.function <- function(i) {
    kmeans( data, centers=4, nstart=i )
}
cl <- makeCluster( mpi.universe.size(), type="MPI" )
clusterExport(cl, c('data'))

results <- parLapply( cl, c(25,25,25,25), fun=parallel.function )

temp.vector <- sapply( results, function(result) { result$tot.withinss } )
result <- results[[which.min(temp.vector)]]
print(result)

stopCluster(cl)
mpi.exit()
```

doSNOW foreach

```
library(foreach)
library(doSNOW)
data <- read.csv('dataset.csv')
cl <- makeCluster( mpi.universe.size(), type='MPI' )
clusterExport(cl,c('data'))
registerDoSNOW(cl)
results <- foreach( i = c(25,25,25,25) ) %dopar% {
    kmeans( x=data, centers=4, nstart=i )
}

temp.vector <- sapply( results, function(result)
    { result$tot.withinss } )
result <- results[[which.min(temp.vector)]]

print(result)
stopCluster(cl)
mpi.exit()
```

snow

```
cluster <- getMPIcluster()

# Print the hostname for each cluster member
sayhello <- function()
{
  info <- Sys.info()[c("nodename", "machine")]
  paste("Hello from", info[1], "with CPU type", info[2])
}

names <- clusterCall(cluster, sayhello)
print(unlist(names))

# stopCluster will call mpi.finalize, no need for mpi.exit
stopCluster(cluster)
```

Installing snow on ARCHER2

- Requires a slightly modified `Rmpi` build to install:
  - Firstly, we need to set up a modified ARCHER2 R build environment (configuring the compilers):

    ```
    mkdir ~/.R
    ```

    - Add this to the file:

    ```
    ~/.R/Makevars
    ```

    - With the contents:

    ```
    CC = cc
    CXX = CC
    FC = ftn
    ```

  - `Rmpi` install:
    - Make sure we have the R module loaded:

    ```
    module load cray-R
    ```

    - Make sure we have the GNU compilers loaded:

    ```
    module load PrgEnv-gnu
    ```

    - And we have the R library path setup to install on to the /work filesystem, i.e.:

    ```
    export R_LIBS_USER=/work/ta055/ta055/$USER/Rinstall
    ```

    - Build `Rmpi`

    ```
    R CMD INSTALL /work/z19/shared/adrianj/Rmpi_0.6-9.2.tar.gz --configure-args=" --with-Rmpi-type=CRAY“
    ```

- Finally, install snow:

  ```
  R -e 'install.packages("snow", repos="https://cran.ma.imperial.ac.uk/")'
  ```

Running snow

```
#!/bin/bash
#SBATCH --job-name=snow
#SBATCH --nodes=2
#SBATCH --tasks-per-node=128
#SBATCH --time=0:5:0
#SBATCH --partition=standard
#SBATCH --qos=short
#SBATCH --account=z19
#SBATCH --hint=nomultithread

module load cray-R
export R_LIBS_USER=/work/z19/z19/adrianj/Rinstall
export PATH=$PATH:/work/z19/z19/adrianj/Rinstall/snow

export OMP_NUM_THREADS=1

srun RMPISNOW < ./simple_parallel_snow.R
```

More complex snow

```
nmax <- as.numeric(Sys.getenv("SLURM_NPROCS"))

cl <- getMPIcluster()

pbday <- function(n) {
  ntests <- 100000
  pop <- 1:365
  anydup <- function(i)
  any(duplicated(sample(pop, n,replace=TRUE)))
  sum(sapply(seq(ntests), anydup)) / ntests
}
clusterExport(cl, list('pbday'))

# print the time to do nmax tests, after distributing them to the workers
system.time( x <- clusterApply(cl, 1:nmax, function(n) { pbday(n) }) )

# compute the theoretical probability for each n
prob <- rep(0.0,nmax)
probnot <- 1.0
for (i in 2:nmax) {
  probnot <- probnot*(366.0-i)/365.0
  prob[i] = 1.0 - probnot
}

# print results, comparing tests to theory
z <- cbind(x,prob)
print(z)

# always include the following to stop the cluster
stopCluster(cl)
```

```
#!/bin/bash
#SBATCH --job-name=snow
#SBATCH --nodes=1
#SBATCH --tasks-per-node=64
#SBATCH --time=0:5:0
#SBATCH --partition=standard
#SBATCH --qos=short
#SBATCH --account=z19
#SBATCH --hint=nomultithread

module load cray-R
export R_LIBS_USER=/work/z19/z19/adrianj/Rinstall
export PATH=$PATH:/work/z19/z19/adrianj/Rinstall/snow

export OMP_NUM_THREADS=1

srun RMPISNOW < ./sample_birthday_snow.R
```

Summary

- R available and optimised on ARCHER2
- Controlling number and placement of workers can help with performance
- Many different mechanisms for parallel R and using multiple nodes
  - Can be configured to scale tasks, access more memory, reduce runtime
  - Choosing the most apprporiate approach can improve performance