Introduction to BiocParallel

Vincent Carey, Michael Lawrence, Martin Morgan*

Edited: May 6, 2015; Compiled: April 24, 2017

Contents

1 Introduction 1
2 Quick start 2
3 The BiocParallel Interface 3
   3.1 Classes ................................................................. 3
      3.1.1 BiocParallelParam ............................................... 3
      3.1.2 register()ing BiocParallelParam instances .................. 4
   3.2 Functions .............................................................. 6
      3.2.1 Parallel looping, vectorized and aggregate operations .......... 6
      3.2.2 Parallel evaluation environment .................................. 6
      3.2.3 Error handling and logging ..................................... 6
4 Use cases 6
   4.1 Single machine .......................................................... 7
      4.1.1 Multi-core .......................................................... 7
      4.1.2 Clusters ............................................................ 7
   4.2 Ad hoc cluster of multiple machines ................................ 11
      4.2.1 Sockets ............................................................ 11
      4.2.2 MPI ............................................................... 12
   4.3 Clusters with schedulers .............................................. 13
      4.3.1 Cluster-centric .................................................... 13
      4.3.2 R-centric .......................................................... 14
   4.4 Bioconductor Amazon Machine Image (AMI) .......................... 15
5 Analyzing genomic data in Bioconductor 17
6 For developers 17
7 sessionInfo() 18

1 Introduction

Numerous approaches are available for parallel computing in R. The CRAN Task View for high performance and parallel computing provides useful high-level summaries and package categorization. http://cran.r-project.org/web/views/HighPerformanceComputing.html Most Task View packages cite or identify one or more of snow, Rmpi, multicore or

*mtmorgan@fhcrc.org
**Introduction to BiocParallel**

`foreach` as relevant parallelization infrastructure. Direct support in R for parallel computing started with release 2.14.0 with inclusion of the `parallel` package which contains modified versions of `multicore` and `snow`.

A basic objective of BiocParallel is to reduce the complexity faced when developing and using software that performs parallel computations. With the introduction of the BiocParallelParam object, BiocParallel aims to provide a unified interface to existing parallel infrastructure where code can be easily executed in different environments. The BiocParallelParam specifies the environment of choice as well as computing resources and is invoked by ‘registration’ or passed as an argument to the BiocParallel functions.

BiocParallel offers the following conveniences over the ‘roll your own’ approach to parallel programming.

- unified interface: BiocParallelParam instances define the method of parallel evaluation (multi-core, snow cluster, etc.) and computing resources (number of workers, error handling, cleanup, etc.).
- parallel iteration over lists, files and vectorized operations: bplapply, bpmapply and bpvec provide parallel list iteration and vectorized operations. bpiterate iterates through files distributing chunks to parallel workers.
- cluster scheduling: When the parallel environment is managed by a cluster scheduler through BatchJobs, job management and result retrieval are considerably simplified.
- support of foreach: The `foreach` and `iterators` packages are fully supported. Registration of the parallel back end uses BiocParallelParam instances.

## 2 Quick start

The BiocParallel package is available at bioconductor.org and can be downloaded via biocLite:

```r
gistfile=1
source("http://bioconductor.org/biocLite.R")
biocLite("BiocParallel")
```

Load BiocParallel.

```r
gistfile=1
library(BiocParallel)
```

The test function simply returns the square root of “x”.

```r
FUN <- function(x) { round(sqrt(x), 4) }
```

Functions in BiocParallel use the registered back-ends for parallel evaluation. The default is the top entry of the registry list.

```r
registered()

# $MulticoreParam
# class: MulticoreParam
# bpisup: FALSE; bpnworkers: 4; bptasks: 0; bpjobname: BPJOB
# bplog: FALSE; bpthreshold: INFO; bpstopOnError: TRUE
# bptimeout: 2592000; bpprogressbar: FALSE
# bpRNGseed:
# bplogdir: NA
# bpsresultdir: NA
# cluster type: FORK
#
# $SnowParam
# class: SnowParam
# bpisup: FALSE; bpnworkers: 4; bptasks: 0; bpjobname: BPJOB
# bplog: FALSE; bpthreshold: INFO; bpstopOnError: TRUE
# bptimeout: 2592000; bpprogressbar: FALSE
# bpRNGseed:
```
Introduction to BiocParallel

Configure your R session to always use a particular back-end by setting options named after the back-ends in an .Rprofile file, e.g.,

```r
options(MulticoreParam=quote(MulticoreParam(workers=4)))
```

When a BiocParallel function is invoked with no BPPARAM argument the default back-end is used.

```r
bplapply(1:4, FUN)
```

Environment specific back-ends can be defined for any of the registry entries. This example uses a 2-worker SOCK cluster.

```r
param <- SnowParam(workers = 2, type = "SOCK")
bplapply(1:4, FUN, BPPARAM = param)
```

### 3 The BiocParallel Interface

#### 3.1 Classes

##### 3.1.1 BiocParallelParam

BiocParallelParam instances configure different parallel evaluation environments. Creating or register()ing a 'Param' allows the same code to be used in different parallel environments without a code re-write. Params listed are supported on all of Unix, Mac and Windows except MulticoreParam which is Unix and Mac only.

- **SerialParam:**
  - Supported on all platforms.
  - Evaluate BiocParallel-enabled code with parallel evaluation disabled. This approach is useful when writing new scripts and trying to debug code.

- **MulticoreParam:**
  - Supported on Unix and Mac. On Windows, MulticoreParam dispatches to SerialParam.
Evaluate _BiocParallel_-enabled code using multiple cores on a single computer. When available, this is the most efficient and least troublesome way to parallelize code. Windows does not support multi-core evaluation (the MulticoreParam object can be used, but evaluation is serial). On other operating systems, the default number of workers equals the value of the global option mc.cores (e.g., getOption("mc.cores")) or, if that is not set, the number of cores returned by parallel::detectCores() - 2. Based on facilities originally implemented in the _multicore_ package and subsequently the _parallel_ package in base _R_.

- **SnowParam**: Supported on all platforms. Evaluate _BiocParallel_-enabled code across several distinct _R_ instances, on one or several computers. This is a straightforward approach for executing parallel code on one or several computers, and is based on facilities originally implemented in the _snow_ package. Different types of _snow_ ‘back-ends’ are supported, including socket and MPI clusters.
- **BatchJobsParam**: Applicable to clusters with formal schedulers. Evaluate _BiocParallel_-enabled code by submitting to a cluster scheduler like SGE.
- **DoparParam**: Supported on all platforms. Register a parallel back-end supported by the _foreach_ package for use with _BiocParallel_.

The simplest illustration of creating BiocParallelParam is

```
serialParam <- SerialParam()
serialParam
## class: SerialParam
## bpisup: TRUE; bpnworkers: 1; bptasks: 0; bpjobname: BPJOB
## bplog: FALSE; bpthreshold: INFO; bpstopOnError: TRUE
## bptimeout: 2592000; bpprogressbar: FALSE
## bplogdir: NA
```

Most parameters have additional arguments influencing behavior, e.g., specifying the number of ‘cores’ to use when creating a MulticoreParam instance

```
multicoreParam <- MulticoreParam(workers = 8)
multicoreParam
## class: MulticoreParam
## bpisup: FALSE; bpnworkers: 8; bptasks: 0; bpjobname: BPJOB
## bplog: FALSE; bpthreshold: INFO; bpstopOnError: TRUE
## bptimeout: 2592000; bpprogressbar: FALSE
## bpRNGseed:
## bplogdir: NA
## bpreresultdir: NA
## cluster type: FORK
```

Arguments are described on the corresponding help page, e.g., ?MulticoreParam.

### 3.1.2 register()ing BiocParallelParam instances

The list of registered BiocParallelParam instances represents the user’s preferences for different types of back-ends. Individual algorithms may specify a preferred back-end, and different back-ends maybe chosen when parallel evaluation is nested.

The registry behaves like a ‘stack’ in that the last entry registered is added to the top of the list and becomes the “next used” (i.e., the default).
registered invoked with no arguments lists all back-ends.

```r
registered()
```

```r
## $MulticoreParam
## class: MulticoreParam
## bpisup: FALSE; bpnworkers: 4; bptasks: 0; bpjobname: BPJOB
## bplog: FALSE; bpthreshold: INFO; bpstopOnError: TRUE
## bptimeout: 2592000; bpprogressbar: FALSE
## bpRNGseed:
## bplogdir: NA
## bpresultdir: NA
## cluster type: FORK
##
## $SnowParam
## class: SnowParam
## bpisup: FALSE; bpnworkers: 4; bptasks: 0; bpjobname: BPJOB
## bplog: FALSE; bpthreshold: INFO; bpstopOnError: TRUE
## bptimeout: 2592000; bpprogressbar: FALSE
## bpRNGseed:
## bplogdir: NA
## bpresultdir: NA
## cluster type: SOCK
##
## $SerialParam
## class: SerialParam
## bpisup: TRUE; bpnworkers: 1; bptasks: 0; bpjobname: BPJOB
## bplog: FALSE; bpthreshold: INFO; bpstopOnError: TRUE
## bptimeout: 2592000; bpprogressbar: FALSE
## bplogdir: NA
```

`bpparam` returns the default from the top of the list.

```r
bpparam()
```

```r
## class: MulticoreParam
## bpisup: FALSE; bpnworkers: 4; bptasks: 0; bpjobname: BPJOB
## bplog: FALSE; bpthreshold: INFO; bpstopOnError: TRUE
## bptimeout: 2592000; bpprogressbar: FALSE
## bpRNGseed:
## bplogdir: NA
## bpresultdir: NA
## cluster type: FORK
```

Add a specialized instance with `register`. When `default` is `TRUE`, the new instance becomes the default.

```r
register(BatchJobsParam(workers = 10), default = TRUE)
```

BatchJobsParam has been moved to the top of the list and is now the default.

```r
names(registered())
```

```r
## [1] "BatchJobsParam" "MulticoreParam" "SnowParam" "SerialParam"
```

```r
bpparam()
```

```r
## class: BatchJobsParam
## bpisup: TRUE; bpnworkers: 10; bptasks: 0; bpjobname: BPJOB
## bplog: FALSE; bpthreshold: INFO; bpstopOnError: TRUE
```
3.2 Functions

3.2.1 Parallel looping, vectorized and aggregate operations

These are used in common functions, implemented as much as possible for all back-ends. The functions (see the help pages, e.g., ?bplapply for a full definition) include

\[ \text{bplapply}(X, \text{FUN}, ...) \]  
Apply in parallel a function \( \text{FUN} \) to each element of \( X \). \( \text{bplapply} \) invokes \( \text{FUN} \) \( \text{length}(X) \) times, each time with a single element of \( X \).

\[ \text{bpmapply}(\text{FUN}, ...) \]  
Apply in parallel a function \( \text{FUN} \) to the first, second, etc., elements of each argument in . . .

\[ \text{bpiterate}(\text{ITER}, \text{FUN}, ...) \]  
Apply in parallel a function \( \text{FUN} \) to the output of function \( \text{ITER} \). Data chunks are returned by \( \text{ITER} \) and distributed to parallel workers along with \( \text{FUN} \). Intended for iteration though an undefined number of data chunks (i.e., records in a file).

\[ \text{bpvec}(X, \text{FUN}, ...) \]  
Apply in parallel a function \( \text{FUN} \) to subsets of \( X \). \( \text{bpvec} \) invokes function \( \text{FUN} \) as many times as there are cores or cluster nodes, with \( \text{FUN} \) receiving a subset (typically more than 1 element, in contrast to \( \text{bplapply} \)) of \( X \).

\[ \text{bpaggregate}(x, \text{data}, \text{FUN}, ...) \]  
Use the formula in \( x \) to aggregate data using \( \text{FUN} \).

3.2.2 Parallel evaluation environment

These functions query and control the state of the parallel evaluation environment.

\[ \text{bpisup}(x) \]  
Query a \( \text{BiocParallelParam} \) back-end \( x \) for its status.

\[ \text{bpworkers}, \text{bpnworkers} \]  
Query a \( \text{BiocParallelParam} \) back-end for the number of workers available for parallel evaluation.

\[ \text{bptasks} \]  
Divides a job (e.g., single call to \(*lapply\) function) into tasks. Applicable to \( \text{MulticoreParam} \) only; \( \text{DoparParam} \) and \( \text{BatchJobsParam} \) have their own approach to dividing a job among workers.

\[ \text{bpstart}(x) \]  
Start a parallel back end specified by \( \text{BiocParallelParam} x \), if possible.

\[ \text{bpstop}(x) \]  
Stop a parallel back end specified by \( \text{BiocParallelParam} x \).

3.2.3 Error handling and logging

Logging and advanced error recovery is available in \( \text{BiocParallel 1.1.25} \) and later. For a more details see the vignette titled "Error Handling and Logging":

\[ \text{browseVignettes}("\text{BiocParallel"}) \]

4 Use cases

Sample data are BAM files from a transcription profiling experiment available in the \text{RNAseqData.HNRNPC.bam.chr14} package.

\[ \text{library(RNAseqData.HNRNPC.bam.chr14)} \]
\[ \text{fls <- RNAseqData.HNRNPC.bam.chr14_BAMFILES} \]
4.1 Single machine

4.1.1 Multi-core

There are substantial benefits, such as shared memory, to be had using multiple cores on a single machine. On a single non-Windows machine the recommended approach is multi-core, or forked processes.

This example counts overlaps between BAM files and a defined set of ranges. First create a GRanges with regions of interest (in practice this could be large).

```r
library(GenomicAlignments) # for GenomicRanges and readGAlignments()
gr <- GRanges("chr14", IRanges((1000:3999)*5000, width=1000))
```

A `ScanBamParam` defines regions to extract from the files.

```r
param <- ScanBamParam(which=range(gr))
```

`FUN` counts overlaps between the ranges in `gr` and the files.

```r
FUN <- function(fl, param) {
  gal <- readGAlignments(fl, param = param)
  sum(countOverlaps(gr, gal))
}
```

All parameters necessary for running a job in a multi-core environment are specified in the `MulticoreParam` instance.

```r
MulticoreParam()
```

4.1.2 Clusters

Both Windows and non-Windows machines can use the cluster approach to spawn processes. `BiocParallel` back-end choices for clusters on a single machine are `SnowParam` for configuring a Snow cluster or the `DoparParam` for use with
the `foreach` package.

To re-run the counting example, `FUN` needs to be modified such that `’gr’` is passed as a formal argument and required libraries are loaded on each worker.

```r
FUN <- function(fl, param, gr) {
  library(GenomicAlignments)
  gal <- readGAlignments(fl, param = param)
  sum(countOverlaps(gr, gal))
}
```

Define a 2-worker SOCK Snow cluster.

```r
snow <- SnowParam(workers = 2, type = "SOCK")
```

A call to `bplapply` with the `SnowParam` creates the cluster and distributes the work.

```r
bplapply(fls[1:3], FUN, BPPARAM = snow, param = param, gr = gr)
```

---

```
# Loading required package: BiocGenerics
# Loading required package: parallel
#
# Attaching package: BiocGenerics
#
# The following objects are masked from package:parallel:
# #
#  clusterApply, clusterApplyLB, clusterCall, clusterEvalQ,
#  clusterExport, clusterMap, parApply, parCapply, parLapply,
#  parLapplyLB, parRapply, parSapply, parSapplyLB
#
# The following objects are masked from package:stats:
# #
#  IQR, mad, sd, var, xtabs
#
# The following objects are masked from package:base:
# #
#  Filter, Find, Map, Position, Reduce, anyDuplicated, append,
#  as.data.frame, cbind, colMeans, colSums, colnames, do.call,
#  duplicated, eval, evalq, get, grep, grepl, intersect, is.unsorted,
#  lapply, lengths, mapply, match, mget, order, paste, pmax, pmax.int,
#  pmin, pmin.int, rank, rbind, rowMeans, rowSums, rownames, sapply,
#  setdiff, sort, table, tapply, union, unique, unsplit, which,
#  which.max, which.min
#
# Loading required package: S4Vectors
# Loading required package: stats4
#
# Attaching package: S4Vectors
#
# The following object is masked from package:base:
# #
#  expand.grid
#
# Loading required package: IRanges
# Loading required package: GenomeInfoDb
# Loading required package: GenomicRanges
# Loading required package: SummarizedExperiment
```
## Loading required package: Biobase
## Welcome to Bioconductor
## Vignettes contain introductory material; view with
## `browseVignettes()`. To cite Bioconductor, see
## `citation("Biobase")`, and for packages `citation("pkgname")`.
## Loading required package: DelayedArray
## Loading required package: matrixStats
## Attaching package: matrixStats
## The following objects are masked from package:Biobase:
## anyMissing, rowMedians
## Attaching package: DelayedArray
## The following objects are masked from package:matrixStats:
## colMaxes, colMins, colRanges, rowMaxes, rowMins, rowRanges
## The following object is masked from package:base:
## apply
## Loading required package: Biostrings
## Loading required package: XVector
## Attaching package: Biostrings
## The following object is masked from package:DelayedArray:
## type
## The following object is masked from package:base:
## strsplit
## Loading required package: Rsamtools
## Loading required package: BiocGenerics
## Loading required package: parallel
## Attaching package: BiocGenerics
## The following objects are masked from package:parallel:
## clusterApply, clusterApplyLB, clusterCall, clusterEvalQ,
## clusterExport, clusterMap, parApply, parCapply, parLapply,
## parLapplyLB, parRapply, parSapply, parSapplyLB
## The following objects are masked from package:stats:
##
## IQR, mad, sd, var, xtabs

## The following objects are masked from package:base:
## Filter, Find, Map, Position, Reduce, anyDuplicated, append,
## as.data.frame, cbind, colMeans, colSums, colnames, do.call,
## duplicated, eval, evalq, get, grep, grepl, intersect, is.unsorted,
## lapply, lengths, mapply, match, mget, order, paste, pmax, pmax.int,
## pmin, pmin.int, rank, rbind, rowMeans, rowSums, rownames, sapply,
## setdiff, sort, table, tapply, unique, unsplit, which,
## which.max, which.min
##
## Loading required package: S4Vectors
## Loading required package: stats4
##
## Attaching package: S4Vectors
##
## The following object is masked from package:base:
## expand.grid
##
## Loading required package: IRanges
## Loading required package: GenomeInfoDb
## Loading required package: GenomicRanges
## Loading required package: SummarizedExperiment
## Loading required package: Biobase
## Welcome to Bioconductor
##
## Vignettes contain introductory material; view with
## 'browseVignettes()'. To cite Bioconductor, see
## 'citation("Biobase")'.
##
## Loading required package: DelayedArray
## Loading required package: matrixStats
##
## Attaching package: matrixStats
##
## The following objects are masked from package:Biobase:
## anyMissing, rowMedians
##
## Attaching package: DelayedArray
##
## The following objects are masked from package:matrixStats:
## colMzs, colMns, colRngs, rowMzs, rowMns, rowRngs
##
## The following object is masked from package:base:
## apply
##
## Loading required package: Biostrings
## Loading required package: XVector
The FUN written for the cluster adds some overhead due to the passing of the GRanges and the loading of `GenomicAlignments` on each worker. This approach, however, has the advantage that it works on most platforms and does not require a coding change when switching between windows and non-windows machines.

### 4.2 Ad hoc cluster of multiple machines

We use the term *ad hoc* cluster to define a group of machines that can communicate with each other and to which the user has password-less log-in access. This example uses a group of compute machines ("the rhinos") on the FHCRC network.

#### 4.2.1 Sockets

On Linux and Mac OS X, a socket cluster is created across machines by supplying machine names as the `workers` argument to a `BiocParallelParam` instance instead of a number. Each name represents an R process; repeat names indicate multiple workers on the same machine.

Create a `SnowParam` with 2 cpus from 'rhino01' and 1 from 'rhino02':

```r
define argument names here.
```

```r
hosts <- c("rhino01", "rhino01", "rhino02")
param <- SnowParam(workers = hosts, type = "SOCK")
```

Execute FUN 4 times across the workers.

```r
> FUN <- function(i) system("hostname", intern=TRUE)
> bplapply(1:4, FUN, BPPARAM = param)
```

```r
[[1]]
[1] "rhino01"

[[2]]
[1] "rhino01"

[[3]]
[1] "rhino02"
```
When creating a cluster across Windows machines, workers must be IP addresses (e.g., "140.107.218.57") instead of machine names.

### 4.2.2 MPI

An MPI cluster across machines is created with `mpirun` or `mpiexec` from the command line or a script. A list of machine names provided as the `-hostfile` argument defines the mpi universe.

The hostfile requests 2 processors on 3 different machines:

```
rhino01 slots=2
rhino02 slots=2
rhino03 slots=2
```

From the command line, start a single interactive R process on the current machine.

```r
mpiexec --np 1 --hostfile hostfile R --vanilla
```

Load `BiocParallel` and create an MPI Snow cluster. The number of workers in `SnowParam` should match the number of slots requested in the hostfile. Using a smaller number of workers uses a subset of the slots.

```r
> library(BiocParallel)
> param <- SnowParam(workers = 6, type = "MPI")

Execute FUN 6 times across the workers.

```r
> FUN <- function(i) system("hostname", intern=TRUE)
> bplapply(1:6, FUN, BPPARAM = param)
```

6 slaves are spawned successfully. 0 failed.

```r
[[1]]
[1] "rhino01"

[[2]]
[1] "rhino02"

[[3]]
[1] "rhino02"

[[4]]
[1] "rhino03"

[[5]]
[1] "rhino03"

[[6]]
[1] "rhino01"
```

Batch jobs can be launched with mpiexec and `R CMD BATCH`. Code to be executed is in ‘Rcode.R’.

```r
mpiexec --hostfile hostfile R CMD BATCH Rcode.R
```
4.3 Clusters with schedulers

Computer clusters are far from standardized, so the following may require significant adaptation; it is written from experience here at FHCRC, where we have a large cluster managed via SLURM. Nodes on the cluster have shared disks and common system images, minimizing complexity about making data resources available to individual nodes. There are two simple models for use of the cluster, Cluster-centric and R-centric.

4.3.1 Cluster-centric

The idea is to use cluster management software to allocate resources, and then arrange for an R script to be evaluated in the context of allocated resources. NOTE: Depending on your cluster configuration it may be necessary to add a line to the template file instructing workers to use the version of R on the master / head node. Otherwise the default R on the worker nodes will be used.

For SLURM, we might request space for 4 tasks (with `salloc` or `sbatch`), arrange to start the MPI environment (with `orterun`) and on a single node in that universe run an R script `BiocParallel-MPI.R`. The command is

```
$ salloc -N 4 orterun -n 1 R -f BiocParallel-MPI.R
```

The R script might do the following, using MPI for parallel evaluation. Start by loading necessary packages and defining FUN work to be done

```
library(BiocParallel)
library(Rmpi)
FUN <- function(i) system("hostname", intern=TRUE)
```

Create a `SnowParam` instance with the number of nodes equal to the size of the MPI universe minus 1 (let one node dispatch jobs to workers), and register this instance as the default

```
param <- SnowParam(mpi.universe.size() - 1, "MPI")
register(param)
```

Evaluate the work in parallel, process the results, clean up, and quit

```
x <- bplapply(1:100, FUN)
table(unlist(xx))
mpi.quit()
```

The entire session is as follows:

```
$ salloc -N 4 orterun -n 1 R --vanilla -f BiocParallel-MPI.R
salloc: Job is in held state, pending scheduler release
salloc: Pending job allocation 6762292
salloc: job 6762292 queued and waiting for resources
salloc: job 6762292 has been allocated resources
salloc: Granted job allocation 6762292
## ...
> FUN <- function(i) system("hostname", intern=TRUE)
> 
> library(BiocParallel)
> library(Rmpi)
> param <- SnowParam(mpi.universe.size() - 1, "MPI")
> register(param)
> xx <- bplapply(1:100, FUN)
> 4 slaves are spawned successfully. 0 failed.
> table(unlist(xx))
```
One advantage of this approach is that the responsibility for managing the cluster lies firmly with the cluster management software – if one wants more nodes, or needs special resources, then adjust parameters to `salloc` (or `sbatch`).

Notice that workers are spawned within the `bplapply` function; it might often make sense to more explicitly manage workers with `bpstart` and `bpstop`, e.g.,

```r
param <- bpstart(SnowParam(mpi.universe.size() - 1, "MPI"))
register(param)
xx <- bplapply(1:100, FUN)
bpstop(param)
mpi.quit()
```

### 4.3.2 R-centric

A more R-centric approach might start an R script on the head node, and use `BatchJobs` to submit jobs from within the R session. One way of doing this is to create a file containing a template for the job submission step, e.g., for SLURM:

```bash
#!/bin/bash
## file: slurm.tmpl
## Job Resource Interface Definition
##
## ntasks [integer(1)]: Number of required tasks.
## ncpus [integer(1)]: Number of required cpus per task.
## walltime [integer(1)]: Walltime for this job, in minutes.
##
## 'resources' is an argument provided to BatchJobsParam()
#SBATCH --job-name=<%= job.name %>
#SBATCH --output=<%= log.file %>
#SBATCH --error=<%= log.file %>
#SBATCH --ntasks=<%= resources$ntasks %>
#SBATCH --cpus-per-task=<%= resources$ncpus %>
#SBATCH --time=0:10:0

## Run R: we merge R output with stdout from SLURM, which gets then
## logged via --output option
R CMD BATCH --no-save --no-restore "<%= rscript %>
```

The R script, run interactively or from the command line, might then look like:

```r
## define work to be done
FUN <- function(i) system("hostname", intern=TRUE)

library(BiocParallel)
library(BatchJobs)
```

1. see [https://github.com/tudo-r/BatchJobs/tree/master/examples/cfSLURM](https://github.com/tudo-r/BatchJobs/tree/master/examples/cfSLURM)
The code runs on the head node until bplapply, where the R script interacts with the SLURM scheduler to request a SLURM allocation, run jobs, and retrieve results. The argument 4 to BatchJobsParam specifies the number of workers to request from the scheduler; bplapply divides the 100 jobs among the 4 workers. If BatchJobsParam had been created without specifying any workers, then 100 jobs implied by the argument to bplapply would be associated with 100 tasks submitted to the scheduler.

Because cluster tasks are running in independent R instances, and often on physically separate machines, a convenient ‘best practice’ is to write FUN in a ‘functional programming’ manner, such that all data required for the function is passed in as arguments or (for large data) loaded implicitly or explicitly (e.g., via an R library) from disk.

4.4 Bioconductor Amazon Machine Image (AMI)

An AMI for running Bioconductor in the Elastic Compute Cloud (EC2) is available at http://www.bioconductor.org/help/bioconductor-cloud-ami/. The documentation provides detailed instructions for setting up accounts, launching instances and starting sessions via RStudio or SSH.

Motivation for running jobs in the cloud may be access to additional CPUs and / or memory. Amazon Web Services (AWS) has a variety of instances ranging from general purpose to those optimized for compute, memory or I/O intensive jobs. See http://aws.amazon.com/ec2/instance-types/ for a full listing of instances.

Single or multiple instances can be requested when starting up the AMI. When a single instance is requested, interaction with the resource is the same as described in the ‘Single Machine’ section above. Requesting multiple instances is essentially creating a cluster. To do this with the Bioconductor AMI the StarCluster toolkit must be installed and a config file must be modified to specify the number and type of instances. Walk-through examples are provided in the Bioconductor AMI web documentation http://www.bioconductor.org/help/bioconductor-cloud-ami/.

This example uses a cluster of three m3.large instances each of which has 2 virtual CPUs. The name of the cluster in the config file is ‘smallcluster’ and can be started with the ‘start’ command:

    starcluster start smallcluster

List the cluster nodes:

    ~ > starcluster listclusters

StarCluster - (http://star.mit.edu/cluster) (v. 0.95.5)
Software Tools for Academics and Researchers (STAR)
Please submit bug reports to starcluster@mit.edu

-----------------------------------------------
smallcluster (security group: @sc-smallcluster)
-----------------------------------------------
Launch time: 2014-07-21 08:44:11
Uptime: 0 days, 00:09:30
Zone: us-east-1b
Keypair: bioc-keypair-vobench
EBS volumes: N/A
Cluster nodes:
Introduction to BiocParallel

smallcluster-master running i-1f757234 ec2-54-91-126-83.compute-1.amazonaws.com
smallcluster-node001 running i-1e757235 ec2-50-16-135-207.compute-1.amazonaws.com
smallcluster-node002 running i-19757232 ec2-54-89-112-24.compute-1.amazonaws.com
Total nodes: 3

Use the hostname for the master node to connect to the cluster via RStudio or SSH.

The AMI cluster workers can communicate via SSH, SunGrid Engine (SGE) or MPI. For MPI, a SnowParam should be configured with type = "MPI".

```r
library(BiocParallel)
param <- SnowParam(workers=3, type = "MPI")
```

Both SSH and SunGrid Engine require a BatchJobsParam but differ slightly in the set-up.

For SSH, the nodes are registered as SSH workers. The 'workers' argument to BatchJobsParam should be the number of nodes and 'ncpus' the number of processors per node.

```r
library(BiocParallel)
library(BatchJobs)
funs <- makeClusterFunctionsSSH(
  + makeSSHWorker(nodename="smallcluster-master"),
  + makeSSHWorker(nodename="smallcluster-node001"),
  + makeSSHWorker(nodename="smallcluster-node002")
)
param <- BatchJobsParam(workers=3,
  + resources=list(ncpus=2),
  + cluster.functions=funs)
```

SunGrid Engine only needs the number of 'workers' and 'ncpus'.

```r
library(BiocParallel)
library(BatchJobs)
param <- BatchJobsParam(3, resources=list(ncpus=2))
```

This example uses 8 paired-end RNA-Seq BAM files, 1 per sequencing run, subset on chromosome 14 only.

```r
library(BiocParallel)
library(RNAseqData.HNRNPC.bam.chr14)
fls <- RNAseqData.HNRNPC.bam.chr14_BAMFILES
```

Reads with more than 2 gaps in the CIGAR are isolated and locateVariants is used to identify where these multi-gap reads fall with respect to the UCSC hg19 known gene model.

```r
FUN <- function(file, ...) {
  library(GenomicAlignments)
  library(VariantAnnotation)
  library(TxDB.Hsapiens.UCSC.hg19.knownGene)
  txdb <- TxDb.Hsapiens.UCSC.hg19.knownGene
  gal <- readGAlignmentPairs(file)
  gal_with_gaps <- gal[njunc(gal) > 2L]
  locateVariants(granges(gal_with_gaps), txdb, AllVariants())
}
```

Define a BatchJobsParam with 3 workers, 2 processors each.

```r
param <- BatchJobsParam(3, resources=(list(ncpus=2)))
```

Execute in parallel over the 8 files.

```r
res <- bplapply(fls, FUN, BPPARAM=param)
```

The return value is a list of GRanges, one for each file. The length of each GRanges will vary.
Introduction to *BiocParallel*

> lengths(res)
ERR127306 ERR127307 ERR127308 ERR127309 ERR127302 ERR127303 ERR127304 ERR127305
  5228  5202  5721  4326  4494  4909  4636  4538

Summarize the LOCATION and TXID output of `locateVariants` with `xtabs`.

> mdat <- lapply(res, function(x) mcols(x)[c("LOCATION", "TXID")])
> xtab <- xtabs(~ LOCATION + TXID, do.call(rbind, mdat))

The `xtab` object can be subset to isolate transcripts that meet a criteria. These are the top 5 transcripts hit by the multi-gap reads.

> xtab[,xtab["spliceSite", ] > 500]

<table>
<thead>
<tr>
<th>TXID</th>
<th>LOCATION</th>
<th>spliceSite</th>
<th>intron</th>
<th>fiveUTR</th>
<th>threeUTR</th>
<th>coding</th>
<th>intergenic</th>
<th>promoter</th>
</tr>
</thead>
<tbody>
<tr>
<td>51581</td>
<td>51582</td>
<td>53506</td>
<td>53507</td>
<td>53508</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>994</td>
<td>994</td>
<td>520</td>
<td>548</td>
<td>548</td>
<td></td>
<td></td>
</tr>
<tr>
<td>spliceSite</td>
<td>994</td>
<td>994</td>
<td>520</td>
<td>548</td>
<td>548</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>intron</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>fiveUTR</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>threeUTR</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>coding</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>intergenic</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>promoter</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Extract the transcripts with multi-gap reads in promoter regions:

> xtab[,xtab["promoter", ] > 0]

<table>
<thead>
<tr>
<th>TXID</th>
<th>LOCATION</th>
<th>spliceSite</th>
<th>intron</th>
<th>fiveUTR</th>
<th>threeUTR</th>
<th>coding</th>
<th>intergenic</th>
<th>promoter</th>
</tr>
</thead>
<tbody>
<tr>
<td>51495</td>
<td>52270</td>
<td>52272</td>
<td>52273</td>
<td>52528</td>
<td>52538</td>
<td>52540</td>
<td>52541</td>
<td>52716</td>
</tr>
<tr>
<td></td>
<td></td>
<td>152</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>46</td>
</tr>
<tr>
<td>spliceSite</td>
<td>152</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>intron</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>fiveUTR</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>threeUTR</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>coding</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>intergenic</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>promoter</td>
<td>38</td>
<td>31</td>
<td>314</td>
<td>314</td>
<td>54</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

5 Analyzing genomic data in Bioconductor

General strategies exist for handling large genomic data that are well suited to R programs. A manuscript titled *Scalable Genomics with R and Bioconductor* ([http://arxiv.org/abs/1409.2864](http://arxiv.org/abs/1409.2864)) by Michael Lawrence and Martin Morgan, reviews several of these approaches and demonstrate implementation with *Bioconductor* packages. Problem areas include scalable processing, summarization and visualization. The techniques presented include restricting queries, compressing data, iterating, and parallel computing.

Ideas are presented in an approachable fashion within a framework of common use cases. This is a beneficial read for anyone tackling genomics problems in R.

6 For developers

Developers wishing to use *BiocParallel* in their own packages should include *BiocParallel* in the DESCRIPTION file

```r
Imports: BiocParallel
```

and import the functions they wish to use in the NAMESPACE file, e.g.,
importFrom(BiocParallel, bplapply)

Then invoke the desired function in the code, e.g.,

```
system.time(x <- bplapply(1:3, function(i) {
  Sys.sleep(i); i })
```

```
## Warning: RSQLite::dbGetPreparedQuery() is deprecated, please switch to DBI::dbGetQuery(params = bind.data).
## Warning: Named parameters not used in query: fun_id, pars, jobname
## Warning: Named parameters not used in query: job_def_id, seed
## Warning in formals(fun): argument is not a function
## Warning in formals(fun): argument is not a function
## Warning in formals(fun): argument is not a function
## user  system elapsed
## 3.632  0.012  9.711

unlist(x)
## [1] 1 2 3
```

This will use the back-end returned by bpparam(), by default a MulticoreParam() instance or the user’s preferred back-end if they have used register(). The MulticoreParam back-end does not require any special configuration or set-up and is therefore the safest option for developers. Unfortunately, MulticoreParam provides only serial evaluation on Windows.

Developers should document that their function uses BiocParallel functions on the man page, and should perhaps include in their function signature an argument BPPARAM=bpparam().

Developers wishing to invoke back-ends other than MulticoreParam need to take special care to ensure that required packages, data, and functions are available and loaded on the remote nodes.

7 sessionInfo()

toLatex(sessionInfo())

- R version 3.4.0 (2017-04-21), x86_64-pc-linux-gnu
- Locale: LC_CTYPE=en_US.UTF-8, LC_NUMERIC=C, LC_TIME=en_US.UTF-8, LC_COLLATE=C, LC_MONETARY=en_US.UTF-8, LC_MESSAGES=en_US.UTF-8, LC_ADDRESS=C, LC_TELEPHONE=C, LC_MEASUREMENT=en_US.UTF-8, LC_IDENTIFICATION=C
- Running under: Ubuntu 16.04.2 LTS
- Matrix products: default
- BLAS: /home/biocbuild/bbs-3.5-bioc/R/lib/libRblas.so
- LAPACK: /home/biocbuild/bbs-3.5-bioc/R/lib/libRlapack.so
- Base packages: base, datasets, grDevices, graphics, methods, parallel, stats, stats4, utils
- Other packages: BBmisc 1.11, BatchJobs 1.6, Biobase 2.36.0, BiocGenerics 0.22.0, BiocParallel 1.10.0, Biostatics 2.44.0, DelayedArray 0.2.0, GenomInfoDb 1.12.0, GenomicAlignments 1.12.0, GenomicRanges 1.28.0, IRanges 2.10.0, RNAseqData.HNRNPC.bam.chr14 0.13.0, Rsamtools 1.28.0, S4Vectors 0.14.0, SummarizedExperiment 1.6.0, XVector 0.16.0, checkmate 1.8.2, matrixStats 0.52.2
- Loaded via a namespace (and not attached): BiocStyle 2.4.0, DBI 0.6-1, GenomInfoDbData 0.99.0, Matrix 1.2-9, RCurl 1.95-4.8, RSQLite 1.1-2, Rcpp 0.12.10, backports 1.0.5, base64enc 0.1-3, bitops 1.0-6, brew 1.0-6, compiler 3.4.0, digest 0.6.12, evaluate 0.10, fail 1.3, grid 3.4.0, htmltools 0.3.5, knitr 1.15.1, lattice 0.20-35, magrittr 1.5, memoise 1.1.0, rmarkdown 1.4, rprojroot 1.2, sendmailR 1.2-1, snow 0.4-2, stringi 1.1.5, stringr 1.2.0, tools 3.4.0, yaml 2.1.14, zlibbioc 1.22.0