

How to use PBS package?

Delta can visualize the interaction loop, TAD, 3D model result through Genome view, Circlet view as well as Physical View.

This document describes a PBS package to run a pipeline by using PBS cluster to get these results from observed interaction matrix file and a genomic feature file.

1. Required software

Delta needs to install the following required software under Linux environment before running the pipeline.

Portable Batch System

Java 1.7

JBrowse package (an embed JBrowse used by Delta, you need to install the JBrowse required modules first)

TADtree (we have embedded the python scripts of TADtree under script directory)

FastHiC (we have embedded the jar package of FastHiC under script directory)

BACH (you need to download the source code of BACH and install it by yourself)

MOGEN (we have embedded the jar package of MOGEN software under script directory)

Tabix (we have embedded the Tabix software under script directory)

2. Download the installation package

Download the stand alone package which is a .tar.gz package. After uncompressed such as /home/test/custom_delta, you will see the file list as the follows:

Name	Description
testdata	A test data directory including all the test files and test configuration files
11_bin_50000.feature	A test feature file
11_bin_50000.matrix	A test matrix file
demo_mogen.properties	A demo configuration file to use MOGEN to call 3D model
demo.properties	A demo configuration file to use BACH to call 3D model
Delta.jar	A required package to run pipeline
How to use.pdf	A description document
reference	A reference directory
scripts	All the scripts to run the pipeline
result	A result directory

3. Prepare the runtime environment

When all the required tools have been installed successfully, you can create a soft link to these tools under the scripts directory such as /home/test/custom_delta/scripts by using Linux command "ln -s".

ln -s BACH installed location/BACH BACH

ln -s java install location/bin/java java

4. Configure the properties file

Delta uses a properties file to store all the parameters which needed by running a pipeline. There is a demo properties file named “delta.properties” which can be modified.

The parameters are described as the following:

Parameter Name	Description	Default Value
delta.pbs.queue	The work queue to submit the task	workq
delta.pbs.memory	The used memory for the task	
delta.pbs.walltime	The need run time for the task	
delta.pbs.subcmd	The submit command for the work queue, such as qsub	qsub
delta.pbs.isautosubmi	Whether submit all task automatically, 1 means yes, 0 means no. If set 0, then users can manually submit the task from the joblist file which located in the result directory.	0
delta.reference_path	A reference path contains the visualization template file which will be used by the pipeline to generate the needed configuration file of each view.	
delta.scripts_path	A script path of pipeline	
delta.matrixfile	An absolute location of the observed interaction matrix file	
delta.organism	The organism of the interaction matrix file belong to, such as human	Two organisms are supported now: human and mouse
delta.cellline	The cell line of the interaction matrix file belong to, such as K562	
delta.binsize	The resolution of the interaction matrix file, such as 50000	
delta.chrom	The chromosome of the interaction matrix file belong to, such as 11	
delta.startbin	The start bin of the interaction matrix file which can be computed by the start position of the first bin/binsize	
delta.endbin	The end bin of the interaction matrix file which can be computed by the start position of the last bin/binsize	
delta.tadtree.bin	The maximum allowable bin size for a TAD	6
delta.tadtree.gamma	the trade-off between sensitivity and specificity	1000

delta.tadtree.number	the total number of TADs allowed on a given chromosome	200
delta.tadtree.p	the minimum scale over which changes in interaction preference can be robustly detected, p is given in units of bins	2
delta.tadtree.q	the minimum scale over which changes in interaction preference can be robustly detected, q is given in units of bins	3
delta.physicalmodel	the software used to call 3D model. Two values provided: bach / mogen	bach
delta.bach.featurefile	A genomic feature file of the genomic location for the interaction matrix file	
delta.bach.k	The number of particles in SIS (-K)	100
delta.bach.mp	The number of enrichment in SIS(-MP)	10
delta.bach.ng	The number of Gibbs sampler iterations (-NG)	5000
delta.bach.nt	The length of tune interval in HMC(-NT)	50
delta.bach.l	The step size of leap frog in HMC(-L)	50
delta.mogen.adjacentedist	maximum distance between 2 adjacent points	1.5
delta.mogen.contactdist	contact distance, points that are in contact should have square distance less than this	6
delta.mogen.posminidist		0.2
delta.mogen.negmaxdist		50
delta.mogen.posmaxdistweight	increase this parameter to improve contact score, but will decrease non-contact score	200
delta.mogen.posminidistweight	increase this parameter if adjacent points are too close to each other	1.0
delta.mogen.nemindistweight	increase this parameter to improve non-contact score, (but will decrease contact score)	40.0
delta.mogen.negmaxdistweight	increase this parameter to prevent the structure from spanning too much (make the structure smaller)	1.0
delta.mogen.learningrate	learning rate for the optimization process	0.01
delta.mogen.maxiterator	maximum iteration numbers	20000

5. Run the pipeline

Use the Delta.jar under the scripts location, type the command as the following:

```
java -jar [Delta.jar location][the properties file][the result output directory]
```

```
java -jar /home/test/custom_delta/DeltaPBS.jar /home/test/
custom_delta/testdata/delta.properties /home/test/custom_delta/result
```

After the pipeline running finished, a result directory will be generated including all the results which needed to be copied into the web project

Result	Description	Operation
A jobid such as 1481540124350	Under this directory, you can check the pipeline result in the following subdirectory: bach the 3d model result directory, the final result includes bach.xyz mogen the 3d model result directory,the final result is .xyz fasthic the interaction loop result directory, the final results include gff3.tabix1,peak.json tadtree the TAD result directory, the final result includes tad.gff3 genome the matrix heat map result directory	Copy the directory into the data directory of the web project
conf	The subdirectories including the configured files(*.conf) for the circlet view and the physical view	Copy the accordingly .conf file into the conf directory of web project separately, and modified the value in the configuration file according to your web project directory
jbrowse	The genome view result	Copy the time stamp directory into the jbrowse directory of web project
userconf	The entry configuration for the circlet view and the physical view	Copy the accordingly *.conf files into the userconf directory of web project separately