
PopCluster (Linux)

Introduction

This document briefly describes how to run PopCluster on a Linux machine. It should be read together with the PopCluster.pdf file, which gives much more details about the methods, inputs and outputs of PopCluster and is thus highly recommended to read before starting the use of PopCluster.

The zipped Linux package includes the following files in 3 subfolders:

- 1) PopClusterLnx
- 2) PopClusterLnx_impi
- 3) PopClusterLnx_openmpi
- 4) Readme.pdf
- 5) PopCluster.pdf
- 6) PopClusterUpdateHistory.txt
- 7) ant377NoScale.dat
- 8) ant377NoScale.PcPjt

The first 3 files are the binaries compiled by Intel's Fortran compiler (2018 Update 3). They are all for 64bit Linux, and may not work for 32bit Linux. The 1st file is statically linked for serial run, the 2nd file is linked with Intel's MPI library (2018 Update 3) and the 3rd file is linked with openMPI library (3.1.4). The latter 2 files are for MPI parallel run, using the corresponding MPI libraries installed on your cluster. The 3 binary files are in the subfolder "Bin".

The 4th file is what you are reading. The 5th is a detailed description of the use of PopCluster program. The 6th file is a brief of the updating history of PopCluster. These 3 documents are in the subfolder "Doc".

The 7th file is an example genotype data file, and the 8th is the corresponding parameter file. These 2 files are in the subfolder "Example".

Serial run

To make a serial run of PopCluster for the example dataset in subfolder Example, simply go to the PopCluster program folder (which contains the 3 subfolders above) and type (in terminal)

```
./Bin/PopClusterLnx INP:./Example/ant377NoScale.PcPjt
```

On finishing the run, analysis results will be in several output files located in the same folder as the parameter file "ant377NoScale.PcPjt". That is subfolder "Example".

In the above command line, the key word "INP:" means INPut file. Other key words are listed and explained in the main documentation, PopCluster.pdf.

To run your own dataset, you need to make a project folder, to prepare a parameter input file and a genotype data file, and to save the 2 files in the project folder. Suppose your project folder with path is "MyPrj", and in this folder you have a parameter file MyPar.PcPjt and a data file MyData.dat. Note the data file name "MyData.dat" must be specified in parameter file "MyPar.PcPjt". You can run the analysis of your data from PopCluster program folder by the X-terminal command line

```
./Bin/PopClusterLnx INP:MyPrj/MyPar.PcPjt
```

On finishing the run, analysis results will be in several output files stored in your project folder, MyPrj.

MPI parallel run with multiple processes

For parallel run with multiple processes, you need either Intel's MPI (2018, Update 3) or openMPI (3.1.4) installed on your Linux machine. Most often, openMPI is already installed. If not, you need to download (openMPI is free) and install it.

There are several different implementations of MPI. Unfortunately, they are not compatible. A binary produced with one MPI implementation may not work with another MPI implementation. Even with the same implementation (say, openMPI), different versions (e.g. 1.8.4 vs 3.1.4) may also be incompatible. For this reason, I have provided two parallel versions of PopCluster, compiled and linked to different MPI implementations.

Choosing the right binary suitable for the MPI implementation and version number on your machine, you can start running the example dataset with 4 processes, *from PopCluster program folder*, by typing:

```
mpirun -np 4 ./Bin/PopClusterLnx_impi INP:MyPrj/MyPar.PcPjt MPI:1
```

or

```
mpirun -np 4 ./Bin/PopClusterLnx_openmpi INP:MyPrj/MyPar.PcPjt MPI:1
```

If you want to use 2 openMP threads per MPI process (4 MPI processes in total), the command line is

```
mpirun -np 4 ./Bin/PopClusterLnx_impi INP:MyPrj/MyPar.PcPjt MPI:1 OMP:2
```

When executing the serial or MPI parallel binaries in the first time, you may see an error message "permission denied". This means the binary needs to be unlocked for execution by issuing the X-terminal command line

```
chmod u+x ./Bin/*
```

in the PopCluster program folder, where * is the binary name.