PopCluster (Mac)

1. Introduction

This document briefly describes how to run PopCluster on a Mac. 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 Mac package includes the following files in 3 subfolders:

1) PopClusterMac
2) PopClusterMac_mpi
3) Readme.pdf
4) PopCluster.pdf
5) PopClusterUpdateHistory.txt
6) ant377NoScale.dat
7) ant377NoScale.PcPjt

The first 2 files are the binaries compiled by Gfortran compiler (GNU fortran 6.3.0). They are all for 64bit Mac, and may not work for 32bit OS. The 1st file is statically linked for serial run, the 2nd file is linked with openMPI library (3.1.0) for parallel run with MPI. The 2 binary files are in the subfolder "Bin".

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

The 6th file is an example genotype data file, and the 7th is the corresponding parameter file. These 2 files are in the subfolder "Example".

Installation and run of PopCluster programs are all better conducted in Mac's x-terminal. It is suggested to open an x-terminal and then to obtain the administrator's privileges by typing

sudo -s

Otherwise, the shell operations (such as unzipping) and PopCluster run may have permission problems.

2. Installation

In x-terminal, unzip the downloaded file, and copy the 3 subfolders (with content files) into your PopCluster program folder on your Mac. Then go to the Bin subfolder, and use command "chmod u+x PopClusterMac" to make the binary executable on your Mac. The same needs to be done for PopClusterMac_mpi as well.

PopClusterMac works no matter Gfortran and openMPI are installed on your Mac or not. However, to run binary PopClusterMac_mpi, you need both Gfortran and openMPI installed on your Mac.

3. Running PopCluster - Serial

To make a serial run of PopCluster for the example dataset, simply go to the PopCluster program folder (using command cd) in the X terminal and type

```
./Bin/PopClusterMac 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`", which acts as the project folder.

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 folder. Suppose your project folder name 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/PopClusterMac INP:MyPrj/MyPar.PcPjt
```

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

4. MPI parallel run with multiple processes

For parallel run with multiple processes, you need openMPI (3.1.0) installed on your Mac. Most often, openMPI is already installed. If not, you need to download (openMPI is free) and install it. Similarly you need gfortran (free) installed on your Mac.

From PopCluster project folder, you can start running the above example dataset with 4 processes by typing:

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

NOTE, the option '`MPI:1`' must be present for MPI run with more than 1 thread.

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

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

Note openMP parallel threads can be used with or without using MPI. In the above command line example, a total number of 8 parallel threads will be used.

When executing the serial or MPI parallel binaries, 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.