gMetapop User Manual: Online Appendix for trouble shooting

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This appendix aims at providing help and describing warnings, error messages, and other possible problems when using the first release of gMetapop (ver 1.0.0). It will be updated regularly from users' feedback and based on next releases. A non-exhaustive list of possible errors is provided in this document, with their most probable and proximal causes and suggestions to solve them. If those explanations are not clear enough, or if you cannot find your error messages here, please don't hesitate to contact Frédéric Raspail (*frederic.raspail@inrae.fr*) or Pauline Garnier-Géré (*pauline.garnier-gere@inrae.fr)*.

1. Trouble shooting for initial conditions, file(s) and path(s) management

1.1 General rules and recommendations

GUI Tabs are connected at different levels when clicking or unclicking the different available *checkboxes*. Although much care has been taken to avoid inconsistent combinations of possible options, some might have been forgotten. These could occur for example when very different *param* xml files are being created without having previously closed an old *param* file. Thus, as a general rule, when you create a new configuration file, prefer **"File/Close param…"** and then **"File/New param…",** which is a way to re-initialize correct combinations (see also **1.1.6** below).

From the GUI, we sometimes constrained input values of some parameters to avoid meaningless scenarios: for example, we prevent the **conf.txt** creation from the GUI if some populations are initially empty and isolated from others (see errors in **2.2.1**). However, if needed, it is generally easy to bypass those constraints with small changes in the GUI and minimal editing of the conf.txt afterwards. This is possible because the CORE part of the program allows more flexibility before launching simulations (e.g. in the "dummy" example before, just allow some migration in the GUI, and edit migration rates by hand in the conf.txt afterwards).

1.1.1 Initial conditions

In general, the files being loaded into the GUI have priority to set initial conditions (e.g. when uploading a genotype file, the initial numbers of individuals will be those indicated in the file).

When exploring scenarios, it might be useful to design initial conditions so that an overview of potential results can be obtained rapidly. Most of the time, this will be straightforward by reducing the time steps or total number of reproductive events for output results. However, some stochastic processes with very rare events might need a large number of replicates to observe the average output patterns. In this case, initial conditions can be changed to reduce the amount of stochasticity in preliminary runs and validate expectations. For example in **test 5.5.2** of the User Manual (i.e. looking at the selection on a recessive advantageous allele), simulating allele frequencies that are initially too low, or using small population sizes, low numbers of loci replicates, or generations that would not be large enough for mutations to occur often enough, might fail in observing any effects. The solution here is to start with a higher initial frequency for the recessive allele. In simulations with added stochasticity, more replicates or generations can be added. See the **tests 5.6** for other similar examples.

Concerning initial demographic conditions, we have tried to group them in 5 general cases with appropriate warnings (see part ***3.5.1.1*** in the User Manual and **tests 5.10.1** for illustrations). Particular cases of interest could be added in future releases of the program, depending on users' feedback.

1.1.2 File names and folder names

Use of special characters for file and folder names:

The use of special characters should be avoided, as it can create various problems at various steps before completing a simulation run, despite some tolerance.

The following special characters should be avoided in names for files or (working) folders (this list is probably not exhaustive): spaces, " ", "=", "&", "%" etc…

If they are used, depending on when they are, various messages may occur:

Message example 1 in the GUI after a simulation: "Exception: ERR Cannot open result file".

Message example 2 when clicking "Run" in the Run Tab: onProgramStarted 'the.path.for.your.working.folder.which.might.be.incomplete' is not recognized as an internal or external command, operable program or batch file. This is likely due to a working folder name that includes a special character, and is thus not read in full.

For output final genotype files, avoid using a dot "." in the name, otherwise the dot will be ignored and only the string before the dash will be used, with the replicate number being added as the suffix in the name.

1.1.3 Opening or renaming file(s)/folder(s) while running simulations

While gMetapop is running, it needs to access many files and folders (e.g. conf.txt, type.txt, output result files, *.bat files etc…). If those files are opened and/or modified during simulations, the programs will probably stop or crash. For example, if you rename working folders previously indicated in the *Run tab* of the GUI, during the current simulation. You may stop a simulation that is too long if needed and examine outputs and *.bat files. *.bat files can be modified (e.g. comment out replicates already performed), and then re-used directly in order to run remaining replicates later.

1.1.4 Opening plot files and re-running plot scripts from the working folder

Default plot files, which are named **plot.perGen.pdf** and/or **plot.perGen.quanti.pdf**, will be printed in the working folder. If they are opened for visualization, they need to be closed for a new **Default plot** request from the File Menu to work. Otherwise, the generic message about plotting errors is shown in the GUI (see **2.3**), and more information issued by R is available in the Log windows, for example:

Error in pdf(file = paste(plot.name, ".pdf", sep = ""), width = 9, height = 9) :
cannot open file 'path.name\plot.perGen.pdf'
Calls: plot.perGen -> pdf

Execution halted

If one want to keep previous *.pdf default plots before re-running the script, these need to be renamed first.

1.1.5 Default plots which are not consistent with simulation performed

This might occur because you did in succession:

a) First, a simulation with statistics requested in the *Output Tab* that led to the creation of the **res1_per_gen1.txt file,**
b) Second, you did a new simulation in the same working folder, but without asking any statistics so no new **res1_per_gen1.txt** result file was created,
c) then you still ran the **Default plot** option.

Since this option uses the **res1_per_gen1.txt** file located in the working folder, the plot provided relates to the simulation in a) and not b). Error messages may appear in the Log window, but only if there are inconsistencies between the **conf.txt** file from simulation b) and the **res1_per_gen1.txt** file from simulation a).

Current solution: keep at least one statistic that will be printed in the new **res1_per_gen_1.txt** file in preliminary new runs (especially when keeping the same working folder for different simulations).

1.1.6 Building very different *param* files without closing previous ones.

In such cases (e.g. you unclick all nuclear loci and simulate cytoplasmic loci only), residual information from previous *param* *.xml files might remain, and in rare cases, create errors linked to possible inconsistencies among Tabs when creating the conf.txt and type.txt files, or when uploading files and checking them (automatically done when creating the conf.txt for example). Although we have done our best to cover this type of cases, we recommend that you close previous *.xml files, and start a new one (see **1.1**). Please let us know if you encounter problems that might be linked to such cases.

1.2 File(s) and path(s) management

1.2.1 Initial files which path(s) are recorded into the GUI

These files, which paths are indicated in the GUI, document for example genetic maps, genotypes, or allele frequencies, and they are used for setting up initial conditions for simulations, along with default or chosen values for various parameters in the GUI.

Their description and use are provided in different parts of the **User Manual** (e.g. in **Chapter 4** and many tutorials of **Chapter 5**), with many examples in tutorials of Chapter 5 of the User Manual. Basic verifications are performed on file formats with various error messages issued (see more in parts **2.** and **3.** below), and their paths (see **2.2.3**).

1.2.2 Genetic map file not saved

Can occur when the path for a genetic map file to save has been modified but not updated in the param xml file (see also **2.2.3**).

1.2.3 Working folder(s) path(s)

If the working folder path is not found: this can occur when the path for a working folder has been modified but not been updated in the current *param* xml file (see also **1.1.2**, **2.2.3** and **2.4**).

Working folders can be chosen by going directly to the *Run Tab* of the GUI (independently to creating a *param* xml file), and by clicking on **Select/Create** in the **Working directory**

window. This may be useful in different cases:

- doing or redoing a Default plot from a folder where results files from a simulation have already been produced.
- Relaunching a simulation from a folder where the conf.txt, type.txt and allele frequency files are available.
- See also **2.2.3** and **3.1** for possible errors linked to the presence/availability of the allele frequency files.

1.2.4 File transfer

param *.xml files that have been saved from gMetapop_GUI are transferrable between different OS, so you can just create one file with the Windows gMetapop_GUI version, copy it to your folder under the Linux OS, and open it with the gMetapop_GUI Linux version, or the reverse.

Conf.txt, type.txt and other text files are also transferable and re-usable among OS. From Linux to Windows, there is usually no compatibility problems. From windows to linux, you usually need to make your files linux-compatible if they have previously been created under Windows. To do that, you can either re-open then save text files with text editors, or use tools such as *dos2unix* (type “dos2unix *.*” in the working folder where the text files have been copied, type “sudo apt install dos2unix” in a terminal for installing it).

1.2.5 Conf.txt editing

User-defined values for various parameters can be uploaded directly from simple text files across the different GUI tabs. Additionally, values in most lines of the configuration file (conf.txt, created from the GUI in the last tab, the *Run tab*) can be edited by hand, as long as they are consistent with the principal settings (i.e. number of populations and loci, at the start of the conf.txt file). This greatly expands the possible range of scenarios and initial conditions. However, this must be done cautiously in order to maintain an original and consistent format.

- *Example 1*: maximum allele numbers for cytoplasmic or nuclear loci can be customized easily, if the three groups of loci already proposed in the GUI are not sufficient for the scenarios simulated. More examples are provided throughout the tutorials (Chapter 5 of the User Manual).
- *Example 2*: particular additive values in the *phenotype=f(genotype) Tab* cannot be chosen directly from the GUI; they are randomly drawn from particular distributions. However, the corresponding lines in the conf.txt can easily be changed, either by hand or using a small R script.
- *Example 3:* see the tutorial **5.3** in **Chapter 5** of the User Manual for an example of editing migration rates lines in the conf.txt with such an R script.

Also, be aware that gMetapop_CORE may run after bypassing some inconsistent values in the conf.txt, but these values can still prevent to obtain default plots in particular cases, as the plot script needs to check the overall consistency of the conf.txt and output files.

1.2.6 Errors when reading the *param* xml file

It should be avoided to edit the *param* *.xml file, after it has been created by the GUI. Otherwise, due to incorrect formatting, error messages can appear:

"Fatal error, send the following message to gMetapop support : etc… with different possible messages"

ERR the param xml file format is not readable or corrupted. Can you please re-create a new one from the GUI. If problems persist, contact gMetapop support"

1.2.7 Windows or radio buttons not accessible when opening a *param* xml file

Multiple options are available in the GUI. Different checking operations are also launched when re-opening previously saved *param* xml files (e.g. if the working folder path still exists).

2. GUI error messages: likely causes and how to deal with them

Various types of errors are provided for helping users of the GUI, which aims at creating the text configuration files needed to run gMetapop_CORE.

Errors listed below are indicated in blue, followed by possible explanations. The list is not exhaustive, and will be updated based on users' feedback.

2.1 Creation of "type.txt" file (i.e. clicking on "Create" in the "Type of Result File" window)

ERR: Construction of kind of result file failed: Cannot open C:/*user-path…/user-working-folder*\type.txt file.

This error occurs if the path of the working folder indicated is not correct anymore, possibly because it was modified before clicking on the "Create" type.txt file.

ERR: The type of results file has not been created, or it can't be found.

This is due for example to clicking on the "Run" button without having previously clicked on the "**Create**" or "**Select**" options from the "**Type of result file**" window of the *Run tab*. Also, the programs looks for a file which name is provided in the small window under "Type of result file", thus if the name is changed and the "**Create**" button is not clicked again, you can also get this error.

2.2 Creation of the Configuration "conf.txt" file (i.e. by clicking on "Create" in the "Prepare Configuration File" window)

NB: Numbers in italics in the ERR messages are just examples and can vary according to cases.

ERR: The configuration file has not been created, or it can't be found.

Due to omitting to click on the "**Create**" or "**Select**" options from the "**Prepare configuration files(s)**" window of the *Run tab*, or the file has been created with the default name conf.txt but its name changed afterwards in the working folder, or in the corresponding GUI window.

Other reasons for failing to create the configuration (conf.txt) file from the GUI include:

- an initial combination of number of individuals across populations and classes which does not allow the simulation to proceed,
- the loading of files (e.g. allele frequency or genotype files) with incorrect formats, which can be due to Inconsistencies between GUI parameter values and corresponding values in those files.

2.2.1 Error due to incorrect population configuration or initial conditions

ERR: Construction of configuration file failed: At least one pop is empty with no migration, please correct.

It occurs if at least one population under the "By hand" option is unclicked with no individuals to start with, and no connections with other populations (no migration). Clicking zygote migration will allow simulation(s) to run.

ERR: Construction of conf file failed: transition_rate: Transition rate + survival rate for classe 2 is > 1.0 : *1.34* Transition rate + survival rate for classe 3 is > 1.0 : *1.66*

These transition rates (defined in the "**Extended Lefkovitch matrix – Class parameters**" window of the *Demography Tab*, see also part **3.5.3** of the User Manual) should be below or equal to 1.

2.2.2 Error due to format problems in loaded files

When building *param* xml files that necessitate the loading of text files, two types of information can be recorded:

- either the files themselves (generally with very simple formats, for example for mutation rates, or selection strength values within populations, etc…),
- or the paths where those files are located. This will be the case for **1)** a genetic map, **2)** an allele frequency file, or **3)** a file documenting all genotypes across populations at the start of simulations. As explained in length in the User Manual (see Chapter 1, Chapter 4 / introduction, Chapter 5 / introduction and many tutorials), the best way to obtain and check the correct formats for these three types of files is to perform a preliminary test run with 0 generation. In this run, use the **Save option** for files in "**1)"** above in the Genome Tab, for files in "**2)"** in the Output Tab, and for files in "**3)"** in the Run Tab. These files just need to be consistent with initial settings chosen in the GUI Tabs (e.g. loci, alleles and populations numbers). Basic checks are performed before creating the conf.txt in the *Run tab*, which may lead to various types of errors in case of inconsistency, as shown in examples below:

2.2.2.1 Allele frequency, genotype files, or genetic maps

ERR: Construction of conf file failed: ERR: The header of the allele frequency file isn't correct. You may also need dos2unix - like app if your file has been created under Windows.

This occurs if the format of the allele frequency file to be loaded is incorrect. This can be due to the following causes (non-exhaustive):

- An incorrect separator between columns of the header (e.g. comma). In the first release 1.0 of gMetapop, the only correct separator is the semi-colon (";"). If your file

is a *.csv, there is an underlying separator which could be different to ";", although not seen from the Xcell sheet. You can change the extension of the file to *.txt and open it in a text editor to change it, or change your language options in Xcell in a Win OS.

- The text format of the allele frequency file is not linux-compatible if they were copied from a Windows OS, while there is usually no problem from linux to windows OS for text files. You then need to run the *dos2unix* application on all text files coming from windows (if not available, install it by typing "sudo apt install dos2unix" in a terminal), just type "dos2unix *.*" in a terminal opened in your working folder.
- Some columns are missing, or too many columns due to too many loci or alleles, compared to values in the GUI *Genome Tab* and/or *Genotype Tab*
- The identifiers of the columns for the type of file loaded are not recognized.

Exception: ERR Incorrect number of rows in the loaded frequency file, 4 are needed.

Occurs if the number of populations (one per row) in the loaded allele frequency file is too low.

Exception: Row 5: pop# is > to the total expected population number in the loaded frequency file.

Occurs if the number of populations (one per row) in the loaded allele frequency file is too high.

Exception: ERR Inconsistency between presence of individuals in pop2 and allele frequency sum <= 0

When loading a frequency file, there is an inconsistency between the presence of individuals in one population, and a value below or equal to "0" for initial allele frequency in that population at one or more loci.

ERR: Construction of conf file failed: The number **of rows** in your file is incorrect, you have *5* and the program needs *4*.

Occurs if the number of population lines in the loaded allele frequency file is too low (or too high in particular cases, for example if one line is replicated with the same population identifier).

ERR: Construction of conf file failed: *Row 5*: pop# is higher than the total expected population number.

Occurs if the number of population lines in the loaded allele frequency file is too high.

ERR: Construction of conf file failed: Line 5: Numbering of populations needs to be in ascending order.

This may occur if the frequency file to load includes populations that are not sorted in ascending order (but this may also be due to the fact that the file includes allele frequency across populations at more than one particular generation, since only one is needed for initial conditions).

ERR: Construction of conf file failed: ERR Row *#1* hasn't got the correct number of columns. Expected=*12* Found=*4*. Check also that semicolons are used as column separators.

This may be due to errors in the format of either the allele frequency file or the genotype data file, when the information in those files is compared to the values entered into the GUI, which also define the content of the conf.txt file (e.g. the header is not correct in terms of number of loci and alleles, data are missing for one population, or 2 alleles exist in the file to be loaded while 10 are indicated for the maximum number of alleles in the GUI/Genotype Tab).

ERR: Construction of conf file failed: ERR at row: 1 at column: 0

ERR: Construction of conf file failed: ERR Cannot convert to integer.

Occurs for an empty genotype data file with an inconsistent header or line structure, compared to what is included into the GUI.

ERR: Construction of configuration file failed: Load Map File: Value(s) above 0.5 in Recombination rates line.

Values above 0.5 do not make sense and are not accepted by the GUI in a loaded map file.

ERR: Construction of configuration file failed: Load Map File: Loci number in the Recombination rates line and in the GUI are different.

The “Recombination rates between the nuclear loci” line in the loaded map file does not contain the expected number of values, or the line has been deleted.

ERR: Construction of configuration file failed: Load Map File: Cannot find the 1st line.”

The “Codominant loci 1:” line has been removed by the user or it has been edited and its syntax is incorrect, while it is compulsory for gMetapop_CORE to run. You can do a test run with a **“save map”** in the *Genome Tab* in order to get the correct genetic map format.

ERR: Construction of configuration file failed: Load Map File: Cannot find the 2nd line.

The “Selected nuclear loci (0=neutral, 1=selected) :” line has been removed by the user, or it has been edited and its syntax is incorrect, while it is compulsory for gMetapop_CORE to run. You can do a test run with a **“save map”** in the *Genome Tab* in order to get the correct format.

ERR: Construction of conf file failed: Load Map File: *5* values in the Selected nuclear loci found in the file while *6* values in the Selected nuclear loci are expected in the current configuration.

One value from the vector of 0 or 1 in the “Selected nuclear loci (0=neutral, 1=selected) :” line has been removed by the user, so the line is incorrect. You can do a test run with a **“save map”** in the *Genome Tab* in order to get the correct format.

ERR: Construction of configuration file failed: Load Map File: a locus under selection is at the same position than a codominant one.

Values of the vector of 0 or 1 in the “Selected nuclear loci (0=neutral, 1=selected) :” line has been incorrectly edited. You can do a test run with a **“save map”** in the *Genome Tab* in order to get the correct format.

ERR: Construction of configuration file failed: Load Map File: Cannot find the 3rd line.

Commenté [P1]: **Put a more explicit one if easy → check of file not possible since no data!!**
No genotype data?? → what would happen if CORE only was launched with an empty file?

Commenté [P2]: Same than above, while if # comment lines with no header or just the header, the message no invidiuals in the CORE is given

SEE also previous message incorrect number of rows → removed parce que jamais dans une config où c’est important sauf si nb max trop grand?? → only for Frequency fil with nb of lines = nb of pop but not for geotype file since regulation applies!! → RECHECK later

The “Selected cytoplasmic loci (0=neutral, 1=selected):” line has been removed by the user, or it has been edited and its syntax is incorrect. It needs to be kept for reading the conf.txt file correctly, even though selection on cytoplasmic loci is not included in this version of the program. You can do a test run with a **“save map”** in the *Genome Tab* in order to get the correct format.

ERR: Construction of configuration file failed: Load Map File: For the codominant line in the file we found *30* value(s) while *11* are expected in the current configuration.

There are inconsistencies between the genetic map file loaded (**load map** option in the *Genome Tab*) and either the allele frequency file or the genotype file which have been loaded, or the parameter values provided for number of loci in the GUI *Genome Tab* for example.

ERR: Construction of conf file failed: Line 9: cla# is higher than the total expected class number.

This error occurs when loading a file of genotypes (“**Load genotypes**” in *Genotype Tab*), if a class number that appears in the file is incorrect, when comparing to the values chosen for the initial settings.

2.2.2.2 Small text files (.csv or *.txt) loaded in the GUI*

The file to load has too few lines.

Occurs when loading text files requiring one line per population (e.g. if loading selection strength values in scenarios with selection on phenotypes, trying to load an empty file, or a file with only one value while two are needed for two populations being simulated, *Selection Tab*).

ERR: Construction of configuration file failed: likely due to formatting errors when loading mutation rate file. Please check the file format in 4.2 of the User Manual.

Occurs if the file has been deleted before the creation of the configuration file, or if there is a format problem with mutation rate values loaded into the GUI (user-defined option), see various examples at https://github.com/gMetapop/gMetapop/tree/master/4-Format.Examples .

2.2.3 Error due to incorrect or absent paths or file names

ERR: Construction of configuration file failed: Cannot copy : *path.name*/*allele.frequency.name* to *working.folder.name**allele.frequency.name*

The path name where the frequency file should be located and/or the frequency file are not found, and thus the creation of the configuration file cannot be completed in the working folder.

NB: *allele.frequency.name* is **allele_frequency.txt** by default unless it has been modified in the conf.txt and in the corresponding working folder

ERR: Construction of configuration file failed: Cannot open map file *path.name.chosen.in.Genome.tab*

Occurs for example if the path name of a genetic map file to load have been changed, or if the corresponding folder have been deleted before launching the simulation.

2.3 File/Default or File/Custom plots

A default plot of the statistics printed in the result file **res1_per_gen_1.txt** is performed by using the **plot.gM.perGen.R** R script, which is called with the **File/Default plot** option in the **GUI** Menu. You can find the last version of this script (date indicated at the start of the script with eventual changes) online at https://github.com/gMetapop/gMetapop/tree/master/7-Plotting.R.scripts. If the default plot cannot be produced, you will get the following message:

Error(s) occurred when plotting statistics from the res1_per_gen_1.txt file. Please check whether a) the plot.gM.perGen.R script is present in the working folder, b) the working folder or result file names are correct, c) result file(s) are present, d) the plot files are not currently open, otherwise close them before asking for Default plot again, and e) other log windows messages…(more information in **3.9.1** of the User Manual, or in the online Appendix about errors)

This generic message can be issued for different reasons:

- the working folder name may have been changed before the end of the simulations, and thus does not exist anymore,
- special characters were accepted in the folder names but they are not processed by R,
- results files have been removed,
- the plot script does not work due to an incorrect conf.txt (maybe because the conf.txt was edited manually before the end of a simulation run, with impossible or inconsistent values with the output result of the current simulation),
- Absence of file **res1_per_gen_1.txt** in the working folder, either because no statistics has been requested in the *Output Tab*, or because those that have been requested are printed into another result file,
- In some rare cases, the plot should be performed correctly, but previous errors in launching it have opened R plot devices which have not been closed properly. In such cases, closing the GUI, re-opening it and relaunching the default plot directly from the working folder might solve the problem. You do not need to redo the simulation, but just need to go directly to the *Run Tab*, open the working folder, and redo the **File/Default plot** option.
- Particular cases which have been omitted and cause problems for the R script, or because of other bugs in the R default plot script or in other R scripts provided in the tutorials, and used in the **File/Custom plot** GUI option. In such cases, please do not hesitate to let us know.

In rare cases where all summary statistics are requested from the *Output Tab*, the *.png default plot legend rectangle might not be high enough to contain the descriptions of all requested statistics. This can be solved by asking for less statistics (see part **4.**). Otherwise, the *.pdf plot should normally include all of them.

Error in pdf(file = paste(plot.name, ".pdf", sep = "")) :
cannot open file "*plot.name.example*.pdf
Execution halted

This type of message appears in the **Run Log** window of the *Run tab* from running either the default or custom R plot scripts. It can be due to reason d) in the generic message above for default plots, or to the fact that the same name was given to a plot file that is already open by your pdf reader for custom plots, so the programs cannot access it. Just close the corresponding *.pdf files and relaunch the plots.

Problem(s) occurred when using the File/Custom plot option, please check the user R script/command line arguments/working folder/file(s) occurrence/ log windows messages…(more information in 3.9.2 of the User Manual, or in the online Appendix about errors)

Please see all the possible causes listed for the File/Default plot options above
Since the second argument that gives the plot filename is compulsory, if it is omitted, plots with "NA.png" name may be produced,

2.4 File/Open interface parameter file

The working directory isn't correct

- occurs when the path of the working folder, which was previously saved in the loaded *param* xml file, is neither correct nor found. In the tutorials, this will occur when reloading the various *param* examples provided. Please update the working folder by clicking on the "**Select/Create**" button of the Run Tab, and by looking for the folder containing downloaded example files.
- occurs if you reload *param* *.xml files from your own folders that you have since renamed.

2.5 Error messages in the Run log window of the *Run Tab*

See part **3.** Below

2.6 EXIT_FAILURE in the GUI

A generic EXIT_FAILURE in the GUI message can be due to:

- Failure to read a "conf.txt" file, which has been edited by hand and shows inconsistencies among values: in this case, an error message probably appears in the **Run log** Windows of the *Run Tab*, and further describes the problem (see messages listed in part **3.** below). Please contact gMetapop support if you cannot fix the problem.
- Many other reasons…most of them explained in this appendix.

3. CORE or other Run log error messages

These messages appear in the **Run Log** window from the GUI *Run Tab*. They generally correspond 1) either to problems in executing gMetapop_CORE when reading the conf.txt file (see **3.1** below), or 2) to errors issued by the R software due to problems when running plot scripts (part **2.3** above and **3.2** below). If the GUI is not used to launch simulations or

run R scripts, these messages are sent to command-line terminals used in your linux of windows OS.

Some errors issued while running gMetapop_CORE can also be the same or linked to similar problems encountered while running gMetapop_GUI.

3.1 gMetapop CORE error messages

These messages can be due to inconsistencies or format errors found throughout all the initial files required to run a simulation (e.g. the conf.txt or the type.txt file or the initial allele Frequency file). The list below is not exhaustive, it will be completed from the users' feedback if needed. If the ERR message that you encounter is not explicit enough or is not listed here, don't hesitate to contact the gMetapop support (F. Raspail and P. Garnier-Géré).

For example if the conf.txt has been edited for the total number of loci, the lines corresponding to the number of alleles, number of selected loci/neutral loci, recombination and mutation rates lines also need to be edited.

ERR: The header of the allele frequency file isn't correct. You may also need dos2unix - like app if your file has been created under Windows.

- An allele_frequency.txt file (looked for by default in the working folder) has been edited by hand for example, producing inconsistencies with the header of the allele_frequency.txt file and the actual number of alleles or loci in the conf.txt file.
- See also other reasons provided for the same error when checking the allele frequency file before creating the conf.txt file (part *2.2.2.1*), while here the conf.txt has already been created, but a verification is also performed before running gMetapop_CORE.

Exception: ERR configuration file cannot be opened: *working.folder.name*\conf.txt

This occurs if the configuration file is not found in the working folder: either it has not been created, or its name has been changed in the working folder or in the GUI *Run Tab*. (after being created with the default conf.txt name)

Exception: ERR Allele frequency file cannot be opened: *working.folder.name**allele.frequency.name*

This can be caused by various situations:

- The allele frequency file (needed to run a simulation from the working folder) is not found or has been renamed.
- The path written in the conf.txt file that points towards the allele frequency file is not correct (or the name of the file is not correct), for example if the conf.txt, type.txt and allele frequency files have been copied from one folder to another (e.g. when transferring among OS) for redoing a simulation. The path name needs then to be updated to go from the working folder to the new location, by editing the conf.txt file, but you might find it easier to redo the *param *.xml* file on the new OS for example.
- A simulation is launched directly from the *Run Tab,* in a working folder where the conf.txt and type.txt files have previously been created, but using a genotype file for initial conditions instead of an allele frequency file. In this case, the allele frequency has not been created at the same time than the conf.txt. Since by default, the last line of the conf.txt is pointing to it (but this line is not read if the command line indicates to

start from a genotype file), the **.bat* re-created from the **GUI** *Run Tab* is searching for it.

- Another case could be that the genotype file loaded has got an incorrect format. In this case the program is looking for an allele frequency instead, but does not find it since it should start from a correct genotype file.

Solution 1: use command lines directly from the previous run_gMetapopCore.bat (/.sh) if it does exist in the working folder. All you need to launch gMetapop_CORE are the conf.txt, type.txt and initial genotype file to indicate with the [***–l***] option (see the **.bat or* *.sh produced by the GUI with a "**Run**" click, and the ***3.8.7.4*** paragraph of the User Manual).

Solution 2: reload the previously saved *param* xml file into the GUI to re-run the simulation, or recreate it from the GUI if it has not been saved, following information stored in the previous conf.txt and type.txt, and reload the initial genotype data file (in the *Genotype Tab*).

NB: *allele.frequency.name* is **allele_frequency.txt** by default unless it has been modified in the conf.txt and in the corresponding working folder

Exception: ERR Nnucl

The integer for the total number of nuclear loci is not found or the line does not have the right format.

Exception: ERR Nalleles[locus]

The line including the number of alleles does not have the correct format (e.g. one allele number is missing for one or more loci) in the conf.txt file

Exception: ERR locus codominant 1

The total number of loci is not consistent with the different lines throughout the conf.txt file describing the first group of codominant loci.

Exception: ERR Row #1 does not have the correct number of columns. Expected=104 Found=102. Check also that semicolons are used as column separators.

There are inconsistencies between the loci and allele numbers in the conf.txt file (as created by the GUI, and eventually edited by users), and the allele frequency file to which it is associated.

Exception: ERR All populations are empty. Nothing can be simulated.

All populations are empty (either from "**By Hand**" option of the *Demography Tab*, or by loading a Genotype data file in the *Genotype Tab*). There can be a correct header but no individuals' line in any populations. However that there may be no individuals in some populations, as long as at least one contains one individual.

case 4

Exception: ERR: During the search for an initial demographic equilibrium distribution, numbers of individuals have converged to zero in all populations and classes (before iteration 10000). This is likely due to demographic values that lead to extinction of populations (e.g. too strong demographic regulation, too low female fecundities). Please

review those values and try again until a non-zero initial equilibrium is reached in at least one population, or until the population and class sizes reached before iteration 10000 allow simulations to proceed. Alternatively, with the "By Hand" option, more or all populations can be unclicked, and new transitory conditions can be tested.

This error corresponds to one of the possible cases of initial demographic conditions, in which demographic parameters values lead to extinction in all populations. Thus new demographic parameter values need to be found for simulations to start from equilibrium conditions with some individuals. Alternatively, those initial conditions can be chosen in the "**By Hand**" option for the simulation to be analyzed. See also **Chapter 3** of the User Manual (part **3.5.1** about population size parameters).

Exception: ERR FORMAT for type of result file at row 4

There is an inconsistency between the number of classes in the *type.txt* file and the conf.txt file, or the *type.txt* file has an incorrect format (if it has been **Select**ed and not **Create**d in the Run Tab for example).

3.2 R plot script error messages

Additionally to the generic GUI error message issued in case of plotting problems (see part **2.3**), the R software specific error or warning messages are printed in the **Run log** window and might give more information about the origins of the problems. However, we suggest that you first perform the checks proposed in the generic message (see in **2.3**) since error messages can sometimes be indirectly linked to the primary cause of the error.

Encoding problems in the Run log window of the Run tab:

If the message « Ex�cution arr�t�e » (or something equivalent in the default language of your computer) occurs in the Run log window instead of « Execution halted » (for example if a default plot cannot be performed), it means that you probably need to modify the language options from your Windows/linux settings: either change to, or add the English language for writing messages. This change can be done independently to the keyboard language.

3.3 CORE not launched

Apart from the many reasons explained in this document that might explain why **gMetapop_CORE** fails to start from the **GUI**, another one is the time between two different clicks:

With a bit of practice, you might click very rapidly to produce a scenario, arrive at the *Run tab*, create the type.txt and the conf.txt, and launch the simulations. In rare cases, if you let very little time (less than a second) between the click on "**Create**" in the "**Preparation Configuration Files**" windows of the *Run tab*, and the click of the "**Run**" button, the writing of the conf.txt might not be completely finished (e.g. if there are hundreds of loci and lines to write for genotype fitness values) , and nothing happens. In such a case, simply click again on "Run".

4. R Default plot script editing

It is straightforward for R users (beginners also) to modify the **plot.gM.perGen.R** script (located in the *.exe folder of the release, with the last updated version online, if any) that produces the default plot from the GUI.

We show here a few examples: In general, open the script in a text editor (*Tinn-R, R-studio*…), go at the end of the script where the plot functions (plot.perGen(), plot.quanti2()) are being called. More information is provided in **part 3.9.1** of the User Manual.

For the plot.perGen() function, the arguments that can be modified are:

def2plot: if TRUE ("=T", default), all statistics except the demographic ones for scale are plotted, i.e. the maximum found in result files within a consistent scale, if "=F", the user can then choose which statistics to plot with the vector argument **list2plot.user** below.

list2plot.user: NULL is the default, otherwise define a vector c() with statistics to plot, using the colnames of the res1_per_gen_1.txt files in quotes "" in the vector. For example use list2plot.user=c("Gstcor_l1","Gstcor_l2") for plotting the Gstcor statistics for loci l1 and l2 only, even if many other loci have been simulated.

stat2rem=c("Generation","St","Nt","Nremt","Nsext","Nclot") by default. This allows to avoid the plot of demography statistics that have a scale range much larger than most genetic diversity statistics. Any statistics that is present in the res1_per_gen_1.txt file can be added to this vector, and the corresponding "colnames" will be absent from the plot.

max.y=1, default, is the maximum bound for the plot of statistics from the res1_per_gen1.txt file and this value can be changed. The actual maximum value for each plot depends on the range for the plotted statistics.

min.y=-1, is the minimum bound for the plot of statistics from the res1_per_gen1.txt file, and this value can be changed. The minimum value for the default plot depends on the actual statistics range.

plot.legend=T, default, can be changed to "=F" (or "=FALSE") for avoiding to plot of the legend.

plot.dev="png" or **"pdf"**, allows to choose the type of plot device, among the ones available in R. Both are provided in the current release, but more can be added to the function arguments with lines conditioning the type of plot (search for "if (plot.dev==" in the script, add your condition and then change the type of plot and you can change it also in the function call at the end of the script).

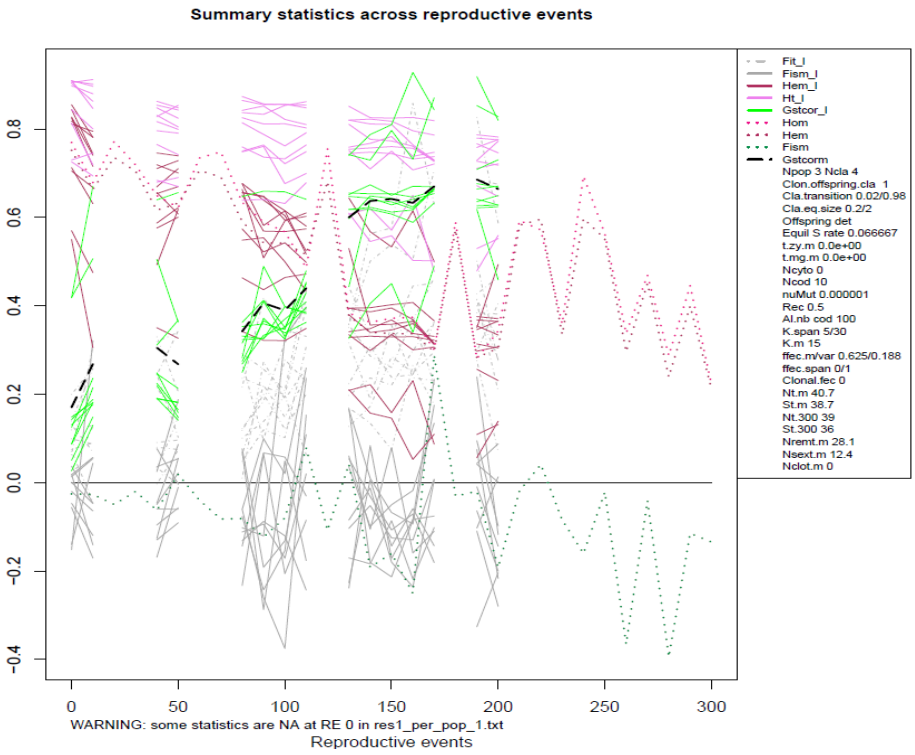
For the function *plot.quanti2(),* the arguments that can be modified are the same (except max.y, min.y=-1, the plot.dev argument is not available but can be changed inside the function, or the function can be edited)

Also many options for the legend attributes or lines properties have been optimized for a large number of plots, but can easily be changed (in particular for the range of possible colours or line types in the corresponding parts of the script).

5. Possible reasons for particular plots

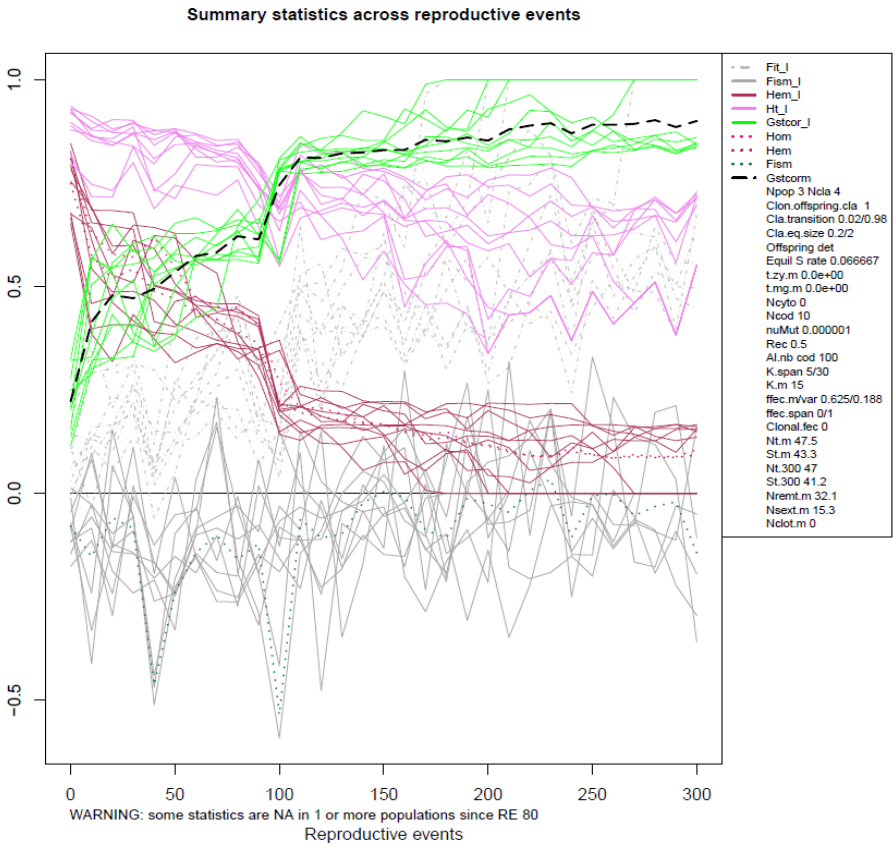
Example 1:

If your plot looks like this:



You can see that the number of individuals in the populations is very small (St=36 at RE 300), so it is possible that at some reproductive steps, the number of individuals is below the minimum number of 10 (used by default) below which summary statistics are not computed (NA in results files).

Solution: change “Minimum population size” in the *Output Tab* to 1, and the plot will look in the same scenario like this:


Summary statistics across reproductive events
1.0
0.5
0.0
−0.5
0
50
100
150
200
250
300
WARNING: some statistics are NA in 1 or more populations since RE 80
Reproductive events
Fit_I
Fism_I
Hem_I
Ht_I
Gstcor_I
Hom
Hem
Fism
Gstcorm
Npop 3 Ncla 4
Clon.offspring.cla 1
Cla.transition 0.02/0.98
Cla.eq.size 0.2/2
Offspring det
Equil S rate 0.066667
t.zy.m 0.0e+00
t.mg.m 0.0e+00
Ncyto 0
Ncod 10
nuMut 0.000001
Rec 0.5
Al.nb cod 100
K.span 5/30
K.m 15
ffec.m/var 0.625/0.188
ffec.span 0/1
Clonal.fec 0
Nt.m 47.5
St.m 43.3
Nt.300 47
St.300 41.2
Nremt.m 32.1
Nsext.m 15.3
Nclot.m 0