

Formation FROGS juillet 2019

Géraldine Pascal, Laurent Cauquil

▶ To cite this version:

Géraldine Pascal, Laurent Cauquil. Formation FROGS juillet 2019: Trainingon Galaxy: Metagenomics / ITS analysisin FROGS? / Trainingon Galaxy: Statistics to explore metagenomics. Master. (Trainingon Galaxy: Metagenomics / ITS analysisin FROGS? / Trainingon Galaxy: Statistics to explore metagenomics), 2019. hal-02790029

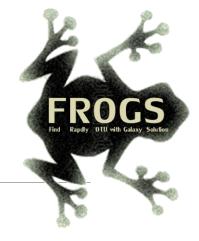
HAL Id: hal-02790029

https://hal.inrae.fr/hal-02790029

Submitted on 5 Jun 2020

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.



Training on Galaxy: Metagenomics July 2019

Find, Rapidly, OTUs with Galaxy Solution

FRÉDÉRIC ESCUDIÉ* and LUCAS AUER*, MARIA BERNARD, LAURENT CAUQUIL, SARAH MAMAN, MAHENDRA MARIADASSOU, SYLVIE COMBES, GUILLERMINA HERNANDEZ-RAQUET, GÉRALDINE PASCAL & MALO LE BOULCH

*THESE AUTHORS HAVE CONTRIBUTED EQUALLY TO THE PRESENT WORK.



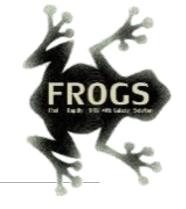












Introduction to Galaxy platform and preparation of FROGS training

July 2019

MALO LE BOULCH, SARAH MAMAN, GÉRALDINE PASCAL









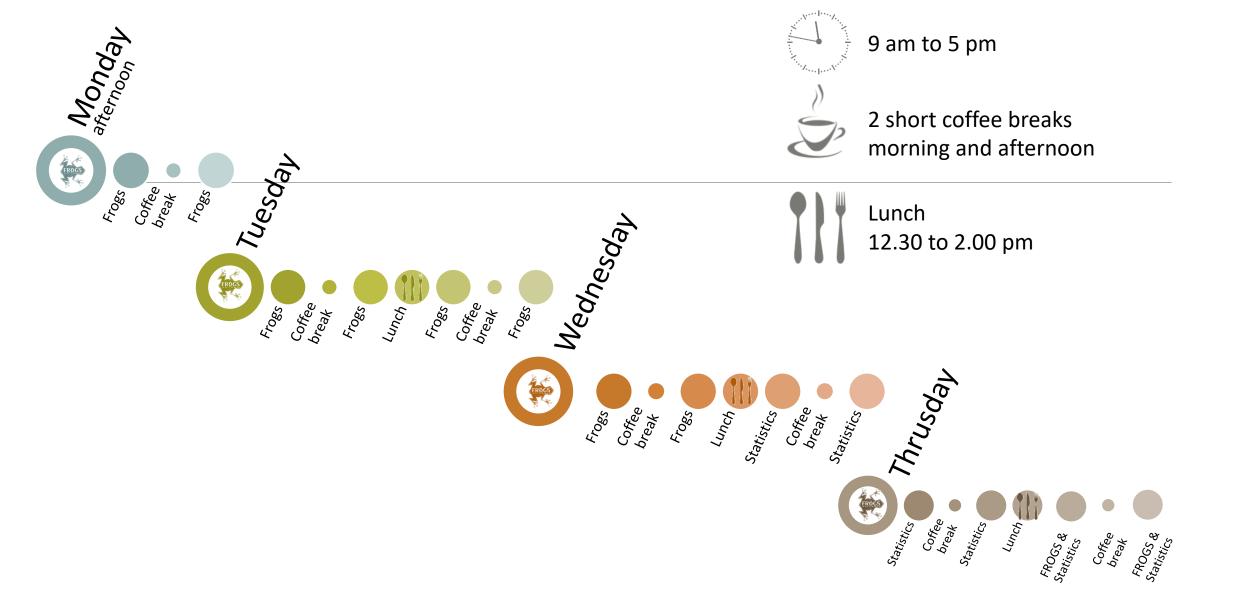


Chitchat time!

- What is your computer skills level?
- Have you ever heard of or used Galaxy?

Feedback on metagenomics:

- What are your needs in "metagenomics"?
- 454 / MiSeq?
- 16S/ITS?
- Your background ?



Objectives of the 1st part

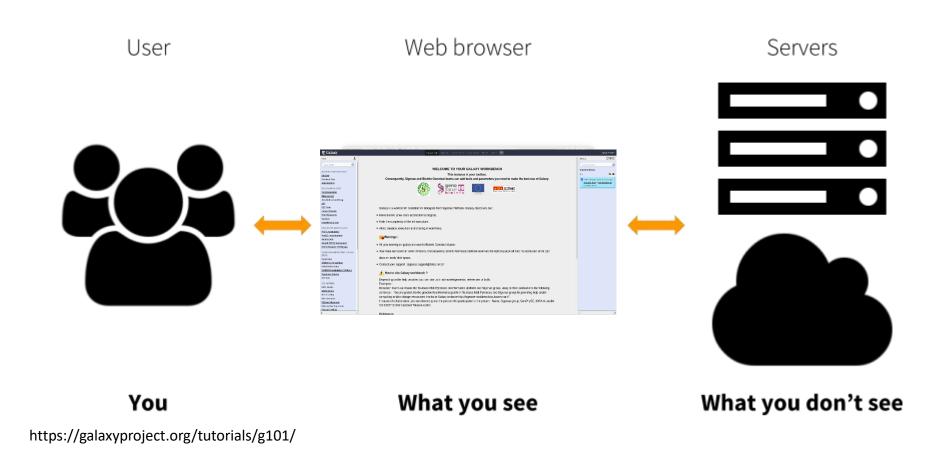
- Learn the basics of Galaxy
- Being independent when using it
- Prepare the datasets for FROGS formation

What is Galaxy?

Galaxy software framework

- Galaxy is an overlay that allows researchers without computer expertise to perform computational analyses online, automate them and share the results easily.
- Developed by the Galaxy Team Project.
- Relies on a computational infrastructure (Server).
- Open source

Galaxy software framework



Where to use Galaxy?

- Galaxy software can be installed and run on powerful server farms (Cluster) or on your individual PC.
- Genotoul Bioinfo



- Cluster: Many computers tightly connected that work together
- High performance computer:
 - More than 5000 cores
 - 34 TB of RAM
 - More than 1 Peta Byte (1024 TB) of hard drive



Where to use Galaxy?

Our Galaxy platform is http://sigenae-workbench.toulouse.inra.fr/galaxy/

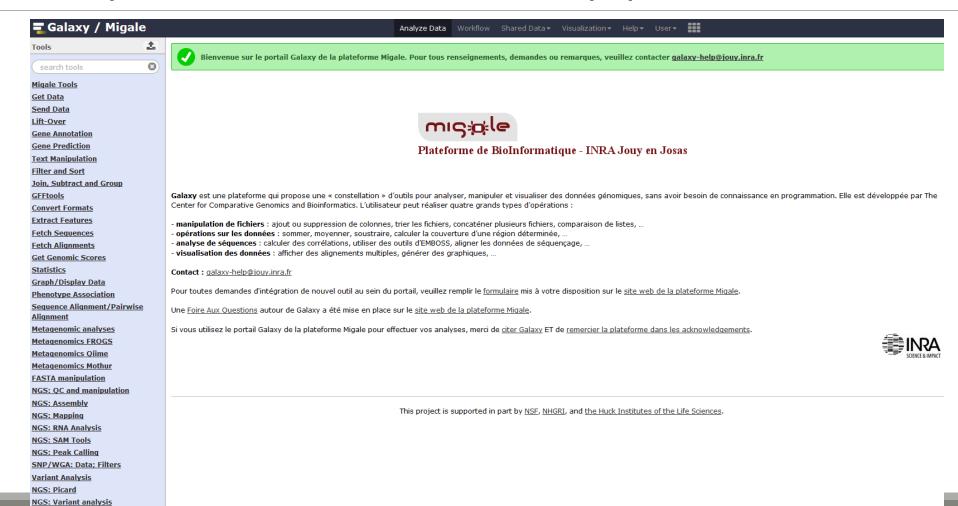
⚠ The different platforms of Galaxy are not connected together

- Galaxy is installed on many clusters across the world.
- Some tools are in <u>our</u> Galaxy platform but not in <u>other</u> platforms.
- Your data is not shared with other Galaxy platforms than ours.

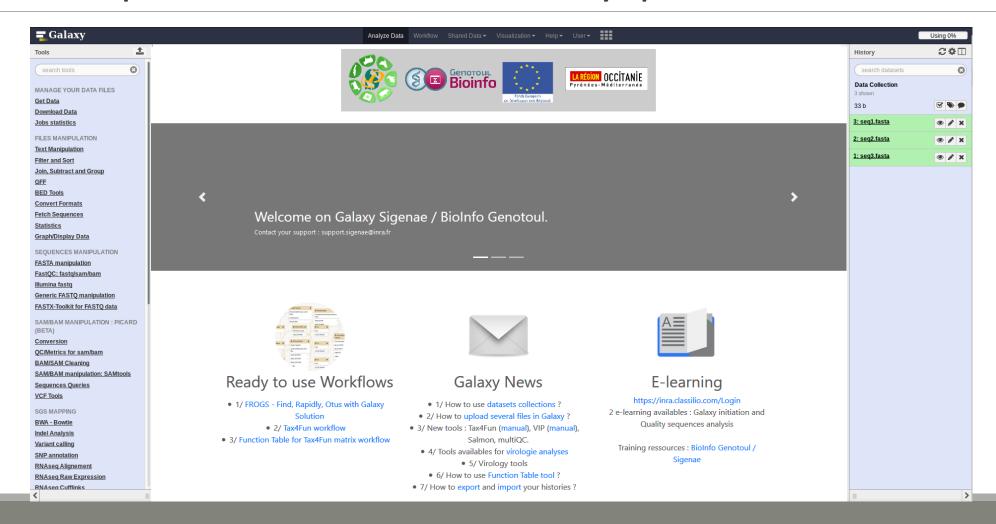
Exemple of 2 INRA Galaxy platforms

Workflows

All workflows



Exemple of 2 INRA Galaxy platforms



Your Turn!

CONNECT TO OUR GALAXY WORKBENCH

During this formation, we will use a remote computer.

Connect to a distant computer by clicking on the remote desktop connection icon in the task bar.

Ask trainers for the address and password.

All your data will be erased at the end of the week of the remote computer

During this formation if you have a personal account, use it.

This account will save all the work done during this week and your future work.

If you don't have a personal account ask us for a temporary account.

You can request a personal account later on : http://bioinfo.genotoul.fr/index.php/ask-

for/create-an-account/

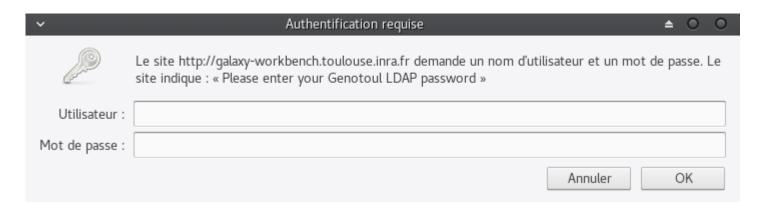
All your data will be erased at the end of the week on a temporary account

Our Galaxy platform is: http://sigenae-workbench.toulouse.inra.fr/galaxy/ Before starting, check if your browser is not already connected to a Galaxy account. If this is the case, log out or use a private browser window! **Risk of data duplication**

Our Galaxy platform is: http://sigenae-workbench.toulouse.inra.fr/galaxy/

Be careful, to fully login you must enter your credentials twice:

The first time in this pop-up window:



And a second time, in the browser:



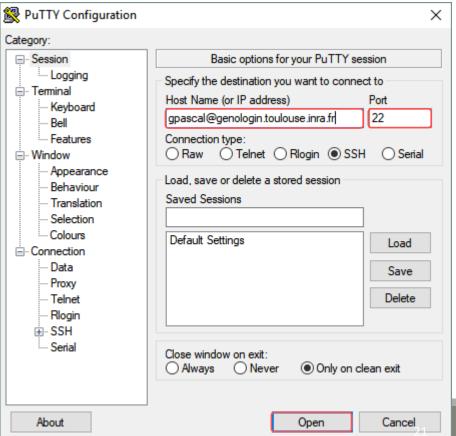
- In order to change your password, you need to download PuTTY: http://www.putty.org/
- PuTTY is a terminal emulator, it allows to connect directly to the server in command line.
- You can not change your password via the Galaxy's interface for the moment.

Launch PuTTY.

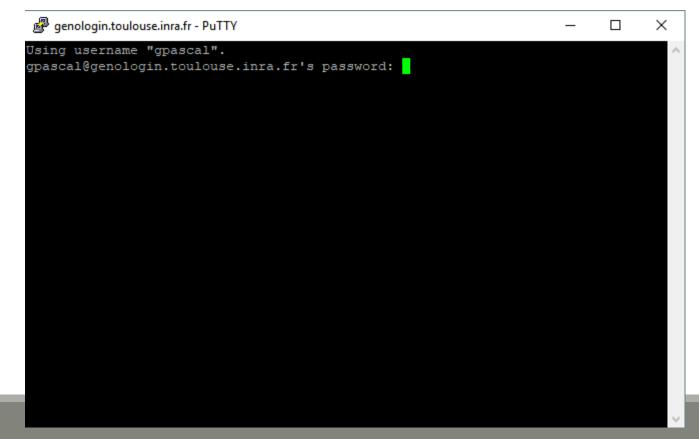
In the following window, you must enter your host <u>name which is:</u>

YourGenotoulName@genologin.toulouse.inra.fr

- The connection type must be SSH.
- Click on « Open » .



- A new window appear, click on « Yes ».
- In the following window, enter your password and hit « Enter ».



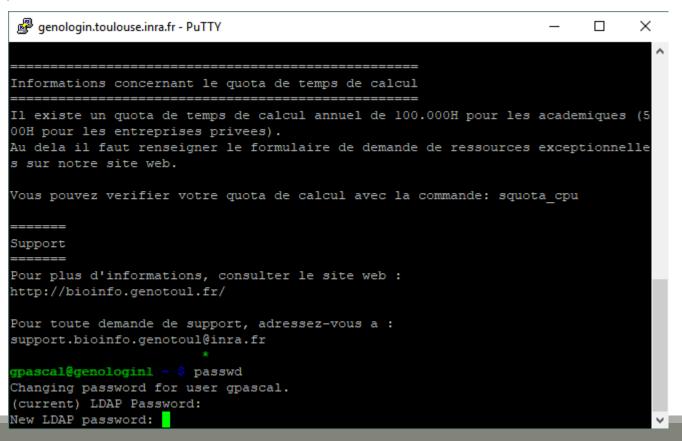
Type « passwd » and hit « Enter ».

```
genologin.toulouse.inra.fr - PuTTY
e cluster).
Pour obtenir plus de memoire, veuillez consulter la FAQ de notre site web (cf +
bas)
Informations concernant le quota de temps de calcul
Il existe un quota de temps de calcul annuel de 100.000H pour les academiques (5
00H pour les entreprises privees).
Au dela il faut renseigner le formulaire de demande de ressources exceptionnelle
s sur notre site web.
Vous pouvez verifier votre quota de calcul avec la commande: squota cpu
 ____
Support
Pour plus d'informations, consulter le site web :
http://bioinfo.genotoul.fr/
Pour toute demande de support, adressez-vous a :
support.bioinfo.genotoul@inra.fr
 pascal@genologinl ~ 💲 passwd
```

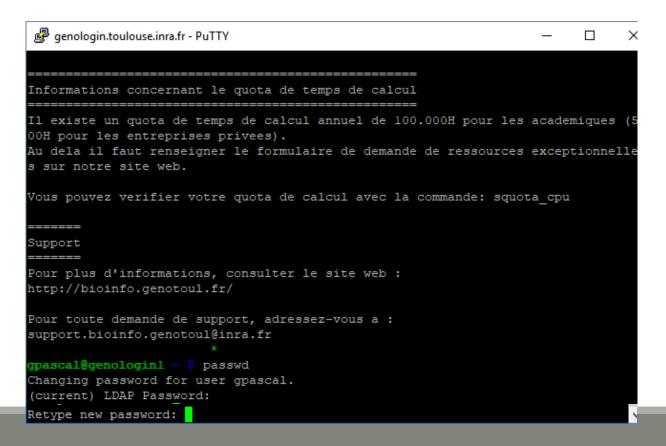
Enter your current password and hit « Enter ».

```
genologin.toulouse.inra.fr - PuTTY
                                                                            \times
Informations concernant le quota de temps de calcul
 _____
Il existe un quota de temps de calcul annuel de 100.000H pour les academiques (5
00H pour les entreprises privees).
Au dela il faut renseigner le formulaire de demande de ressources exceptionnelle
s sur notre site web.
Vous pouvez verifier votre quota de calcul avec la commande: squota cpu
Support
Pour plus d'informations, consulter le site web :
http://bioinfo.genotoul.fr/
Pour toute demande de support, adressez-vous a :
support.bioinfo.genotoul@inra.fr
pascal@genologinl ~ $ passwd
Changing password for user gpascal.
(current) LDAP Password:
```

Enter your new password (with an upper case, a number and a special character in it) and hit « Enter ».



Enter a second time your new password and hit « Enter ». You have changed your Genotoul password, you can close PuTTY.





Vocabulary of Galaxy

Tools:

- A tool has a function which is explained when you click on it.
- Each Galaxy platform has its own tools.

Dataset:

- A dataset is a file, uploaded to Galaxy by you or produced by a tool.
- Be careful: a dataset has a datatype.

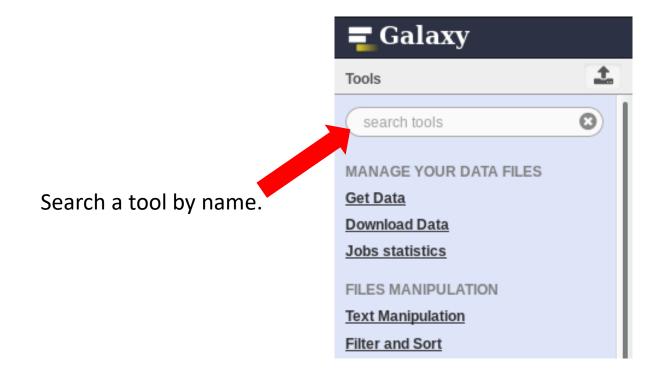
History:

- A tool generates datasets and these datasets are stored in the current history.
- Everything is permanently saved.
- If you log off your computer or browser, it's ok, everything will keep running and be saved!

Your Turn!

DISCOVER GALAXY

- 1. Visit the Galaxy Platform.
- 2. Look at the tool list.
- 3. Display only FROGS tools.
- 4. Display all tools concerning fastq files.



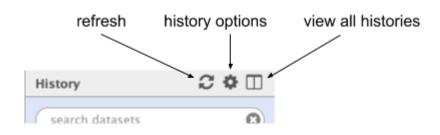
Manipulate Histories

Your Turn!

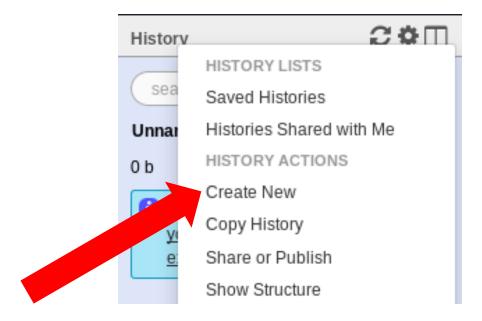
CREATE THE 4 HISTORIES NEEDED FOR THE FROGS FORMATION

To create a new history:

Click on the wheel.



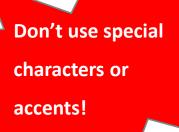
Click on « create new ».



To rename a history:

- Click on the history name (at the top).
- Enter « multiplex ».

Hit « Enter » to validate.



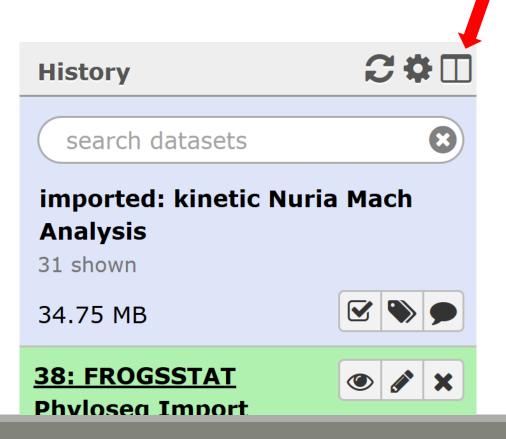


Exercise

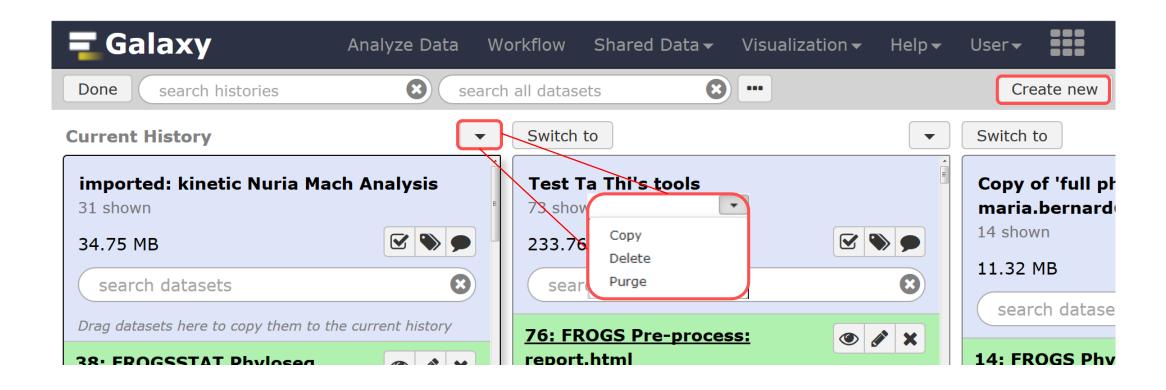
- Create histories named:
 - 454 or ITS
 - merged
 - temp
- Switch to the history named « multiplex » as current history.
- Go back to the main interface.

How to list all histories?

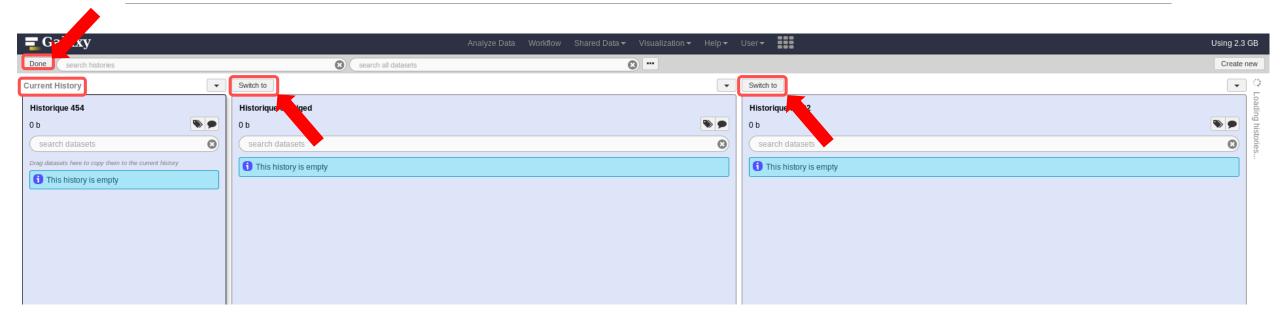
To view all histories, click on this icon.



Explore the « View all histories » section



Switch current history



- Switch to the history named « multiplex » as current history.
- Click on "Done" to go back to the main interface.

Data import

How to import your data to Galaxy

- 5 ways to upload your data to Galaxy:
 - From your computer



By URL



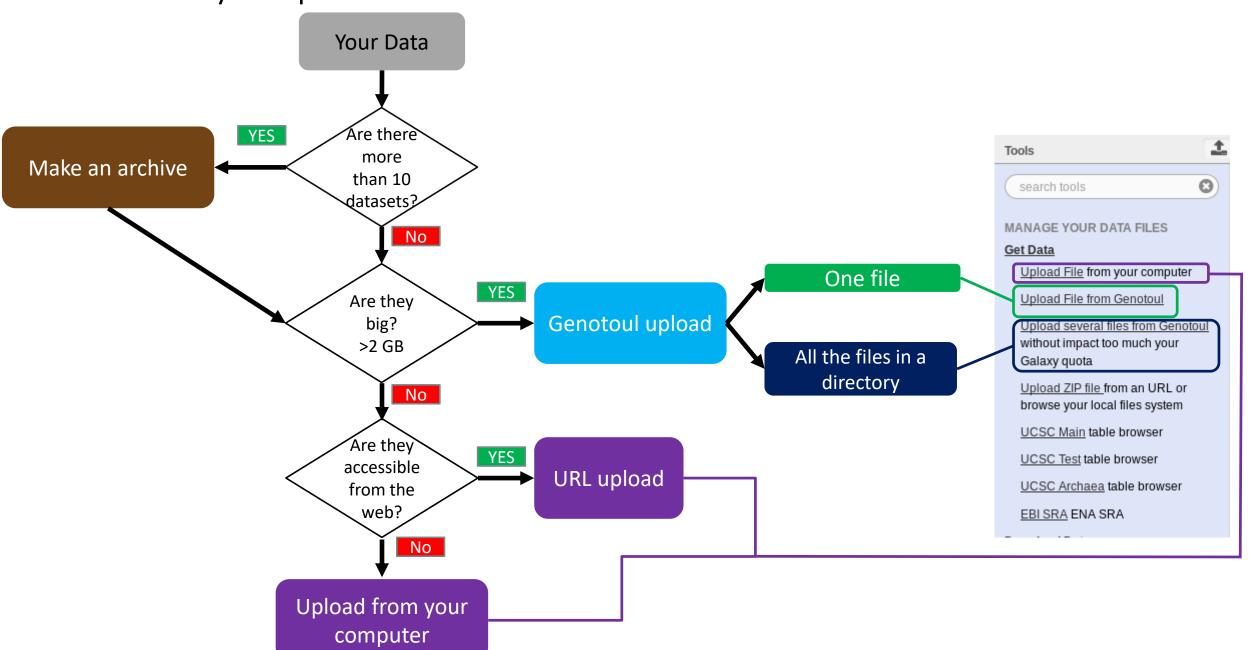
From Genotoul Bioinfo clusters



Shared by other users of Galaxy



How to choose your upload method?

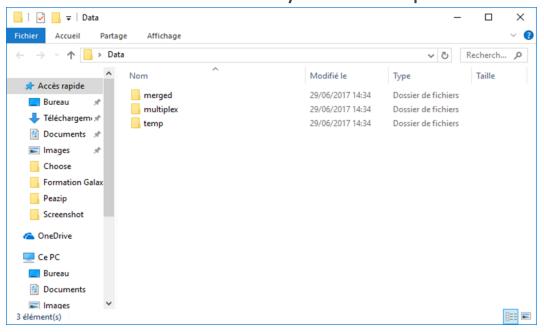


Your Turn!

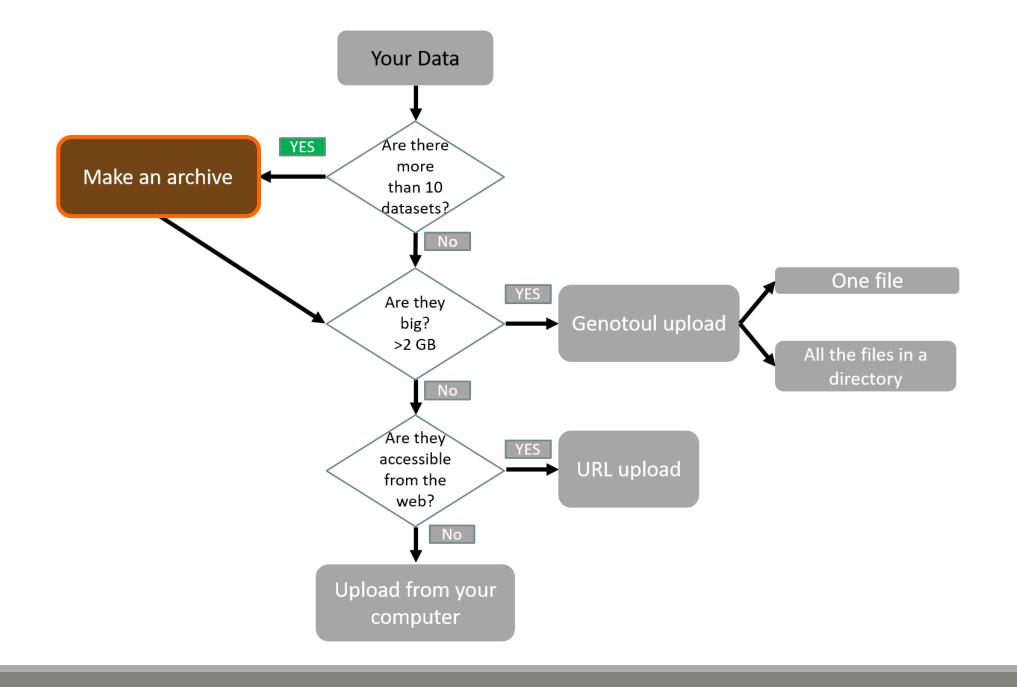
PREPARE FILES

Formation data

All the formation data are in the Data folder on your desktop.

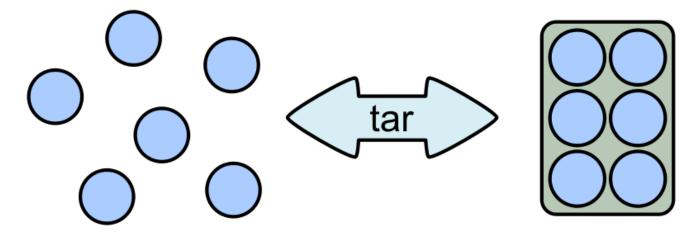


- If you don't have this directory on your desktop, ask us.
- You can find all the formation data online on: http://genoweb.toulouse.inra.fr/~formation/15 FROGS/FROGS ini/DATA/Dataset/



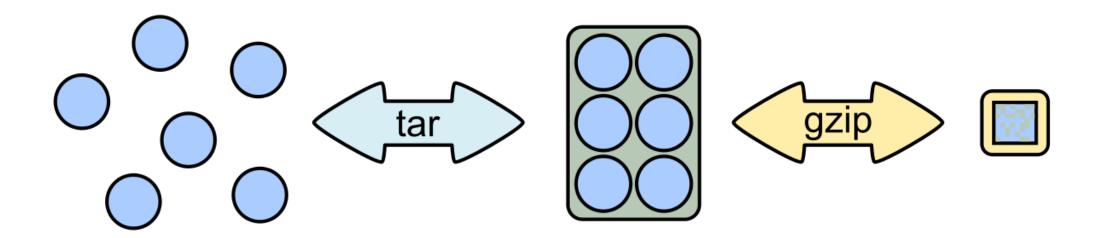
Create a Tar file

- Uploading multiple local files is time consuming.
- Solution: put all your files in an archive!
- What is a tar file?



Create a Tar.gz

Moreover, we can compress the archive to free up space.



Your Turn!

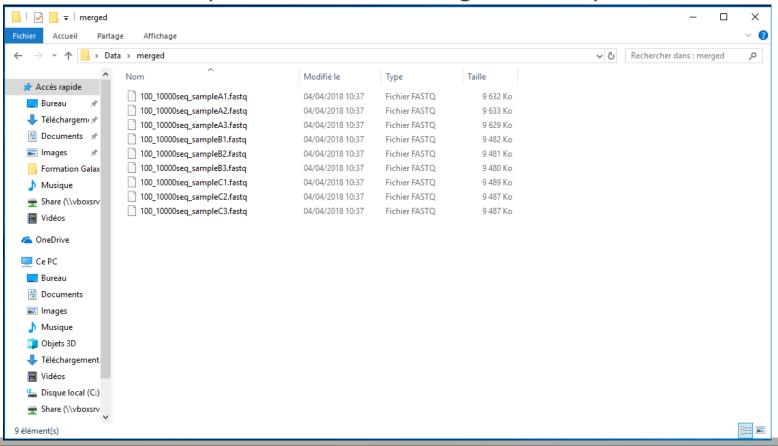
CREATE AN ARCHIVE WITH THE FILES IN MERGED

7-Zip

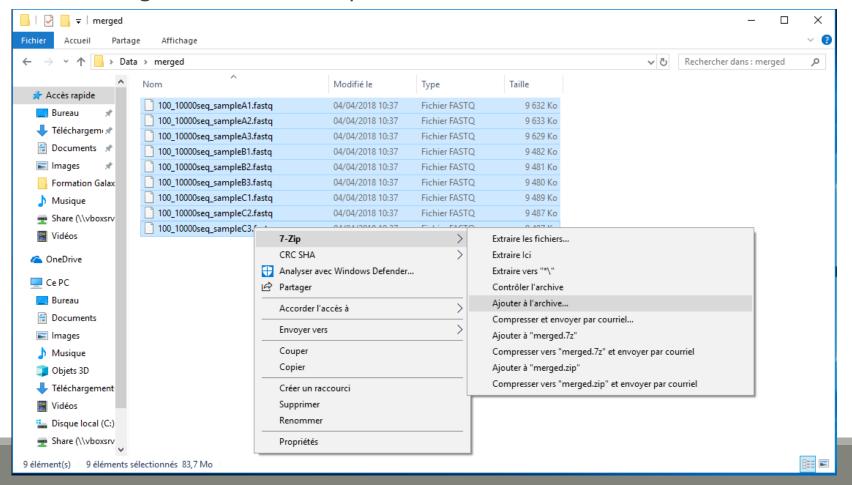
- 7-Zip is a software called a file archiver.
- Can archive and compress files.
- Open source
- At the lab, you could download it at: http://www.7-zip.org/



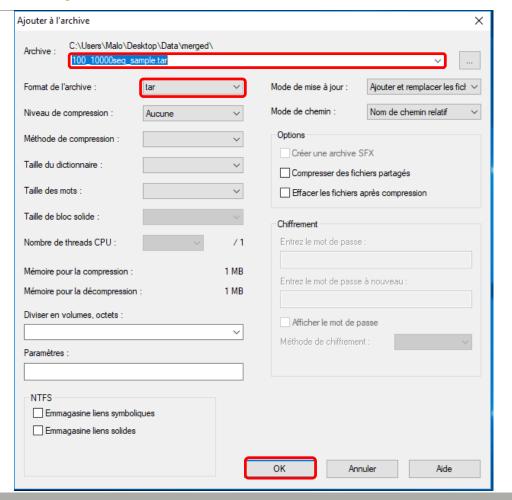
Browse into the Data directory and next into the merged directory.



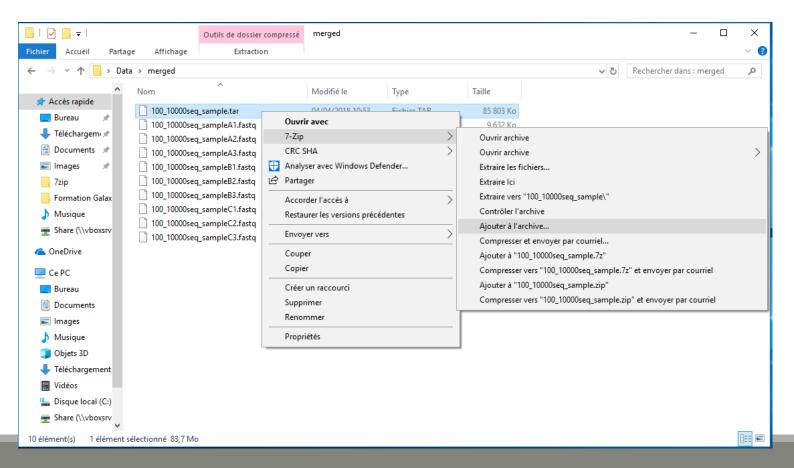
Select all files and right click on it > 7-Zip > Add to archive . . .



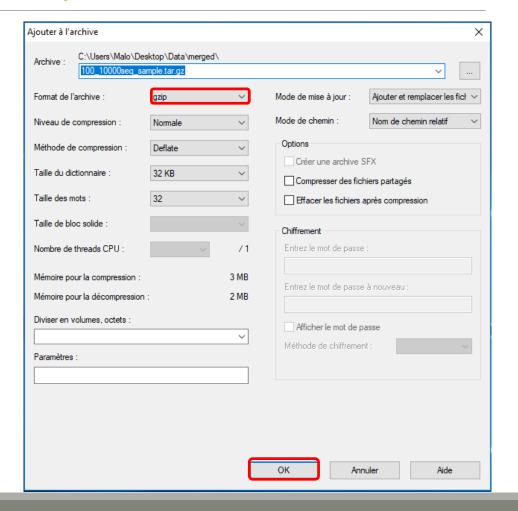
- Change the name of the archive to:
- « 100_10000seq_sample.tar »
- Choose « tar » as archive format .
- Click on OK.

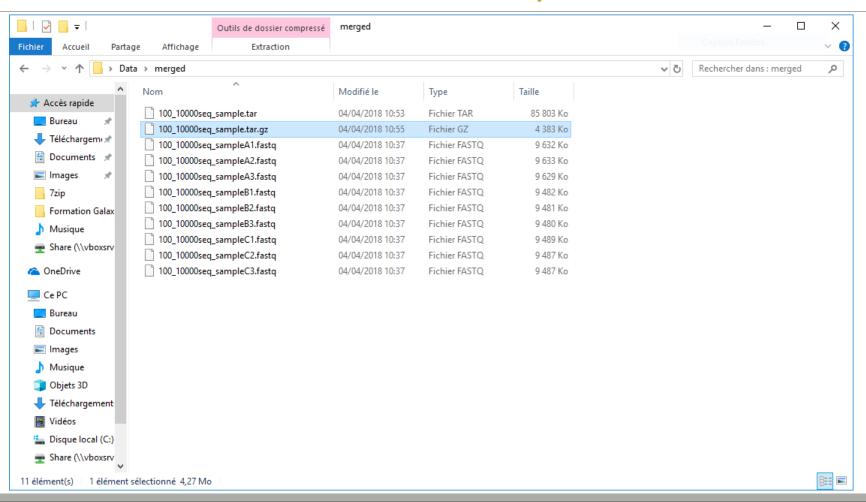


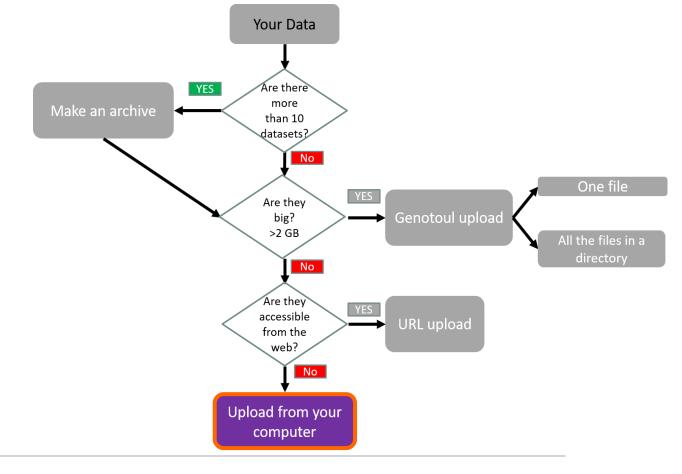
Select the newly created archive and right click on it > 7-Zip > Add to archive . . .



- Choose « gzip » as archive format .
- Click on OK.





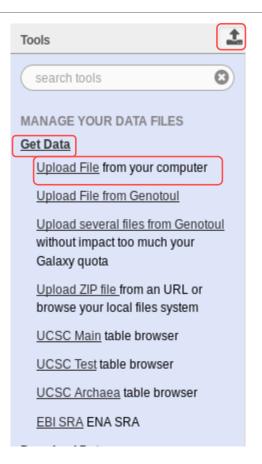


Your Turn!

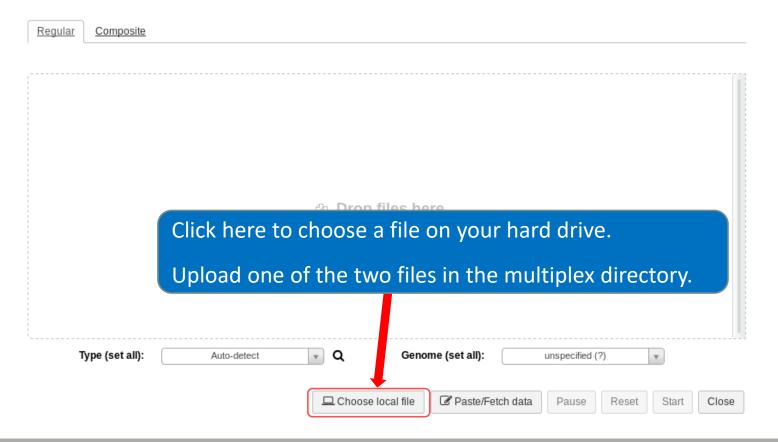
UPLOAD FILES FROM YOUR COMPUTER

- In Galaxy, your current history must be multiplex.
- Click on the « Get Data » tool.
- Upload file from your computer.

↑ For files smaller than 2 GB



Download from web or upload from disk



The datatype of a file indicates the content of it.

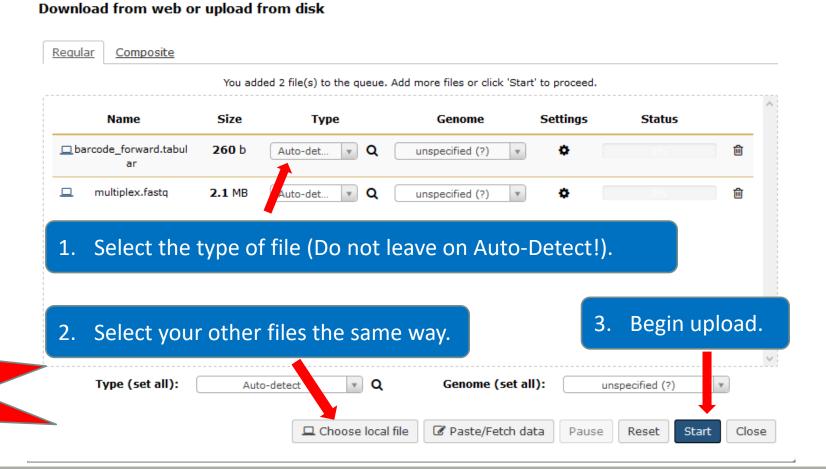
.fasta = fasta

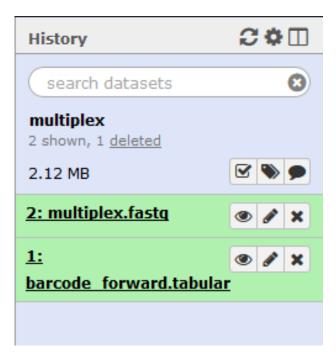
.fastq = fastq

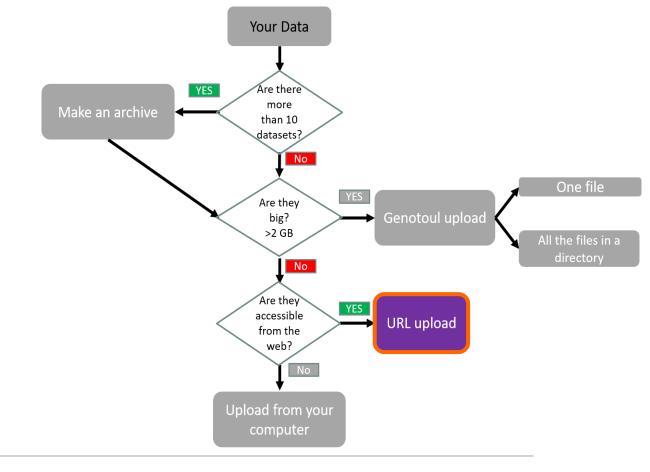
.tar = tar

Select the type corresponding to your file.

Do no not trust blindly the auto-detect!







Your Turn!

UPLOAD FILE FROM AN URL

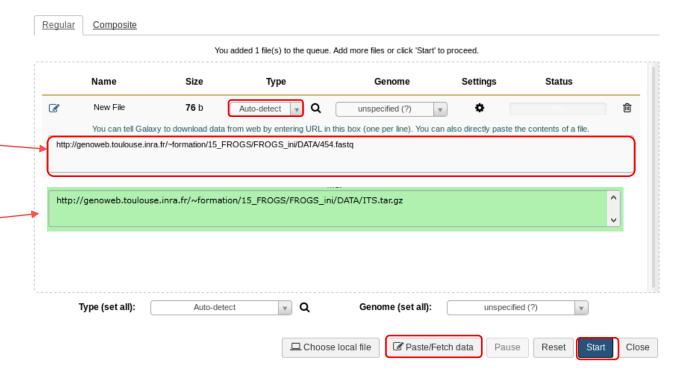
Upload file from URL

- 1. Switch to 454 or ITS history as current history.
- 2. Go to **Get Data** > **Upload File from your computer**
- 3. Click on **Paste/Fetch Data**
- 4. Copy the address of the file: http://genoweb.toulouse.inra.fr/~formation/15_FROGS/FROGS_ini/DATA/454.fastq

Or

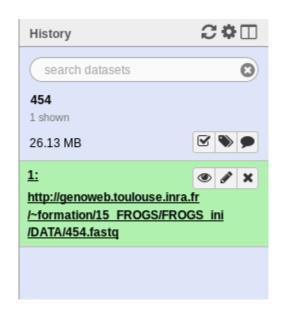
http://genoweb.toulouse.inra.fr/~formation/15 FROGS/FROGS ini/DATA/ITS.tar.gz

- 1. Change the type!
- 2. Click on Start.
- 3. You can put one address per line for multiple uploads.

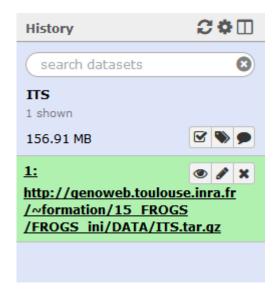


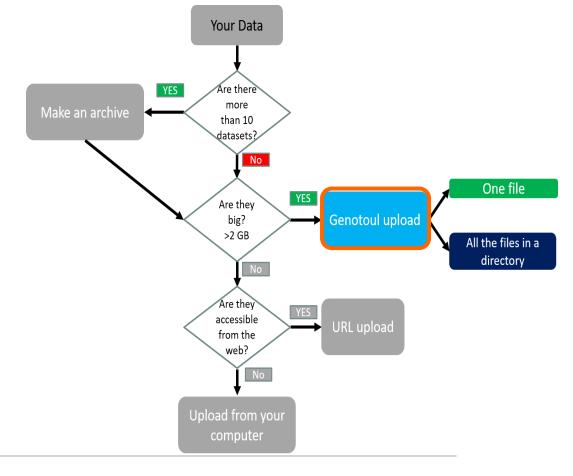
Download from web or upload from disk

Upload file from URL



OR

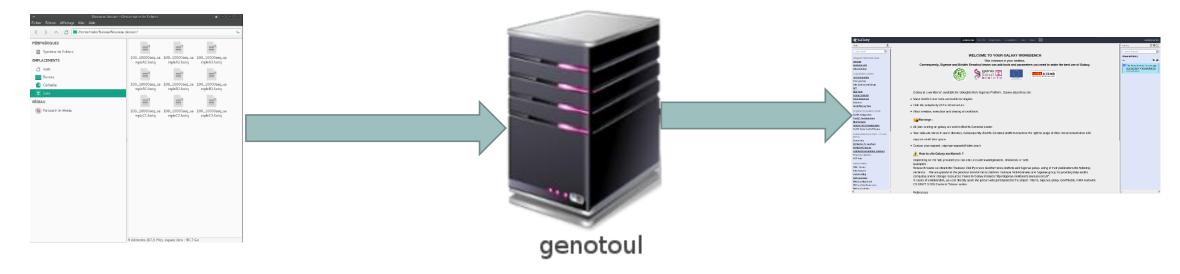




Your Turn!

UPLOAD FILES TO GENOTOUL AND LINK IT TO GALAXY

Objectives

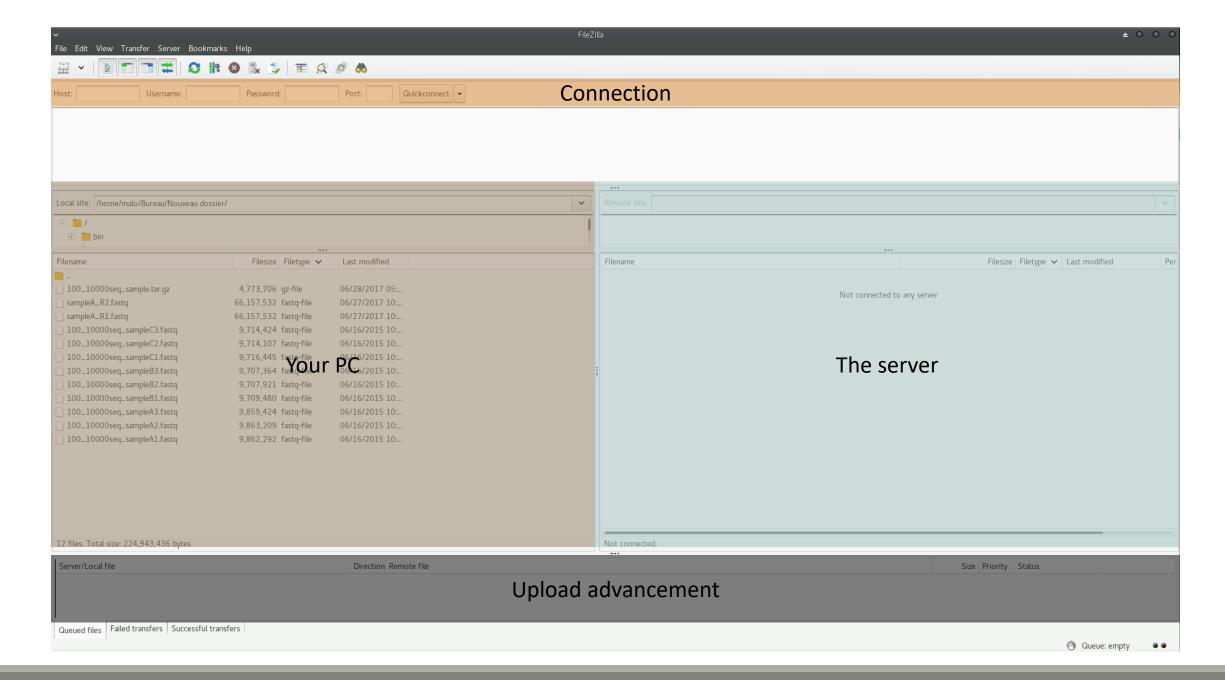


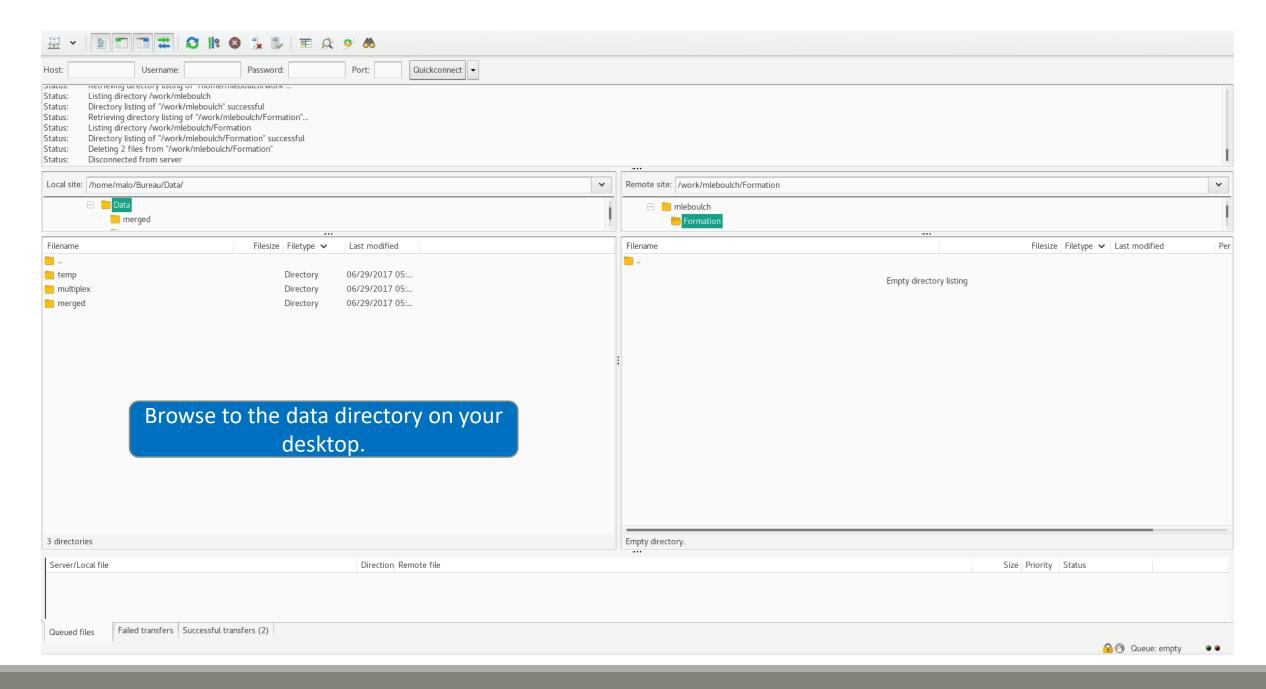
Transfer your files to your Genotoul account and link the file to Galaxy.

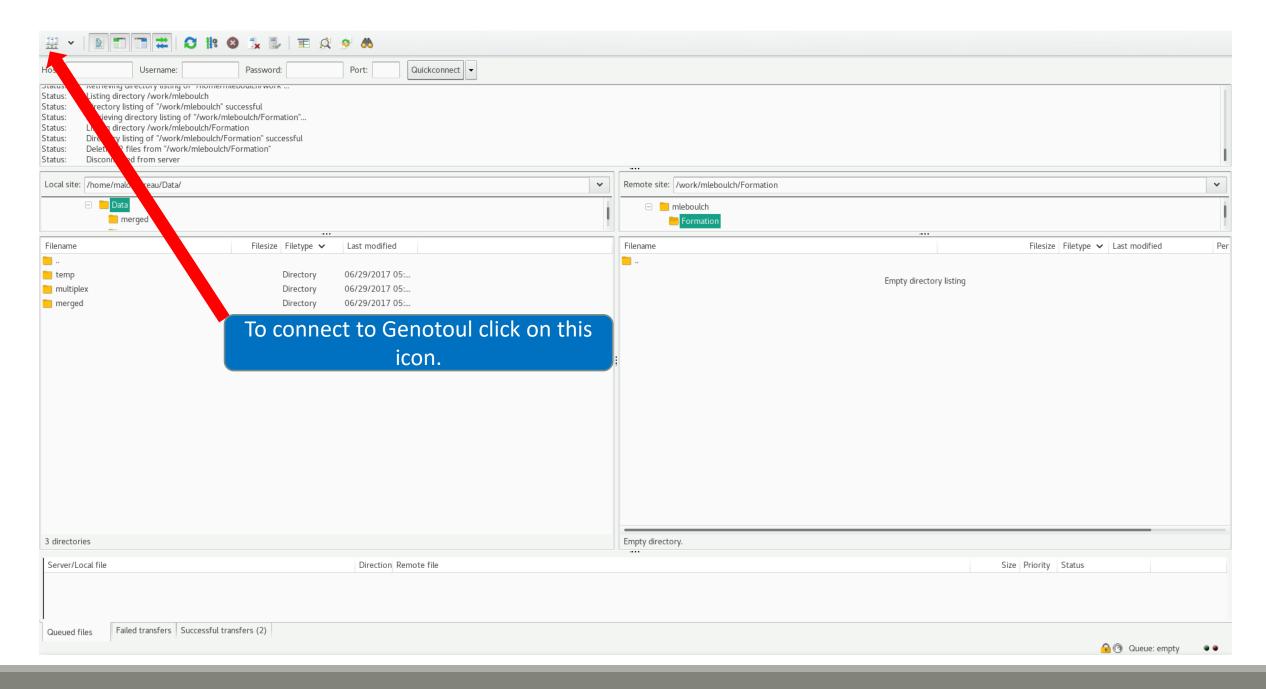
Preparation

- Open the data directory on your desktop.
- Launch Filezilla.
 - Filezilla is a FTP client *i.e.* can transfer files to a distant server.
 - You can download it on : https://filezilla-project.org/









Host: genologin.toulouse.inra.fr

Port: 22

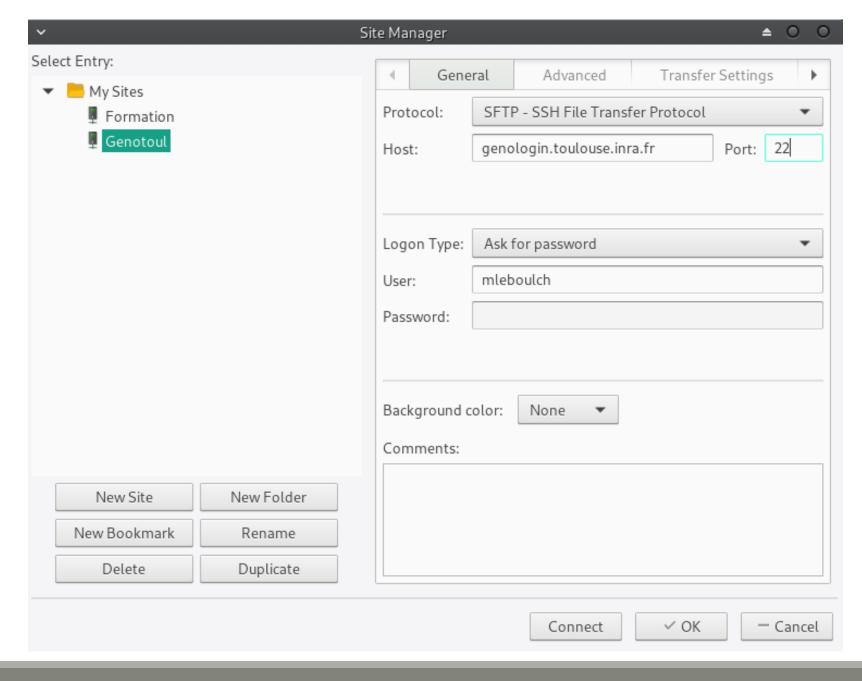
Protocol: SFTP

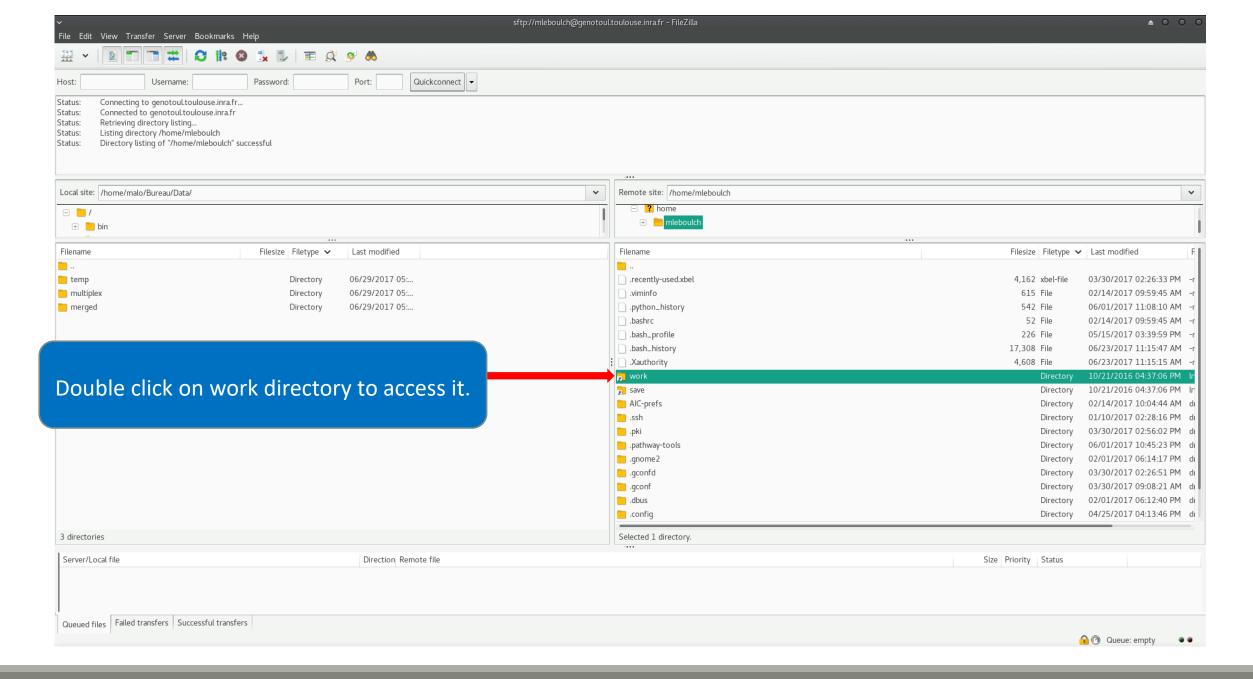
User: your Genotoul login

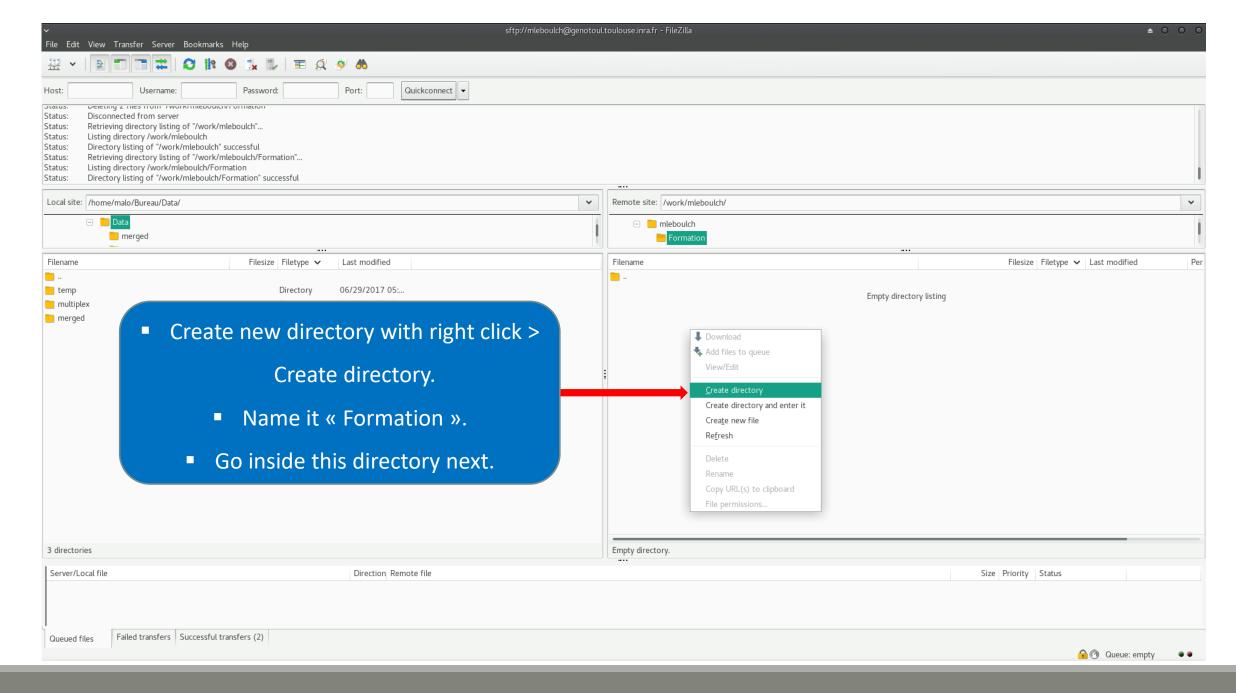
Logon Type: Ask for password

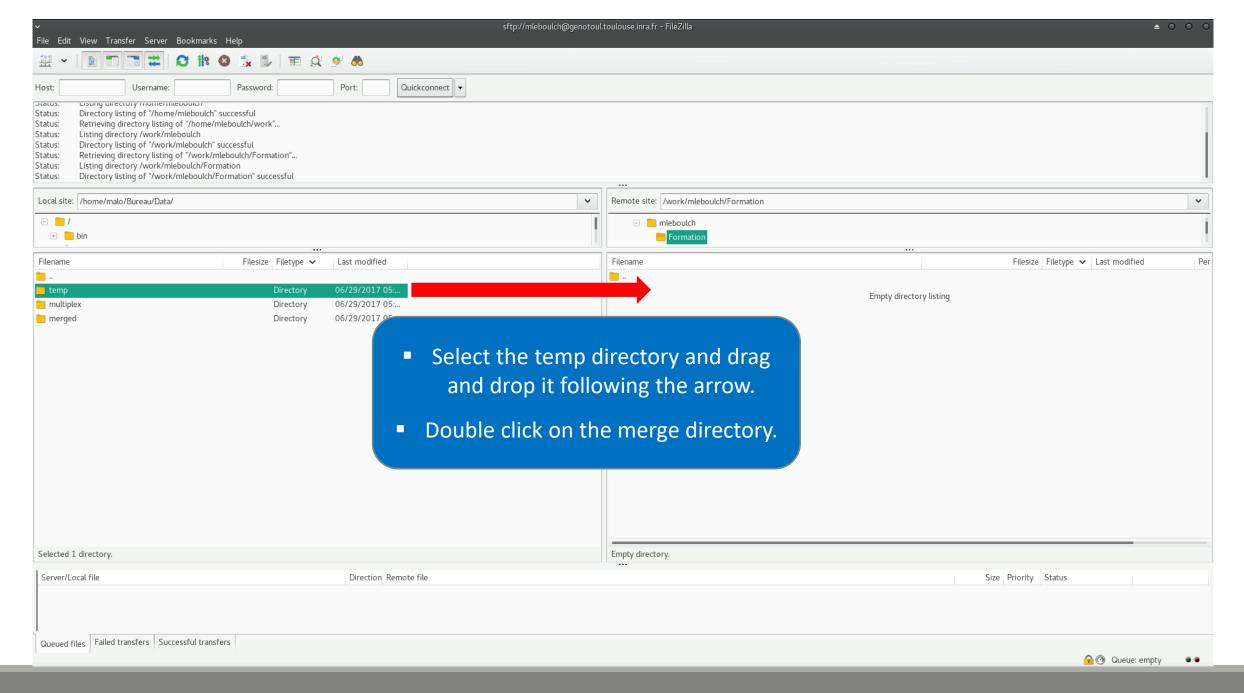
Click on connect.

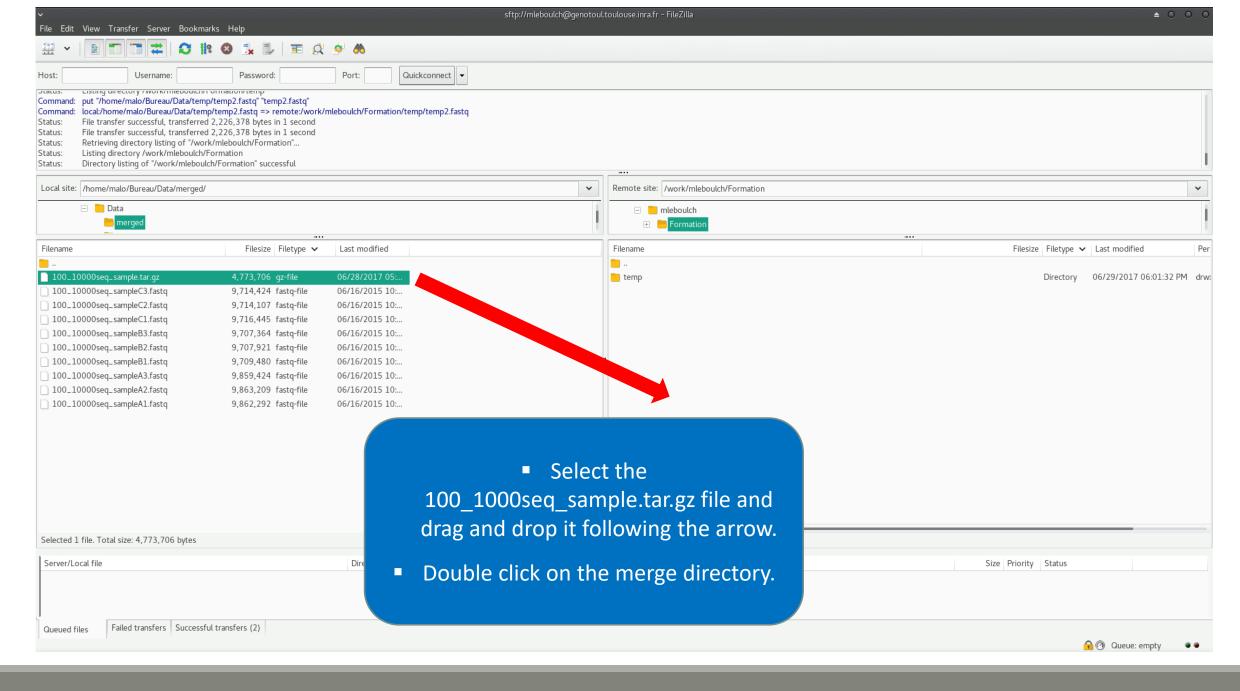
Password: your password

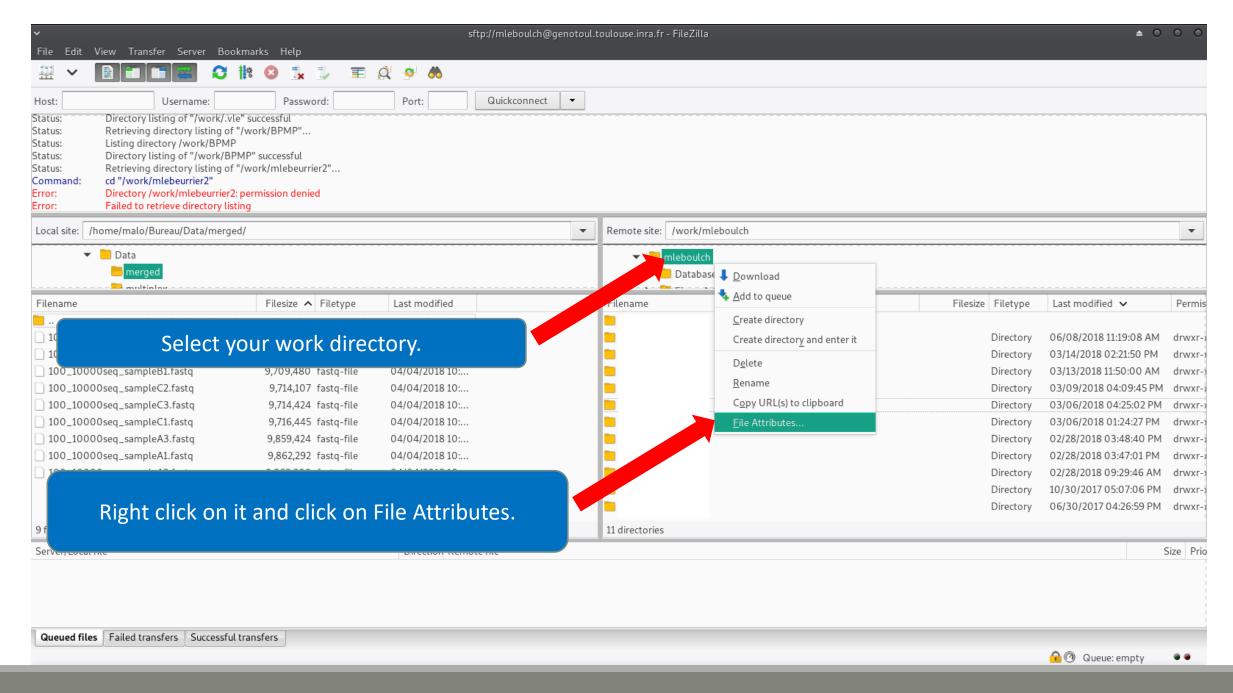


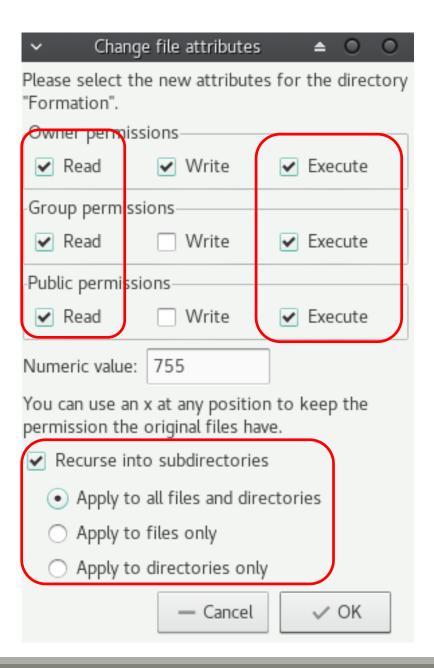






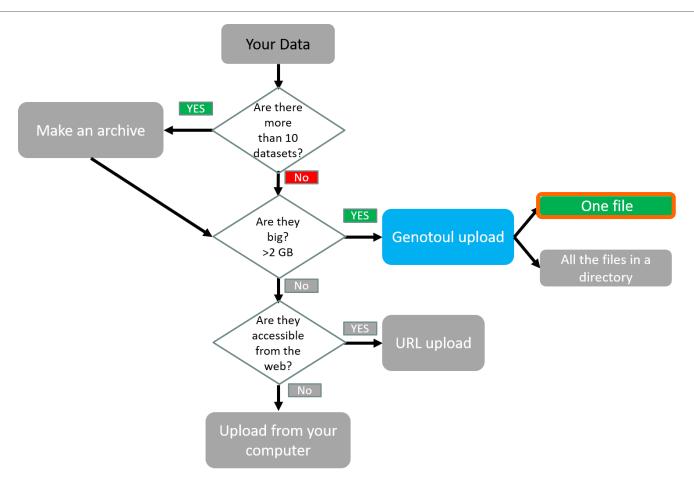


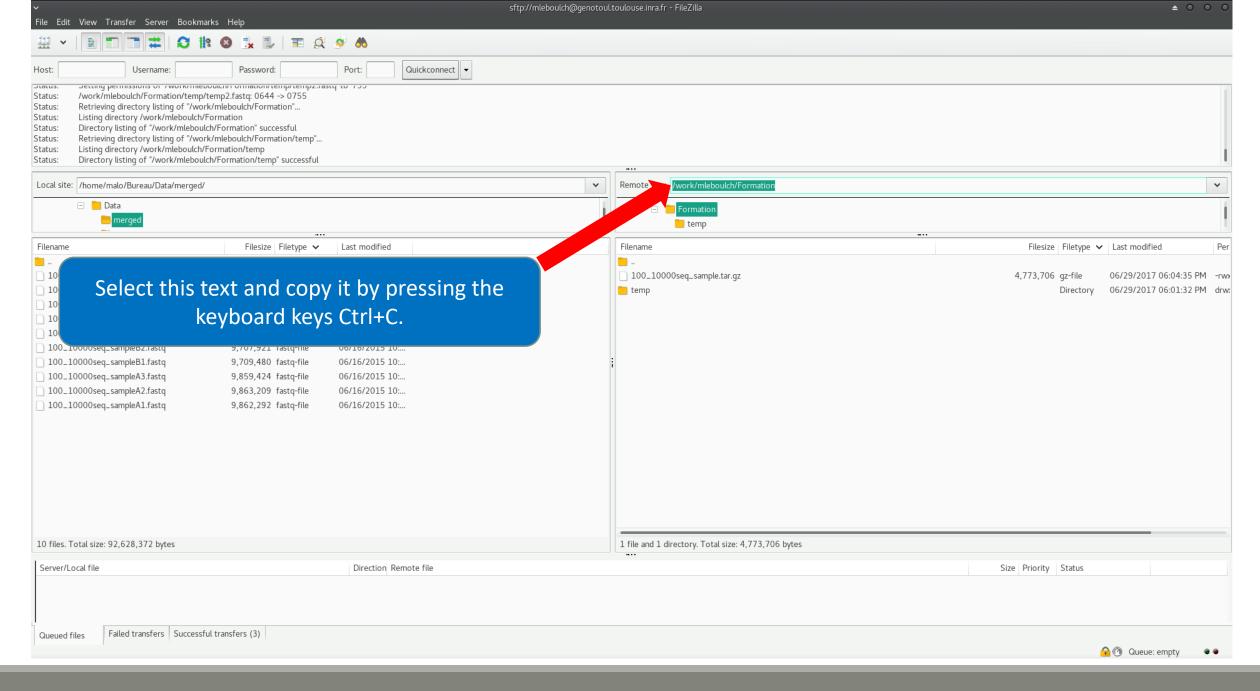


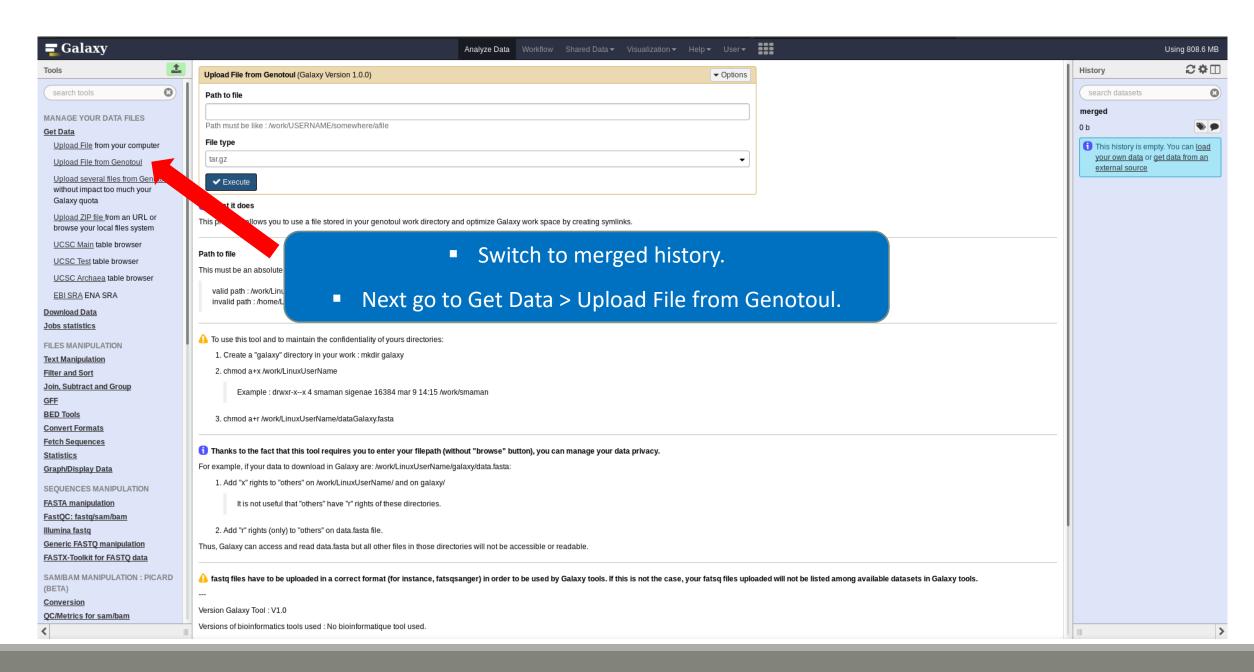


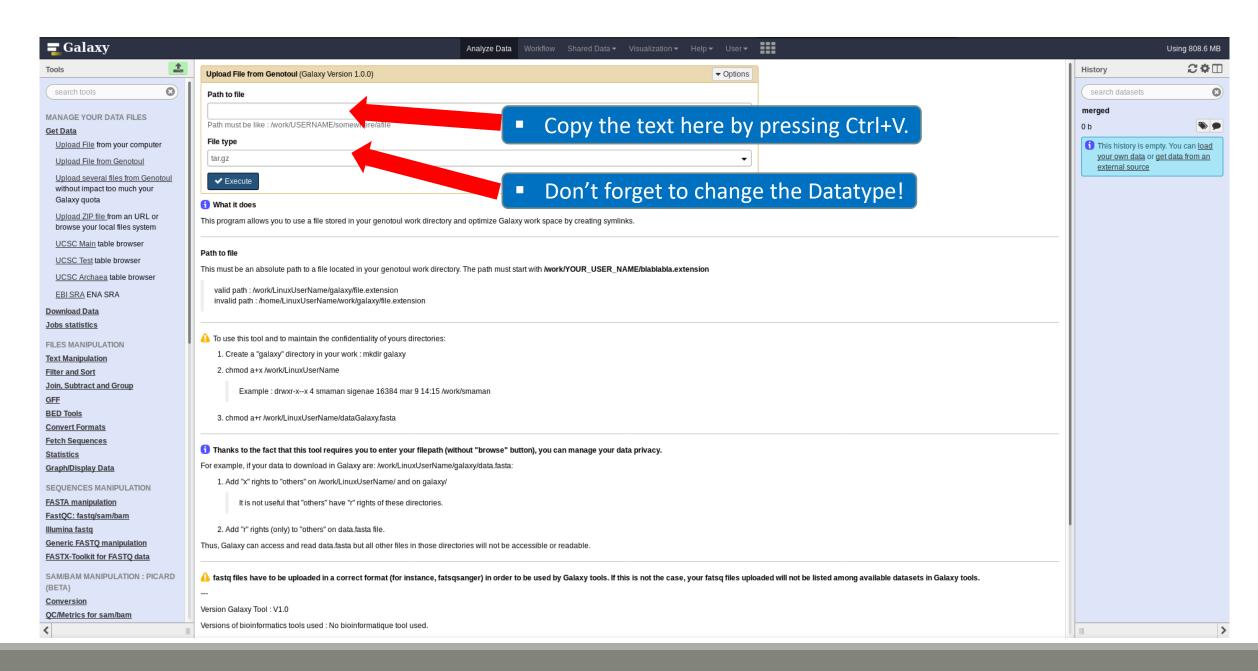
- Check that all boxes for execute and read are checked.
 - Recurse this action to all files and subdirectories.
- That allows Galaxy to access your files on Genotoul.
 - Click on Ok.

Upload files from Genotoul



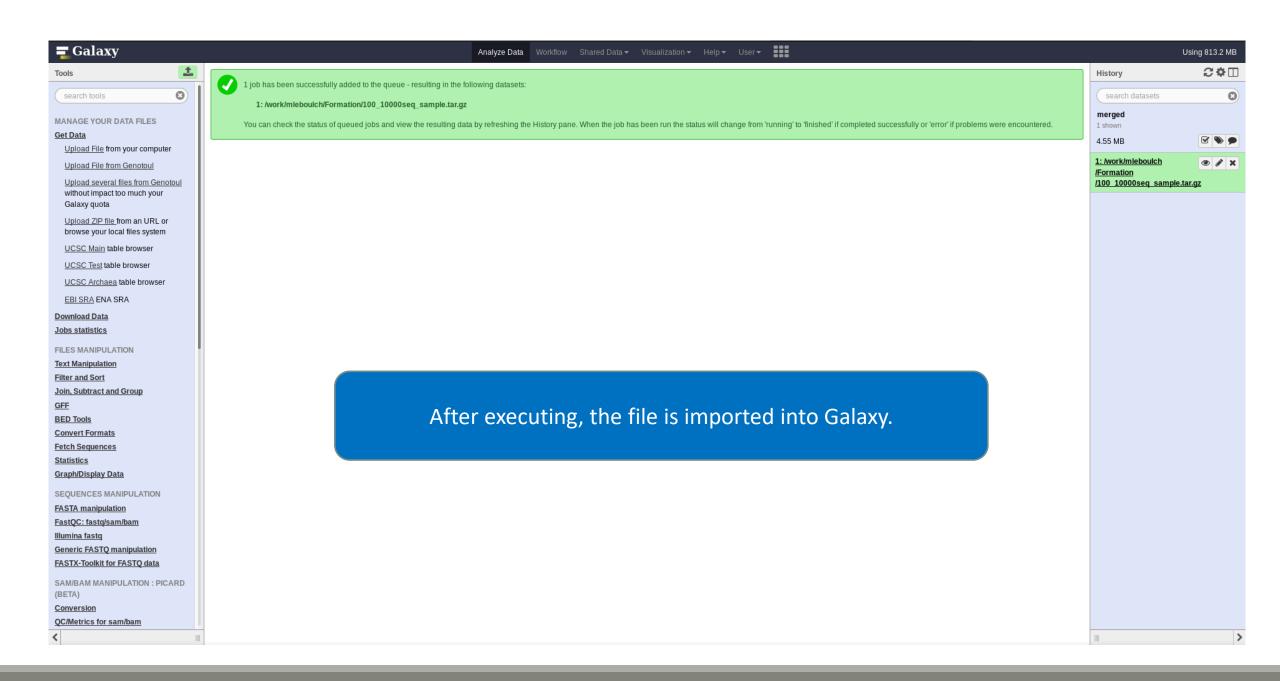




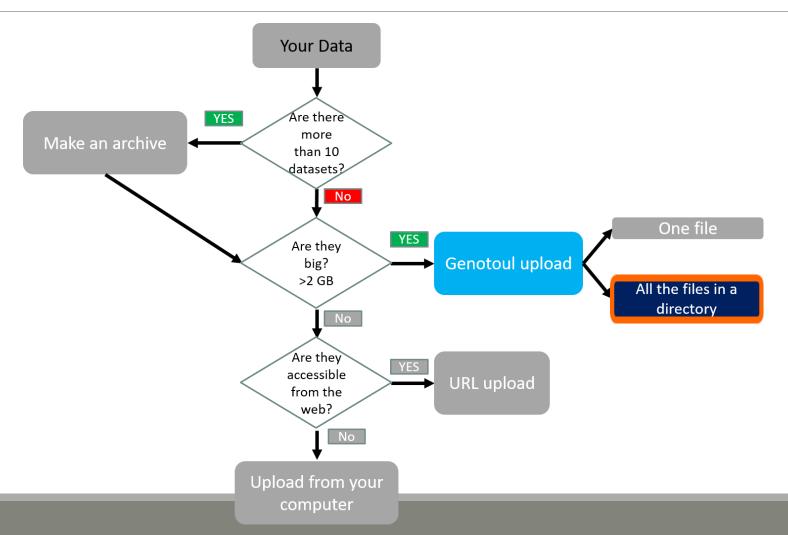


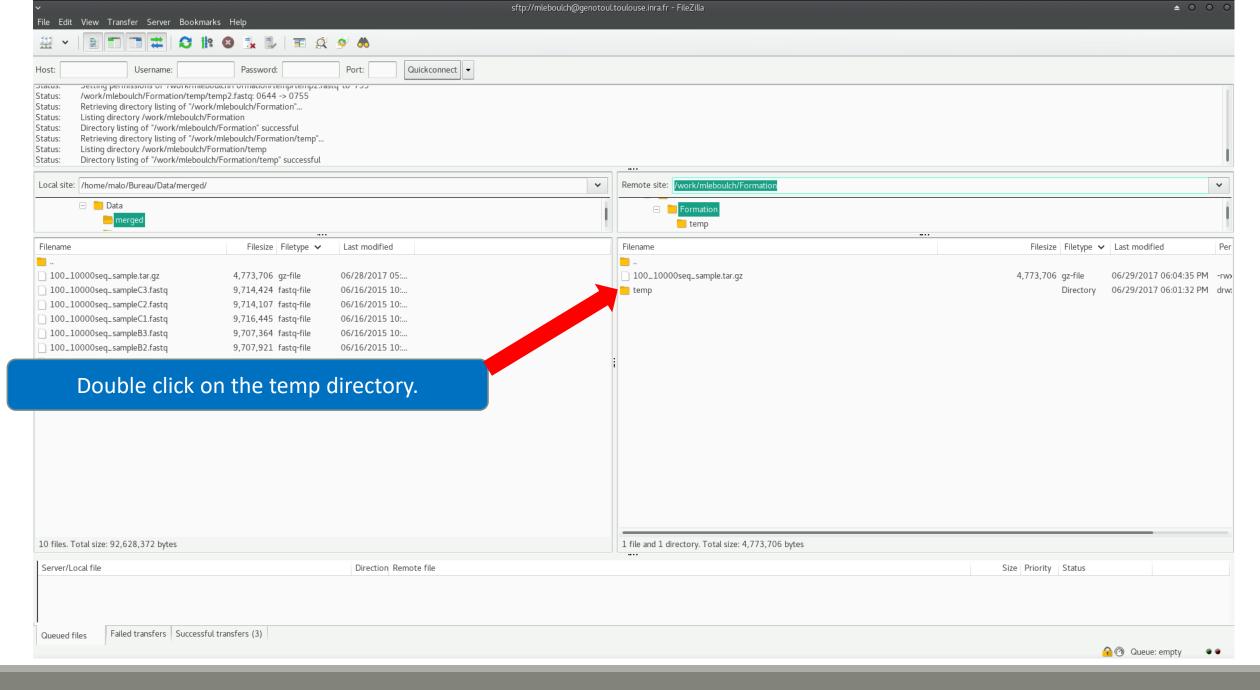


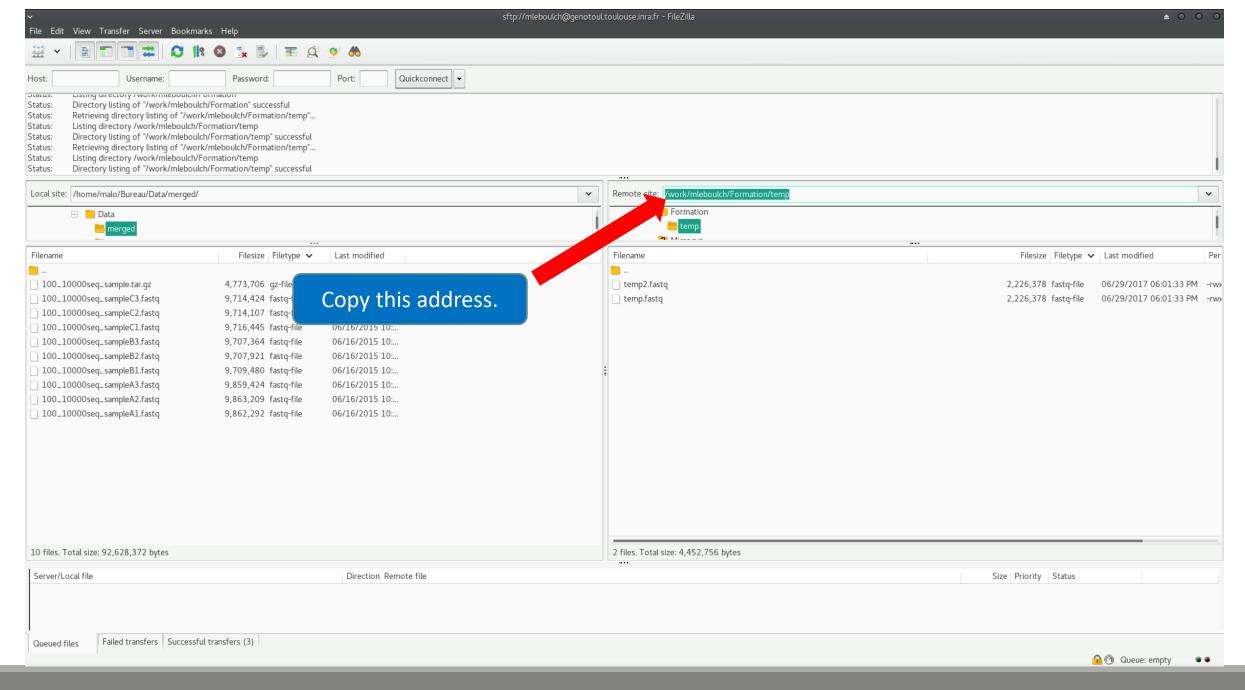
You must add « / » and the name of the file at the end of the text.

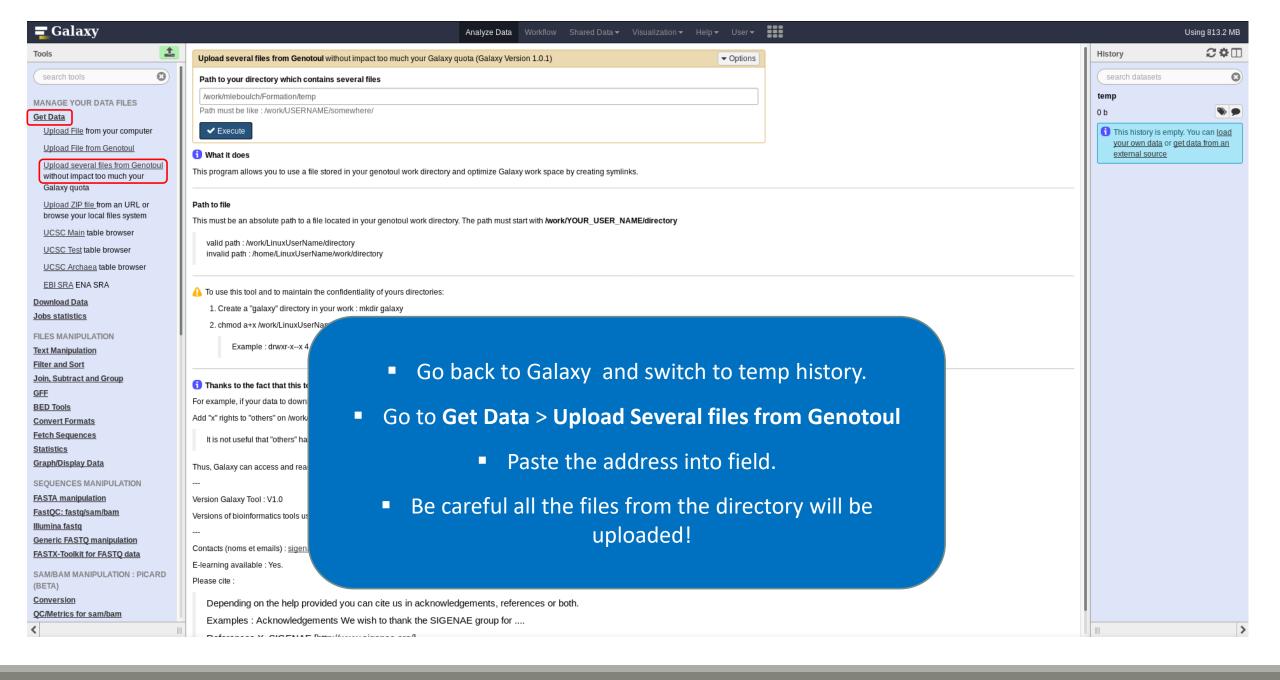


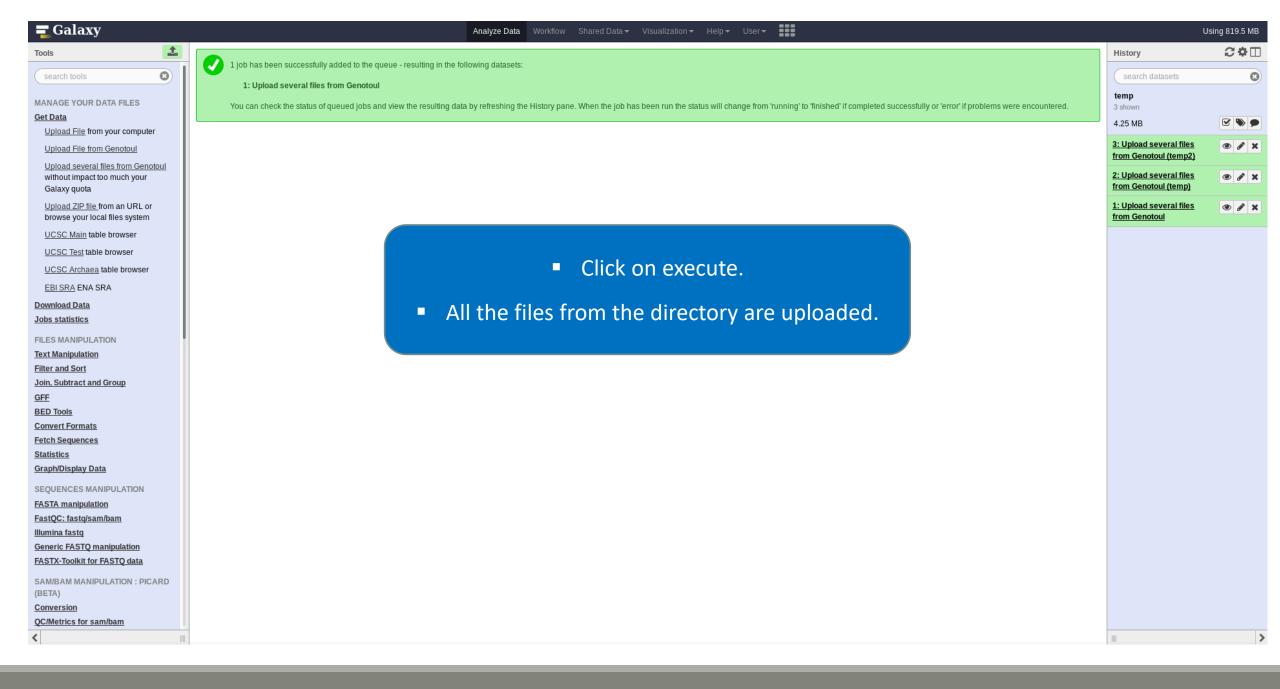
Upload files from Genotoul



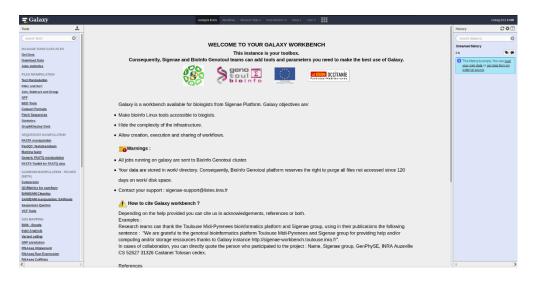








Upload by Genotoul



1TB of space



/work: 1TB (1024GB) of space

/save: 250GB of space

- This method allows you to have more disk space and to upload bigger files.
- Files not used in the last 180 days can be purged at any time.

Share a History

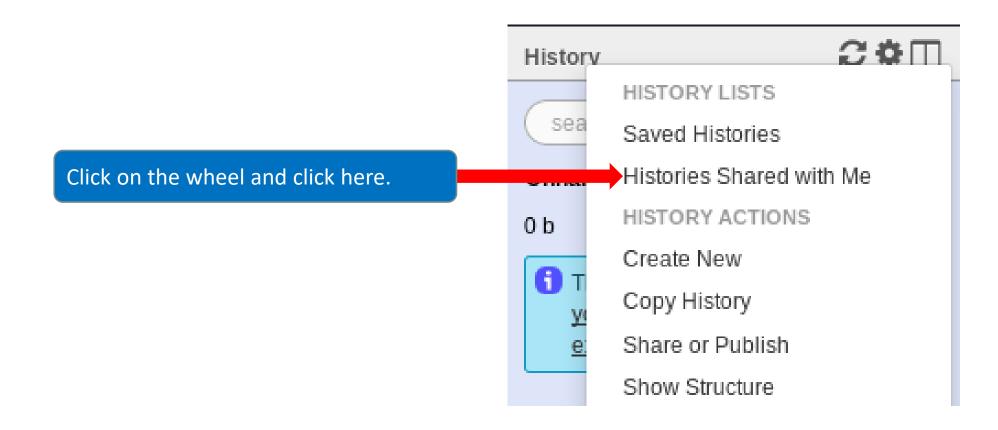
Share a history

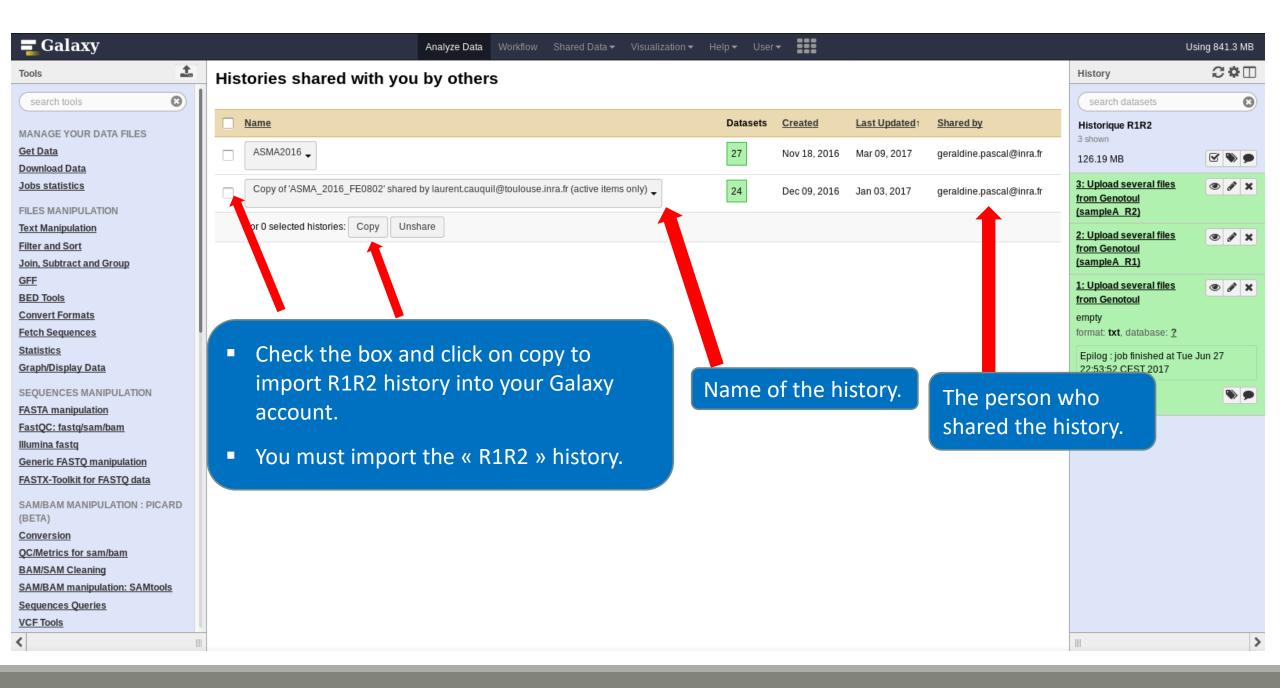
- You can share a history with another Galaxy user:
 - For working with your colleague.
 - For support, so we can help you better and faster.
- You can import shared history to your account too.

Your Turn!

IMPORT A SHARED HISTORY TO YOUR ACCOUNT

Import a shared history

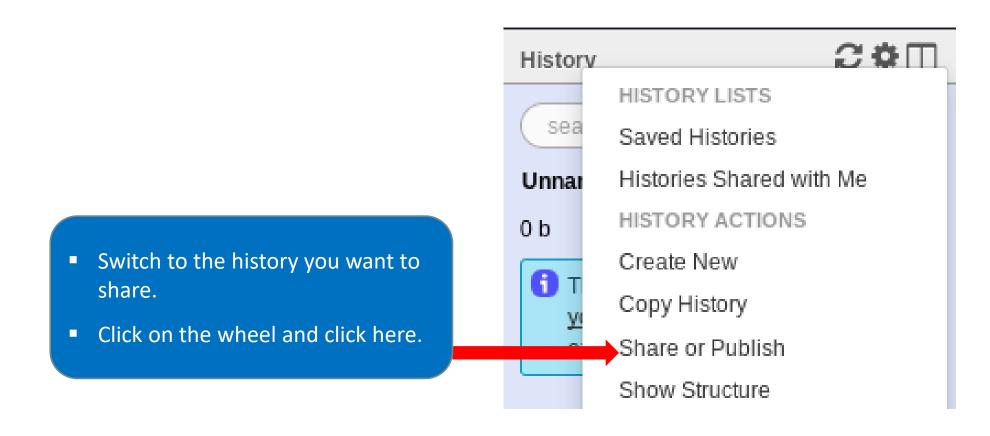


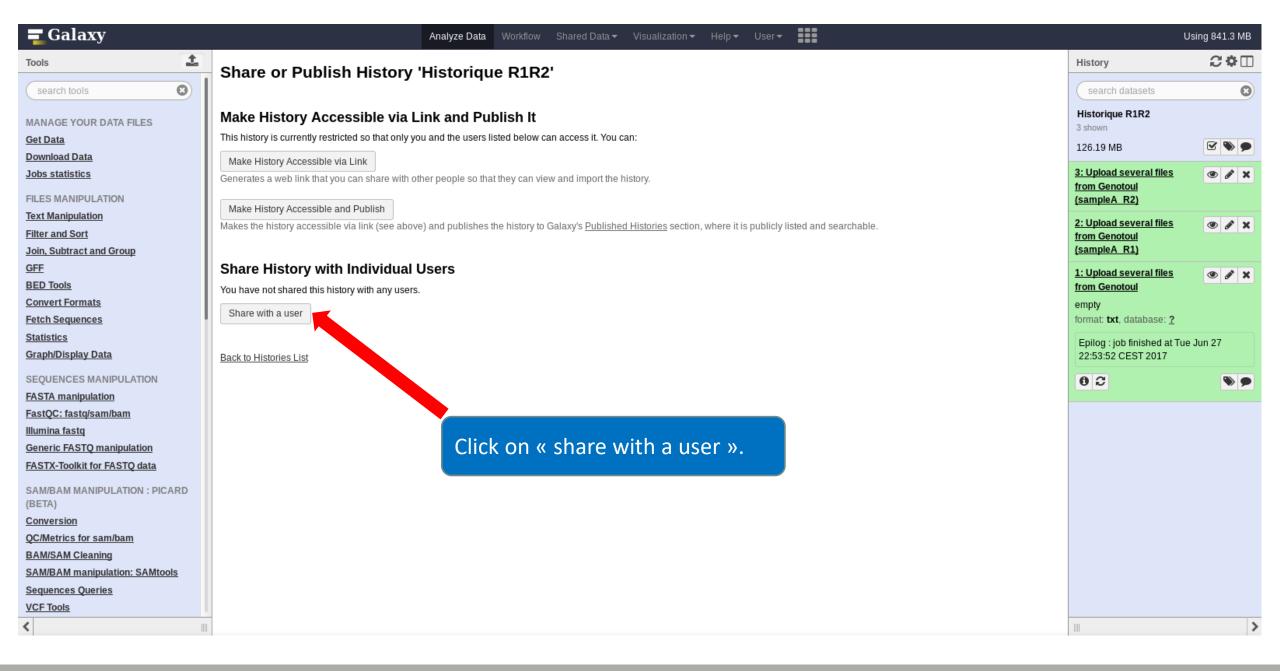


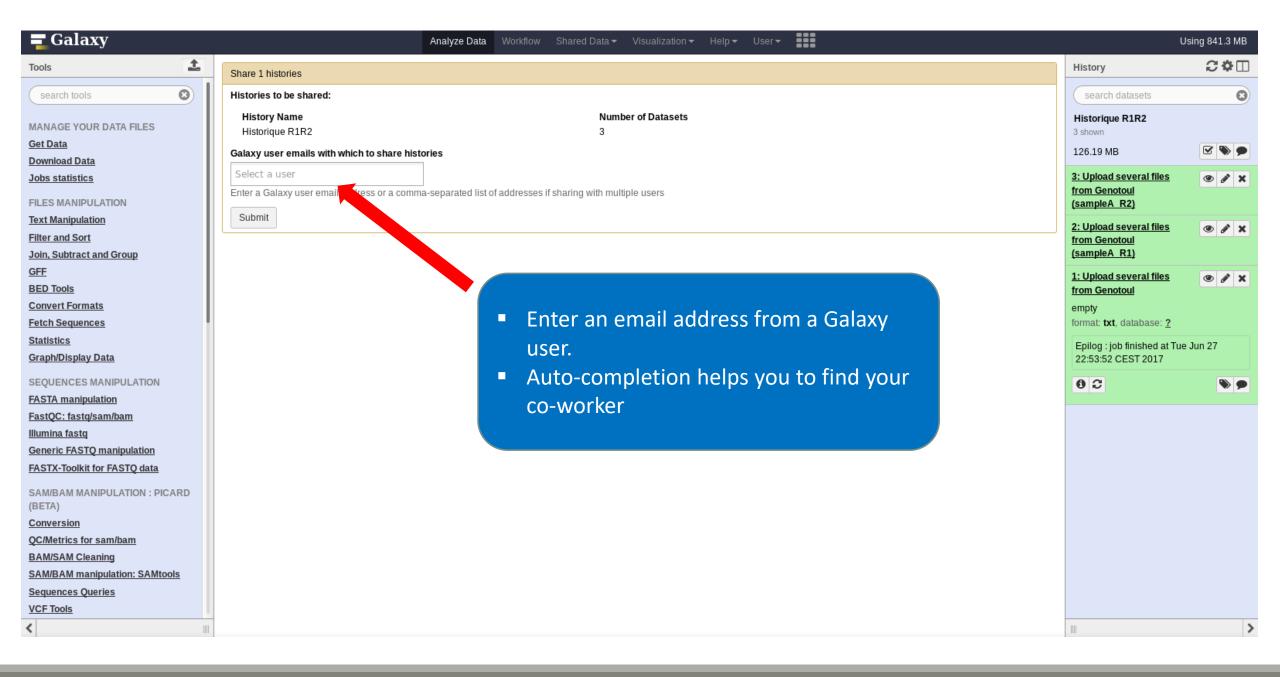
Your Turn!

SHARE A HISTORY WITH YOUR NEIGHBOUR

Share a history







Galaxy user emails with which to share histories



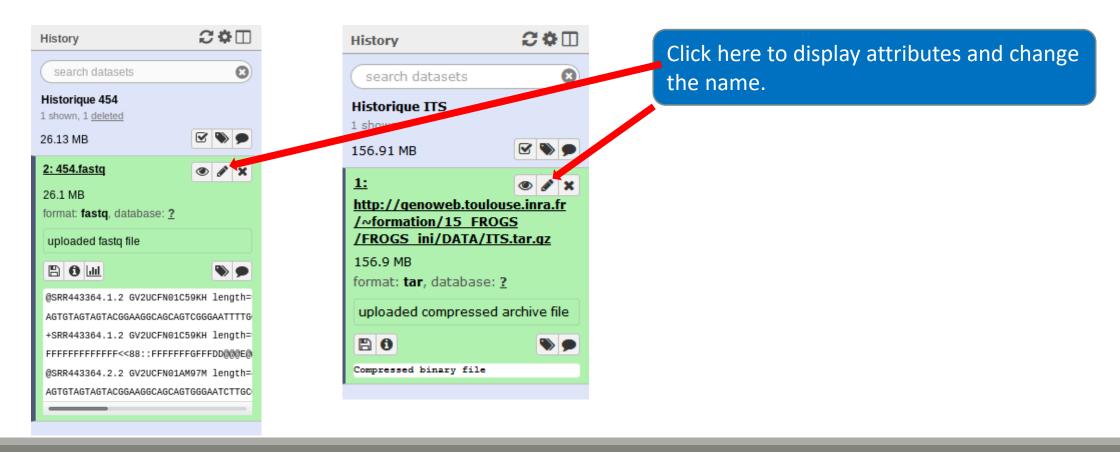
- You must click on the address in the dropdown menu.
- Click on submit.
- The history will appear in your coworker's history.

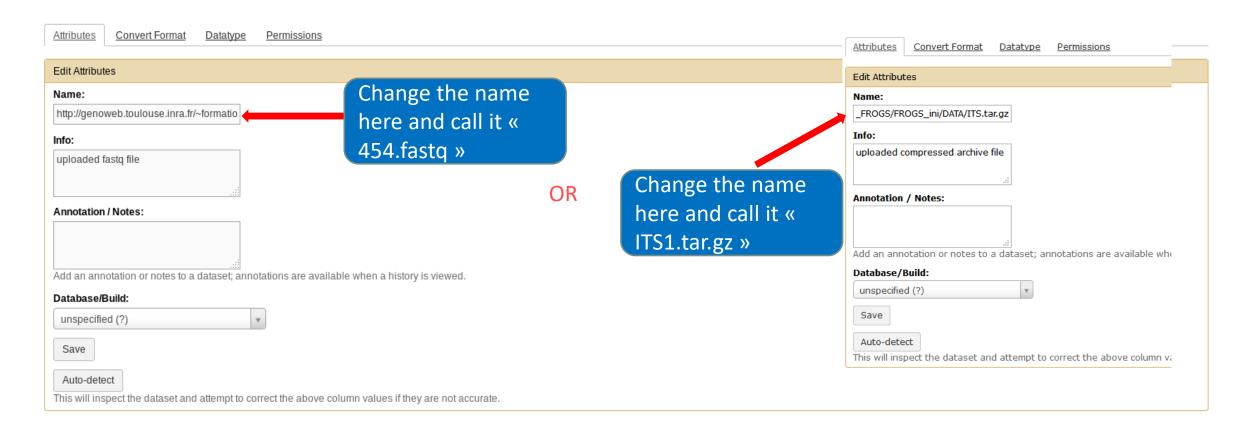
Manipulate datasets

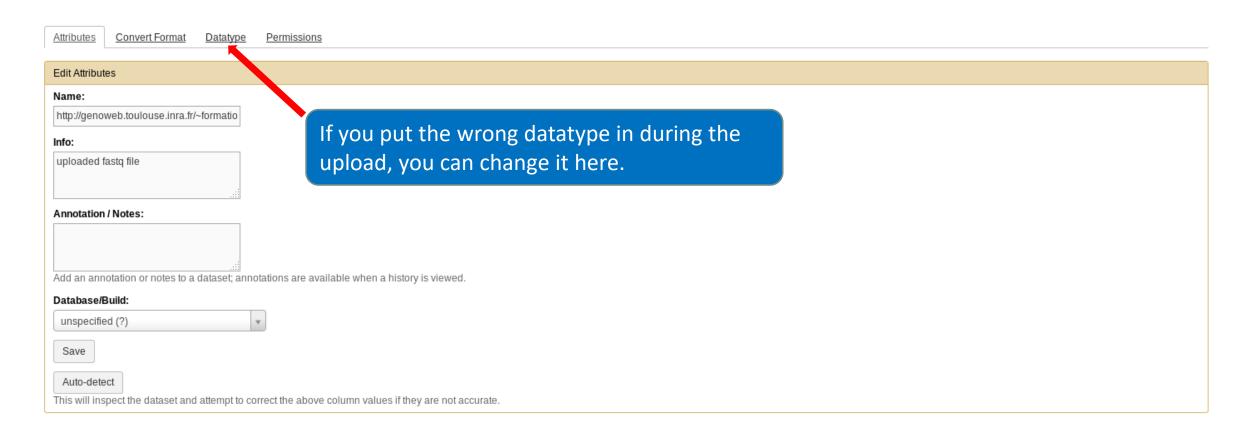
Your Turn!

RENAME A DATASET

Switch to 454 history or ITS history







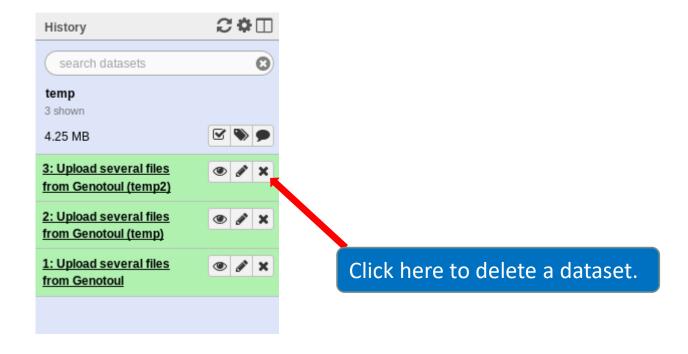
- Do the same with the merged history:
 - Switch to the merged history.
 - Change the name of the file to «100_10000seq_sample.tar.gz ».

Your Turn!

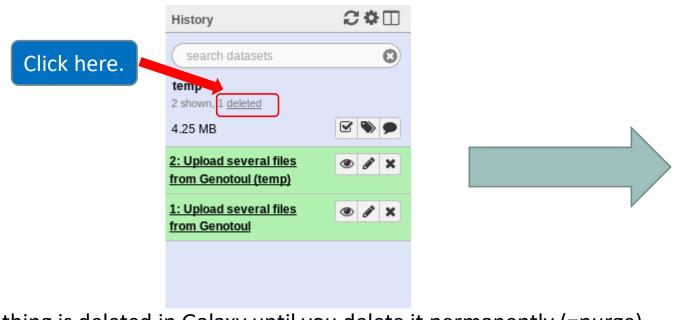
DELETE A DATASET

Delete a dataset

Switch to temp history.



Delete a dataset



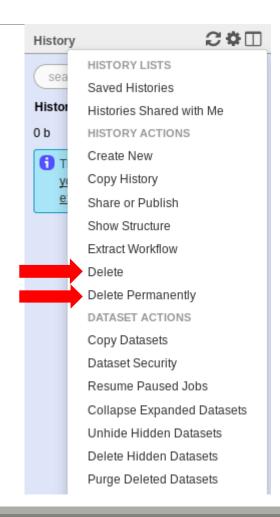
History search datasets temp 3 shown, hide deleted 4.25 MB This dataset has been deleted Undelete it Permanently remove it from disk 3: Upload several files **(9**) from Genotoul (temp2) 2: Upload several files ● 🖋 🗙 from Genotoul (temp) 1: Upload several files ● 🖋 🗙 from Genotoul

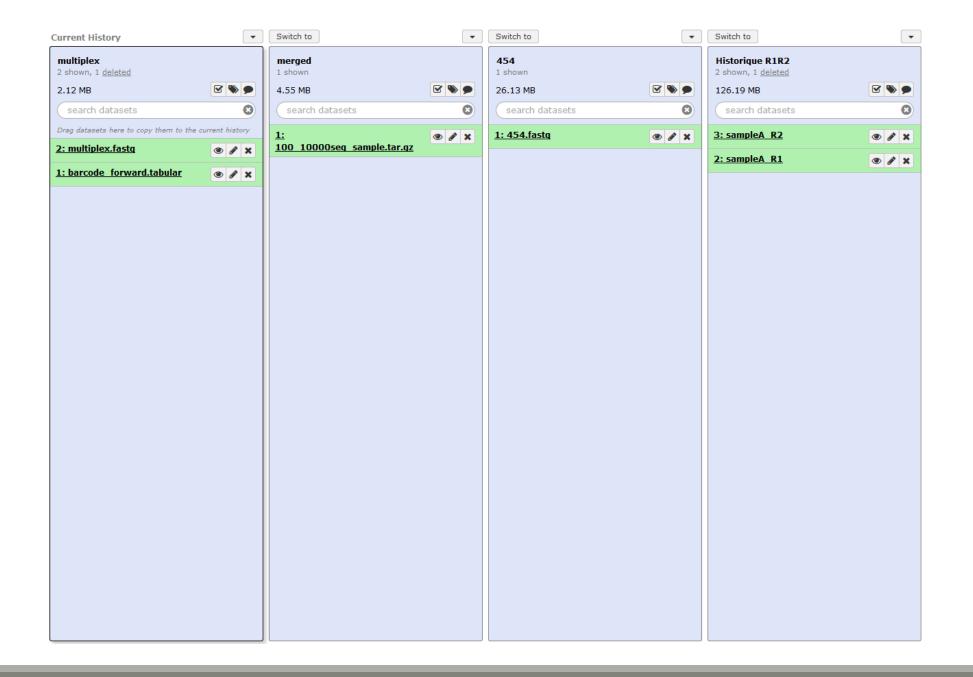
Delete this dataset permanently.

Nothing is deleted in Galaxy until you delete it permanently (=purge).

How to delete a history?

- Stay in the temp history.
- Click on the wheel.
- Click on delete.
- A deleted item on Galaxy is recoverable.
- To definitively delete it: click on « Delete Permanently ».

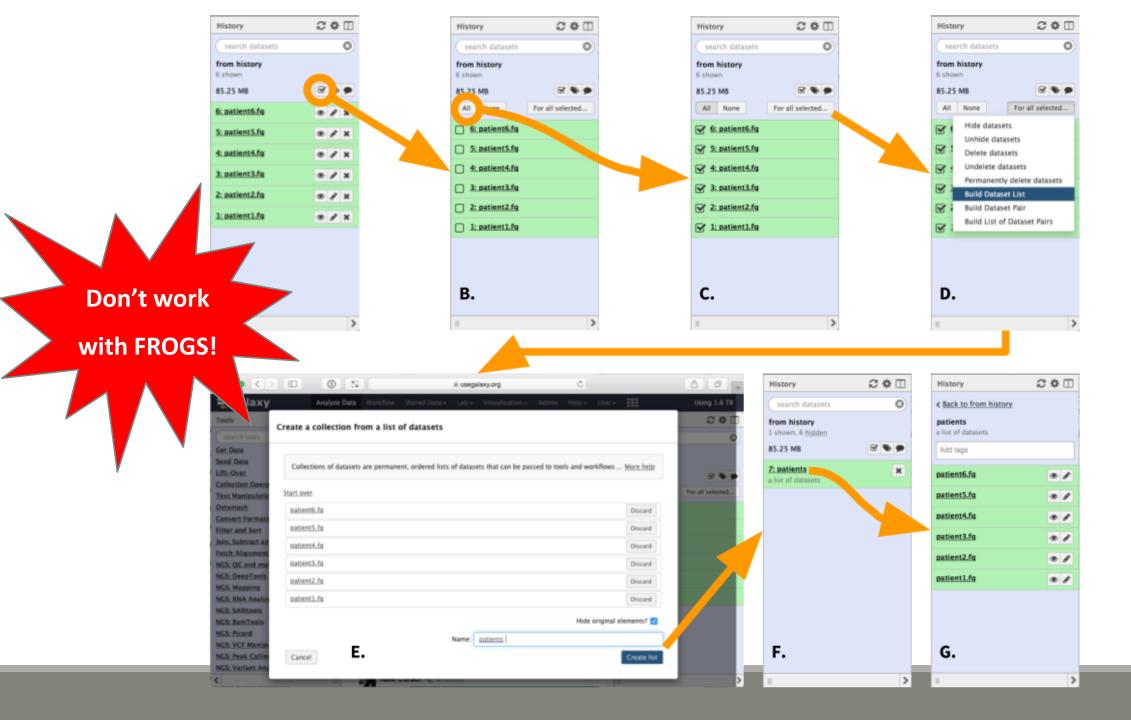




One word about data collections

- Used to perform the same analysis on multiple files.
- Gather multiple datasets in one collection.





Others tools available on galaxy

- Text Manipulation
- Filter and Sort
- FASTA manipulation

Galaxy support

- Mail: <u>support.sigenae@inra.fr</u>
- If you need more training about bioinformatics and Galaxy, please connect to Sigenae e-learning platform: http://sig-learning.toulouse.inra.fr/

How to cite Galaxy?

- Goecks, J, Nekrutenko, A, Taylor, J and The Galaxy Team. "Galaxy: a comprehensive approach for supporting accessible, reproducible, and transparent computational research in the life sciences." Genome Biol. 2010 Aug 25;11(8):R86.
- Blankenberg D, Von Kuster G, Coraor N, Ananda G, Lazarus R, Mangan M, Nekrutenko A, Taylor J. "Galaxy: a web-based genome analysis tool for experimentalists". Current Protocols in Molecular Biology. 2010 Jan; Chapter 19:Unit 19.10.1-21.
- Giardine B, Riemer C, Hardison RC, Burhans R, Elnitski L, Shah P, Zhang Y, Blankenberg D, Albert I, Taylor J, Miller W, Kent WJ, Nekrutenko A. "Galaxy: a platform for interactive large-scale genome analysis." Genome Research. 2005 Oct; 15(10):1451-5.

How to cite Genotoul Galaxy workbench?

- Research teams can thank the Toulouse Midi-Pyrenees bioinformatics platform and Sigenae group, using in their publications the following sentence: "We are grateful to the genotoul bioinformatics platform Toulouse Midi-Pyrenees and Sigenae group for providing help and/or computing and/or storage resources thanks to Galaxy instance http://sigenae-workbench.toulouse.inra.fr".
- In cases of collaboration, you can directly quote the person who participated to the project: Name, Sigenae group, GenPhySE, INRA Auzeville CS 52627 31326 Castanet Tolosan cedex.