# Formation intégration d'outils sous Galaxy

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#### **PLAN**

Présentation du toolshed

L'arborescence du serveur Galaxy

Exemple d'outil: Logol

La syntaxe des descripteurs

TP1. Préparation de l'environnement

TP2. Les différentes étapes de l'intégration

TP3. Intégration d'un outil

TP4. Intégration d'un outil avec plusieurs entrées

TP5. Intégration d'un outil avec plusieurs sorties

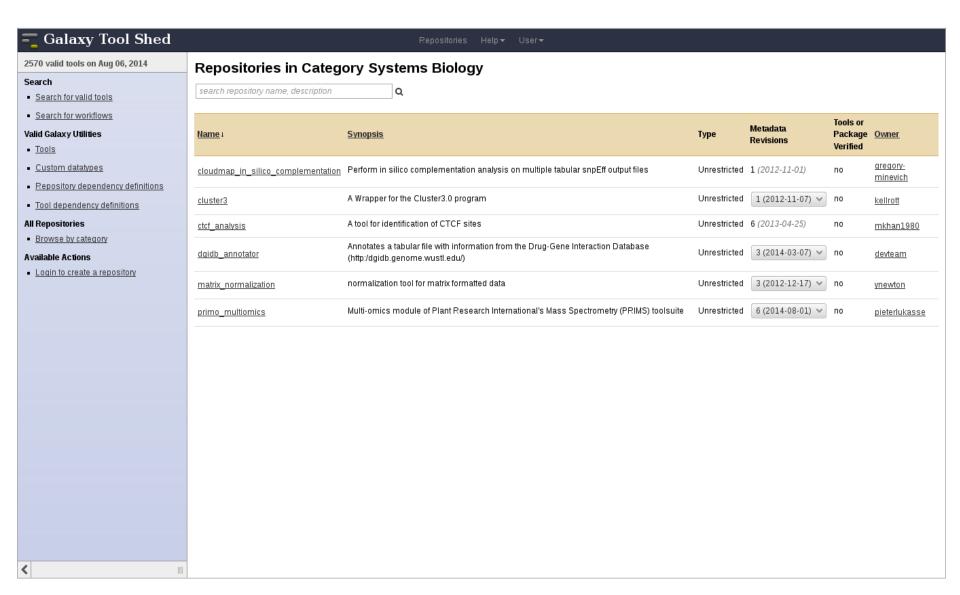
TP6. Intégration de dépendances



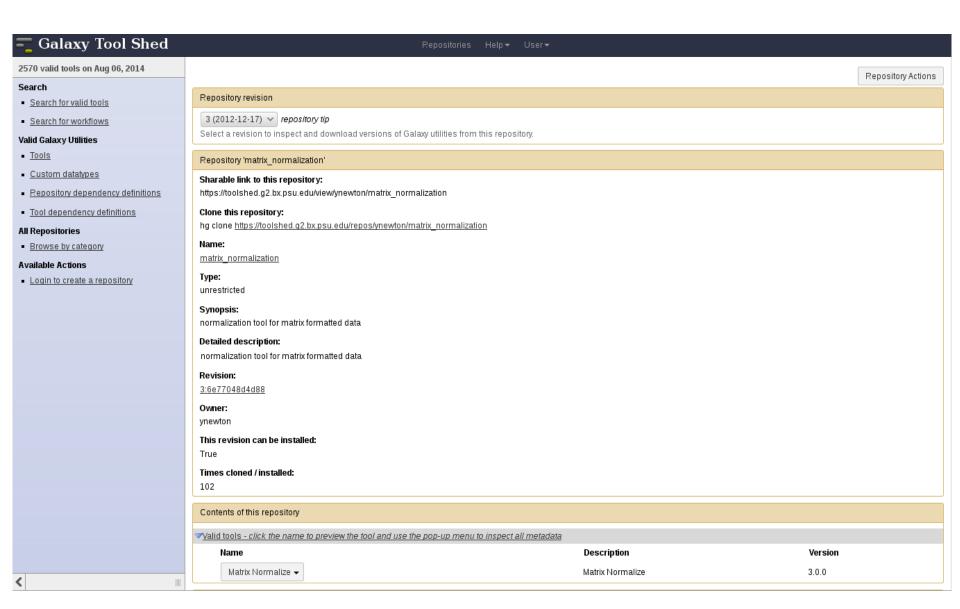
#### Le toolshed Galaxy

- Appstore d'outils pour Galaxy
  - centralisation des outils
  - intégration rapide dans son instance
- Contient des répertoires contenant :
  - des outils
  - des datatypes
  - des workflows
  - des data managers
- Deux toolsheds principaux
  - toolshed main -> https://toolshed.g2.bx.psu.edu
  - toolshed test -> https://testtoolshed.g2.bx.psu.edu/

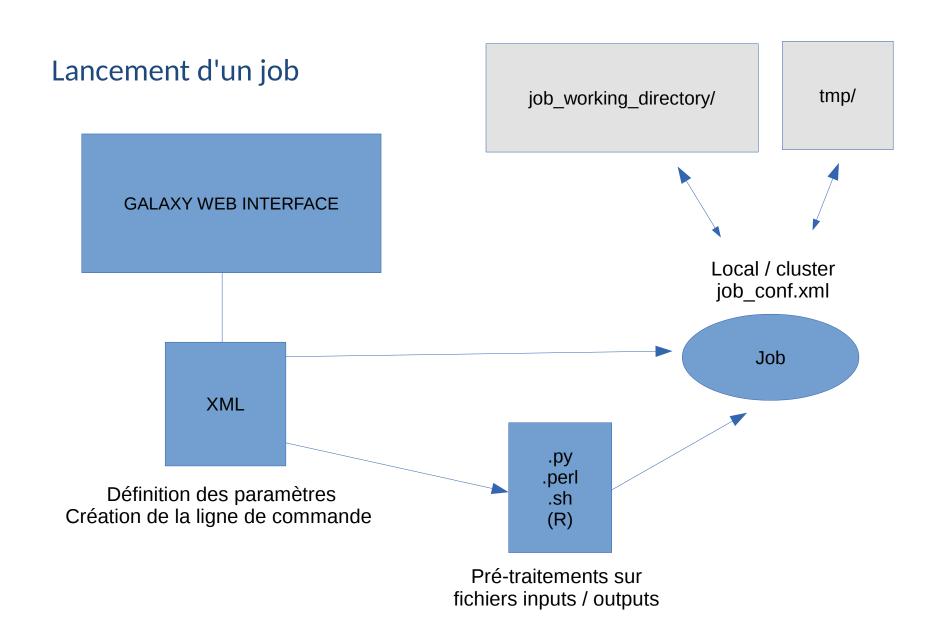
# Catégorie "Systems Biology"



### Outil "matrix\_normalization"







#### Serveur Galaxy : /opt/galaxy-dist

- universe\_wsgi.ini
- fichier de configuration (database, admin, server, ...)

- tool\_conf.xml
- shed\_tool\_conf.xml
- datatypes\_conf.xml
- · database/
  - files/
    - 000/
    - 001/
- tools
  - alignment/
    - outil1.xml
    - outil1.py
    - outil2.xml
    - outil2.sh
  - mapping/

#### Serveur Galaxy : /opt/galaxy-dist

- universe\_wsgi.ini
- tool\_conf.xml
- shed\_tool\_conf.xml
- datatypes\_conf.xml
- database/
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    - 001/
- tools
  - alignment/
    - outil1.xml
    - outil1.py
    - outil2.xml
    - · outil2.sh
  - mapping/



ensemble des tools (emplacements des descripteurs xml, structure du panel)

#### 1 Tools 0 search tools Get Data Send Data Lift-Over Convert genome coordinates between assemblies and genomes Text Manipulation Filter and Sort Join, Subtract and Group Convert Formats Extract Features Fetch Sequences Fetch Alignments Get Genomic Scores Statistics Graph/Display Data Evolution Motif Tools NGS: QC and manipulation NGS: Mapping NGS: RNA Analysis NGS: SAM Tools NGS: Simulation Phenotype Association NCBI Blast+ NGS: Bed Tools NGS: Assembly NGS: SNP Analysis STACKS toolsuite Archives Manipulation Workflows All workflows

# lopt/galaxy-dist

tool conf.xml

tools/descripteur.xml

shed\_tool\_conf.xml

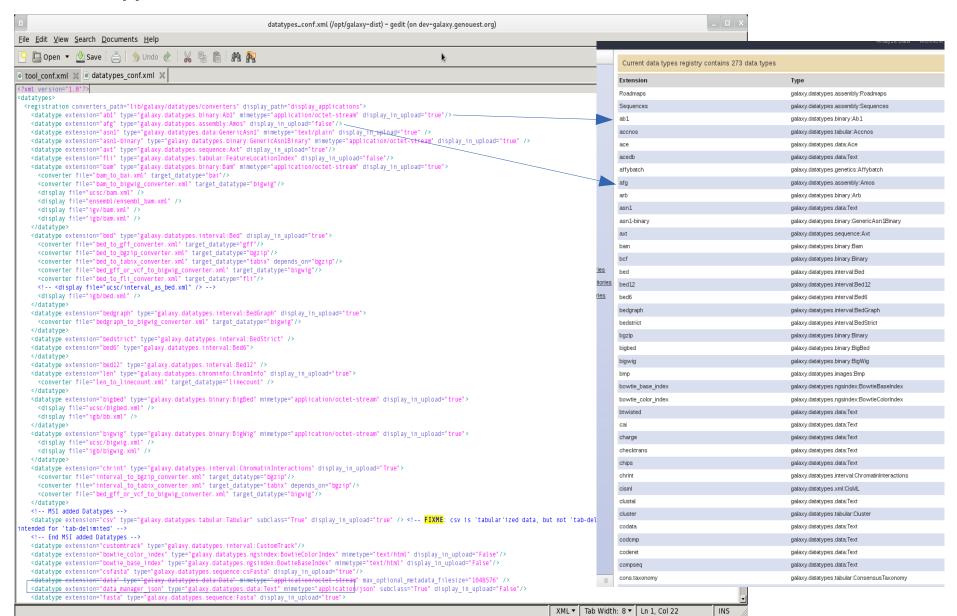
```
<section id="getext" name="Get Data" version="">
  <tool file="cloud-
45.genouest.org/toolshed/repos/cmonjeau/test/e0266fbac9ec/test/discoSNP.xml"
guid="cloud-45.genouest.org/toolshed/repos/cmonjeau/test/discosnp/1.0.0">
        <tool_shed>cloud-45.genouest.org/toolshed</tool_shed>
            <repository_name>test</repository_name>
            <repository_owner>cmonjeau</repository_owner>
            <installed_changeset_revision>e0266fbac9ec</installed_changeset_revision>
            <id>cloud-45.genouest.org/toolshed/repos/cmonjeau/test/discosnp/1.0.0</id>
            </or>
            </rool>
            </section>
```

# Serveur Galaxy : /opt/galaxy-dist

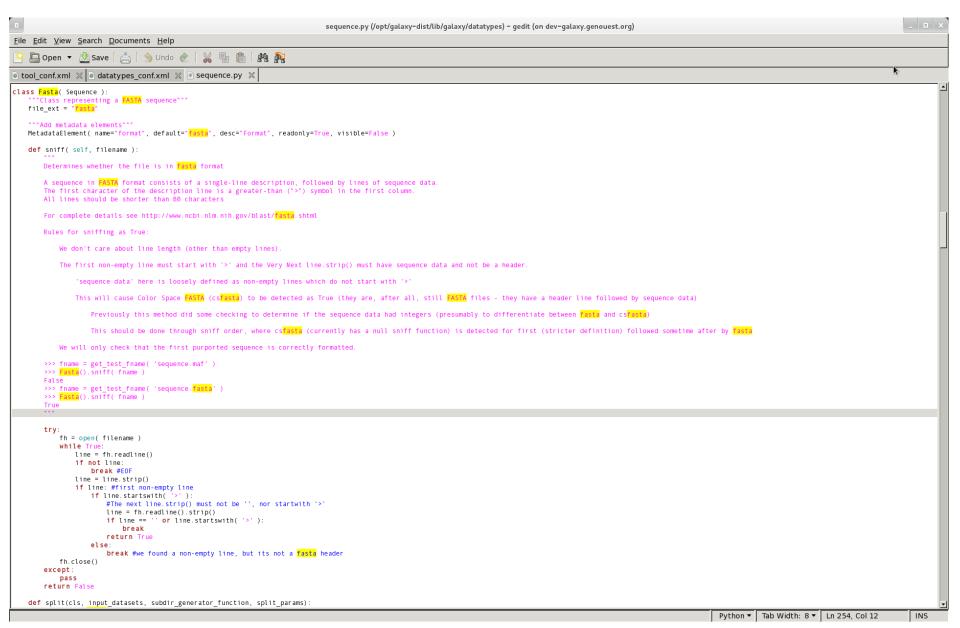
- universe\_wsgi.ini
- tool\_conf.xml
- shed\_tool\_conf.xml
- datatypes\_conf.xml
- · database/
  - files/
    - 000/
    - 001/
- tools
  - alignment/
    - outil1.xml
    - outil1.py
    - outil2.xml
    - · outil2.sh
  - mapping/

ensemble des datatypes (emplacements vers des classes python)

#### datatypes\_conf.xml



### lib/galaxy/datatypes/sequence.py



### Serveur Galaxy : /opt/galaxy-dist

- universe\_wsgi.ini
- tool\_conf.xml
- shed\_tool\_conf.xml
- datatypes\_conf.xml
- · database/
  - · files/
    - . 000/
    - . 001/
- tools
  - alignment/
    - outil1.xml
    - outil1.py
    - outil2.xml
    - · outil2.sh
  - mapping/

ensemble des fichiers de données (input/output)

# Serveur Galaxy : /opt/galaxy-dist

- universe\_wsgi.ini
- tool\_conf.xml
- shed\_tool\_conf.xml
- datatypes\_conf.xml
- database/
  - files/
    - 000/
    - 001/
- · tools
  - · alignment/
    - · outil1.xml
    - · outil1.py
    - · outil2.xml
    - · outil2.sh
  - mapping/

Emplacement des descripteurs / wrappers intégrés directement dans Galaxy

#### Partie toolshed : /opt/shed\_tools

- /opt/shed\_tools/
  - cloud-45.genouest.org/ Source du toolshed

Propriétaire du repository

Repositories

**Outils** 

- toolshed/repos/
  - cmonjeau/
  - ylebras/
    - discosnp/
    - · takeabreak/
      - e45d1faade2c/ → Révision
        - takeabreak
          - · takeabreak.xml
          - takeabreak.py

Exemple d'outil : Logol

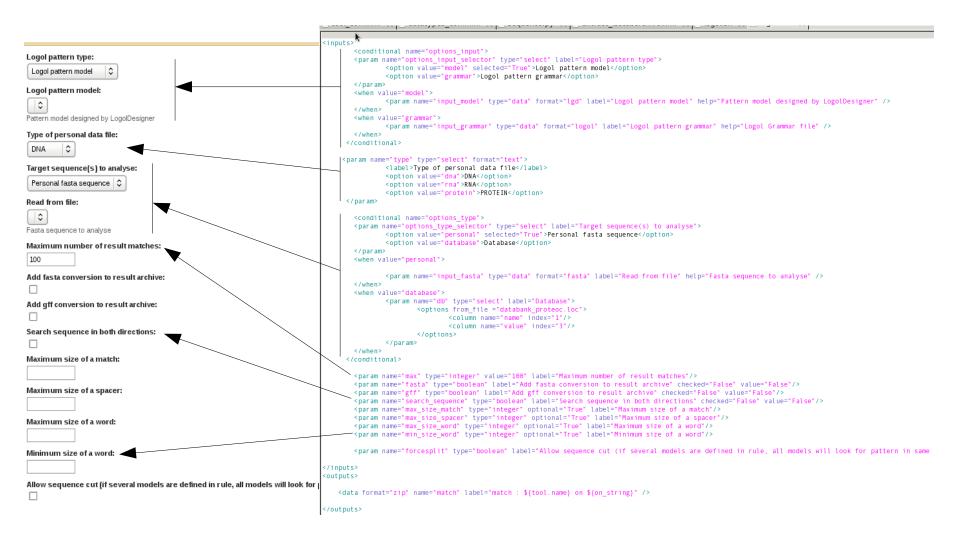
#### Le descripteur : logol.xml

```
<tool id="logol_wrapper" name="Logol">
  <description>Biological patterns matching</description>
 <command interpreter="bash">
logol.sh -sge
#if str( $options_input.options_input_selector ) == "model":
 -m $input_model
#else
 -g $input_grammar
#end if
#if str( $options_type.options_type_selector ) == "personal":
-s $input fasta
#else
-s $options_type.db
#end if
-out $match -max $max
#if $fasta:
-fasta
#end if
#if $gff:
-gff
#end if
#if $search_sequence:
#end if
#if $max size match:
-maxmatchsize $max size match
#if $max size spacer:
-maxspacer $max_size_spacer
#end if
#if $max size word:
-lmax $max_size_word
#end if
#if $min size word:
-lmin $min_size_word
#end if
#if $forcesplit:
-forcesplit
#end if
```

</command>

```
inputs>
        <conditional name="options input">
        <param name="options_input_selector" type="select" label="Logol pattern type">
                <option value="model" selected="True">Logol pattern model</option>
                <option value="grammar">Logol pattern grammar</option>
       </param>
        <when value="model">
                <param name="input_model" type="data" format="lgd" label="Logol pattern model" help="Pattern model designed by LogolDesigner"</pre>
        </when>
        <when value="grammar">
               <param name="input grammar" type="data" format="logol" label="Logol pattern grammar" help="Logol Grammar file" />
       </when>
     </conditional>
     <param name="type" type="select" format="text">
               <label>Type of personal data file</label>
               <option value="dna">DNA</option>
               <option value="rna">RNA</option>
                <option value="protein">PROTEIN</option>
     </param>
       <conditional name="options type">
       <param name="options_type_selector" type="select" label="Target sequence(s) to analyse">
               <option value="personal" selected="True">Personal fasta sequence</option>
               <option value="database">Database
       </param>
       <when value="personal">
                <param name="input_fasta" type="data" format="fasta" label="Read from file" help="Fasta sequence to analyse" />
       </when>
        <when value="database">
                <param name="db" type="select" label="Database">
                       <options from_file ="databank_proteoc.loc">
                               <column name="name" index="1"/>
                               <column name="value" index="3"/>
                       </options>
                </param>
       </when>
     </conditional>
       <param name="max" type="integer" value="100" label="Maximum number of result matches"/>
       <param name="fasta" type="boolean" label="Add fasta conversion to result archive" checked="False" value="False"/>
       <param name="gff" type="boolean" label="Add gff conversion to result archive" checked="False" value="False"/>
       <param name="search_sequence" type="boolean" label="Search sequence in both directions" checked="False" value="False"/>
       <param name="max_size_match" type="integer" optional="True" label="Maximum size of a match"/>
       <param name="max size spacer" type="integer" optional="True" label="Maximum size of a spacer"/>
       <param name="max size word" type="integer" optional="True" label="Maximum size of a word"/>
       <param name="min_size_word" type="integer" optional="True" label="Minimum size of a word"/>
        <param name="forcesplit" type="boolean" label="Allow sequence cut (if several models are defined in rule, all models will look for pat</pre>
</inputs>
<outputs>
   <data format="zip" name="match" label="match : ${tool.name} on ${on string}" />
</outputs>
```

#### Le descripteur : logol.xml



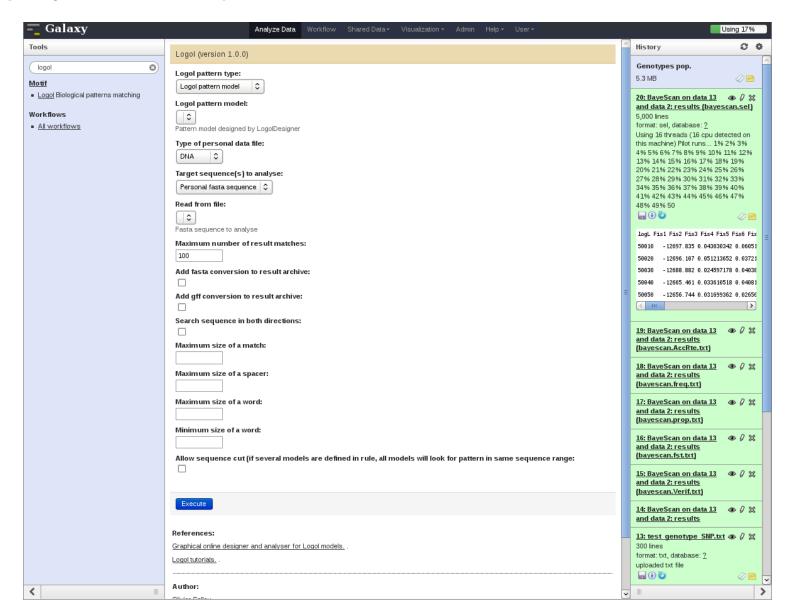
#### Le wrapper : logol.sh

```
#!/bin/bash
# ./LogolMultiExec.sh -h for usage
. /local/env/envjava-1.6.0_05.sh
#. /local/env/envlogol.sh
#. /local/env/envvmatch.sh
# Installation directory
export LOGOL HOME=/local/logol/LogolMatch
export VMATCH_HOME=/local/vmatch/vmatch.distribution
export PATH=/local/logol/LogolMatch: $PATH: $VMATCH HOME
export LD LIBRARY PATH=$LD LIBRARY PATH:/usr/local/sge/lib/lx24-amd64
echo "calling logol with parameters "$*
java -Xms512m -Xmx4096m -Dlogol.install=$LOGOL HOME -Dlog4j.configuration=file://$LOGOL HOME/log4j.properties -classpath
$LOGOL HOME/lib/xalan.jar:$LOGOL HOME/lib/xercesImpl.jar:$LOGOL HOME/lib/xml-apis.jar:$LOGOL HOME/lib/mail.jar:$LOGOL HOME/lib/
activation.jar:$LOGOL HOME/lib/biojava.jar:$LOGOL HOME/lib/bytecode:$LOGOL HOME/lib/drmaa.jar:$LOGOL HOME/lib/commons-
configuration-1.5.jar: $LOGOL HOME/lib/LogolExec.jar: $LOGOL HOME/lib/commons-cli-1.1.jar: $LOGOL HOME/lib/commons-
collections-3.2.1.jar: $LOGOL HOME/lib/commons-lang-2.4.jar: $LOGOL HOME/lib/commons-logging-1.1.1.jar: $LOGOL HOME/lib/
log4j-1.2.15.jar:$LOGOL_HOME/lib/antlrworks-1.4.2.jar org.irisa.genouest.logol.dispatcher.Dispatch $* -conf /home/genouest/admin/
galaxy/dependencies/logol/logol.dev.properties
```

#### Le fichier de configuration : tool\_conf.xml

```
<tool Tile="TastaZotu/summary.tax.xml" />
 <tool file="fasta2otu/trim graph.xml" />
 <tool file="fasta2otu/trim.seqs.xml" />
 <tool file="fasta2otu/unique.seqs.xml" />
</section>
<section name="Dev MB" id="devmb">
 <tool file="fasta2otu/tool to come.xml" />
 <tool file="fasta2otu/r test.xml" />
</section>
<section name="454 data Manipulation" id="454data">
 <tool file="454utilities/extractFastaFromSff.xml" />
 <tool file="454utilities/extractQualFromSff.xml" />
 <tool file="454utilities/extractSff.xml" />
 <tool file="454utilities/concatenateSff.xml" />
 <tool file="454utilities/trimByPromotor.xml" />
 <tool file="454utilities/trimByMid.xml" />
 <tool file="454utilities/clean454data.xml" />
 <tool file="454utilities/generateMidFile.xml" />
</section>
<section name="Motif" id="motif_symbiose">
 <tool file="symbiose/logol.xml"/>
 <tool file="symbiose/protomata.xml"/>
 <tool file="symbiose/protomatch.xml"/>
 <section name="Primer design and test" id="primer">
 <tool file="data source/primer3.xml" />
 <tool file="data_source/oligoanalyzer.xml" />
 </section>
 <section name="Alignment" id="alignment_symbiose">
 <tool file="symbiose/gassst.xml"/>
 <tool file="symbiose/gassst to sam.xml"/>
 <tool file="alignment/glint.xml"/>
 </section>
<section name="NGS: Assembly" id="ngs-assembly">
  <tool file="symbiose/minia.xml"/>
```

### Aperçu dans Galaxy



# La syntaxe des descripteurs

http://wiki.galaxyproject.org/Admin/Tools/ToolConfigSyntax

#### Balises les plus importantes

| </help>

```
<tool id="logol_wrapper" name="Logol">
                                                                                                                 Motif
   <description>Biological patterns matching</description>
                                                                                                                    Logol Biological patterns matching
   <command interpreter="bash">
          logol.sh $options.input.options input selector $option input.input model $type > $match
                                                                                                                 Workflows
   </command>

    All workflows

   <inputs>
       <conditional name="options input">
             <param name="options_input_selector" type="select" label="Logol pattern type">
               <option value="model" selected="True">Logol pattern model
               <option value="grammar">Logol pattern grammar</option>
             </param>
             <when value="model">
              | <param name="input model" type="data" format="lgd" label="Logol pattern model" help="Pattern model designed by LogolDesigner" />
             </when>
       </conditional>
       <param name="type" type="select" format="text" label="type">
          <option value="dna">DNA</option>
          <option value="rna">RNA</option>
          <option value="protein">PROTEIN</option>
      </param>
      <param name="max" type="integer" value="100" label="Maximum number of result matches"/>
       <param name="fasta" type="boolean" label="Add fasta conversion to result archive" checked="False" value="False"/>
   </inputs>
   <outputs>
        <data format="text" name="match" label="match : ${tool.name} on ${on string}" />
   </outputs>
   <help>
```

Tools

logol

0

```
<tool id="logol wrapper" name="Logol">
   <description>Biological patterns matching</description>
   <command interpreter="bash">
          logol.sh $options.input.options input selector $option input.input model $type > $match
   </command>
   <inputs>
       <conditional name="options input">
             <param name="options_input_selector" type="select" label="Logol pattern type">
               <option value="model" selected="True">Logol pattern model
               <option value="grammar">Logol pattern grammar</option>
             </param>
             <when value="model">
              | <param name="input model" type="data" format="lgd" label="Logol pattern model" help="Pattern model designed by LogolDesigner" />
             </when>
       </conditional>
       <param name="type" type="select" format="text" label="type">
          <option value="dna">DNA</option>
          <option value="rna">RNA</option>
          <option value="protein">PROTEIN</option>
      </param>
      <param name="max" type="integer" value="100" label="Maximum number of result matches"/>
       <param name="fasta" type="boolean" label="Add fasta conversion to result archive" checked="False" value="False"/>
   </inputs>
   <outputs>
        <data format="text" name="match" label="match : ${tool.name} on ${on string}" />
   </outputs>
   <help>
   </help>
</tool>
```

```
Tools

logol

Motif

Logol Biological patterns matching

Workflows

■ All workflows
```

```
<tool id="logol wrapper" name="Logol">
   <description>Biological patterns matching</description>
   <command interpreter="bash">
          logol.sh $options.input.options input selector $option input.input model $type > $match
   </command>
   <inputs>
       <conditional name="options input">
             <param name="options_input_selector" type="select" label="Logol pattern type">
               <option value="model" selected="True">Logol pattern model
               <option value="grammar">Logol pattern grammar</option>
             </param>
             <when value="model">
              | <param name="input model" type="data" format="lgd" label="Logol pattern model" help="Pattern model designed by LogolDesigner" />
             </when>
       </conditional>
       <param name="type" type="select" format="text" label="type">
          <option value="dna">DNA</option>
          <option value="rna">RNA</option>
          <option value="protein">PROTEIN</option>
      </param>
      <param name="max" type="integer" value="100" label="Maximum number of result matches"/>
       <param name="fasta" type="boolean" label="Add fasta conversion to result archive" checked="False" value="False"/>
   </inputs>
   <outputs>
        <data format="text" name="match" label="match : ${tool.name} on ${on string}" />
   </outputs>
   <help>
   </help>
</tool>
```

```
Pattern model designed by LogolDesigner
<tool id="logol wrapper" name="Logol">
                                                                                                                  Type of personal data file:
    <description>Biological patterns matching</description>
                                                                                                                   DNA V
    <command interpreter="bash">
                                                                                                                   Target sequence(s) to analyse:
                                                                                                                   Personal fasta sequence 🗸
           logol.sh $options.input.options input selector $option input.input model $type > $match
                                                                                                                   Read from file: 🗅 省
    </command>
                                                                                                                   21: fasta: Check_sense on data 17
                                                                                                                  Fasta sequence to analyse
    <inputs>
                                                                                                                  Maximum number of result matches:
        <conditional name="options input">
               <param name="options input selector" type="select" label="Logol pattern type">
                                                                                                                  Add fasta conversion to result archive:
                 <option value="model" selected="True">Logol pattern model
                                                                                                                   Add gff conversion to result archive:
                 <option value="grammar">Logol pattern grammar</option>
                                                                                                                  Search sequence in both directions:
               </param>
               <when value="model">
                                                                                                                  Maximum size of a match:
                <param name="input model" type="data" format="lgd" label="Logol pattern model" />
                                                                                                                  Maximum size of a spacer:
               </when>
        </conditional>
                                                                                                                   Maximum size of a word:
        <param name="type" type="select" format="text" label="type">
                                                                                                                   Minimum size of a word:
           <option value="dna">DNA</option>
                                                                                                                  Allow sequence cut (if several models are defined in rule, all models will look for pattern in same sequence range:
           <option value="rna">RNA</option>
            <option value="protein">PROTEIN</option>
       </param>
       <param name="max" type="integer" value="100" label="Maximum number of result matches"/>
        <param name="fasta" type="boolean" label="Add fasta conversion to result archive" checked="False" value="False"/>
    </inputs>
    <outputs>
          <data format="text" name="match" label="match : ${tool.name} on ${on string}" />
   </outputs>
    <help>
   </help>
</tool>
```

Logol pattern type:

Logol pattern model

Logol pattern model:

```
<tool id="logol wrapper" name="Logol">
   <description>Biological patterns matching</description>
   <command interpreter="bash">
         logol.sh $options.input.options input selector $option input.input model $type > $match
   </command>
   <inputs>
      <conditional name="options input">
             <param name="options_input_selector" type="select" label="Logol pattern type">
               <option value="model" selected="True">Logol pattern model
              <option value="grammar">Logol pattern grammar
             </param>
             <when value="model">
              | <param name="input_model" type="data" format="lgd" label="Logol pattern model" help="Pattern model designed by LogolDesigner" />
             </when>
      </conditional>
                                                                                                          Maximum number of result matches:
      <param name="type" type="select" format="text" label="type">
         <option value="dna">DNA</option>
                                                                                                          Add fasta conversion to result archive:
         <option value="rna">RNA</option>
          <option value="protein">PROTEIN</option>
      </param>
      <param name="max" type="integer" value="100" label="Maximum number of result matches"/>
      <param name="fasta" type="boolean" label="Add fasta conversion to result archive" checked="False" value="False"/>
   </inputs>
   <outputs>
        <data format="text" name="match" label="match : ${tool.name} on ${on string}" />
   </outputs>
   <help>
   </help>
</tool>
```

```
<tool id="logol wrapper" name="Logol">
   <description>Biological patterns matching</description>
   <command interpreter="bash">
          logol.sh $options.input.options input selector $option input.input model $type > $match
   </command>
                                                                                                          Logol pattern type:
   <inputs>
                                                                                                           Logol pattern model
       <conditional name="options_input">
                                                                                                          Logol pattern model:
              <param name="options_input_selector" type="select" label="Logol pattern type">
               <option value="model" selected="True">Logol pattern model
                                                                                                          Pattern model designed by LogolDesigner
               <option value="grammar">Logol pattern grammar</option>
              </param>
              <when value="model">
              | <param name="input model" type="data" format="lgd" label="Logol pattern model" help="Pattern model designed by LogolDesigner" />
              </when>
       </conditional>
       <param name="type" type="select" format="text" label="type">
          <option value="dna">DNA</option>
          <option value="rna">RNA</option>
          <option value="protein">PROTEIN</option>
      </param>
      <param name="max" type="integer" value="100" label="Maximum number of result matches"/>
       <param name="fasta" type="boolean" label="Add fasta conversion to result archive" checked="False" value="False"/>
   </inputs>
   <outputs>
        <data format="text" name="match" label="match : ${tool.name} on ${on string}" />
   </outputs>
   <help>
   </help>
</tool>
```

</tool>

```
<tool id="logol wrapper" name="Logol">
   <description>Biological patterns matching</description>
   <command interpreter="bash">
          logol.sh $options.input.options input selector $option input.input model $type > $match
   </command>
   <inputs>
      <conditional name="options input">
             <param name="options input selector" type="select" label="Logol pattern type">
               <option value="model" selected="True">Logol pattern model
               <option value="grammar">Logol pattern grammar
             </param>
             <when value="model">
              | <param name="input model" type="data" format="lgd" label="Logol pattern model" help="Pattern model designed by LogolDesigner" />
             </when>
      </conditional>
      <param name="type" type="select" format="text" label="type">
          <option value="dna">DNA</option>
          <option value="rna">RNA</option>
          <option value="protein">PROTEIN</option>
      </param>
      <param name="max" type="integer" value="100" label="Maximum number of result matches"/>
      <param name="fasta" type="boolean" label="Add fasta conversion to result archive" checked="False" value="False"/>
   </inputs>
   <outputs>
        <data format="text" name="match" label="match : ${tool.name} on ${on string}" />
   </outputs>
   <help>
   </help>
```

0.0

@ # X

● # ×

● # ×

● # ×

@ # X

● # ×

● 🖋 🗙

History

on data 12 13: log: Listseqs on

<u>data 12</u> <u>12: names:</u>

16: log: Get.seqs on data 1, data 14, and

14: accnos: Listseqs

Unique.seqs on data 5

11: fasta: Unique.seqs

10: log: Unique.seqs on data 5

9: Summary.tax on

8: Summary.tax on

7: Strip headers on

6: KMeans cluster on 💿 🥒 🗶

5: fasta: Check sense

Remove unclassified on data 3

data 2: logfile

on data 1
4: simplified

tax.summary:

2: taxonomy:

1: UCSC Main on

(chrY:1-59373566) 452 sequences

Human: knownGene

format: fasta, database: hg19

>hg19\_knownGene\_uc011nae.2 range=chrY

GTTTTAGGAAGAGTGTCCCGCAGAGACCCGGCGGGAGC TGGGATTCCAGCGGCTGGAAGgtgagtgtgtctacccc

gcaagtcccctacgggggacgtggcgggtgccgtctgt ctqqqaatcaqqaacccqcqcttccqtcattqaqqctc

ctgggacccttagctgggggcacgggcagggggttcag

Classify.seqs on data

3: tax.summary: Classify.seqs on data

data 2: summary

</tool>

```
<tool id="logol wrapper" name="Logol">
   <description>Biological patterns matching</description>
   <command interpreter="bash">
          logol.sh $options.input.options input selector $option input.input model $type > $match
   </command>
   <inputs>
      <conditional name="options input">
             <param name="options input selector" type="select" label="Logol pattern type">
               <option value="model" selected="True">Logol pattern model
               <option value="grammar">Logol pattern grammar
             </param>
             <when value="model">
              | <param name="input model" type="data" format="lgd" label="Logol pattern model" help="Pattern model designed by LogolDesigner" />
             </when>
      </conditional>
      <param name="type" type="select" format="text" label="type">
          <option value="dna">DNA</option>
          <option value="rna">RNA</option>
          <option value="protein">PROTEIN</option>
      </param>
      <param name="max" type="integer" value="100" label="Maximum number of result matches"/>
      <param name="fasta" type="boolean" label="Add fasta conversion to result archive" checked="False" value="False"/>
   </inputs>
   <outputs>
        <data format="text" name="match" label="match : ${tool.name} on ${on string}" />
   </outputs>
   <help>
   </help>
```

0.0

@ # X

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History

on data 12 13: log: Listseqs on

<u>data 12</u> <u>12: names:</u>

16: log: Get.seqs on data 1, data 14, and

14: accnos: Listseqs

Unique.seqs on data 5

11: fasta: Unique.seqs

10: log: Unique.seqs on data 5

9: Summary.tax on

8: Summary.tax on

7: Strip headers on

6: KMeans cluster on 💿 🥒 🗶

5: fasta: Check sense

Remove unclassified on data 3

data 2: logfile

on data 1
4: simplified

tax.summary:

2: taxonomy:

1: UCSC Main on

(chrY:1-59373566) 452 sequences

Human: knownGene

format: fasta, database: hg19

>hg19\_knownGene\_uc011nae.2 range=chrY

GTTTTAGGAAGAGTGTCCCGCAGAGACCCGGCGGGAGC TGGGATTCCAGCGGCTGGAAGgtgagtgtgtctacccc

gcaagtcccctacgggggacgtggcgggtgccgtctgt ctqqqaatcaqqaacccqcqcttccqtcattqaqqctc

ctgggacccttagctgggggcacgggcagggggttcag

Classify.seqs on data

3: tax.summary: Classify.seqs on data

data 2: summary

/help></tool>

```
<tool id="logol wrapper" name="Logol">
    <description>Biological patterns matching</description>
                                                                                                                                                                                                     2 0
                                                                                                                                                                               History
    <command interpreter="bash">
                                                                                                                                                                               16: log: Get.seqs on
                                                                                                                                                                                                @ # X
                                                                                                                                                                               data 1, data 14, and
                                                                                                                                                                               data 12
            logol.sh $options.input.options input selector $option input.input model $type > $match
                                                                                                                                                                               14: accnos: Listseqs
    </command>
                                                                                                                                                                               on data 12
                                                                                                                                                                               13: log: List.seqs on
                                                                                                                                                                                                @ # X
    <inputs>
                                                                                                                                                                               data 12
                                                                                                                                                                               12: names:
        <conditional name="options input">
                                                                                                                                                                               Unique.segs on data 5
                <param name="options input selector" type="select" label="Logol pattern type">
                                                                                                                                                                               11: fasta: Unique.seqs
                                                                                                                                                                                                ● & ×
                                                                                                                                                                               <u>on data 5</u>
                  <option value="model" selected="True">Logol pattern model
                                                                                                                                                                               10: log: Unique.seqs
                                                                                                                                                                                                @ # X
                                                                                                                                                                               on data 5
                  <option value="grammar">Logol pattern grammar</option>
                                                                                                                                                                               9: Summary.tax on
                                                                                                                                                                                                 ● # ×
                                                                                                                                                                               data 2: summary
                </param>
                                                                                                                                                                               8: Summary.tax on
                                                                                                                                                                                                ● & ×
                                                                                                                                                                               data 2: logfile
                <when value="model">
                                                                                                                                                                                                 ● # ×
                                                                                                                                                                               data 6
                 sparam name="input model" type="data" format="lgd" label="Logol pattern model" help="Pattern model designed by LogolDesigner" />
                                                                                                                                                                               6: KMeans cluster on
                                                                                                                                                                                                @ # X
                </when>
                                                                                                                                                                               5: fasta: Check_sense 🌑 🥒 🗶
        </conditional>
                                                                                                                                                                               <u>on data 1</u>
                                                                                                                                                                                                ● # ×
        <param name="type" type="select" format="text" label="type">
                                                                                                                                                                               tax.summary:
                                                                                                                                                                               Remove unclassified on data 3
            <option value="dna">DNA</option>
                                                                                                                                                                               3: tax.summarv:
                                                                                                                                                                               Classify.seqs on data
            <option value="rna">RNA</option>
            <option value="protein">PROTEIN</option>
                                                                                                                                                                               2: taxonomy:
                                                                                                                                                                                                 ● # X
                                                                                                                                                                               Classify.seqs on data
        </param>
                                                                                                                                                                               1: UCSC Main on
                                                                                                                                                                                                ◎ 🖋 🗙
        <param name="max" type="integer" value="100" label="Maximum number of result matches"/>
                                                                                                                                                                               Human: knownGene
                                                                                                                                                                               (chrY:1-59373566)
                                                                                                                                                                               452 sequences
        <param name="fasta" type="boolean" label="Add fasta conversion to result archive" checked="False" value="False"/>
                                                                                                                                                                               format: fasta, database: hg19
                                                                                                                                                                               ₿ 6 2 11
    </inputs>
                                                                                                                                                                               >hg19_knownGene_uc011nae.2 range=chrY:
    <outputs>
                                                                                                                                                                               GTTTTAGGAAGAGTGTCCCGCAGAGACCCGGCGGGAGC
                                                                                                                                                                               TGGGATTCCAGCGGCTGGAAGgtgagtgtgtctacccc
          <data format="text" name="match" label="match : ${tool.name} on ${on_string}" />
                                                                                                                                                                               gcaagtcccctacgggggacgtggcgggtgccgtctgt
                                                                                                                                                                                ctgggaatcaggaacccgcgcttccgtcattgaggctc
    </outputs>
                                                                                                                                                                                ctgggacccttagctgggggcacgggcagggggttcag
    <help>
```

</tool>

```
<tool id="logol wrapper" name="Logol">
                                                                                                                               Syntax
    <description>Biological patterns matching</description>
                                                                                                                               The filter tool allows you to restrict the dataset using simple conditional statements
                                                                                                                              Columns are referenced with c and a number. For example, c1 refers to the first column of a tab-delimited file
    <command interpreter="bash">
                                                                                                                              Make sure that multi-character operators contain no white space ( e.g., <= is valid while < = is not valid )
                                                                                                                               When using 'equal-to' operator double equal sign '==' must be used ( e.g., c1=='chr1' )
            logol.sh $options.input.options input selector $option input.input model $type > $match
                                                                                                                              Non-numerical values must be included in single or double quotes (e.g., c6=='+')
                                                                                                                              Filtering condition can include logical operators, but make sure operators are all lower case (e.g., {c1!='chrX' and c1!='chrY')
    </command>
    <inputs>
                                                                                                                              Example
        <conditional name="options input">
                                                                                                                               c1=='chr1' selects lines in which the first column is chr1
                                                                                                                              c3-c2<100*c4 selects lines where subtracting column 3 from column 2 is less than the value of column 4 times 100</p>
                 <param name="options input selector" type="select" label="Logol pattern type">
                                                                                                                              len(c2.split(',')) < 4 will select lines where the second column has less than four comma separated elements
                                                                                                                              c2>=1 selects lines in which the value of column 2 is greater than or equal to 1
                    <option value="model" selected="True">Logol pattern model
                                                                                                                              Numbers should not contain commas - c2<=44.554.350 will not work, but c2<=44554350 will
                                                                                                                              Some words in the data can be used, but must be single or double quoted (e.g., c3=='exon')
                   <option value="grammar">Logol pattern grammar</option>
                 </param>
                 <when value="model">
                  | <param name="input model" type="data" format="lgd" label="Logol pattern model" help="Pattern model designed by LogolDesigner" />
                 </when>
        </conditional>
        <param name="type" type="select" format="text" label="type">
             <option value="dna">DNA</option>
             <option value="rna">RNA</option>
             <option value="protein">PROTEIN</option>
        </param>
        <param name="max" type="integer" value="100" label="Maximum number of result matches"/>
        <param name="fasta" type="boolean" label="Add fasta conversion to result archive" checked="False" value="False"/>
    </inputs>
    <outputs>
           <data format="text" name="match" label="match : ${tool.name} on ${on string}" />
    </outputs>
    <help>
    </help>
```

Oouble equal signs, ==, must be used as "equal to" (e.g., c1 == 'chr22')

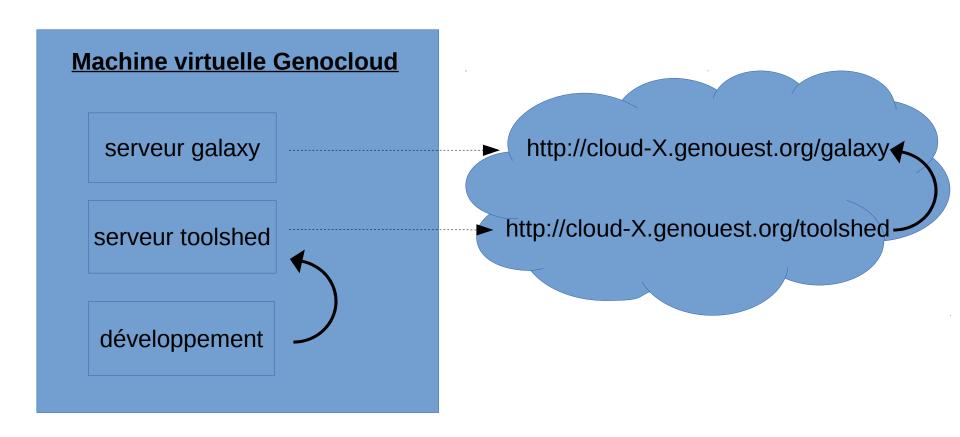
1 TIP: If your data is not TAB delimited, use Text Manipulation->Convert

1 TIP: Attempting to apply a filtering condition may throw exceptions if the data type (e.g., string, integer) in every line of the column a line, that line is skipped as invalid for the filter condition. The number of invalid skipped lines is documented in the resulting histor

# TP1. Préparation de l'environnement

Genocloud

#### **Environnement**

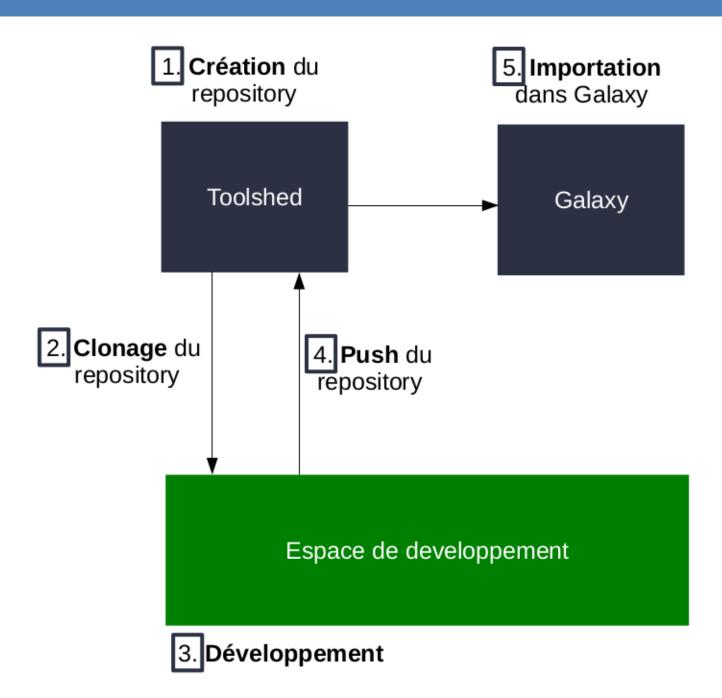


### Installation de l'environnement

cf. document PDF

# TP2. Les différentes étapes pour l'intégration

Toolshed & première intégration d'un outil : discoSNP



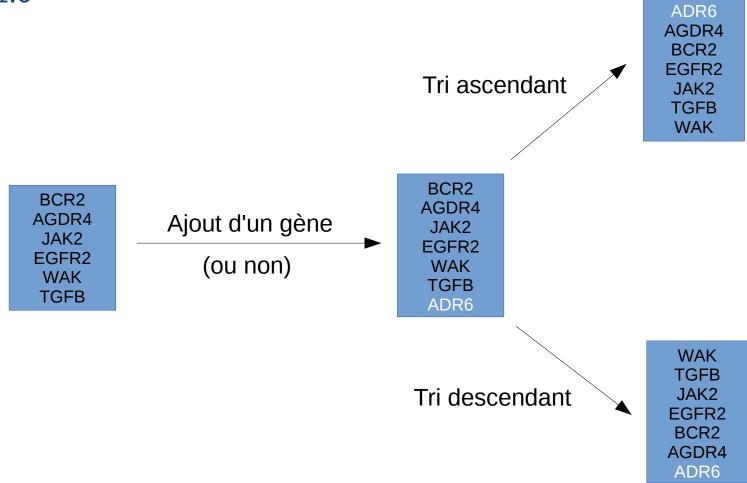
## Intégration de TakeABreak

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# TP3. Intégration d'un outil simple

Tri d'une liste de gènes





Difficultés : aucune

# TP4. Intégration d'un outil avec plusieurs entrées

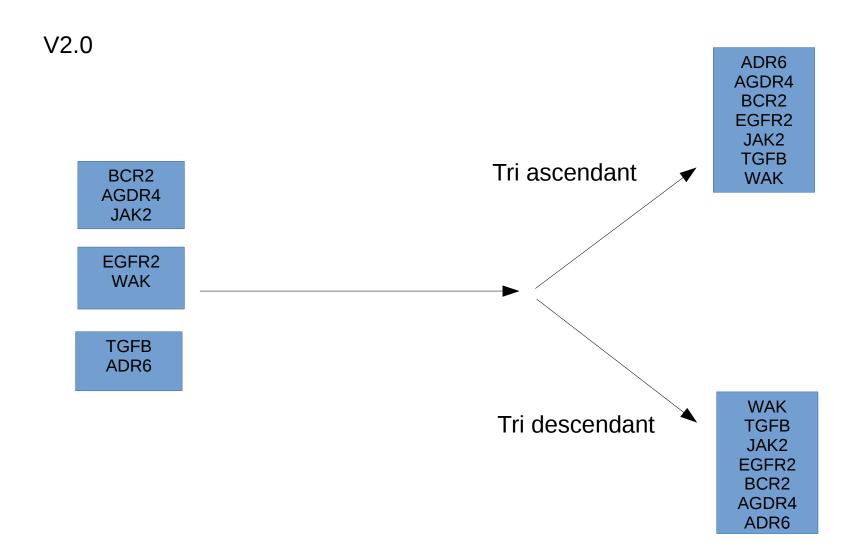
Tri d'une liste de gènes issus de plusieurs fichiers

### Utilisation du multi-input files

- <param name="gene files list" type="data" multiple="true" format="txt" label="Gene list file" />
  - Passage directement de \$gene\_files\_list dans la ligne de commande
  - Dans le wrapper, récupération d'une chaine de caractère du type :
    - /opt/galaxy-dist/database/files/000/dataset\_001.dat,/opt/galaxy-dist/database/files/000/dataset\_002.dat
- <param name="gene\_files\_list" type="data" multiple="true" format="txt" label="Gene list file" />
   <configfiles>
   <configfile name="gene\_files\_list\_config" >

```
#for $file in $data_list_file:
    ${file}::${file.display_name}
#end for
</configfile>
</configfiles>
```

- Passage de \$gene\_files\_list\_config dans la ligne de commande
- · Dans le wrapper, récupération d'un fichier (chemin) à traiter
  - · Contenu du fichier :
    - /opt/galaxy-dist/database/files/000/dataset 001.dat::nom1
    - /opt/galaxy-dist/database/files/000/dataset 002.dat::nom2



Difficultés : multi-input

# TP5. Intégration d'un outil avec plusieurs sorties Tri d'une liste de gènes issus de plusieurs fichiers et limitation d'un nombre de gène par fichier de sortie

### Utilisation du multi-output files avec nombre de fichiers inconnus

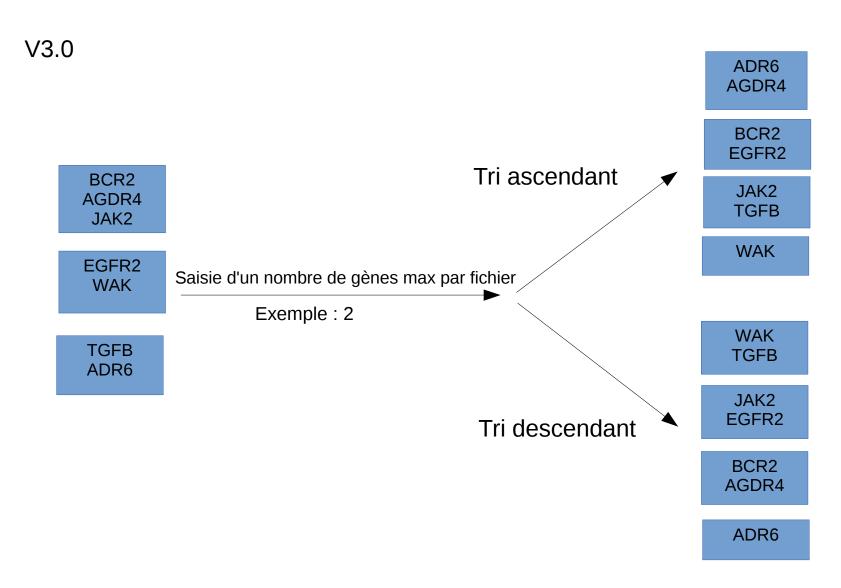
```
    <outputs>

            <data format="txt" name="output" label=" log.txt" />
            <outputs>

    --output $output

            --output_id $output.id
            --new_file_path $__new_file_path__
```

- \$\_\_new\_file\_path\_\_ correspond à un répertoire temporaire définit dans universe\_wsgi.ini
- · Dans le wrapper, les fichiers de sorties doivent être envoyé dans ce répertoire
  - new\_file\_path/primary\_output.id\_name\_visible\_txt



Difficultés : multi-output

# TP6. Intégration de dépendances

Exemple de takeabreak

### Les dependencies : étape 1/3

- · Intégration d'un package spécial dans le toolshed
  - type = tool dependencies
- · Le repository nommé « commet dependencies » contient uniquement un fichier tool\_dependencies.xml définissant un package
- · Dans ce fichier s'applique une succession d' «actions» :

```
<?xml version="1.0"?>
<tool dependency>
  <package name="galaxy_commet" version="24.7.14">
    <install version="1.0">
    <actions>
        <action type="download_by_url">http://github.com/pierrepeterlongo/commet/archive/master.zip</action>
        <action type="shell_command">make</action>
        <!-- move directories into $INSTALL DIR -->
       <action type="move_directory_files">
           <source directory>bin</source directory>
           <destination_directory>$INSTALL_DIR/bin</destination_directory>
       </action>
       <!-- move files into $INSTALL DIR -->
       <action type="move_file">
           <source>dendro.R</source>
           <destination>$INSTALL DIR/Rscript</destination>
       </action>
       <!-- create env.sh -->
       <action type="set_environment">
          <environment_variable name="PATH" action="prepend to">$INSTALL DIR/bin/environment variable>
          <environment_variable name="RSCRIPTS" action="set to">$INSTALL DIR/Rscript//environment variable>
     </action>
    </actions>
    </install>
  </package>
                             Création d'un fichier env.sh embarqué par l'outil lors de l'exécution
</tool_dependency>
```

### Les dependencies : étape 2/3

 Au sein du repository contenant l'outil Galaxy développé doit s'ajouter un fichier tool\_dependencies.xml

• Installation du package lors de l'installation de l'outil

### Les dependencies : étape 3/3

Au sein du descripteur de l'outil :

```
<requirements>
<requirement type="package" version="24.7.14">galaxy_commet</requirement>
</requirements>
```

Nécessaire pour l'embarquement automatique de l'environnement

### Intégration de la dependance de TakeABreak

Takeabreak depend de galaxy\_takeabreak

- Chercher les sources
- Compiler (make)

- Dans le dossier d'installation (\$INSTALL\_DIR):
  - Le script TakeABreak.sh
  - Le dossier bin/ et son contenu
- Une variable "DIR" correspondant au contenu de \$INSTALL DIR
- Ajout de \$INSTALL\_DIR/bin/ dans le PATH