

➤ Introduction aux Galaxy Interactive Tools

Principes et Concepts

Au menu de l'introduction

Les sujets à partager.

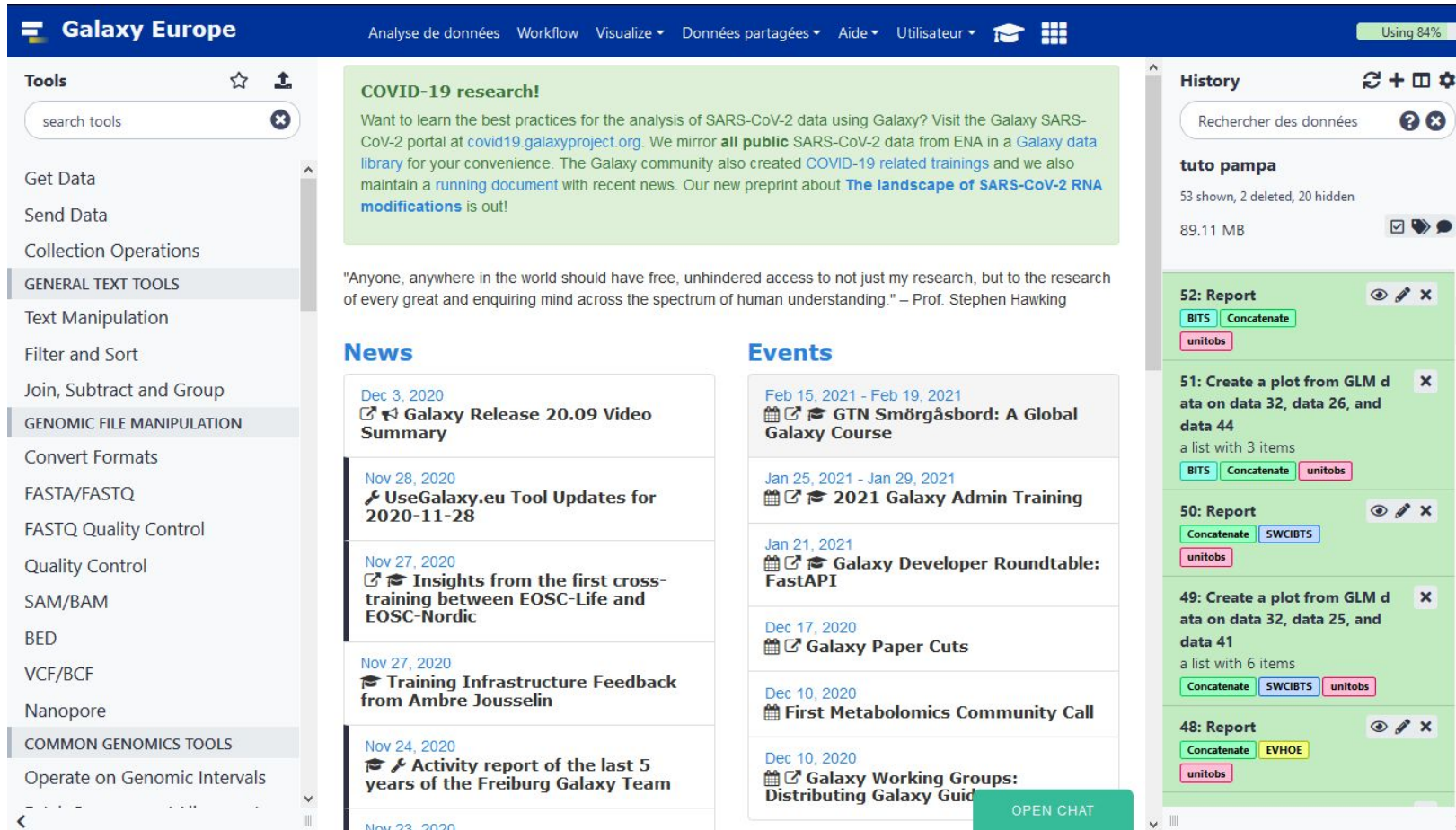
- Intro de l'intro
- Les avantages fonctionnels des interactives tools
- Le type d'applications éligibles à être déployées sous cette forme
- L'architecture informatique sous-jacente
- Le principe des interactions entre Galaxy et les interactives tools
- Les enjeux du point de vue de la ressource de calcul
- Les compétences et les étapes pour développer et déployer les IT

Au cours de la présentation, toutes les interventions sont les bienvenues.

In fine une démo ?

Des Galaxy tools aux Interactive tools

Les outils Galaxy, au top pour la reproductibilité, mais.... comment aller plus loin ?



The screenshot displays the Galaxy Europe web interface. On the left, a sidebar lists various tool categories: 'Tools' (with a search bar), 'Get Data', 'Send Data', 'Collection Operations', 'GENERAL TEXT TOOLS' (including Text Manipulation, Filter and Sort, Join, Subtract and Group), 'GENOMIC FILE MANIPULATION' (including Convert Formats, FASTA/FASTQ, FASTQ Quality Control, Quality Control, SAM/BAM, BED, VCF/BCF, Nanopore), and 'COMMON GENOMICS TOOLS' (including Operate on Genomic Intervals). The main content area features a 'COVID-19 research!' announcement, a quote by Prof. Stephen Hawking, and sections for 'News' and 'Events'. The 'History' panel on the right shows a list of recent jobs, including '52: Report', '51: Create a plot from GLM d', '50: Report', '49: Create a plot from GLM d', and '48: Report', each with associated tool names like 'BITS', 'Concatenate', 'unitobs', 'SWCIBTS', and 'EVHOF'.



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Des Galaxy tools aux Interactive tools

Les outils Galaxy, au top pour la reproductibilité, mais... comment aller plus loin ?

The screenshot displays the Galaxy Europe web interface. The top navigation bar includes links for 'Analyse de données', 'Workflow', 'Visualize', 'Données partagées', 'Aide', 'Utilisateur', and a 'Using 84%' status indicator. The left sidebar lists various tool categories: 'Tools' (with a search bar), 'Get Data', 'Send Data', 'Collection Operations', 'GENERAL TEXT TOOLS' (Text Manipulation, Filter and Sort, Join, Subtract and Group), 'GENOMIC FILE MANIPULATION' (Convert Formats, FASTA/FASTQ, FASTQ Quality Control, Quality Control, SAM/BAM, BED, VCF/BCF, Nanopore), and 'COMMON GENOMICS TOOLS' (Operate on Genomic Intervals). The main content area shows a workflow for 'Get species occurrences data' from GBIF, ALA, iNAT and others (Galaxy Version 0.9.0). The workflow includes input fields for 'Scientific name of the species', 'Data source to get data from' (with a 'Select/Unselect all' checkbox), 'Number of records to return' (set to 500), and an 'Email notification' section with 'Yes' and 'No' buttons. An 'Execute' button is at the bottom. The right sidebar shows a 'History' panel with a search bar and a list of recent workflows, including '52: Report', '51: Create a plot from GLM data on d', '50: Report', '49: Create a plot from GLM data on d', '48: Report', and '47: Create a plot from GLM data on d'.



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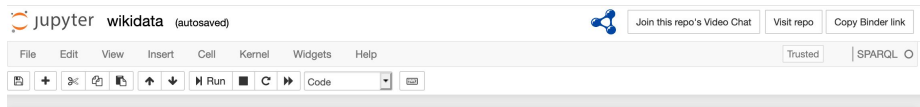
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Jupyter notebook, RStudio, R Shiny apps...

Which algorithms or formulas in Wikidata do not have an image yet?

```
In [1]: %endpoint http://query.wikidata.org/sparql
%display table
%show all

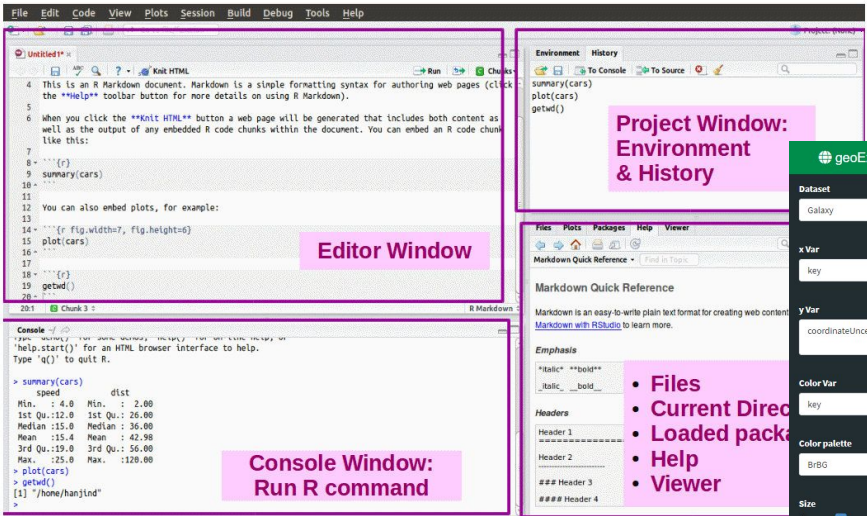
SELECT DISTINCT ?item ?itemLabel ?formula WHERE {
  {
    SELECT DISTINCT ?item ?formula WHERE {
      { ?item ((wdt:P31*)/wdt:P279) wd:Q8366. } UNION { ?item wdt:P2534 ?formula. }
      FILTER(NOT EXISTS { ?item wdt:P18 ?image. })
      FILTER(NOT EXISTS { ?item wdt:P31 wd:Q1266546. })
      FILTER(NOT EXISTS { ?item wdt:P373 ?category. })
    }
    LIMIT 5
  }
  SERVICE wikibase:label { bd:serviceParam wikibase:language "[AUTO_LANGUAGE],en". }
}
ORDER BY ASC(?item)
```

Endpoint set to: <http://query.wikidata.org/sparql>
 Display: table
 Result maximum size: unlimited

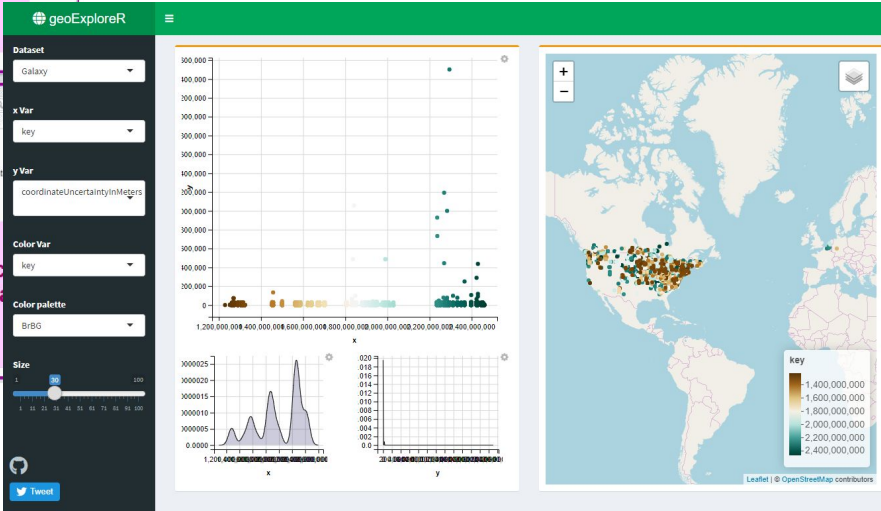
Item	ItemLabel	formula
http://www.wikidata.org/entity/Q116076	CORDIC	
http://www.wikidata.org/entity/Q130762	multiplication algorithm	
http://www.wikidata.org/entity/Q140770	General number field sieve	
http://www.wikidata.org/entity/Q71746	Trachtenberg system	
http://www.wikidata.org/entity/Q93593	common subexpression elimination	

Total: 5, Shown: 5

https://commons.wikimedia.org/wiki/File:Screenshot_of_a_Jupyter_Notebook_with_SPARQL_kernel_after_running_a_query_to_the_Wikidata_Query_Service_as_of_21_September_2020.png



https://commons.wikimedia.org/wiki/File:Structure_of_Rstudio.jpeg



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Jupyter notebook, RStudio, R Shiny apps...

Et l'interactivité !

Développement de Plugins basés sur D3

The screenshot shows the Galaxy Europe web interface. On the left is a sidebar with categories like 'Tools', 'GENERAL TEXT TOOLS', 'GENOMIC FILE MANIPULATION', and 'COMMON GENOMICS TOOLS'. The main area displays a search for visualizations, listing several tools based on NVD3 and jqPlot libraries. A 'History' panel on the right shows a list of recent analyses, including 'tuto pampa' and '33: GLM - Results from your community analysis on data 32 and data 23'.



Trackster

Fast, interactive visualization for large, NGS/HTS datasets using only a web browser.



OpenLayers map

A viewer to show maps using OpenLayers from <https://openlayers.org/>



PV Protein Viewer

PV is a pdb/protein viewer hosted at <https://biasmv.github.io/pv/>.



Cytoscape

A viewer based on graph theory/ network library for analysis and visualisation hosted at <http://js.cytoscape.org>.



Phyloviz

Phylogenetic data analysis from multiple data sources.



Image annotator

An image annotator built using PaperJS at <https://github.com/paperjs/paper.js>.

Des Galaxy tools aux Interactive tools

Via les GIE

Galaxy Interactive Environments



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Des Galaxy tools aux Interactive tools

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Tools
~~Galaxy Interactive Environments~~



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Galaxy Interactive Environments



Tools
~~Galaxy Interactive Environments~~



Galaxy Europe Analyse de données Workflow Visualize ▾ Docs

Galaxy Interactive Environment Launcher

Galaxy Interactive Environments (GIEs) launch embedded, dockerized versions of popular data analysis suites such as Jupyter and RStudio, right from within Galaxy. They allow you to dynamically interact with your data, right on the server. No more uploading and downloading between various platforms just to get your work done!

[Admin Docs](#)

GIE:

Image:

Datasets:



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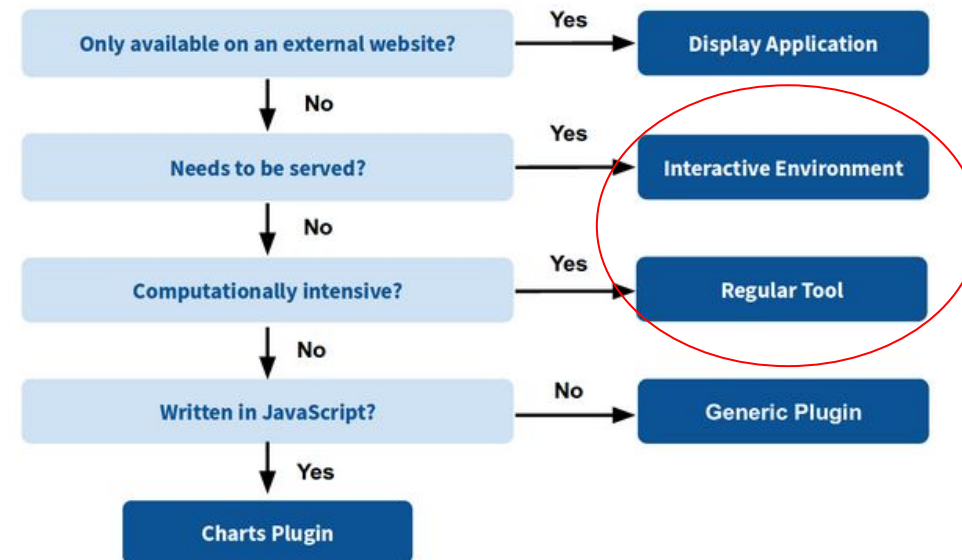
Via les GIE

Galaxy Interactive Environments



~~Galaxy Interactive Environments~~

Tools



Des Galaxy tools aux Interactive tools

Via les GIE



Development

- Not hard to build!
- All the magic is in:

```
$GALAXY/config/plugins/interactive_environments/$ie_name/
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Component	File
Visualization Plugin Configuration	../config/\${ie_name}.xml
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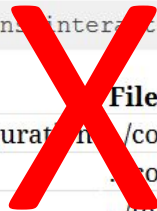


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Galaxy Interactive Environments

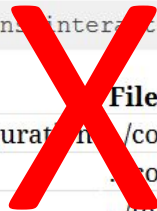


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There is an InteractiveTool result view available, waiting for view to become active...
You may also access all active InteractiveTools from the **User menu**.

Executed **Interactive Jupyter Notebook** and successfully added 1 job to the queue.
The tool uses this input:

- 32: **Regex Find And Replace on data 31**

It produces this output:

- 74: **Executed Notebook**

You can check the status of queued jobs and view the resulting data by refreshing the History panel. When the job has been run the status will change from 'running' to

History

Rechercher des données

tuto pampa
52 shown, 2 deleted, 20 hidden
89.11 MB

74: Executed Notebook

52: Report
BITS Concatenate unitobs

51: Create a plot from GLM data on data 32, d ata 26, and data 44

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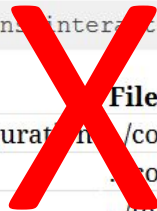
Name	Job Info	Created	La
<input type="checkbox"/> Jupyter Interactive Tool	running	2 minutes ago	a f
<input type="checkbox"/> Openrefine visualisation	running	a few seconds ago	a f

On the right, a user menu is open, showing options like 'Authentifié en tant que yvan.le-bras@mnhn.fr', 'Préférences', 'Mes génomes Builds de référence', 'Déconnexion', 'Datasets', 'Histories', 'Histories shared with me', 'Pages', 'Workflow Invocations', 'Visualisations', and 'Active InteractiveTools'.

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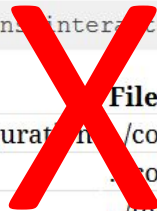


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Des Galaxy tools aux Interactive tools

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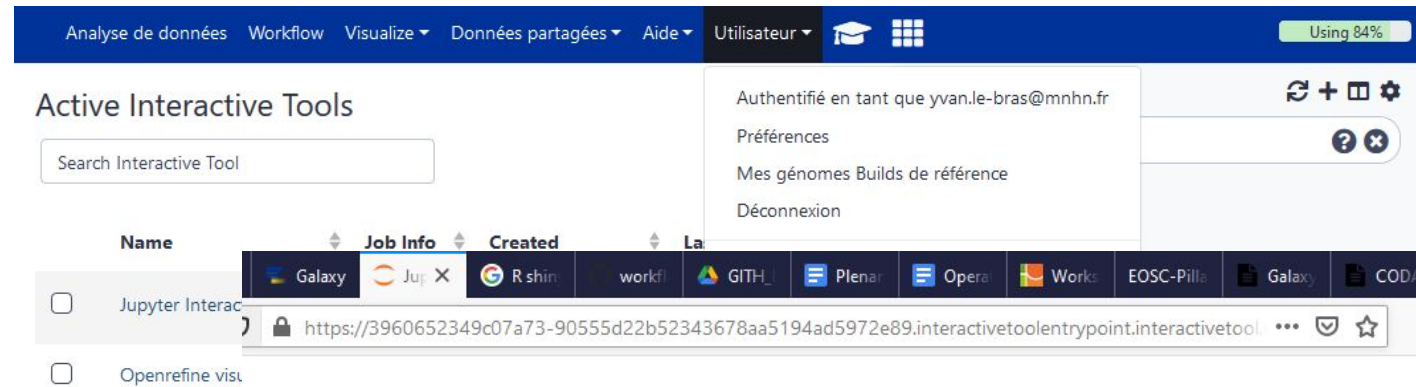
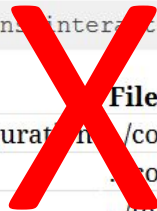


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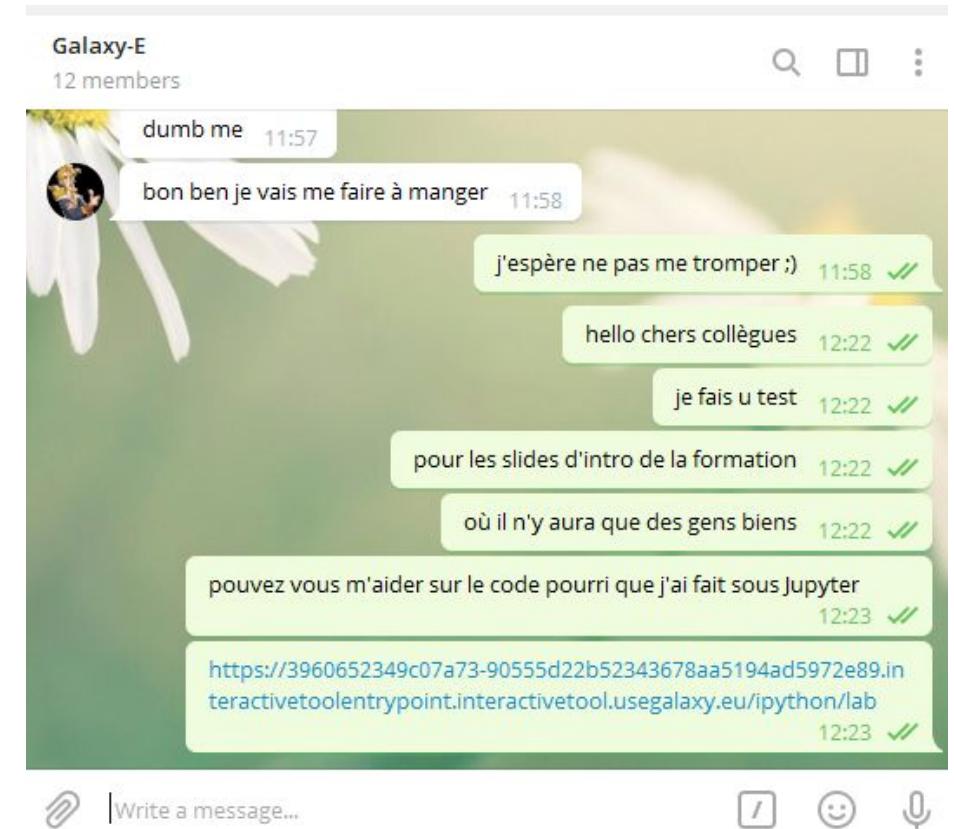
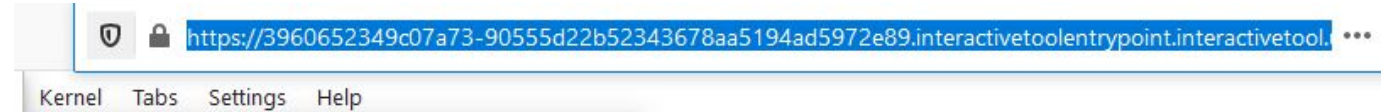
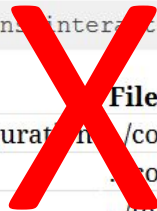


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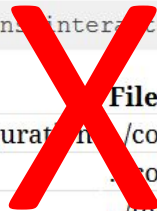


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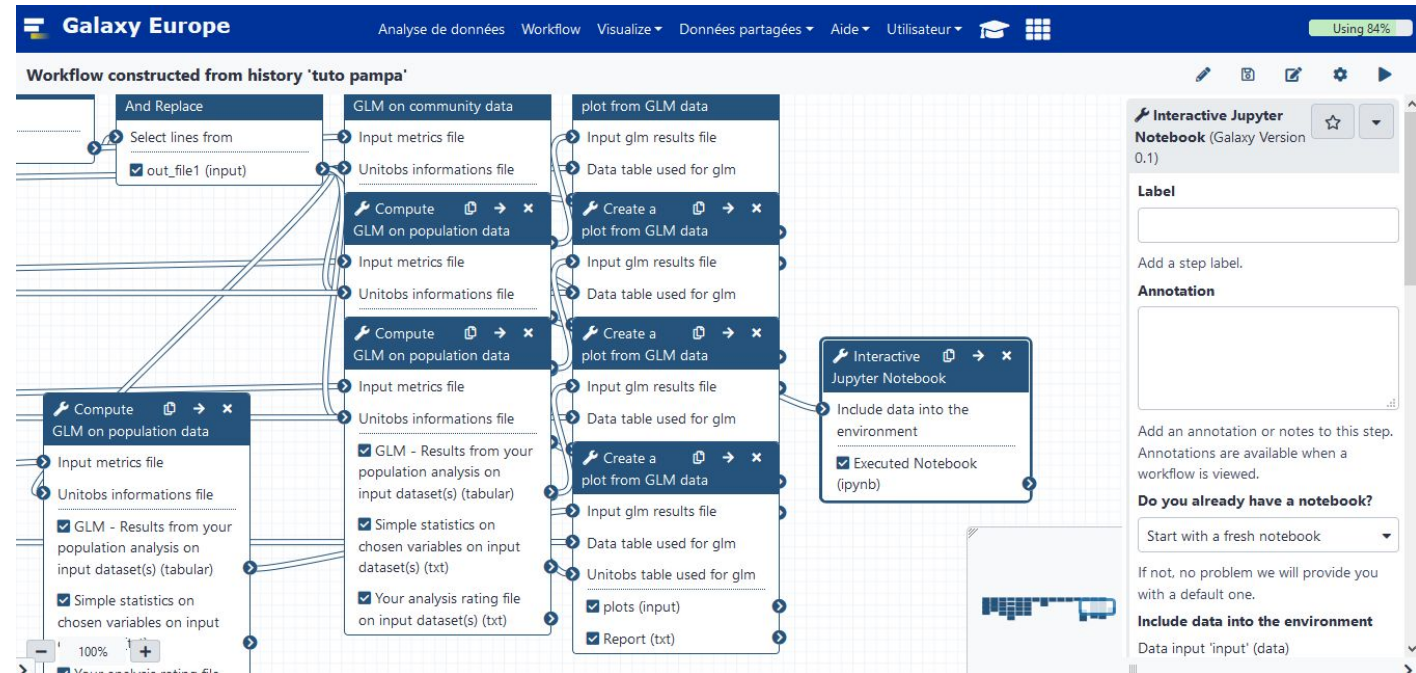


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Les atouts des interactives tools

En particulier par rapport aux “tools” classiques

- L'utilisateur bénéficie d'une interface graphique
- Les outils peuvent bénéficier de paramètres dynamiques
- Visualisations graphiques et complexes

Les IT bénéficient de toutes les propriétés des “tools” qui encapsulent des containers

- Paramétrables par formulaires
- Gestion des dépendances par containerisation
- Packaging & Toolshed



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Les limites des interactives tools

En particulier par rapport aux “tools” classiques

- L'absence de persistance d'une session de travail avec un IT
- Interaction entre les IT et les objets Galaxy (liens input/output histories)
- Interaction entre les IT et d'autres services hébergés ailleurs



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Les applications et les technologies éligibles à devenir des IT

Toutes les applications Web? Les clients lourd ?

- Jupyter
- Rstudio
- ShinY
- ...

Le domaine des possibles semble extrêmement grand.



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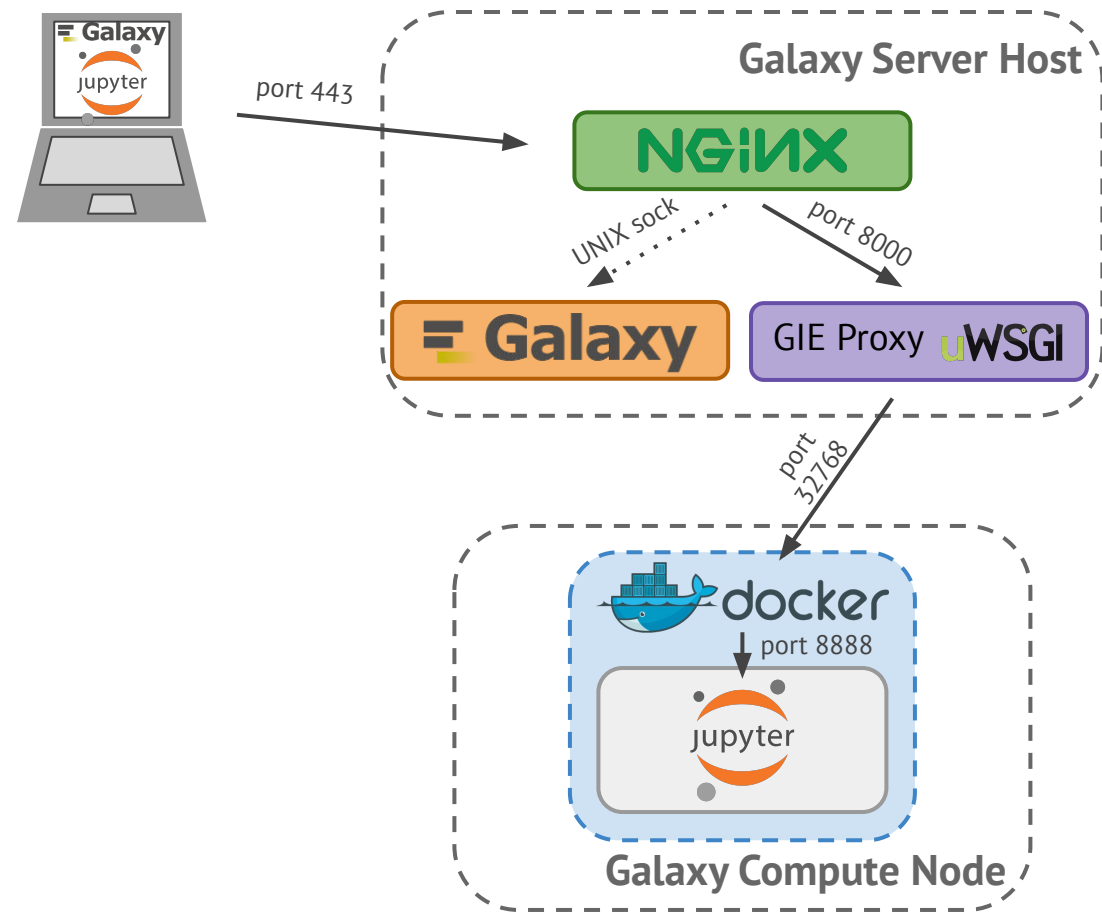
L'architecture du système des interactives tools

socle technologique

- Serveurs Webs
 - Galaxy
 - Containers
- Proxy
- Containerisation
- DNS générique

Quelques étapes pendant le

1. Lancement d'un Job std
2. Prise en charge du mapping de port
3. Gestion des informations propre à la session utilisateur
4. Système de fichier partagé
5. Prise en compte des paramètres du formulaire
6. Exécution du container
7. Monitoring du container

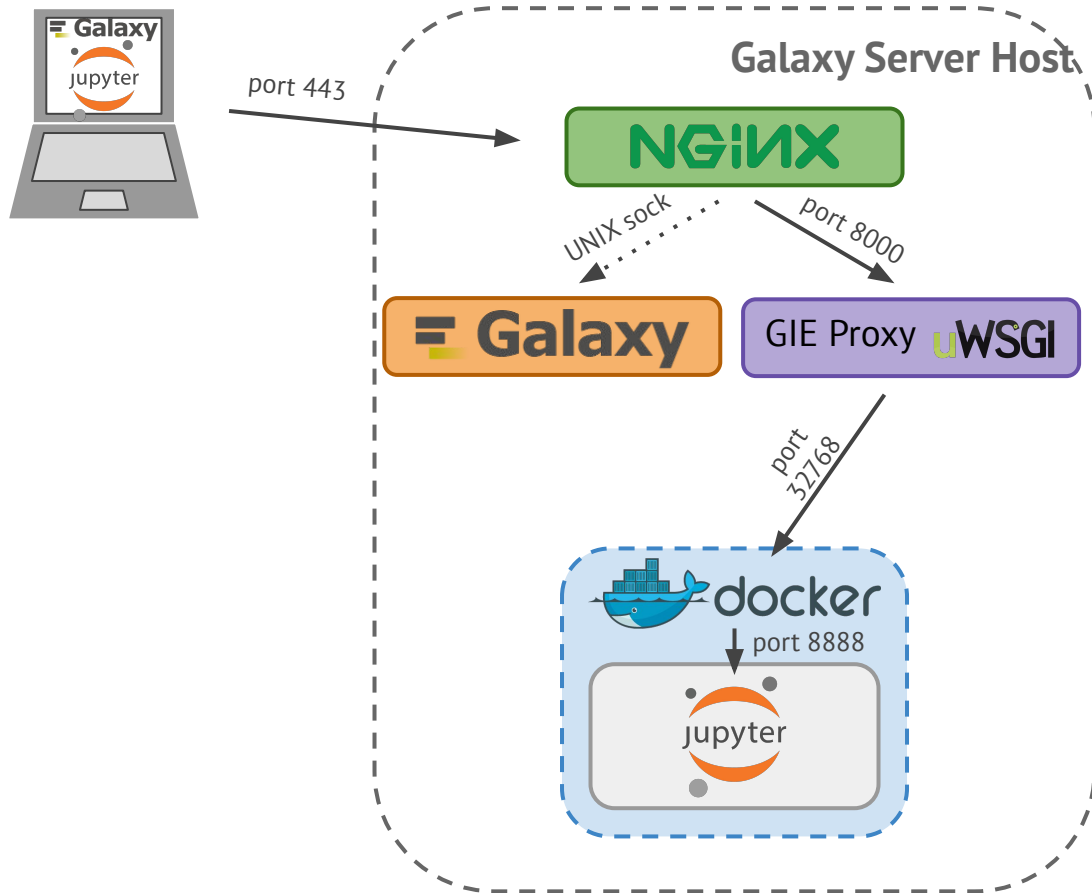


Version originale:

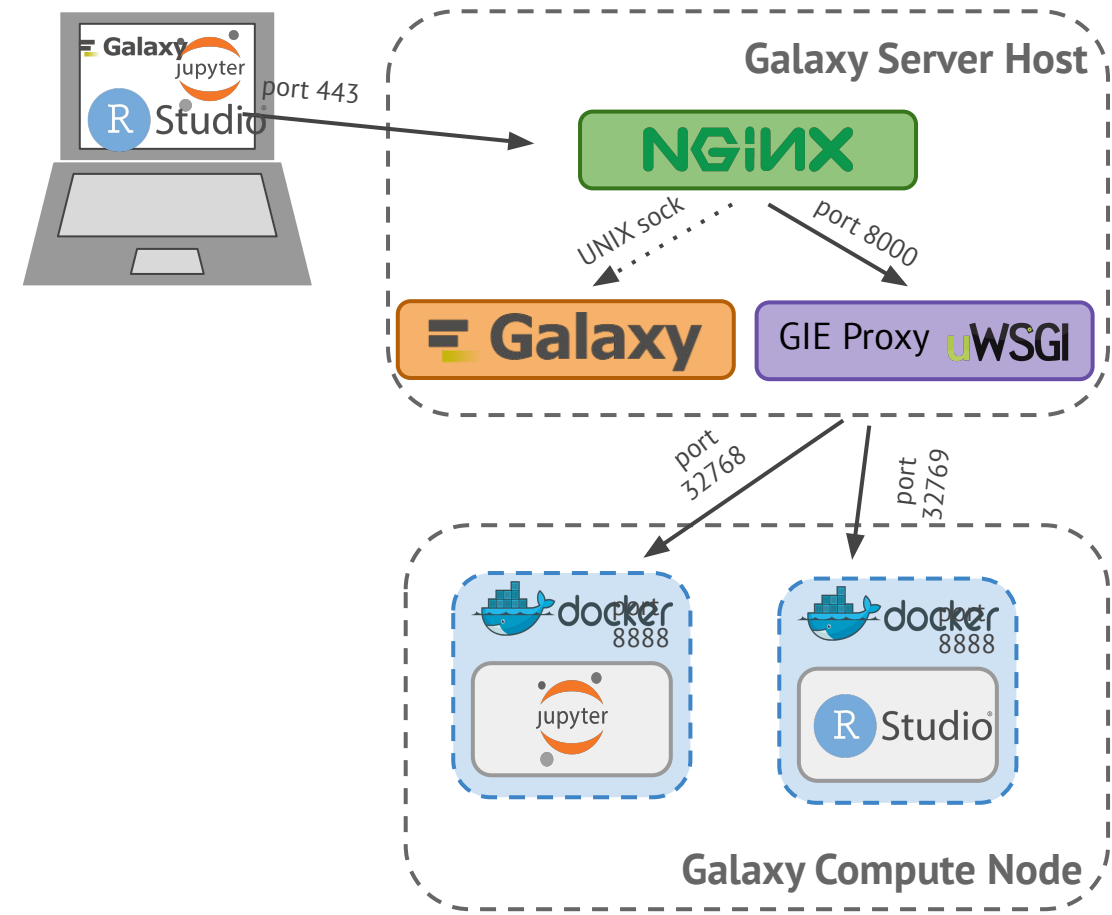
https://docs.google.com/presentation/d/1_4PtM6A4mOxOIgGh6OGWvzFcxD1bdw4CydEWtm5n8k/

L'architecture du système des interactives tools

Single Host



Multi IT



Version originale: https://docs.google.com/presentation/d/1_4PtFM6A4mOxOlGh6OGWvzFcxD1bdw4CydEWtm5n8k/

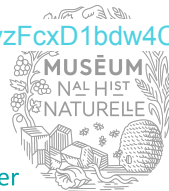


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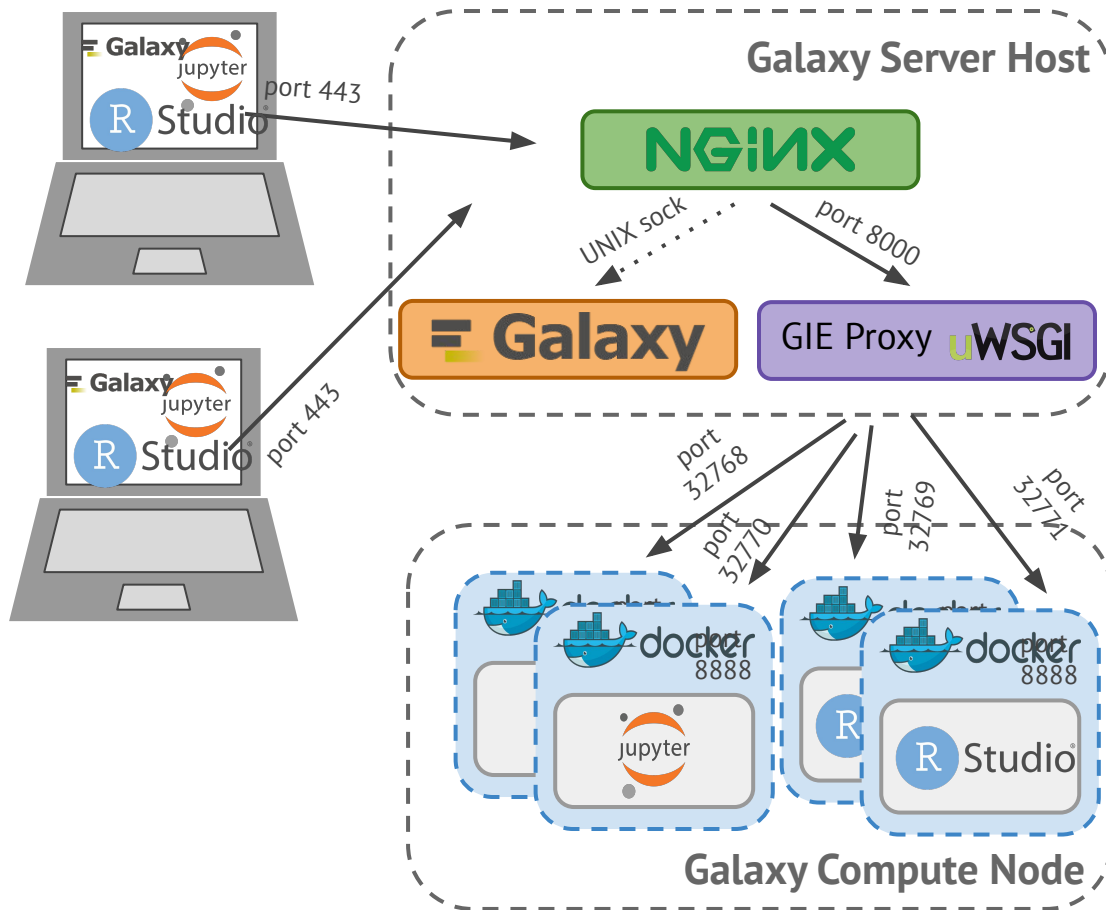
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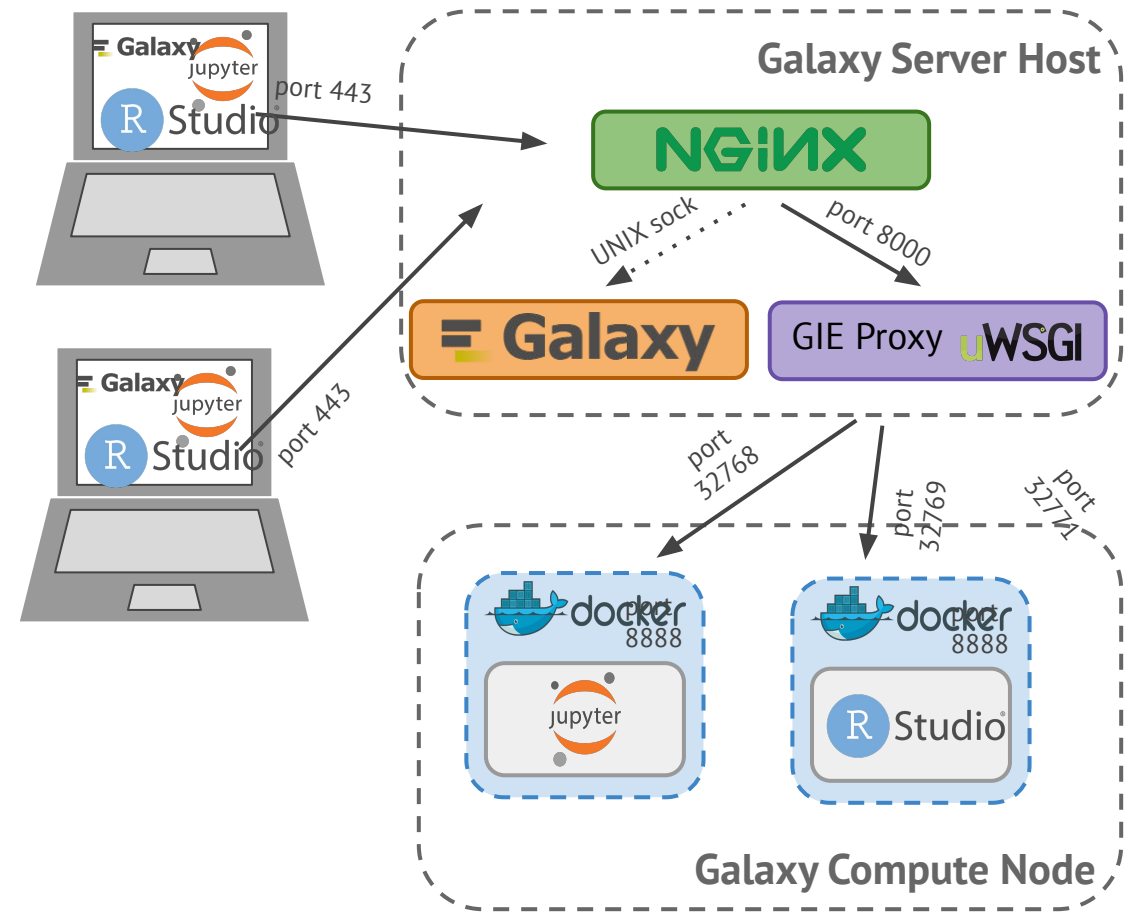


L'architecture du système des interactives tools

Multi User & multi IT



Multi User & Shared IT



Version originale: https://docs.google.com/presentation/d/1_4PtfM6A4mOxOlGh6OGWvzFcxD1bdw4CydEWtm5n8k/



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Interactions entre les IT et Galaxy

Les Entrées/Sorties

Accès aux historiques et aux fichiers (2 approches) :

- en amont à l'aide des formulaires
- pendant la session

1. Wrapper XML std tool + scripting
2. Utilisation de l'API Python Galaxy

Système de fichier partagé entre le serveur Galaxy et les Containers

Upload et Download directement au travers de l'IT



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Les IT et les ressources de calcul

Que savons nous à ce sujet

- Espace disque
- CPU
- La mémoire
- Bande passante
- Montée en charge
- Docker et les cluster
- Mécanismes de limitations



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Les compétences nécessaires

+ de compétences sont-elles nécessaires?

- Pour les administrateurs systèmes

- sécurité
- monitoring des ressources
- complexité des paramètres réseau
- Réseau

- Pour les développeurs

- Compétences propre à l'application
- Containerisation
- API Python
- Développement WEB

