3<sup>rd</sup> Course on Bioinformatics tools for Next Generation Sequencing data mining: use of bioinformatics tools for typing pathogenic *E. coli* 

IT infrastructure and user interface:
The Galaxy architecture and
ARIES cluster





# https://galaxyproject.org/



Communi

Educ

Deploy & Develop

Support <del>-</del>

Search Galaxy

Q

### Data intensive biology for everyone

Galaxy is an open, web-based platform for accessible, reproducible, and transparent computational biomedical research.

- · Accessible: Users without programming experience can easily specify parameters and run tools and workflows.
- Reproducible: Galaxy captures information so that any user can repeat and understand a complete computational analysis.
- Transparent: Users share and publish analyses via the web and create Pages, interactive, web-based documents that describe a complete analysis.

Welcome to the Galaxy Community Hub, where you'll find community curated documentation of all things Galaxy.

#### News

Galaxy Release 18.05 – Style update, Unlimited uploads, Rule-based uploader

GCCBOSC 2018 Childcare Update – eLife Sponsorship & ISB Microgrant lower costs

GCCBOSC 2018 Call for BoFs – Birds of feather flock together in Portland

#### Blog

Coding in the Winter Wonderland: Galaxy Admin Training in Oslo. 2018

Galaxy R Markdown Tools – Using R Markdown as a framework to develop Galaxy tools

#### Events

Galaxy @ ASMS 2018

Galaxy @ Research Bazaar Brisbane (GVL & Alveo – RNA-

Seq & Language Analysis

PhenoMeNal Gateway: Portal to metabolomics data analysis in the cloud – an introduction to metabolomics data analysis

in a cloud computing environment

16S Microbial Analysis with Mothur

Strategic Partnership for Advanced Cyber Infrastructure @ Minority Serving Institutions (SPACI@MSIs) – building a regional community of practitioners that supports next-generation networking

#### @galaxyproject



### Galaxy core values

### Accessibility

 Users without programming experience can easily upload/retrieve data, run complex tools and workflows, and visualize data

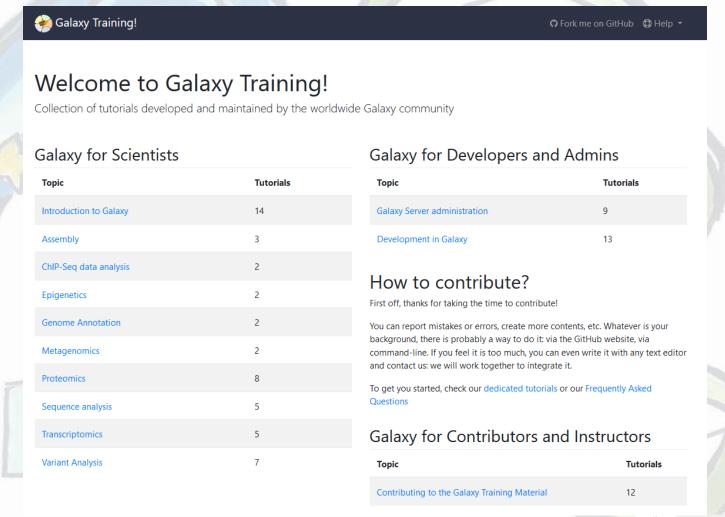
### Reproducibility

 Galaxy captures information so that any user can understand and repeat a complete computational analysis

### Transparency

Users can share or publish their analyses (histories, workflows, visualizations)

# You're not alone: the Galaxy community



### Galaxy vs Command line



- Graphical user interface
- Remote access
- Data organisation
- Easy to share
- Visual workflow editor



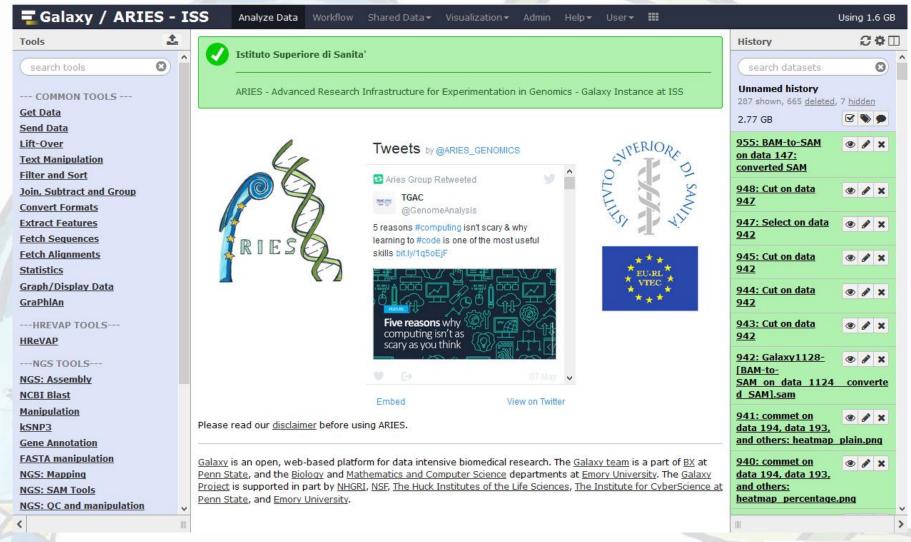
- Command-line interface
- Full control
- Flexibility
- Debugging

# Client-server architecture

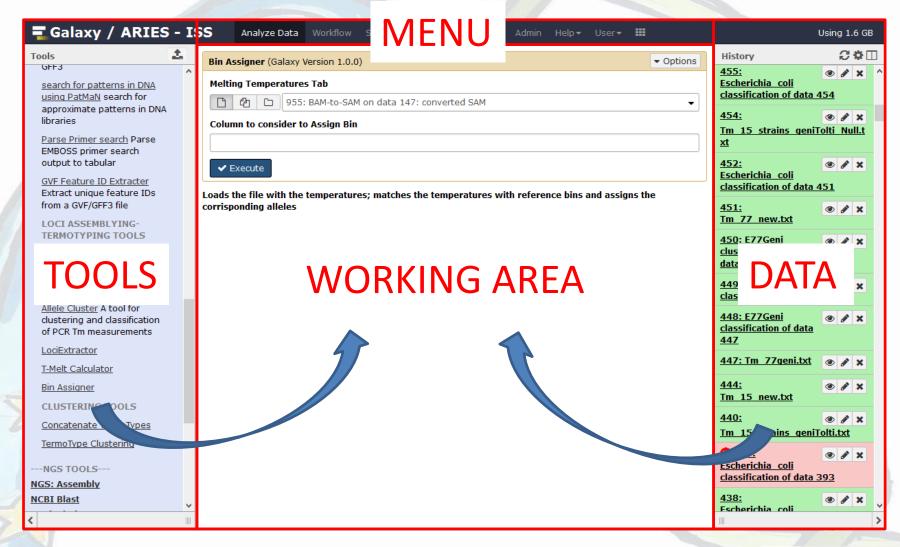


18-19/06/2018

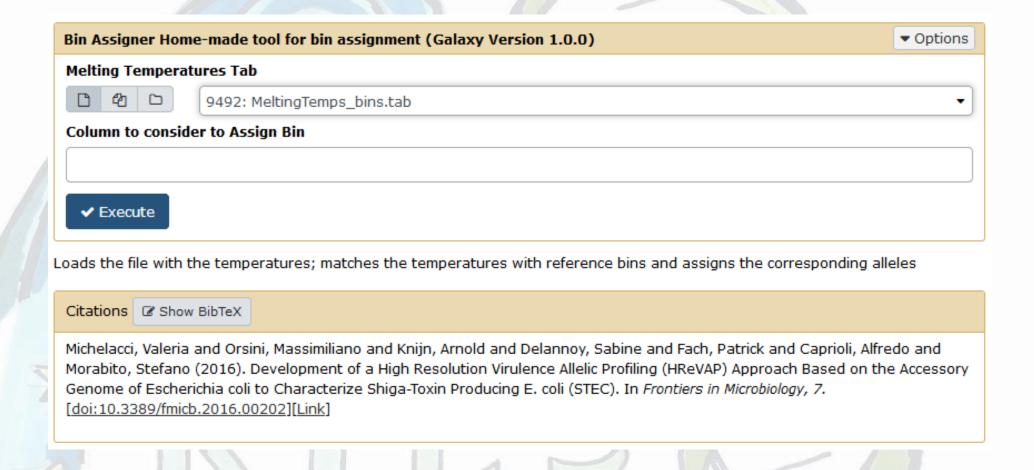
# Galaxy user interface



# Galaxy user interface



## Intuitive and self-documenting

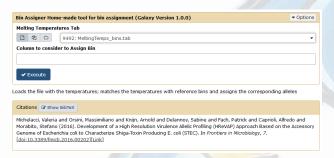


IT infrastructure and user interface: The Galaxy architecture and ARIES cluster

### Home-made tools

```
<tool id="binassigner" name="Bin Assigner">
 <description>Home-made tool for bin assignment</description>
 <requirements>
   <requirement></requirement>
 </requirements>
 <command interpreter="python">
   BinAssigner.py -t $tmstab -o $output -c $columntab > $logfile
 </command>
 <inputs>
  <param name="tmstab" type="data" format="tabular" label="Melting Temperatures Tab"/>
  <param name="columntab" type="text" format="integer" label="Column to consider to Assign Bin" />
 </inputs>
 <outputs>
  <data format="tabular" name="output" label="Allele Table"/>
  <data format="txt" name="logfile" label="BinAssigner Log File" />
 </outputs>
 <help>
   Loads the file with the temperatures; matches the temperatures with reference bins and assigns
   the corrisponding alleles
 </help>
 <citations>
   <citation type="doi">10.3389/fmicb.2016.00202</citation>
 </citations>
/tool>
```

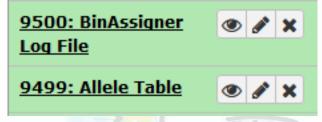
### Behind the scenes



Galaxy

principalities again principal of \$1.2 × 0.2 × 0.4 × 0.0 × 0

### wrapper







### Job runner



# Which Galaxy flavour?

Public server (90+)



- Own computer
- Appliance Galaxy Edition
- Data Center
- Cloud









#### ARIES

Analysis of genomic data in the field of public health and food safety, with the aim of deploying a comprehensive bioinformatics approach to the study of food-borne zoonoses and infectious diseases at the human and animal interface.

This is a **Domain specific server**.

#### Links

ARIES

#### Comments

- The web portal is termed ARIES (Advanced Research Infrastructure for Experimentation in genomicS)
- - o Development of an Information System for the collection of genomic and epidemiological data to enable the Next Generation Sequencing (NGS)-based surveillance of infectious epidemics, foodborne outbreaks and diseases at the animal-human interface.
  - o Development of analytical pipelines enabling harmonized, real time multi-genome comparisons, to improve the detection of clusters of cases of infections and allowing the global bio-tracing of pathogens.
  - o Development of metagenomics models for the culture-independent detection and typing of pathogens and the study of their interactions with the microbiota in human and animal samples and in the vehicles of infections.

#### User Support

- Email support: aries@iss.it
- The system can be rebooted any time for service purposes, although generally a warning will be published with some advance on the ARIES site and through the @ARIES GENOMICS Twitter account.
- No backup of data is performed on our servers

#### Ouotas

An account is required. Contact aries@iss.it to request an account.

#### Citation(s)

- Advanced Research Infrastructure for Experimentation in Genomics (ARIES): A concept of a bioinformatics framework for the analysis of genomic data from zoonotic agents, Valeria Michelacci, Arnold Knijn, Massimiliano Orsini, Stefano Morabito, 4th Med-Vet-Net Association International Conference.
- ARIES tagged publications in Galaxy Publication library.

#### Sponsor(s)

• Set up and maintained at the [Istituto Superiore di Sanità (ISS Rome)] by a collaboration between the European Union Reference Laboratory for VTEC and the Data Management Sector.





### ISS IT infrastructure



Blade server technology







Storage



Networking

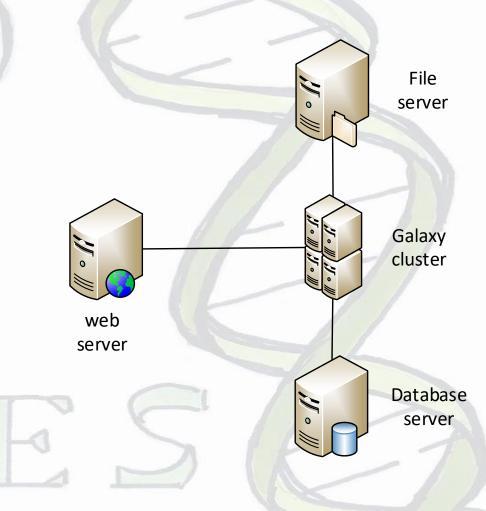


# Galaxy components

- Web server
- Job runner
- File server

18-19/06/2018

Database server





### Default vs production installation

### All-in-one (default)

- ✗ Internal file system
- SQLite
- Built-in HTTP server for all tasks
- Local job runner
- Single process
- ✓ Simplest error-proof configuration

### **Production (scalable)**

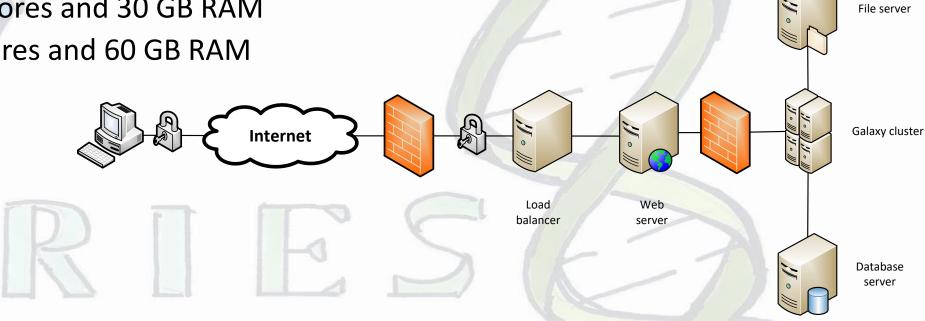
- ✓ External file server
- ✓ External database
- ✓ External HTTPS server for many tasks
- ✓ Cluster job runner
- ✓ Multi process
- More complex configuration



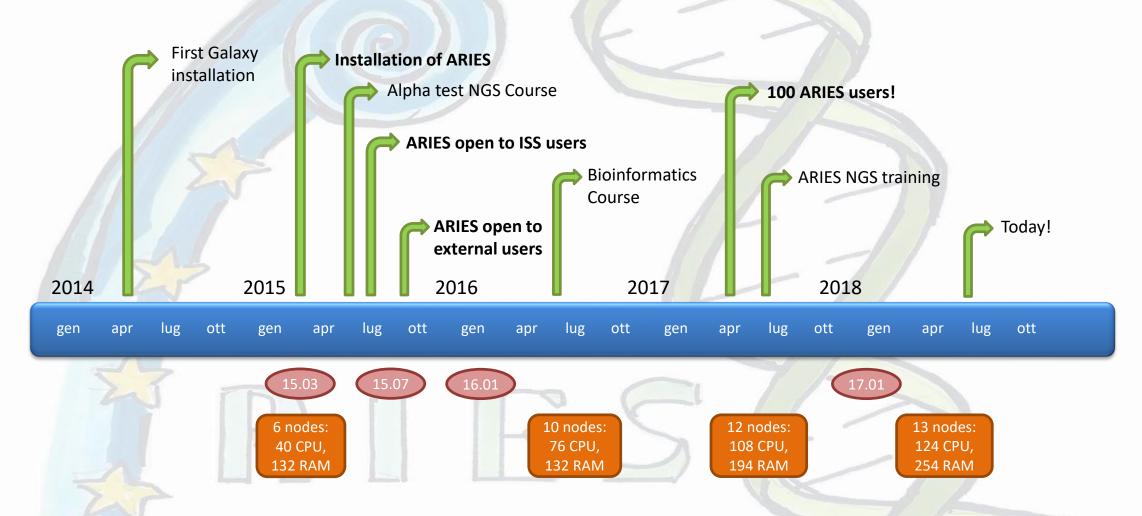


### ARIES cluster

- Cluster is made up of 13 nodes:
- Master node: 8 cores and 8 GB RAM
- 1 node: 4 cores and 4 GB RAM
- 8 nodes: 8 cores and 15 GB RAM
- 2 nodes: 16 cores and 30 GB RAM
- 1 node: 16 cores and 60 GB RAM



# Galaxy in ISS

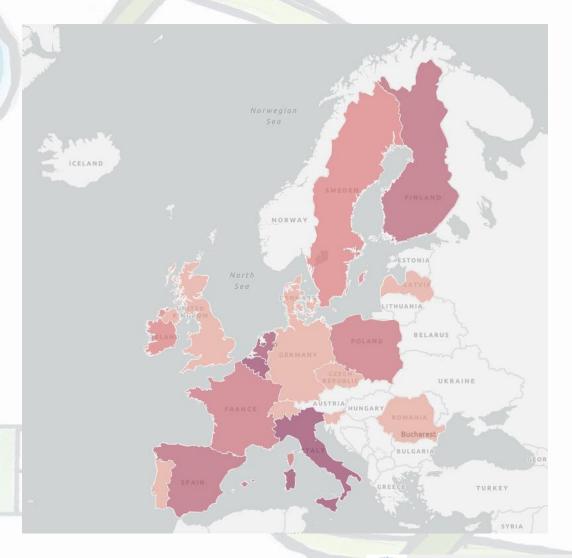


### ARIES users

#### Currently 105 users:

- 4 Belgium
- 1 Czech Republic
- 1 Denmark
- 4 Finland
- 3 France
- 1 Germany
- 2 Ireland
- 51 Italy (37 ISS)
- 1 Latvia
- 1 Luxembourg
- 6 The Netherlands
- 3 Poland
- 1 Portugal
- 1 Romania
- 1 Slovenia
- 2 Spain
- 2 Sweden
- 1 Switzerland
- 1 United Kingdom

- 2 Argentina
- 1 Australia
- 3 China
- 1 India
- 2 Iran
- 3 USA





### ARIES use

**Jobs Per Month** 1 2 3 -Click Month to view details. Graph goes from the 1st to the last of the month.

Month ↑	<u>User and Monitor Jobs</u>	
May 2018	2534	
<u>April 2018</u>	2031	
March 2018	3059	
February 2018	716	
January 2018	1386	
December 2017	571	li
November 2017	2973	lin
October 2017	1218	
September 2017	496	
August 2017	793	
<u>July 2017</u>	1077	
June 2017	2808	<u> </u>

### Questions?



https://w3.iss.it/site/aries





aries@iss.it

- Stefano Morabito
- Valeria Michelacci
- Arnold Knijn
- Massimiliano Orsini
- IZS delle Venezie



@ARIES GENOMICS