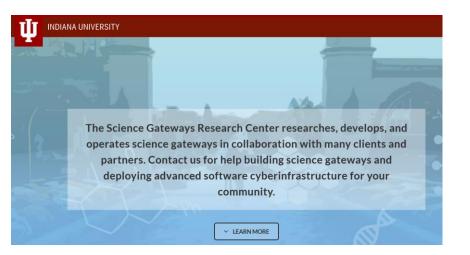
APSEM2019 : éco-systèmes pour la science ouverte et recherche par les données

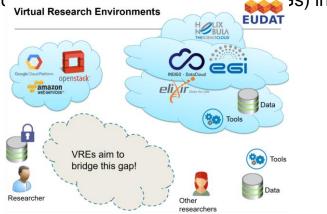
Petit tour d'horizon et comparatif des VREs



Yvan LE BRAS, MNHN Pôle national de données de biodiversité (UMS PatriNat)

Virtual Research Environments (VREs) are increasingly being used to support a more dynamic approach to collaborative working in systematics and taxonomy. Researchers who are not co-located are seeking to work dynamically together at various scales from local to international. These shared infrastructures are funded as VREs in Europe, Virtual Laboratories (VLs) in Attractional Science Cotours (CSs) in the USA and all have similar objectives.





Detasets * Training Support

Welcome to the Biodiversity & Climate Change Virtual Lab



In fact VREs have a very long history in Europe. The UK Open University has used the term as an ICT support environment for students for many (at least 20) years. JISC (an organisation in UK supporting ICT across higher education) worked on VREs for higher education in 2004 and subsequently. Currently the EC (European Commission) favours the term VRE for systems or offerings that we also know as VLs or SGs. The term 'researcher workbench' has also been used widely since the 1980s and basically has the same concept as a VRE.

Key aspects seem to be (from the research I have done):

1. virtualisation (hiding complexity from the user);

2. access to useful resources such as datasets, software, computing power, instruments/detectors (the latter for control as well as data taking) and scholarly publications (including grey literature technical reports etc.) as well as collaboratively with other persons and organisations;

3. interoperability across resources;

4. support for the 'researcher workflow' from research idea (and checking the literature etc.) through observations/experiments to publication and subsequent discussion with citation and accreditation (maybe including management functions such as proposals and reporting to funders).

5. support for workflow composition (or even autonomic composition) of (2) and ideally deployment on virtualised resources (e.g. GRIDs, CLOUDs);

- 1. VRE = Virtual lab
- Online
- Central point of a distributed ecosystem, the e-Science one
- 2. e-Science
- Research + TIC
- « Research done through distributed global collaboration enabled by the internet, using very large data collections, terascale computing resources and high performance visualization » (Sir John Taylo – 2001)
- Three parts
 - Computing : HPC, grid, cloud
 - Storage
 - Collaboration
- 3. From infra to communities through softwares
- Research lifecycle

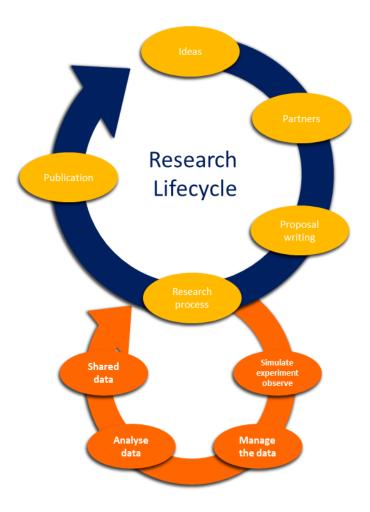
« Research done through distributed global collaboration enabled by the internet, using very large data collections, terascale computing resources and high performance visualization » (Sir John Taylo – 2001)

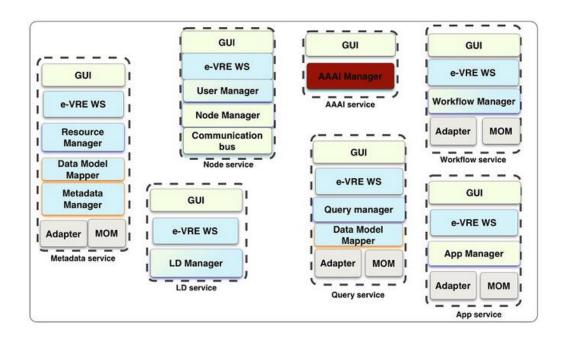
« A VRE comprises a set of online tools and other network resources and technologies interoperating with each other to facilitate or enhance the processes of research practitioners within and across institutional boundaries» <u>JISC</u> <u>definition</u>

« Virtual Research Environments are innovative, web-based, community-oriented, comprehensive, flexible, and secure working environments conceived to serve the needs of modern science» (<u>Candela et al. 2013</u>)

- Web based
- Serve the needs of researchers communities (VRCs)
- Open and **flexible**

VRE, for which purpose ?





VRE « Tools »

- 1. Collaboration oriented tools
- Built on existing platform
 - HUBzero (using Joomla)
 - Sakai (a first demonstrator project so old ;))
 - VRE4EIC e-VRE
- Specific VRE framework
 - gCube
 - Microsoft Sharepoints VRE Toolkits
 - OpenDreamkit for mathematic
 - <u>Parthenos</u> for Humanities
 - <u>Phenomenal</u> on-demand VRE for metabolomics
 - Apache Airavata software framework
- VRE OSF ?

Apache Airavata is a software framework which is dominantly used to build Webbased science gateways and assist to compose, manage, execute and monitor large scale applications and workflows on distributed computing resources such as local clusters, supercomputers, national grids, academic and commercial clouds. Airavata mainly supports long running applications and workflows on distributed computational resources.



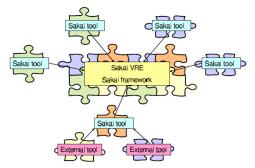


Figure 1. Pluggable Sakai VRE architecture.

Yang et al. 2006 (Integration of Existing Grid Tools in Sakai VRE)

Cloudflare Let's the file Calaxy Coole ANSIBLE (Coole ANSIBLE Cloudflare Coole ANSIBLE COOLE ANSI

Statistical Algorithms Importer (SAI)

DataMiner

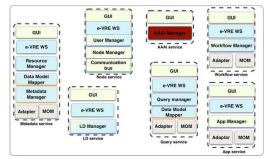




Dependencies management







Cloud

VRE « Tools »

1.

gCube

Specific VRE framework

Built on existing platform

Collaboration oriented tools

VRE4EIC e-VRE

- Microsoft Sharepoints VRE Toolkits
- **OpenDreamkit** for mathematic
- Parthenos for Humanities

HUBzero (using Joomla)

Phenomenal on-demand VRE for metabolomics

Sakai (a first demonstrator project so old ;))

- Apache Airavata software framework
- VRE OSF ? puppet CHEF SALT**STACK** Terraform ANSIBLE infrastructure

manage « infrastructure as code »





Workflow manager





Analyze through GUI

VRE « Tools »

- 1. Collaboration oriented tools
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2. VRE and Virtual / Learning Environments / Virtual Research Communities (VRCs)

External tool

Sakai to

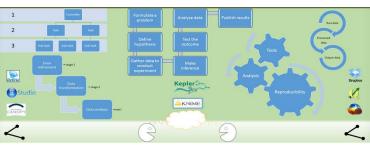
Sakai VRE

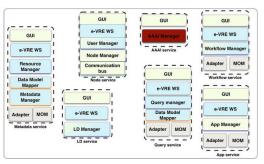
Sakai framework

Figure 1. Pluggable Sakai VRE architecture.

Sakai tool

Yang et al. 2006 (Integration of Existing Grid Tools in Sakai VRE)



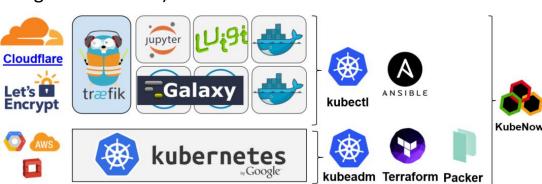




VRE components

- 1. Stack
- Comparing gcube / HUBzero and <u>Phenomenal VRE</u>
- 2. Links
- Gateway -> VREs
- 3. Granulometry
- Size / subject of communities ?
- Genericity of tools as VRE commonents
- 4. Important questions
- Who will use it? Not only needs are important but also particularities of communities (ie Biologist don't code)









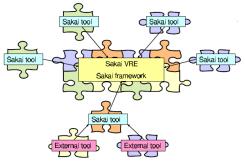


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Yang et al. 2006 (Integration of Existing Grid Tools in Sakai VRE)

Please, do take into account that there six projects officially supported by the EC in 2016 to develop VREs (<u>https://ec.europa.eu/programmes/horizon2020/en/news/six-new-projects-e-i</u>...):

* BlueBRIDGE - Building Research environments for fostering Innovation, Decision making, Governance and Education to support Blue growth

- * MuG Multi-Scale Complex Genomics
- * OpenDreamKit Open Digital Research Environment Toolkit for the Advancement of Mathematics
- * VI-SEEM VRE for regional Interdisciplinary communities in Southeast Europe and the Eastern Mediterranean

* VRE4EIC - A Europe-wide Interoperable Virtual Research Environment to Empower Multidisciplinary Research Communities and Accelerate Innovation and Collaboration

* West-Life - World-wide E-infrastructure for structural biology

* The EVER-EST Horizon 2020 project will create a state of the art virtual research environment (VRE) focused on the earth sciences. <u>https://ever-est.eu/</u>



Wf4Ever Research Object Model 1.0

EVER-EST example

H2020 project for Earth-science





The solution is based on the integration of Earth Science e-infrastructures technologies - developed over 15 years with the innovative concept of Research Object

Enabling reproducible, transparent research.

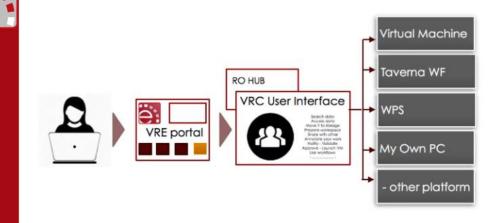
ArcGIS





Wf4Ever Research Object Model 1.0

The system can be easily integrated with different mechanisms to process Earth Science data



It takes full advantage of ES data cloud processing capabilities



EVER-EST example

EVER-COL-040	Project Management Tools	Highly Desirable
Requirement	EVER-EST e-infrastructure shall provide project planning and management tools to be used by the VRCs communities that includes presentation and editing of Gantt charts, reporting and recording of minutes and actions.	
Source	VRE Use Cases (VM, SS)	
Verification Method	Verification Methods: Validated	
Note	not implemented yet, VRCs use as <i>project plann</i> ALFRESCO	ing and management tools

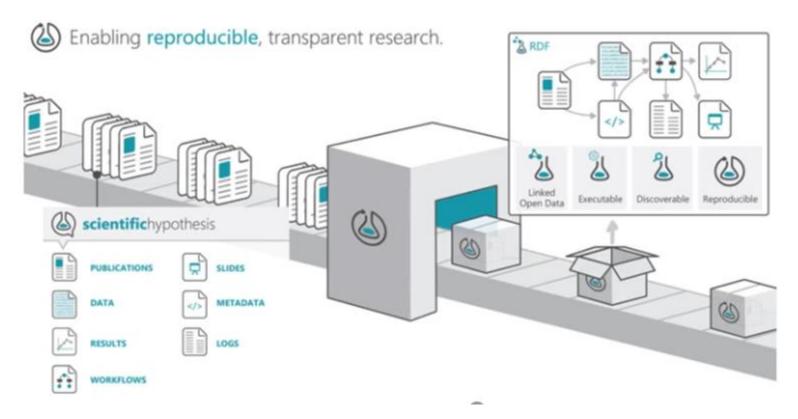
"VRE as a Services" is the response to the impelling need for an e-Science infrastructure supporting: reproducibility, reuse and interdisciplinarity insights and cross-fertilisation of scientific investigation and scholarly data, by developing and operating an Virtual Research Environment sustaining Open Science and implementing FAIR Guiding Principles for scientific data management and stewardship

Open Science covers the following aspects:

- Open Discovery, tools able to increase the efficiency of research as well as of its diffusion;
- Open Access to scientific inputs and outputs as research outcomes;
- Open Data, freely to available to everyone to use and publish, without restrictions from copyright, patents or other mechanisms of control;
- Open Methodology related to research strategy that outlines the way in which research is to be undertaken;

• Open Educational, allowing the broaden access to the learning and training traditionally offered through formal education systems.

EVER-EST example -> what is particularly of interest



RO must be associated to metadata -> here we see the interest of the « completude » of EML as this standard seems to be perfect to inform about each component of ROs EVER-EST example -> what is particularly of interest

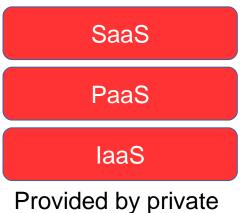


RO must be associated to metadata -> here we see the interest of the « completude » of EML as this standard seems to be perfect to inform about each component of ROs Some issues for me

Tool/Software/Script

Developped by communities of practices -free -usable only in local PC

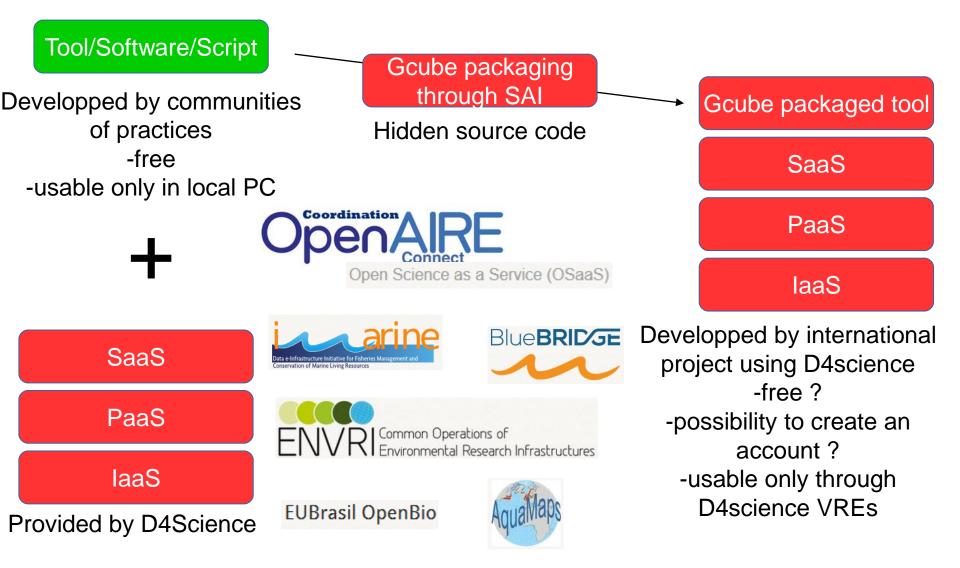
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companies



Developped by international project with « business » delivrables such as H2020 -not free -usable only through private compagnies services Some issues for me





Ref: OpenScience Data Analytics Technologies, AGINFRA+ wiki <u>https://support.d4science.org/projects/aginfraplus_wiki/wiki/D31_- Open_Science_Data_Analytics_Technologies#SAI</u>

EU projects related to gcube: •IMARINE - Data e-Infrastructure Initiative for Fisheries Management and Conservation of Marine Living Resources (283644) •BlueBRIDGE - Building Research environments for fostering Innovation, Decision making, Governance and Education to support Blue growth (675680)

•EGI-Engage - Engaging the EGI Community towards an Open Science Commons (654142)

•PARTHENOS - Pooling Activities, Resources and Tools for Heritage E-research Networking, Optimization and Synergies (654119)

•D4SCIENCE-II - Data Infrastructure Ecosystem for Science (239019)

•EUBRAZILOPENBIO - EU-Brazil Open Data and Cloud Computing e-Infrastructure for Biodiversity (288754)

•ENVRI PLUS - Environmental Research Infrastructures Providing Shared Solutions for Science and Society (654182)

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•D4SCIENCE - DIstributed colLaboratories Infrastructure on Grid ENabled Technology 4 Science (212488)

•ENVRI - Common Operations of Environmental Research Infrastructures (283465)

•SoBigData - SoBigData Research Infrastructure (654024)

DataMiner

"Required packages are assumed to be preinstalled on the backend system"

Java / Maven / Eclipse -> not for ecologs who develop scripts, need for IT JAVA guys



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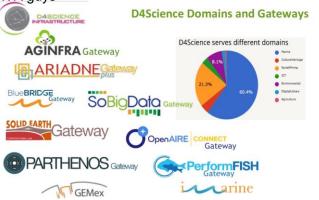
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https://services.d4science.org/thematic-gateways AGINFRA

WWW.PLUS.AGINFRA.EU

https://www.slideshare.net/aginfra/realising-a-science-gateway-for-the-agrifood-the-aginfraplus-experience?next_slideshow=1

Massimiliano Assante CNR IWSG 2019 Realising a Science Gateway for the Agri-food: the AGINFRAplus Experience



Ref: OpenScience Data Analytics Technologies, AGINFRA+ wiki https://support.d4science.org/projects/aginfraplus_wiki/wiki/D31_- Open_Science_Data_Analytics_Technologies#SAI



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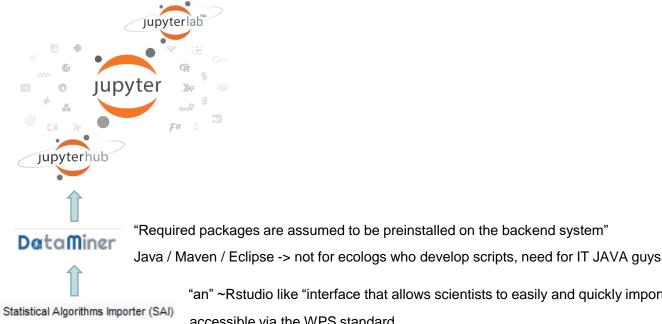
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"an" ~Rstudio like "interface that allows scientists to easily and quickly import R scripts onto DataMiner" accessible via the WPS standard

"The algorithms installer manage a list of users with visibility rights on an algorithm"



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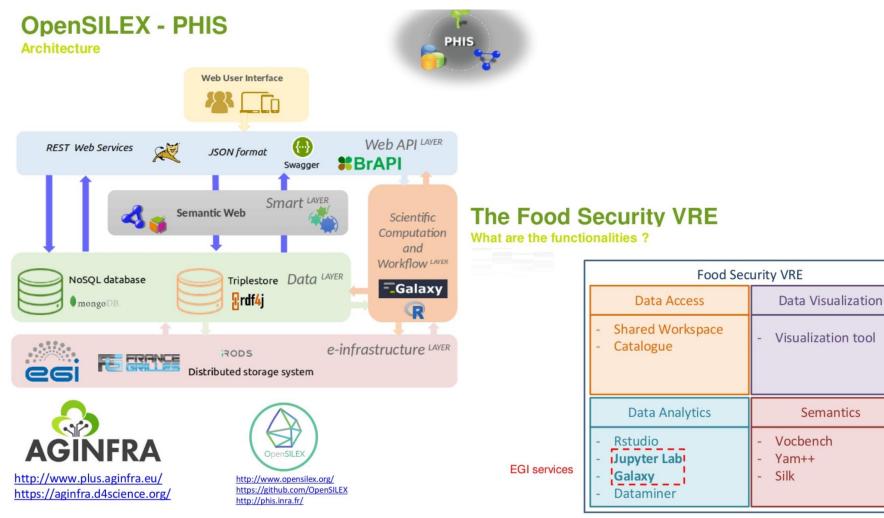


Workflow orientation -> Limitation for HPC or not open source



Ref: OpenScience Data Analytics Technologies, AGINFRA+ wiki https://support.d4science.org/projects/aginfraplus_wiki/wiki/D31_- Open_Science_Data_Analytics_Technologies#SAI

And now, linking Galaxy to D4Science through RapidMiner WPS services available on Galaxy and more!



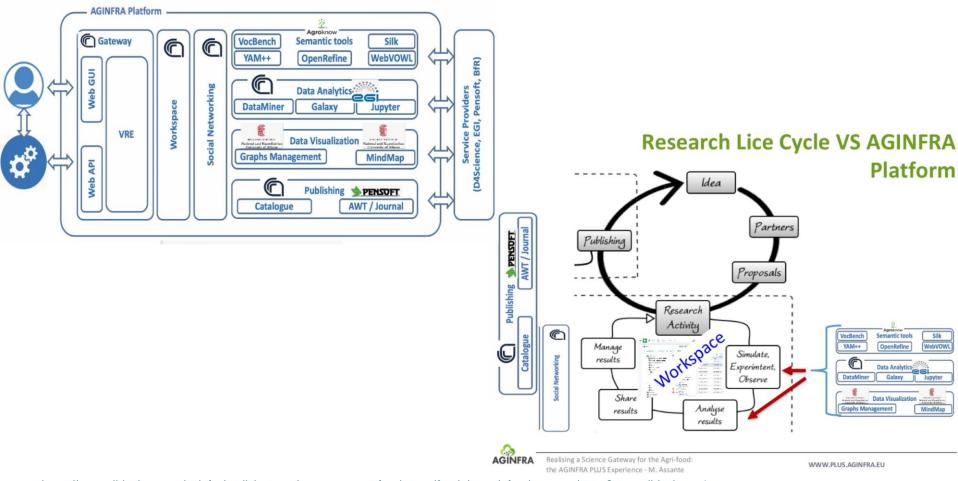
https://www.slideshare.net/aginfra/data-intensive-agricultural-sciences-requirements-based-on-aginfra-project-and-high-throughput-phenotyping-infrastructure Vincent Negre Data intensive agricultural sciences : requirements based on Aginfra+ Project and high throughput phenotyping infrastructure



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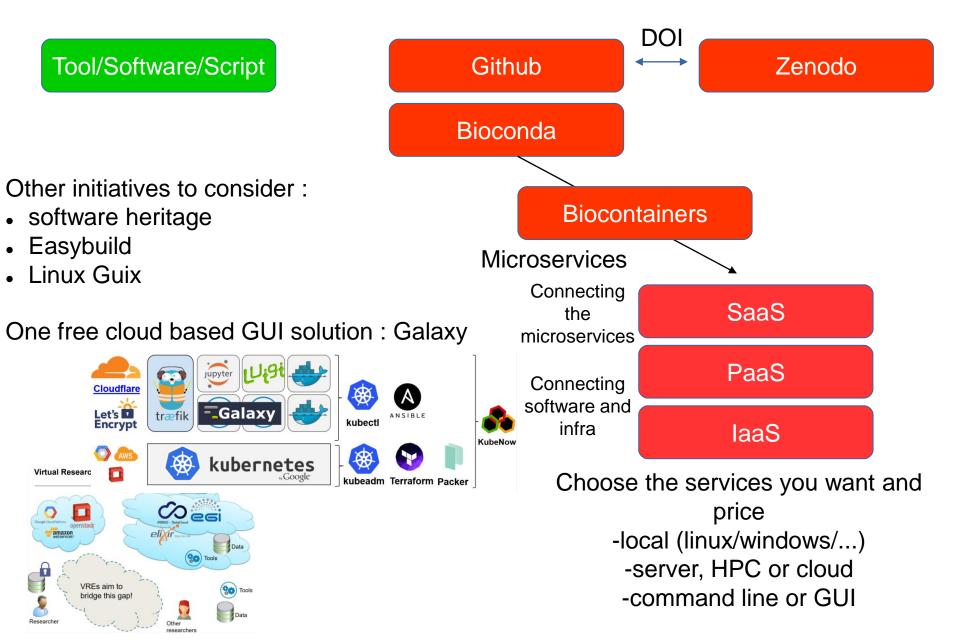
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AGINFRA Plus Platform Architecture



https://www.slideshare.net/aginfra/realising-a-science-gateway-for-the-agrifood-the-aginfraplus-experience?next_slideshow=1 Massimiliano Assante CNR IWSG 2019 Realising a Science Gateway for the Agri-food: the AGINFRAplus Experience

One personal proposal for ecology communities





What is GenomeSpace? Tools Recipes Documentation Developers Support About

User Login

Q

The GenomeSpace project is ending

The GenomeSpace project ends on November 15, 2019 due to expiration of its NHGRI funding and we will be shutting down the GenomeSpace servers on that date. We would like to thank all GenomeSpace users for their support and for all the important science they have done on the platform over the last nine years.

<u>GenomeSpace-enabled tools</u> are separately funded and will continue to be available subject to their own lifecycles, but any connection to GenomeSpace or GenomeSpace-hosted files will cease with the termination of the servers. If you do not remember your login credentials for any individual tools that you rely on, you should use the 'forgot password' links on their websites to reset your login credentials.

NOTE: We are unable to archive any data you have in your GenomeSpace account. Therefore, if you wish to retain copies of such data **you should transfer them to your own storage** from GenomeSpace before the termination date. After that time they will be deleted from the GenomeSpace servers as part of the shutdown process. Data that you host on other platforms (Dropbox, S3, Google Drive) and have connected to your GenomeSpace account will not be affected.

If you have any questions, please contact the GenomeSpace team at gs-help@broadinstitute.org.

The GenomeSpace Team

Merci de votre attention

ATMOSPHERE

SURFACES CONTINENTALES

BIOSPHERE

OCEAN

TERRE INTERNE