Data storage, protection and management for the Life Science community

<u>M. A. Tangaro</u>, G.Donvito, F. Zambelli CNR-IBIOM and INFN-Bari



GIBIOM

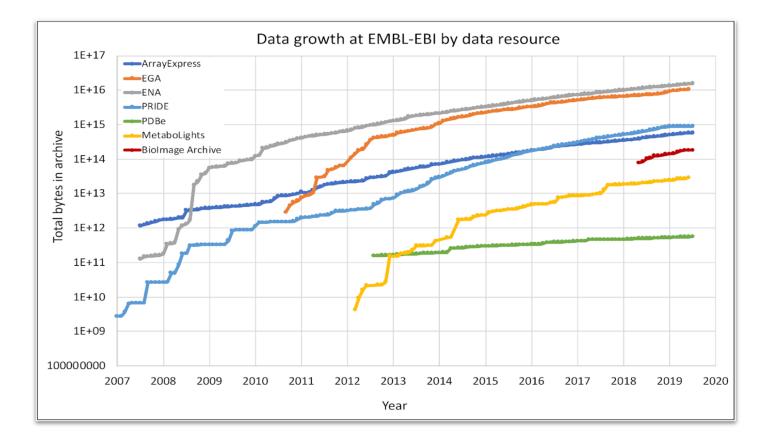
Istituto di Biomembrane, Bioenergetica e Biotecnologie Molecolari



Data in Life Science

Data volume is doubling every six months.

Not only in quantity but also in variety.



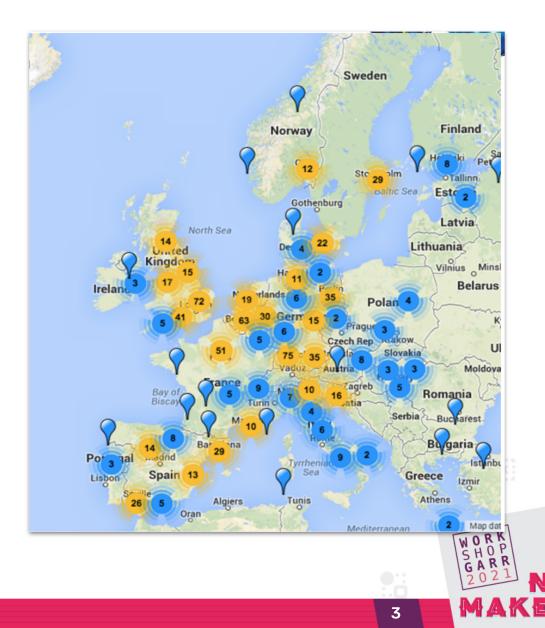
Data growth at EMBL-EBI Source: Charles E. Cook et al. Nucl. Acids Res. 2020; Volume 48, Issue D1, Pages D17-D23

WORK SHOP GARR

Data in Life Science

Genomic data are distributed across several sequencing centres and/or IT infrastructures.

Discipline	Data size	# devices	
HEP-LHC	15PB/year	1	
Astronomy	15PB/year	1	
Genomics	0.4TB/genome	>1000	



Data in Life Science

The GDPR explicitly recognizes the sensitive nature of the collected genetic data (Article 9), but at the same time permits sensitive genetic data processing for scientific research purposes (Article 89(1)) without explicit consent, provided this is allowed by EU or Member States law framework and appropriate safeguards measures are in place.



WORK SHOP GARR 2021 NET MAKERS

Outline

Different use cases for number of users, resource location and data sensitivity Many users Different research domain Distributed resources

The Pulsar Network:

distributed compute and storage across Europe

Sensitive data:

the European Genome-phenome Archive

Data Encryption on-demand:

the Laniakea use case

A "simple" use case:

CNR.BiOmics sequencing facility

Few users dedicated resources

Marco Antonio Tangaro - IBIOM-CNR and INFN-Bari



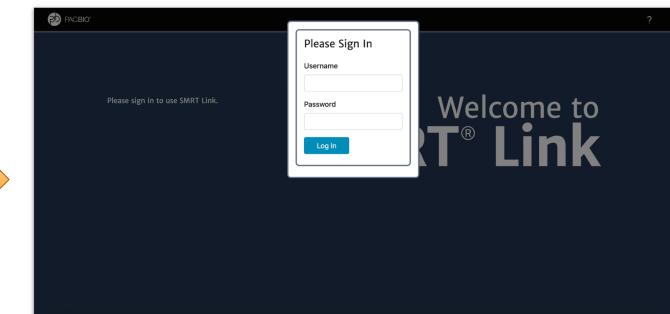
CNR.BiOmics

The CNR.BiOmics project ("National Research Center in Bioinformatics for Omics Sciences", PIR01_00017 14.5 M€ and CIR01_00017 2M€), currently on-going, which aims to strengthen the Italian node of the European Research Infrastructure ELIXIR in the southern regions.



CNR.BiOmis





PacBio Sequel2:

- 2-3 TB output per sample
- 4 sample per run
- 1 run per week.

The sequencing facility is housed at IBIOM-CNR (Bari)

The analysis facility is housed at ReCaS-Bari datacenter.

Data are moved from the PacBio to the analysis server, where PacBio SMRT-Link have been configured for analysis.

WOR

7

70 TB Lustre storage are currently supporting the config.





https://laniakea-elixir-it.github.io

LANIAKEA is a cloud based Galaxy instance provider.

Developed by ELIXIR-ITALY

By hiding the technical complexity behind a user-friendly web front-end, Laniakea allows its users to configure and deploy virtual Galaxy instances with a handful of clicks.

No need for the end user to know the underlying infrastructure.

No need for maintenance of the hardware and software infrastructure.



Laniakea paper



Laniakea@ReCaS paper



Laniakea – Storage encryption on-demand



The user data privacy is granted through LUKS storage encryption as a service: data are isolated from any other instance on the same platform and from the cloud service administrators.

The encryption procedure has been completely automated in order to simplify the user experience: the user can encrypt storage on-demand, using a strong random alphanumerical passphrase.

This has been achieved integrating the key management system Hashicorp Vault (vaultproject.io) to store encryption keys, which are shown in the Laniakea Dashboard only if explicitly requested by the user.



On-demand encryption: user experience

Templete, geland und versi	Q ☆ 🎱 :	PaaS Orche	strator Dashboard Home SLAs Settin		ŧ
Template: galaxy-vault.yaml				LUKS passphrase ×	
Description: Deploy Galaxy on a single Virtual Machine installing it from scratch (SLOW). The basic configuration includes CentOS 7, the selected Galaxy flavour, companion software and reference data. Configure, click on the "Submit" button and wait for the confirmation e-			11e99696-e14e-8185-a	4XTxGXFgN18b1wRWx9C8kheEwPBx1OAdp1ieaeWbt	← Back
mail(s) with instructions on how to provide your passphrase (if encryption is enabled) and log in to your new Galaxy instance. If after some hours you do not receive any e-mail please be sure to check your SPAM BOX.			Description: vault test	Cancel	
Instance description			Overview Input values Outp	Du values Links	
Instance description			STATUS CREATE_COMPLETE		
Virtual hardware Galaxy Advanced			CREATED AT 2019-06-24 15:43:00		
Instance flavour			DEPLOYED AT provider-RECAS-BARI		
Small (1 cpu, 2 GB RAM, 20 GB dsk)	-				
CPUs, memory size (RAM), root disk size			A Retrieve LUKS passphrase		
Galaxy instance SSH public key					
Paste here your SSH public key					
Enable encryption					
On					
Encrypt storage					
Storage volume size					
50 GB	7				
Select storage size					
Submit 🗲 Back					

The user can enable the storage encryption using a switch toggle in the Instance "Virtual hardware" configuration tab.

The procedure is completely automated. The storage is encrypted and the User can retrieve his random passphrase from the Instance overview page.

On-demand encryption: the infrastructure

A bash script (now pypi package) is used to encrypt the storage using a random passphrase and then store it on Hashicorp Vault.

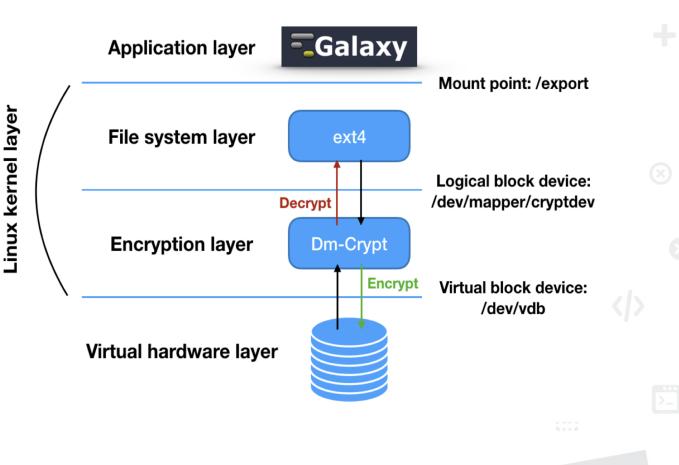
The encryption layer sits between the physical disk and the file system.

Galaxy is unaware of storage encryption.

Galaxy exploits a specific mount point in order to store and retrieve files. Files are encrypted when stored to disk and decrypted when read.

Default encryption algorithm:

- aes-xts-plain64 encryption
- 256 bit key
- sha256 as hash algorithm used for key derivation.

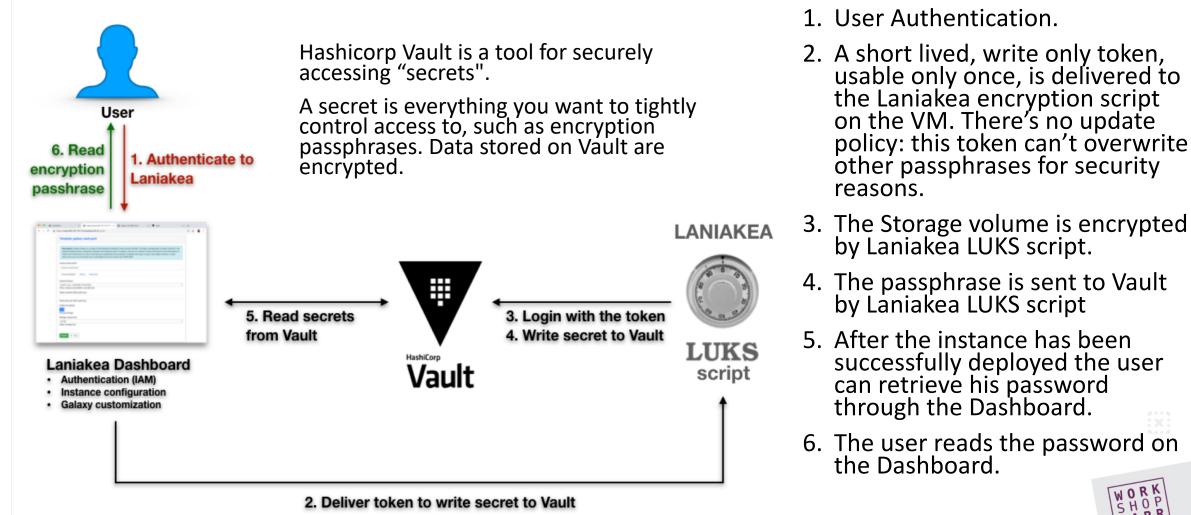


11



On-demand encryption: the infrastructure





2. Deliver token to write secret to Vault

Marco Antonio Tangaro - IBIOM-CNR and INFN-Bari

GARR

The European Genome-phenome Archive



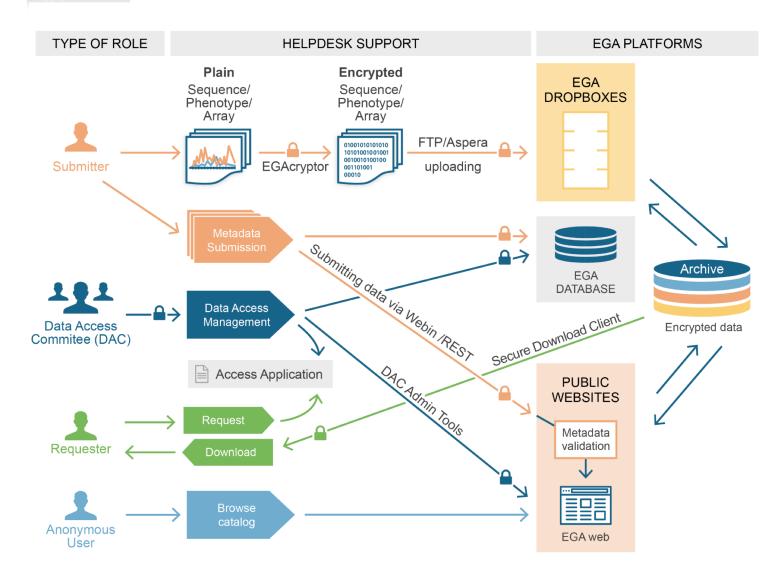
The European Genome-phenome Archive (EGA) is a service for permanent archiving and sharing of all types of personally identifiable genetic and phenotypic data resulting from biomedical research projects.

Data at EGA was collected from individuals whose consent agreements authorise data release only for specific research use to bona fide researchers.

Strict protocols govern how information is managed, stored and distributed by the EGA project.



The European Genome-phenome Archive



Studies and datasets can be browsed by anonymous users.

EUROPEAN

ARCHIVE

GENOME-PHENOME

Data access committee is responsible for approving access to single of multiple datasets.

Data are encrypted. Trusted users exploit a user-specific key to decrypt data.

WOR

G

HOP

Local EGA

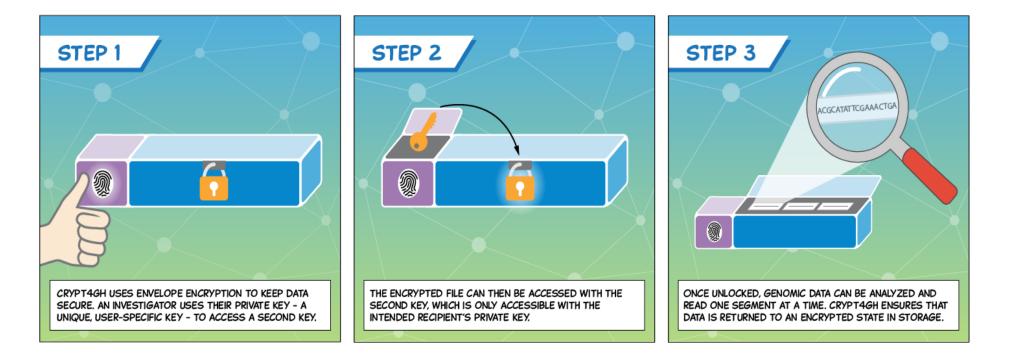


It aims at solving the issue where sensitive data cannot move across borders (cf to GDPR), while public metadata can. Files will be stored encrypted in the Local EGAs located in different countries, while public metadata stays at Central EGA.

- 1. Submitters upload encrypted files into a Local EGA inbox, located in the relevant country.
- 2. Encrypted files are moved from to long-term storage, and information are saved in Local EGA database.
- 3. In the process, each ingested file obtain an Accession ID, which identifies it uniquely across the EGA.
- 4. The distribution system allows requesters to access securely the encrypted files in the long-term storage, using the accession id, if permissions are granted by a Data Access Commitee (DAC).

The European Genome-phenome Archive





The GA4GH Crypt4GH format:

- No re-encryption upon ingestion (only decryption).
- Minimal re-encryption for data distribution.
- Shipping only selected segments for data distribution.

WORK SHOP GARR 2021 NG MAKER

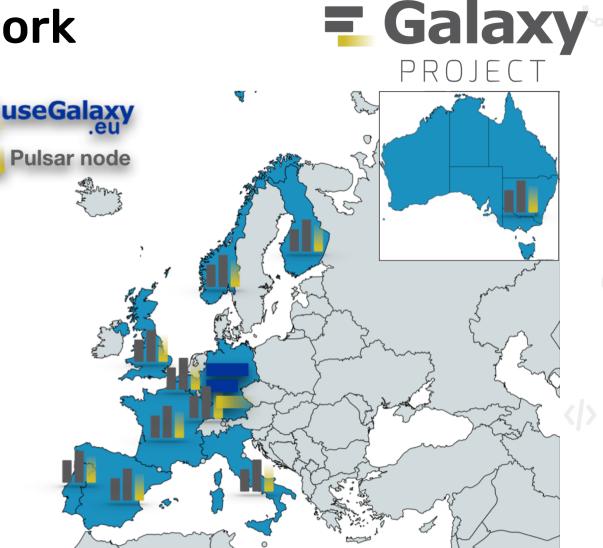
Marco Antonio Tangaro - IBIOM-CNR and INFN-Bari

The European Pulsar Network

The most innovative computing centers across Europe are currently interested to share their remote computation power to support the UseGalaxy.eu load.

- DE, de.NBI cloud
- IT, ReCaS-Bari and GARR Cloud
- BE, Vlaams Supercomputer Centrum (VSC)
- PT, Tecnico ULisboa
- ES, Barcelona Supercomp. Center (INB-BSC)
- NO, University of Bergen
- CZ, CESNET
- FI, CSC
- UK, Diamond Light Source
- FR, GenOuest

https://pulsar-network.readthedocs.io/





The European Pulsar Network



The Galaxy front-end

Galaxy Europe	🚷 Workflow Visualize - Shared Dat	ta 👻 Help 👻 Login or Register 🛛 💼	Using 0 byte				
Tools	COVID-19 Research!	History 记 🗘					
search tools	Want to learn the best practices for the analysis of S	search datasets 🛛 🕄 😒					
1 Upload Data	CoV-2 portal. We mirror all public SARS-CoV-2 dat The Galaxy community has created COVID-19 dedi for more details.	Unnamed history					
Get Data	If you need help submitting your data to public archi sharing your data.	(empty) This history is empty. You can load your own data or get data from an external source					
Send Data							
Collection Operations	"Annone encoders in the world should have free unb						
GENERAL TEXT TOOLS	"Anyone, anywhere in the world should have free, unh every great and enquiring mind across the spectrum of	an external source					
Text Manipulation	anipulation						
ilter and Sort	News	Events					
oin, Subtract and Group	Nov 6, 2021 کر UseGalaxy.eu Tool Updates for	Nov 2, 2021 - Nov 23, 2021 ∰					
ENOMIC FILE MANIPULATION	2021-11-06						
convert Formats	Oct 30, 2021	Nov 8, 2021 - Nov 12, 2021 ∰ C [®] ELIXIR BioHackathon Europe					
ASTA/FASTQ	لا UseGalaxy.eu Tool Updates for 2021-10-30						
uality Control		Nov 11, 2021					
AM/BAM	Oct 23, 2021 UseGalaxy.eu Tool Updates for	Separated data PVC: How it works and potential missed implications					
ED	2021-10-23						
/CF/BCF	Oct 18, 2021 Fraining Infrastructure Feedback	Nov 16, 2021 - Nov 17, 2021 5. NRZ-Authent Expertinnen- und Expertenworkshop					
lanopore	from Dr. Theodora Tsirka						
	Oct 16, 2021	Nov 18, 2021 OPEN CHAT					

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



Marco Antonio Tangaro - IBIOM-CNR and INFN-Bari

The European Pulsar Network





Pulsar allows a Galaxy server to automatically interact with remote systems, ensuring job and provenance information are correctly exchanged.

- Compute: submits and manages jobs. -
- Data: stages user data. -

Data needs to be moved from Galaxy to the remote compute nodes, impacting negatively on the job's execution time in case of large amounts of data.



Provides reference data and Galaxy dependencies (read only).



The Cern-VM FileSystem

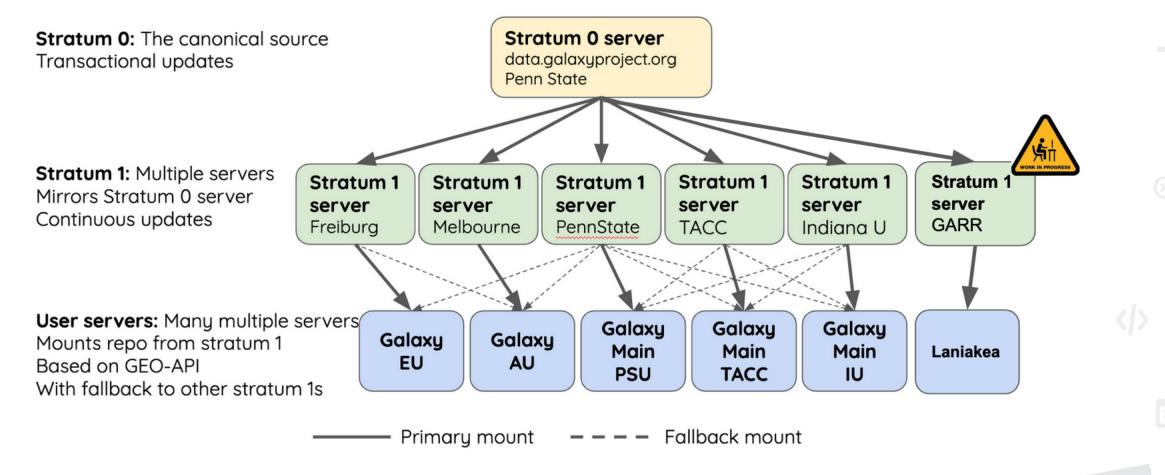


- Needed a method of sharing reference data, e.g. genomic sequences, across countries efficiently
- **CVMFS** is an efficient method for read only data sharing between systems
 - Originally designed for distributed software installation at CERN
 - \circ $\,$ Turns out it's really useful for read only data sets as well
 - HTTP-based, firewall friendly
- All nodes of Galaxy Main get their reference genomes and indices from CVMFS
 - \circ $\,$ Shared via mirroring and caching across the country $\,$
- It's also really useful to share data **globally**
 - The **usegalaxy.*** and **Laniakea** initiatives has taken full advantage of this.



The Cern-VM FileSystem







The Pulsar Network: optimizing resource usage

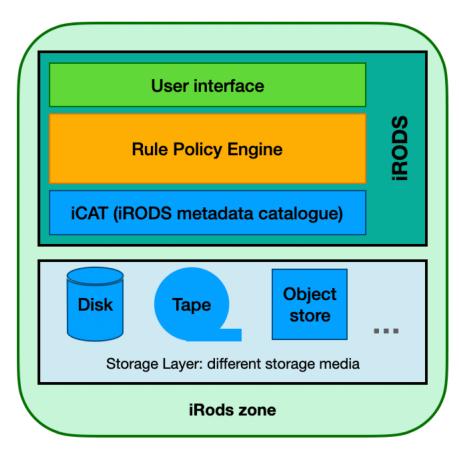


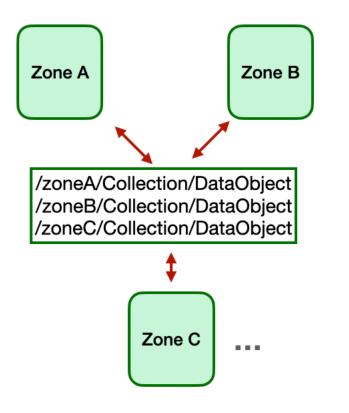
This work is still in early stage development. There is an ELIXIR Implementation plan and other initiatives at EOSC level working on this.

We are still evaluating technologies to support the Pulsar Network and also funding opportunities.



The Pulsar Network: optimizing resource usage





- Independent Administrative domains
- Users can access shared data and metadata in other zones
- No passwords
 needed,
 authenticated to
 local zone

Distributed file systems like iRODS (or similar solution) are keeping track of objects (files, metadata, etc.) and their locations.

WORK

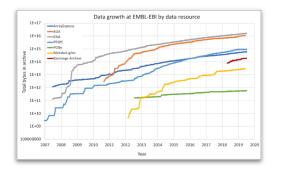
The Pulsar Network: optimizing resource usage

- The job-staging is dependent on the specific tool and analysis and can become the dominating part of the job runtime.
- A network-wide caching layer can accelerate job-staging times and thus job runtimes.
- Objects can be located in different physical locations and can be replicated into other locations before a job starts.
- Adding iRODS or similar solution support would allow replicating data wherever it's needed on the filesystem level without changing logic at the application level. However, this would require that all partners support a single distributed file system, which in turn would make it harder to contribute to the network.
- In case files are already available in a Pulsar destination, the staging step will take this into account.



Conclusions

Data rapid growth, distributed across Europe and often under GDPR.

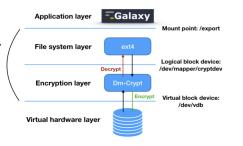






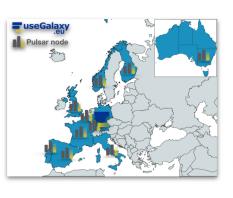
On-demand solution for rapidly store and analyse data, also in case of sensitive data.





Distributed Storage (and compute) solution across Europe.







Thank you for your attention!

Contacts

- ELIXIR: elixir-europe.org
- ELIXIR Italy: elixir-Italy.og
- Head of Node: g.pesole@ibiom.cnr.it
- Technical Coordinator: federico.zambelli@unimi.it
- Compute platform : giacinto.donvito@ba.infn.it

Backup

Marco Antonio Tangaro - IBIOM-CNR and INFN-Bari

WORK SHOP GARR 2021

Net

MAKERS

ELIXIR Italy compute platform upgrade

- A multi-institution, distributed and federated compute and storage infrastructure
- Providing most advanced technologies in the fields of Cloud and HPC
 - Able to support the most modern Artificial Intelligence and Big Data analysis solutions
- Flexible and expandable in the future aiming to support future bioinformatics use cases
- The overall infrastructure will leverage about:
 - 27'000 Cpu/cores
 - About 20Pyte of disk storage
 - 20 NVIDIA V100 GPU
- Distributed over 4 different sites in Italy