

Data Management S2: Experimental data (1)-Storage

Monday 27/11/2023 - 14:00-16:00 (CET)

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EUROPEAN INFRASTRUCTURE FOR PLANT PHENOTYPING

General objectives: Overview of data management for plant phenotyping - focus on FAIR data

Session 2

Experimental Data:

Storage & Data Management Policies



Overview

- Quick review of Session 1
- Data Storage Introduction
- Cloud Computing
 - Data Storage Services
 - Data processing Services
- Data Management Policies
 - DMP Data Management Plan
 - GDPR General Data Protection Regulation



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Phenotyping experiments : Dealing with a big mess!

- Complex & massive data: source, type, operator, scale, transformations, etc.
 - > Breeding, genomic, weather, soil, observations, sensors, internet, etc
- Bad habits dealing with this mess
 - > Dispersed, unstable and highly customized excel sheets
 - > Personal storage solutions
 - > No description on data (Metadata)
 - > Data processing steps and provenance not defined/tracked
 - > No link, no structure, no context



Phenotyping experiments : Dealing with a big mess!

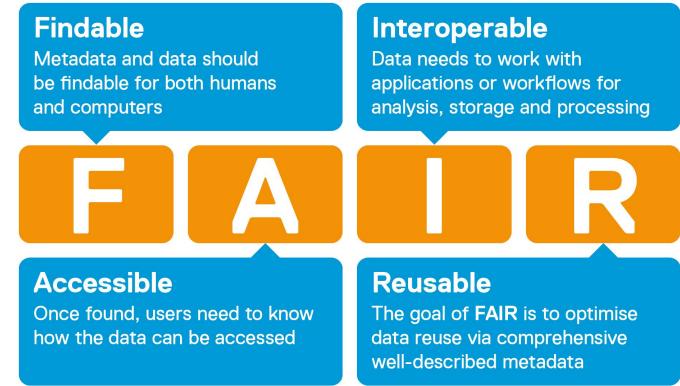
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EMPHASIS

Zed excel sheets

Phenotyping data : No stress, we're going to make it!

Understand, adopt and apply FAIR principles



https://scibite.com/



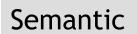
FAIR data

Data structure \Rightarrow store, retrieve, process data and Implement good practices

Based on two key elements:



- Standardized & unambiguous identification
 - Strategy and appropriate tools





- Based on Ontology:
 - Data understanding (definition)
 - Data organization



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FAIR data

MetaData in phenotyping experiments

Metadata is: Data 'reporting'

- WHO created the data?
- WHAT is the content of the data?
- WHEN were the data created?
- WHERE is it geographically?
- HOW were the data developed?
- WHY were the data developed?





What is Metadata



MetaData management in 6 levels



1: Description

No need to any special tool \Rightarrow Only human readable



description2014Bp45.txt

Id : http://www.inrae.fr/PechRouche/2014Bp45
Plot Beausoleil
Site = Pech Rouge
Position = « R4-P5 »
Carignan
The plot is supervising by Jean
planted : 2014

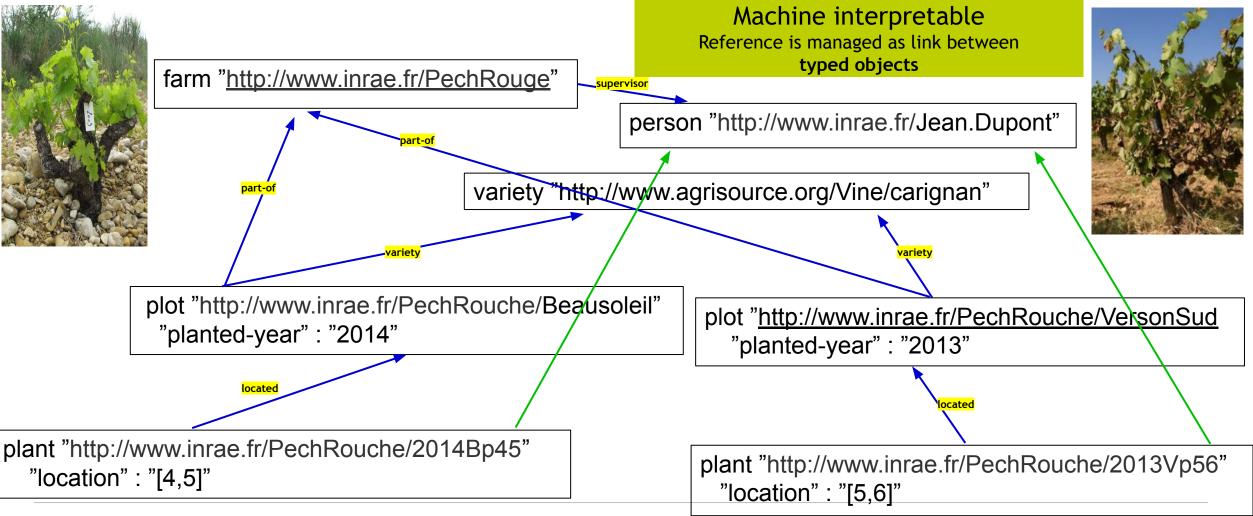
description2013Vp56.txt

ID : http://www.inrae.fr/PechRouche/2013Vp56 Verson Sud Farm = Pech-Rouge Location = [5,6] Carignan The plot manager Jean Dupont planted : 2013



MetaData management in 6 levels

6: Description+Syntax+Vocabulary+Link+ Inference (reasoning)



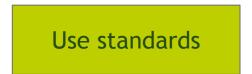


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MetaData management in 6 levels

6: Description+Syntax+Vocabulary+Link+ Inference (reasoning)

- Semantic resources
 - Ontology / Thesaurus
 - Rules
 - Standard term sets
- Specific tools
 - RDF (Subject-Predicate-Object)
 - Language (OWL / SWRL)
 - Graph DB systems
 - Reasons





Common framework to share and reuse data



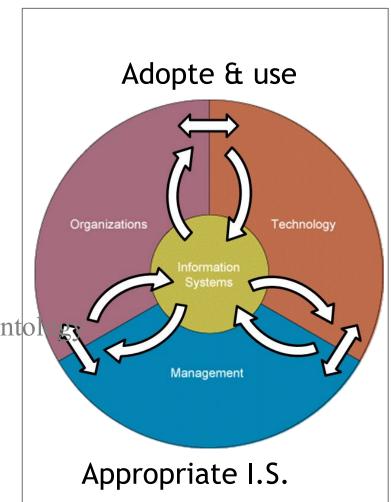
FAIR data: What do we need?

- Data base management system \Rightarrow SGBD, NoSQL, RDF storage
- . Representation language \Rightarrow XML or JSON
- Use standards \Rightarrow MIAPPE, BrAPI
- Access (Web pages, Web Services) \Rightarrow BrAPI
- Knowledge representation (ontology, thesaurus, taxonomy): \Rightarrow Crop Ontology
- Analysis and visualisation tools (R, python,)



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Data Storage - Introduction

Data Challenge

- Context: more and more data!
 - Cheap storage capacity and high speed network
 - e.g. 1 Gigabyte price : \$400K in 1980, \$10K in 1990, \$10 in 2000,
 now less than \$0.01
 - > Heterogeneous devices, simulations, machine learning, Internet data sources (Open, collaborative, etc) are available

Make data valuable!

- Knowledge discovery
- Decision support
- Artificial Intelligence and machine learning (predict, detect, recognize, diagnostic, etc)

Share and Reuse Data



Data Storage - Introduction

Data Challenge

- Volume: massive data and exponential growing size
 - Hard to Store, Manage & Analyze
- Variety, Vocabulary and complexity (differents sources, scales, disciplines, semantics, schema,

format, etc)

- Hard to understand, combine & Integrate
- Velocity : rate of data generation
 - Have to be processed on-line
- Veracity, Validity, Variability, Vulnerability, Volatility, Visibility, Visualisation, Vagueness, etc.
- VALUE



Data storage - Introduction

Phenomics data : Massive & shared data

- No personal computer
 - ⇒ Managing physical servers needs:
 - Admin group with specific skills
 - > Flexibility (variations in data production)
 - ➤ Specific rooms & facilities



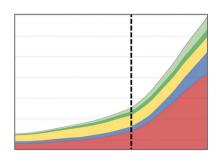


Data Storage - Introduction

Phenomics data : Massive & shared data

But exponential growth of data requires continuous change for physical servers:

- a lot of effort for administrator group
- difficult because discontinuous resources
- and harder to manage

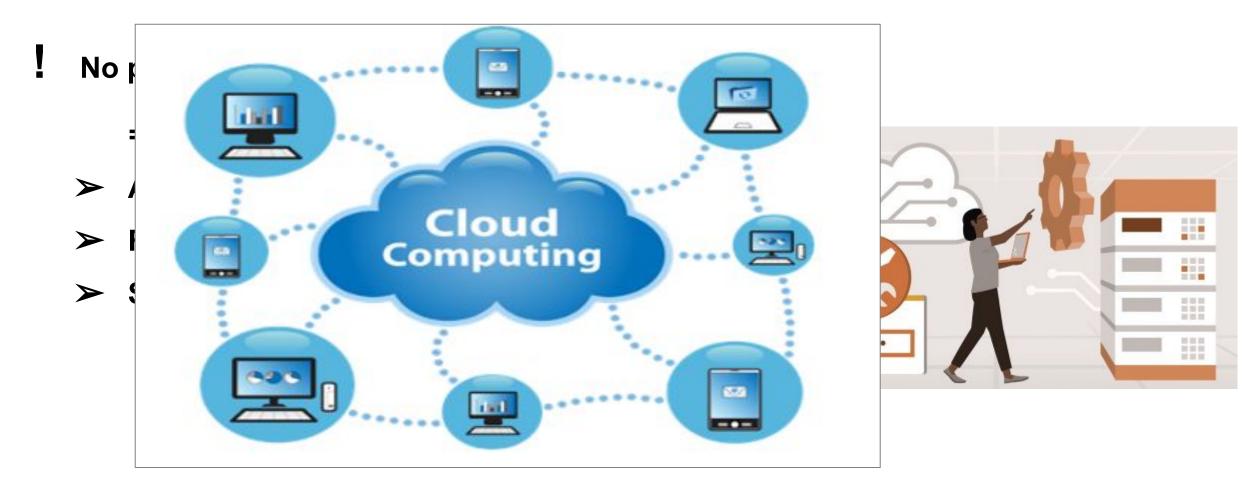






Data Storage - Introduction

Phenomics data : Massive & shared data





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Questions & Survey



On-demand: A consumer can provision (anticipate and use) computing capabilities (storage, VM, etc.) as needed automatically without requiring human interaction with a provider

Network access: Capabilities are available over the network and accessed through standard and use by light clients (phones, tablets, laptops, etc.)

Resource pooling and elasticity: resources are dynamically assigned and reassigned according to consumer demand.

Capabilities can be elastically provisioned and released to scale rapidly with demand. To the consumer, the capabilities available for provisioning often appear unlimited and can be appropriated in any quantity at any time

Measured service: Cloud systems automatically control and optimize resource use. Resource usage can be monitored, controlled, and reported





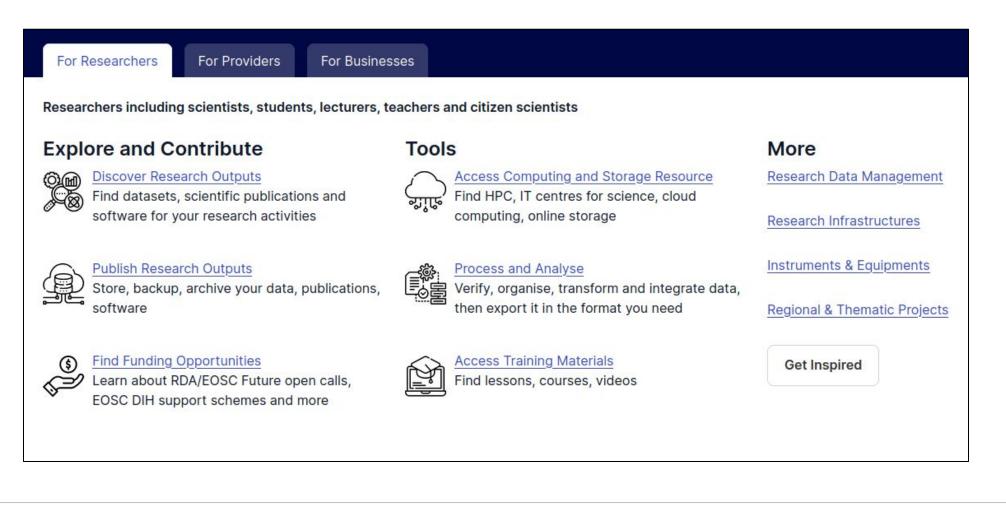
Relevant services for data management

- > Storage
- > Backup, Archiving
- > Virtual Machine
- > High Performance Computing (HPC), High Throughput Computing (HTC)
- > DataHub
- > Virtual Research Environment
- **Coordination of cloud services for research: EOSC**

Academic European providers: EGI, EUDAT

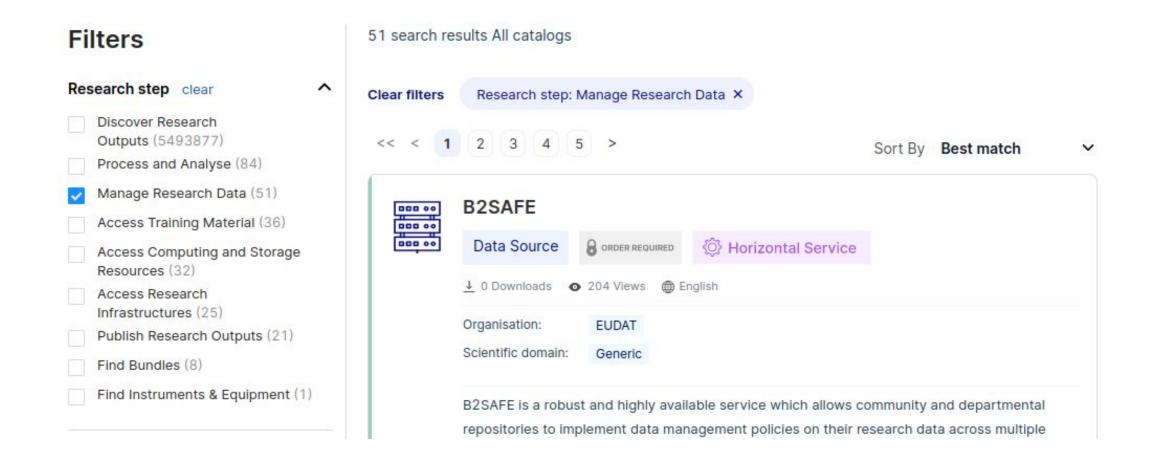


EOSC: European Open Sciences Cloud



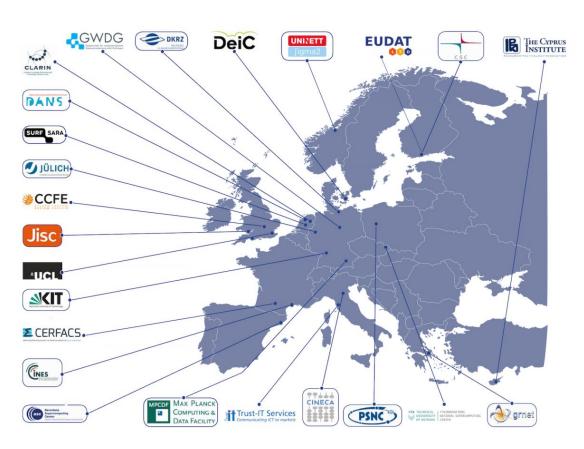


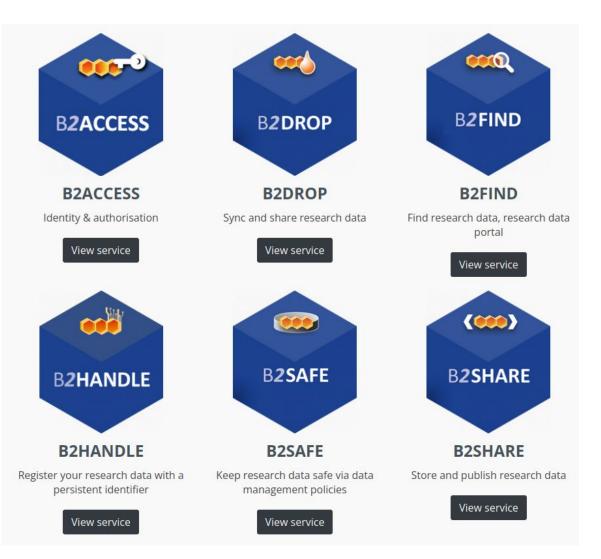
EOSC: Data management services





EUDAT services







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EGI services

ACOnet

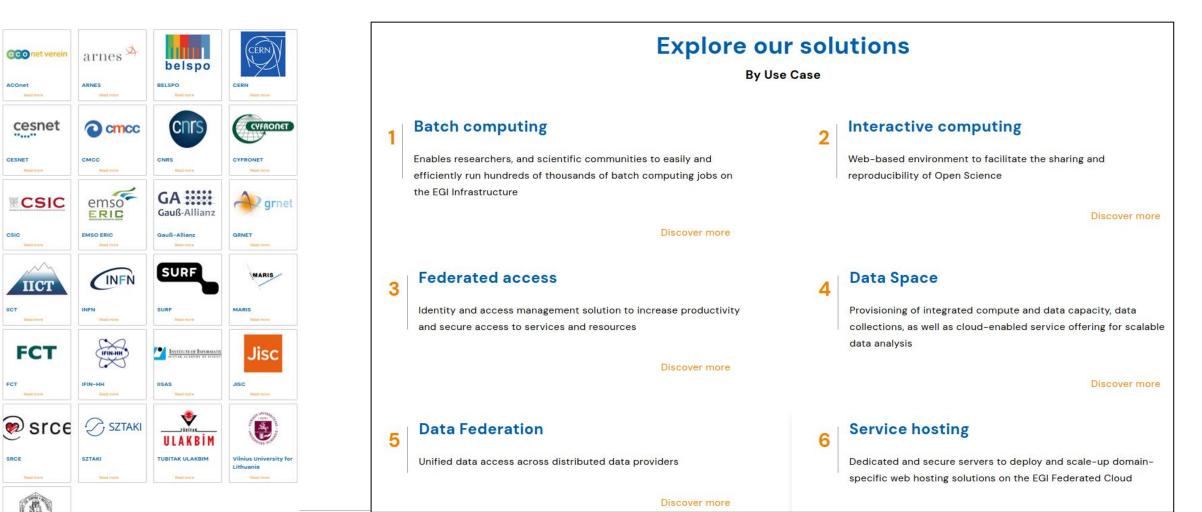
CESNET

CSIC

ECT

SRCE

LIKIM

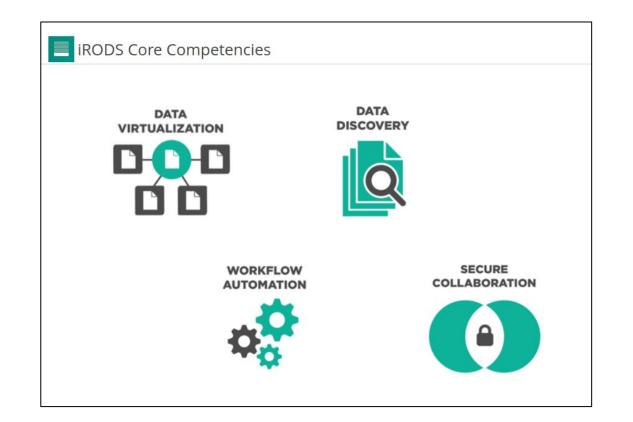


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Storage Service

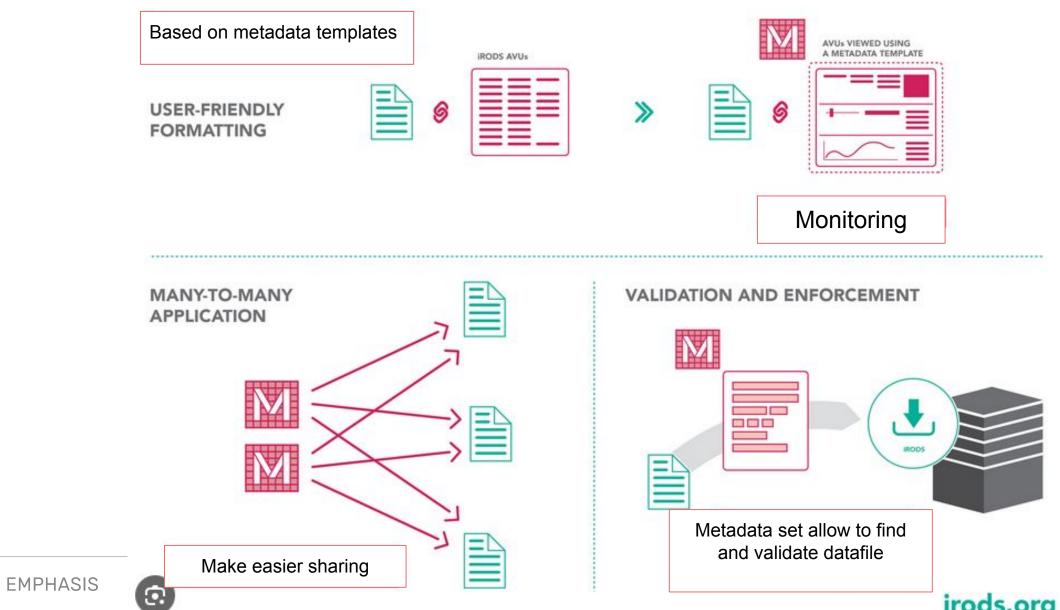
Technological solutions for data storage: iRODS, OneDATA, S3

- Access Authentication, Authorization, Revocation
- Description Standards for discovery, compliance
- Integrity Confidence that nothing has changed
- Replication Multiple copies, multiple locations
- Availability If things are down, nothing else matters
- Migration Hardware changes, format changes
- Recovery Robust plans for when things go wrong
- Provenance Full record of all related activity
- Retention Deleting data on a defined schedule





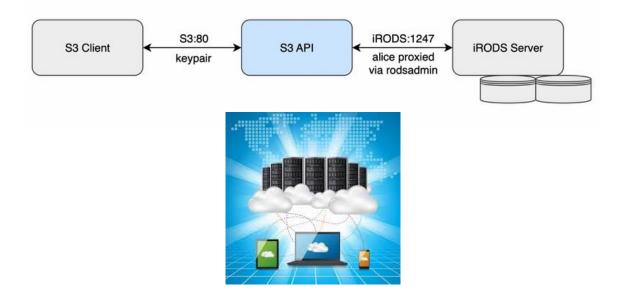
Storage Service



Storage Service

Technological solutions: iRODS, OneDATA, S3

• Tools are available for the interoperability between technologies



Implementation and use via API, Web interfaces, virtual hard disk



EUROPEAN INFRASTRUCTURE FOR PLANT PHENOTYPING

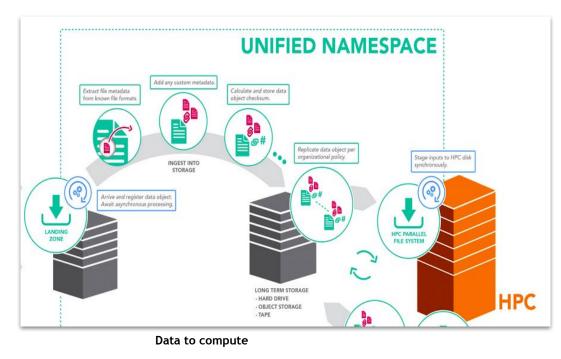
Questions?

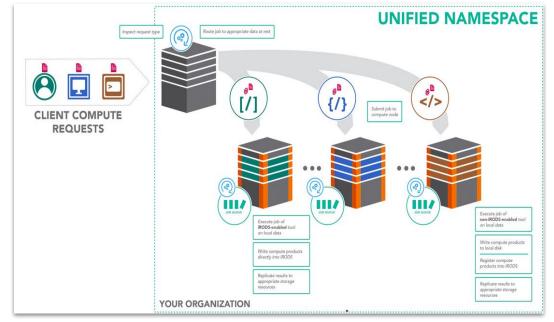


Storage & Computing Considerations

Multiples data access patterns according different usages

- Data to compute (classic approach) : Transfer data to computes nodes and execute tasks
- Compute to data : Distributes and execute computing tasks near the data nodes





Compute to data



Computing Services

HPC -> rather focus complex computing

HTC -> rather focus a large number a data (Data-Based same operation on different data)







Computing Services

HPC	HTC
High-Performance Computing	High Throughput Computing
use of multiple computer processors in order to perform complex computations parallelly.	parallelly executes a large number of simple and computationally independent tasks.
running large-scale, complex, and computationally intensive applications that need significant resources and memory.	running a large number of tasks that does not require a large amount of memory and resources.
designed to provide speed for large tasks.	designed to increase the number of tasks
Centralized management	Distributed management
Try to reduce the risk of data loss and data corruption	Do not affect any other running processes.
Few users are running together	Scale horizontally for simple tasks .
Complex decision support, weather forecasting .	Bioinformatics or Phenomics.



Questions?



Datahub Service

A datahub homogenizing data and possibly serving data in multiple desired formats with features such as de-duplication, quality, security, and standardized set of query services. Datahub is more structured than data lake.

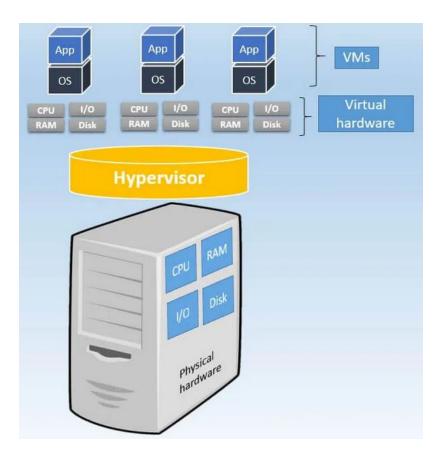
• Unique (virtually) data source





Virtual Machine

- Virtual machine (VM) is the emulation of computer systems
- Provides same functionalities as physical machine
- Several virtual machines on one physical machines
- Can run different Operating Systems
- Hardware abstraction





Virtual Machine

Physical services	Virtual Machines
Large upfront costs	Small upfront costs
Physical servers and additional equipment take a lot of space	A single physical server can host multiple VMs, thus saving space
Has a short life-cycle	Supports legacy applications
No on-demand scalability	On-demand scalability
Hardware upgrades are difficult to implement and can lead to considerable downtime	Hardware upgrades are easier to implement; the workload can be migrated to a backup site for the repair period to minimize downtime
Difficult to move or copy	Easy to move or copy
Poor capacity optimization	Advanced capacity optimization is enabled by load balancing
Doesn't require any overhead layer	Overhead is required for running VMs
Running stable services and operations which require highly productive computing hardware Running multiple services for multiple users, which plan to e	
EMPHASIS EUROPEAN INFRASTRUCTURE FOR PLANT PHENOTYPING 38	



Insurance against human error, technical failure, disaster

Protect your current work

Incremental (difference management)

Overwritten

Restore process





Archive Service

Build an historical record

Valuable content to keep

Permanent record

Eco friendly (low energy)





Backup vs Archive

	Backup	Archive
Definition	COPY -> PASTE	CUT -> PASTE
Purpose	Disaster Recovery Accidental Data Loss Compliance	Storage Cost Compliance Analytics
Performance	Significantly drops the performance	Drastically improve the performance
Retention	Short-term	Long-term
Cost	More costly day by day	Significantly save storage cost



Questions?



Data Infrastructures

Data Challenge

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VALUE



Data Management Challenge : Velocity

- Green House platforms produce tens of thousands images/day \Rightarrow (200 days/year)
- Field platforms produce tens of thousands images/day \Rightarrow (100 days/year)
- Omic platforms produce tens of Gbytes/day \Rightarrow (300 days/year)
- Approaches:
 - Scientific Workflow (consists of an orchestrated and repeatable pattern of tasks of information processing (depicted as a sequence of operations)
 - Galaxy
 - Cloud workflow services
- Allows to share and to store data treatment

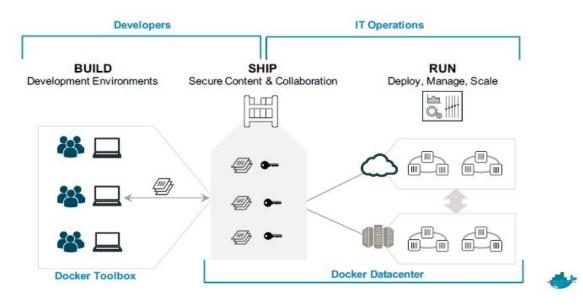


Container Service

Container : Code and dependencies (libraries, DB) and configuration inside a single package

Container service:

- Provide an easy-to-use and reproducible execution environment
- Simplified integration, deploy and management of applications
- Deploy scalable and secure applications
- Allow developers to focus on user features, not on infrastructure management







A virtual research environment (VRE) or virtual laboratory is an online system for research collaboration

Can be based on virtual desktop Standard features:

Forum, Data Publication

Data exploration, Data visualisation

Set of tools for data analytics

Set of discipline-specific tools



Virtual Research Environment

to access, share and collaborate





Data storage - Conclusion

- On-demand infrastructure and Elasticity
- Virtualization technologies
- Many services available: complementaries with overlaps

Coordination of metadata and data services requires DMP



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Questions & survey



How to formalise your data management?

In a research project or structure

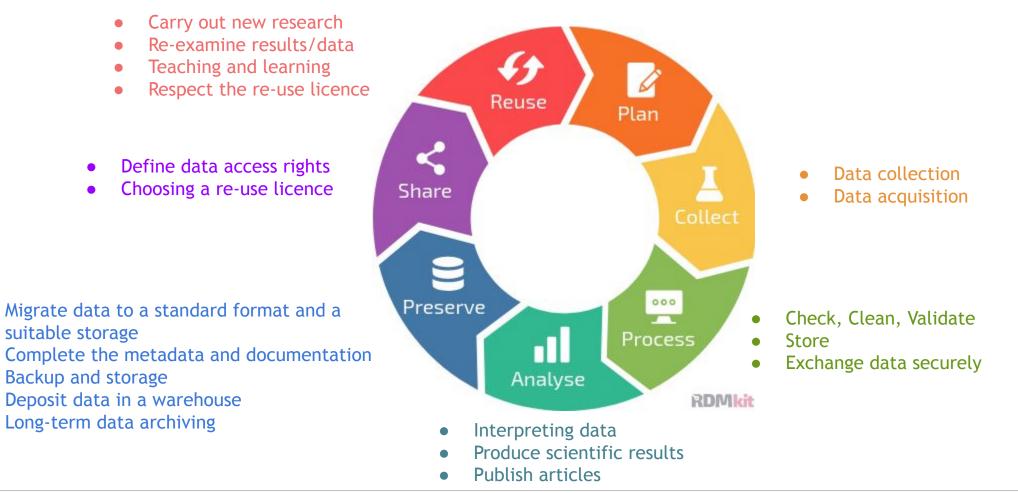
You need to describe:

- Various sources and types of data
- Various processing steps applied to data
- Storage resources and duration
- Data protection, rights of use
 - ⇒ That's why we need **Data Management Plan**!



What is a Data Management Plan (DMP)?

A DMP is a **document** that describes how the data of a research project or structure will be managed throughout its lifecycle.



What is it for?

Implementing **best practice**, respecting the **FAIR principles**

- Ensuring the **reproducibility of experiments** by describing the data and how it was obtained
- Enabling data to be understood and therefore re-used
- Avoid loss of data by appropriate storage
- Establish the **roles and responsibilities** of each party
- **Respect the law and individuals** by clarifying the legal and ethical framework (link to GDPR)
- Clarify re-use rights and sharing arrangements



How to set it up?

- A pragmatic approach
 - Simple to understand, implement, evaluate and develop
 - Text document for the time being, but "actionable machine" versions are appearing
- Models available
 - Beware of national specificities!
 - Frameworks defined by supervisory bodies (National Institutes, Universities, etc.), funders (HORIZON 2020, etc.), computing/storage centres (IN2P3), etc.
 - More or less rich information (INRAE framework = 40 questions, ANR framework = 15 questions, H2020 framework = 9 questions)
 - Little or no specificity about the type of data
 - The format and proposed aids change, but the content remains the same!
- Tools to create DMP:
 - DSW (Data Stewardship Wizard): <u>https://ds-wizard.org</u>
 - B2SAFE: https://www.eudat.eu/b2safe
 - French tool DMP OPIDoR: <u>https://dmp.opidor.fr</u>
 - RDMkit https://rdmkit.elixir-europe.org/data_life_cycle



Project DMP vs. research structure DMP

Project DMP

- Funded or unfunded research project
- Specific scope and fixed duration
- Mandatory

Research structure DMP

- Research platform, Collective Scientific Infrastructure (EU, CRB, Platforms, etc.), Research Infrastructure
- Broader scope and indefinite duration
- Not compulsory, voluntary for the moment
- Distancing practices
- Identification of areas for improvement
- Formalisation of our requirements and commitments: linked to quality approach
- Centralisation of information
- Facilitate the creation of other DMP



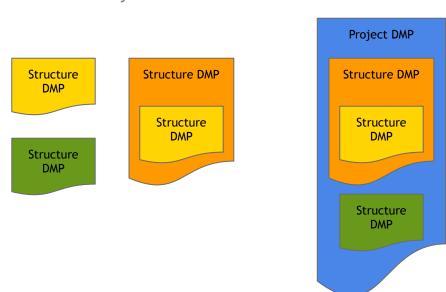
Project DMP vs. research structure DMP

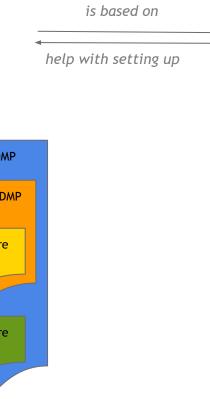
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Mandatory

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DMP - Phenotyping data issues





Questions?



Personal Data: a specific case

What is General Data Protection Regulation (GDPR)

- G General
- D Data
- P Protection
- R Regulation

European Union law implemented 25th May 2018

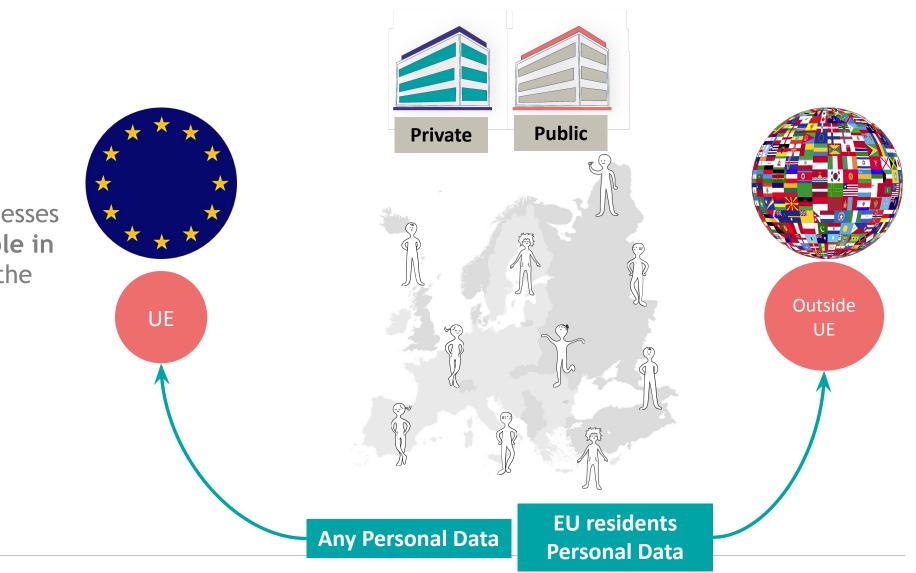
European reference text on personal data protection for EU residents.



GDPR - General Data Protection Regulation

Who is involved?

Any organization that processes the **personal data of people in the EU** must comply with the GDPR.





GDPR - General Data Protection Regulation

EU National Data Protection Authorities (DPA)

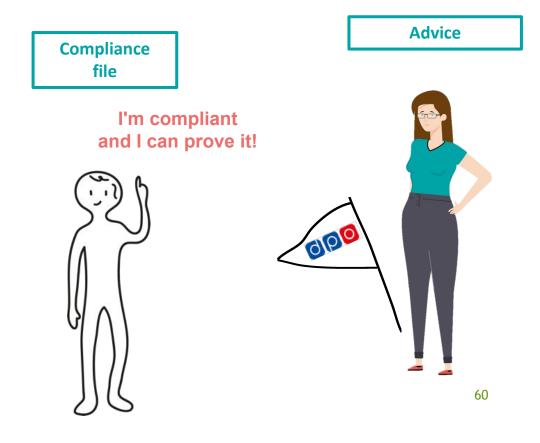
- DPAs are **independent public authorities** that supervise, through investigative and corrective powers, the application of the data protection law.
- As in the case of the DMP, the implementation of the GDPR has **specific national characteristics**
- DPA provide expert advice on data protection issues and handle complaints lodged against violations of the General Data Protection Regulation **and the relevant national laws.**
- There is one DPA in each EU Member State :

https://edpb.europa.eu/about-edpb/about-edpb/members en



Data Protection Officer (DPO)

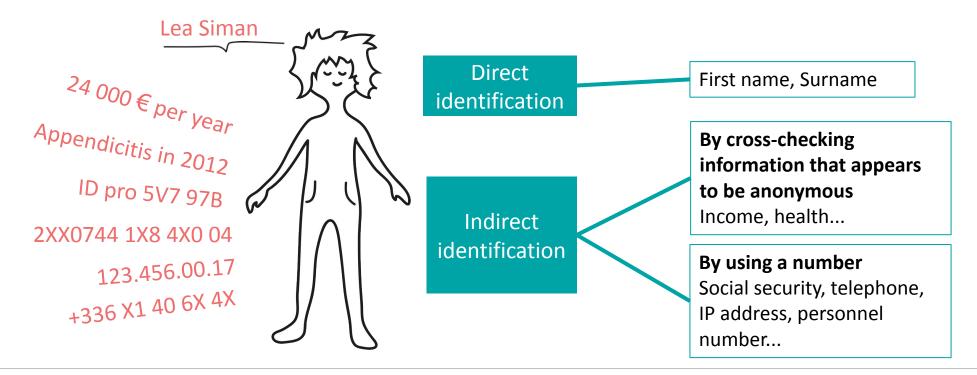
- DPO handles personal data and GDPR compliance
- DPA must be informed and have easy access to DPO contact details
- DPO must be provided with the **necessary resources** to carry out his duties effectively and **independently**.
- "The controller and the processor shall ensure that the data protection officer is involved, properly and in a timely manner, in all issues which relate to the protection of personal data." (GDPR Article 38)



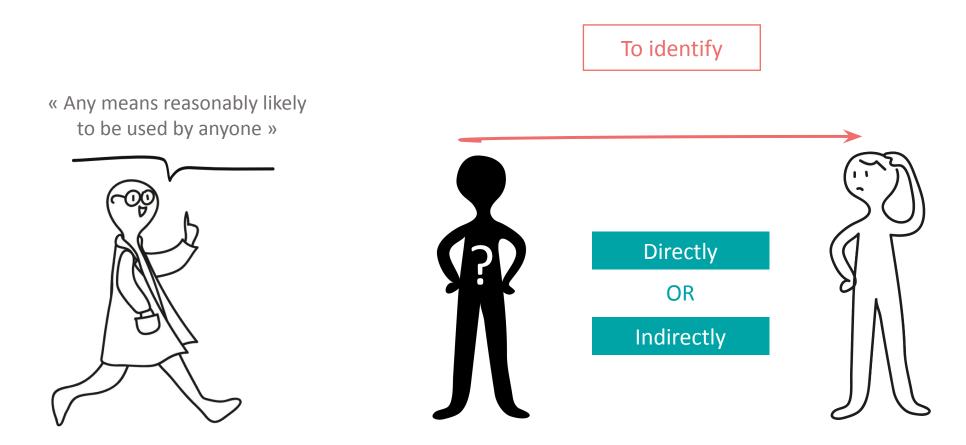


Personal data (PD)

• **Personal data** – Personal data is any information that relates to an individual who can be directly or indirectly identified. Names and email addresses are obviously personal data. Location information, ethnicity, gender, biometric data, religious beliefs, web cookies, and political opinions can also be personal data. Pseudonymous data can also fall under the definition if it's relatively easy to ID someone from it.



Personal data (PD) - Determining whether a person is identifiable



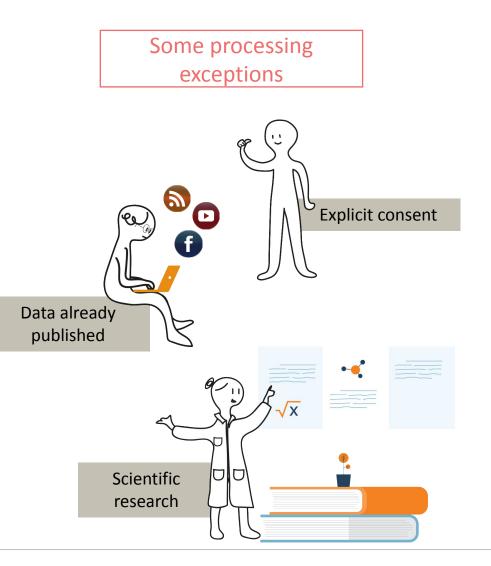


Personal data (PD) - Sensitive data

Prohibited from processing

- Racial or ethnic origin
- Political opinions
- Philosophical or religious beliefs
- Trade union membership
- Health
- Sex life
- Genetic and biometric data

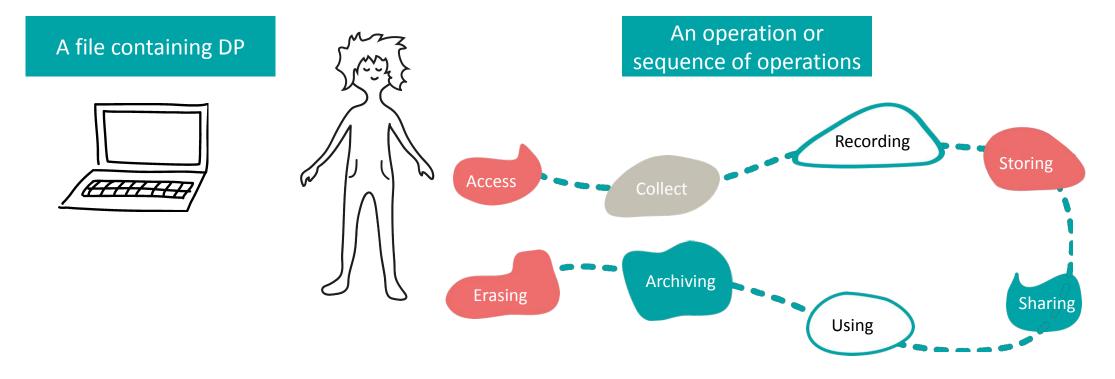
(for identification purposes)





Data processing

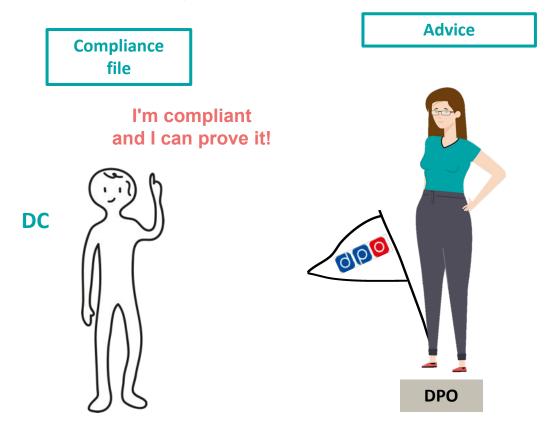
• Data processing – Any action performed on data, whether automated or manual. The examples cited in the text include collecting, recording, organizing, structuring, storing, using, erasing... so basically anything.



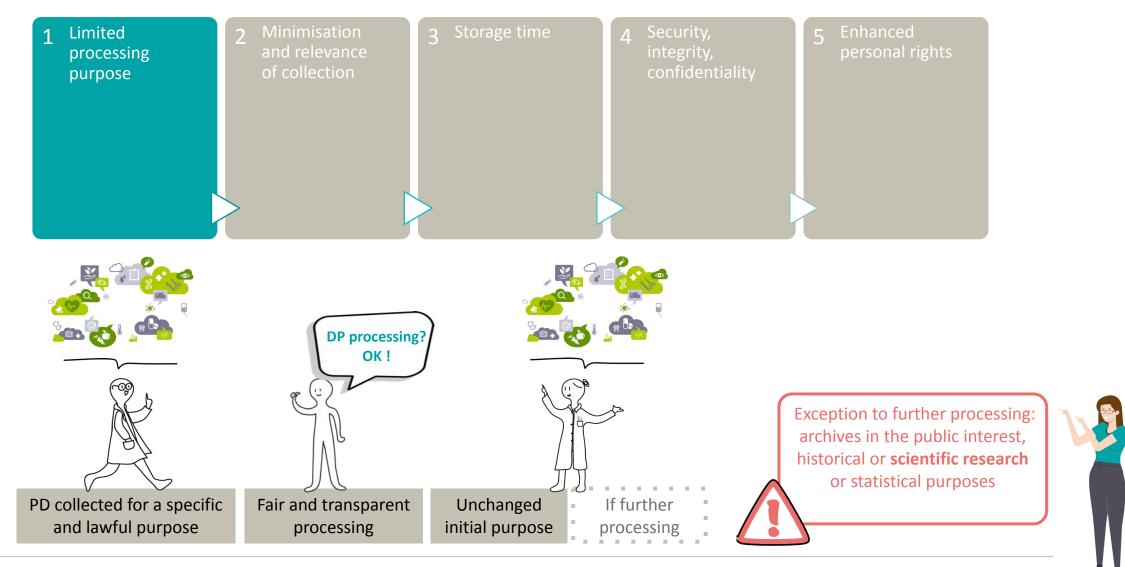


Data controller (DC)

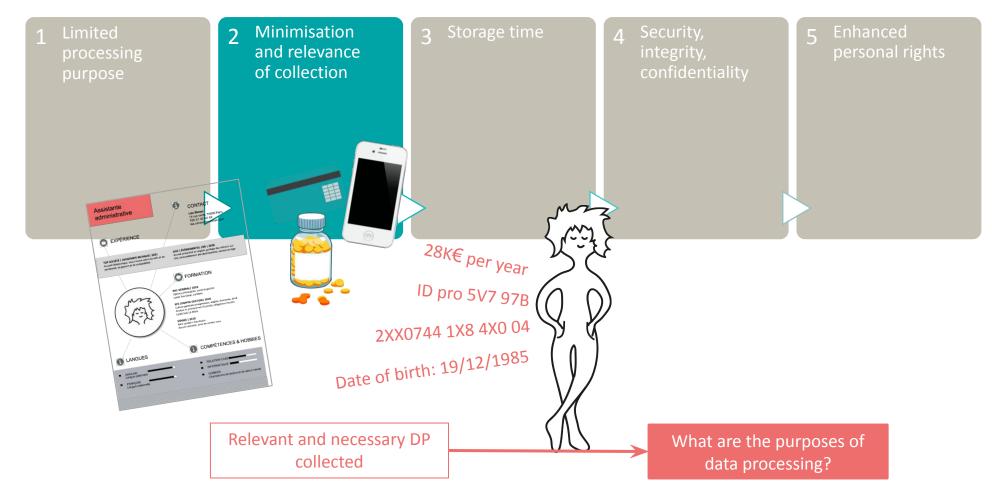
• Data controller – The person who decides why and how personal data will be processed. If you're an owner or employee in your organization who handles data, this is you.



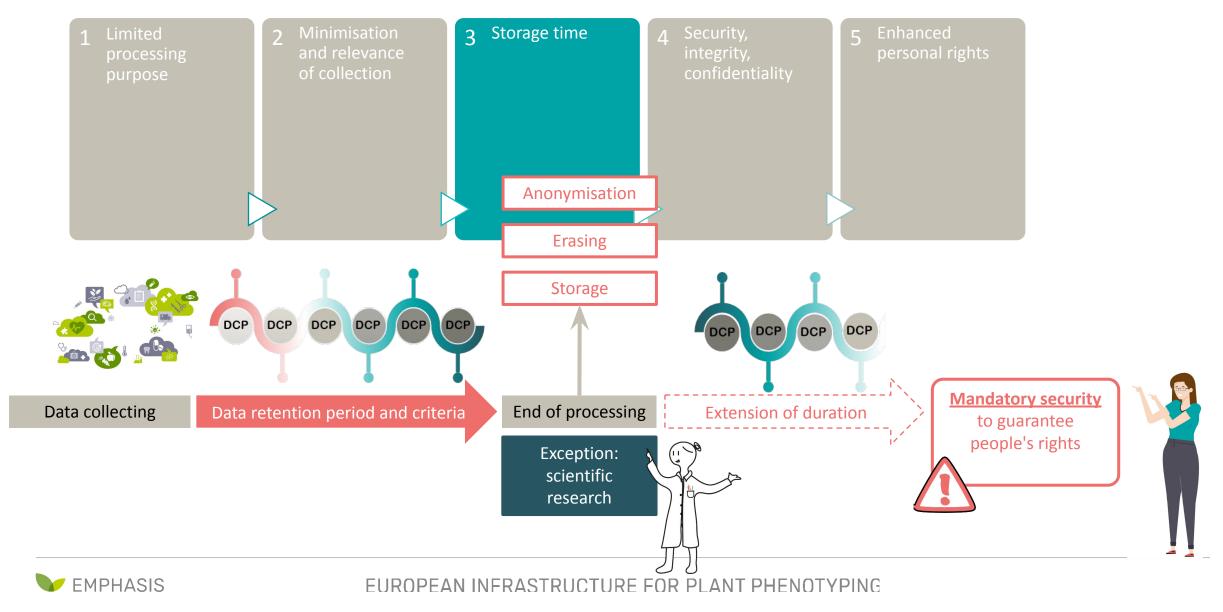


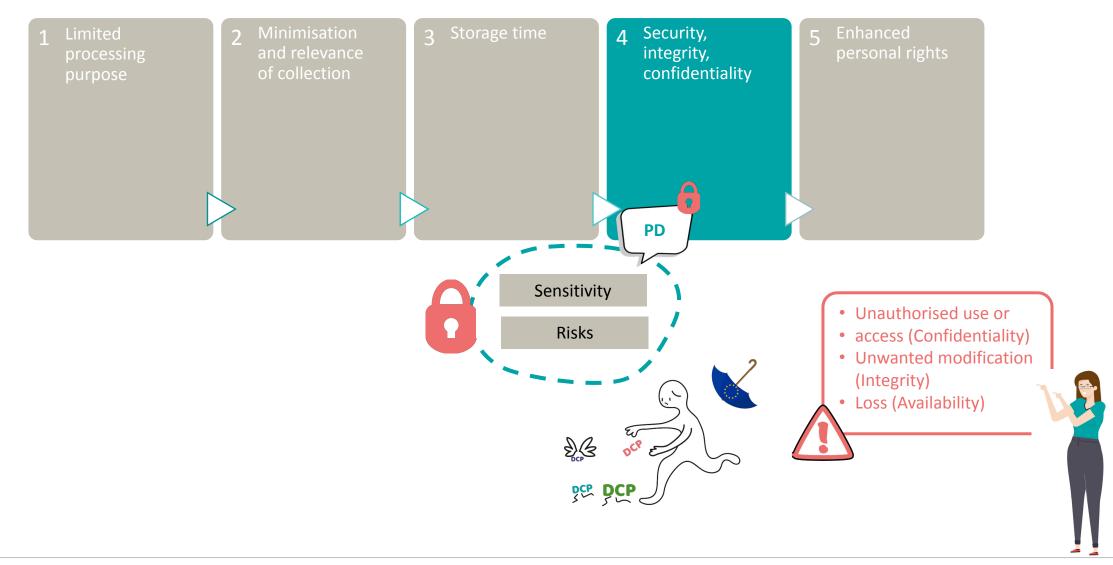




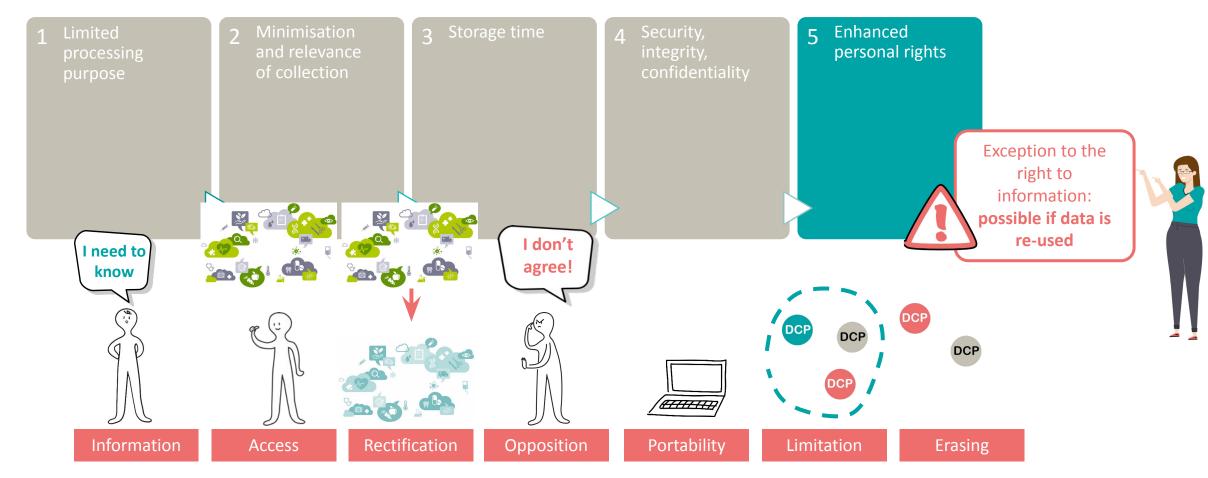








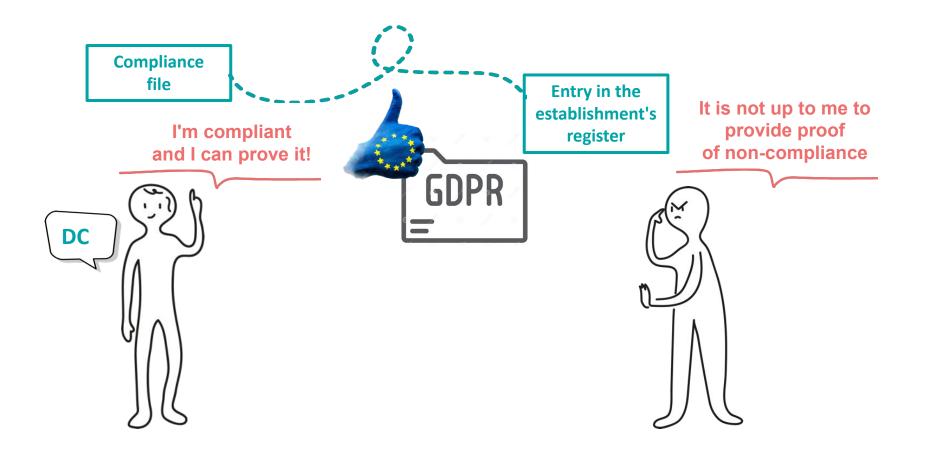






GDPR Main Concepts: more responsibilities

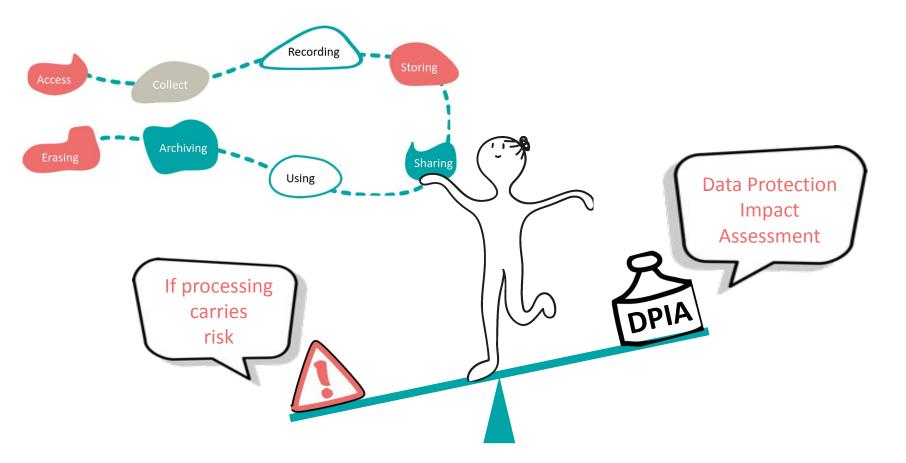
Accountability principle: Change in practices, not in principles





GDPR Main Concepts: more responsibilities

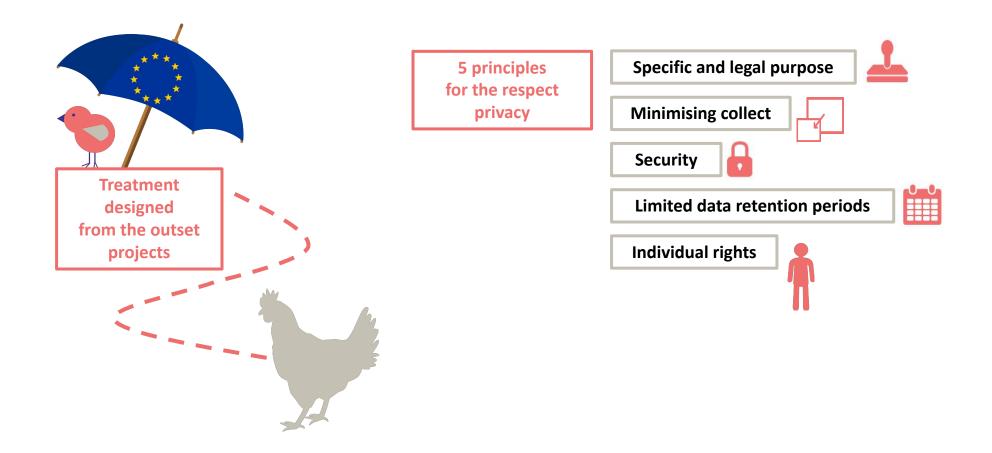
Privacy Impact Assessment





GDPR Main Concepts: more responsibilities

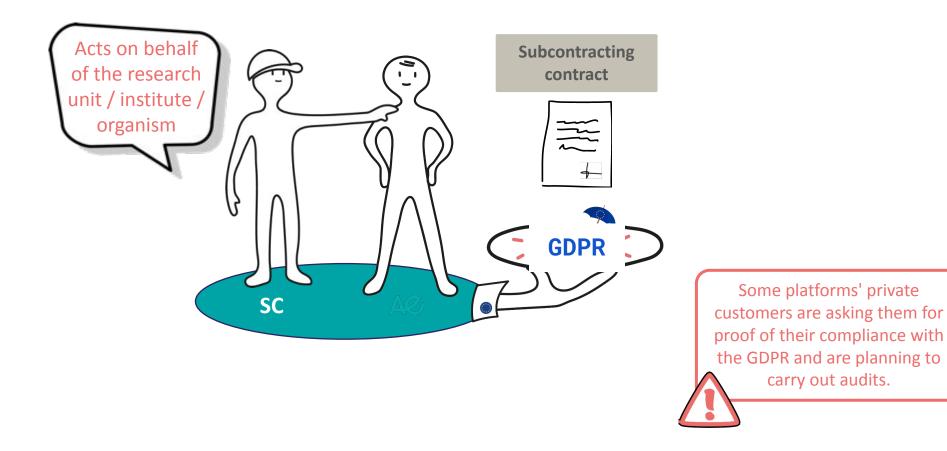
Privacy by design





GDPR Main Concepts: more responsibilities

New status for subcontractors









Subject		Financeurs Margino acceleration Margino ac
1 Role of partners	Who handles PD and how? Diagram the flow of data between partners	Partenaire 0 Poconsenerse a devotes s advectes Processeners s advectes Processeners s advectes Processeners s advectes Processeners s advectes Processeners s advectes Processeners s advectes Processeners proces processeners proces processeners proces
Check partners' nationality	If appropriate: OK If not: contract complementary to the consortium agreement	
Joint liability agreement between partners	Even between European partners	X X X
Verification of the place of residence of the people whose data you are going to process	If outside Europe, check whether there is a national law on personal data: to be checked with local partners	





	Subject		Please note!
2	Legal basis for processing PD	Depending on the purpose and partners (public, private): consent, public interest G mission, legitimate interest	Different rights
3	Ethics committee	Certain types of project (particularly research involving humans) may need to be submitted to an ethics committee. Some journals also require a favourable opinion from the committee before publishing an article.	
4	People selection	Transparent inclusion/exclusion criteria	
5	Nature of PD handled and level of impact (1 / no risk 4 / high risk)	Possible justification? Remember to use "categories" for answers	
6	Reuse of pre-existing PD	From which partner? Will you need to <u>re-inform people or not</u> ?	BMI > 3



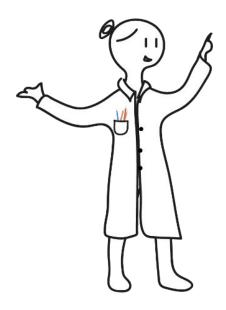


SubjectQuestions et actions7Tools usedWhat collection tools? For storage? Processing? Is it subcontracted? Read the GCU/GTC Does it involve a transfer outside the EU (subcontractor's parent company outside the EU or appropriate country)?8IT securityTo be adapted according to the nature of the data. If level 3 to 4: risk analysis Storage, access procedure9Retention period and future of dataWhat is the useful life until future publications? What happens to the data (anonymisation / archiving / destruction)?10Information and people's rightsIf consent: proof and withdrawal procedure to be provided for Generic alias for exercise of rights			
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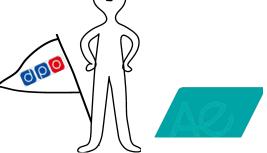








Subject	Questions et actions	,
Registering the project	Internal process for each partner	000
Compliance	Variable duration - 1 month for simple cases Take into account the complexity of the project and the nature of the risks to people. 	









GDPR - Research Project Good Practice



Sujet	Questions et actions	R
Open data	 PD may not be made available in open data unless : the persons concerned have given their consent, a legislative or regulatory text allows it (such as a decree on the publication of certain administrative documents without anonymisation), the data is rendered anonymous, so it is no longer personal, but there will be the inevitable loss of all the criteria enabling individuals to be identified, particularly by cross-referencing. 	(REB
The project has a website	Don't forget the legal notices, terms and conditions and information on cookies.	
Non-permanent staff	Get them to sign a <u>confidentiality agreement</u>	
Transcription / translation of interviews	In addition to the order form for the transcription/translation service, it is preferable to have an GDPR rider signed.	



Non-compliance GDPR: What are the risks?

Examples of offences:

- Treatment despite opposition of the individual
- Diversion of purpose
- Lack of impact assessment
- Failure to cooperate with the supervisory

Image impact	Financial impact	Conformity impact
Public Warning	Criminal and	Stop treatment
	administrative	(=stopping
Loss of confidence	fines	research)
as a partner		
establishment	Compensation for	Criminal
	damages	conviction
Loss of appeal to		
volunteers		

Legal action possible via group actions





Research project - Questions to ask...

... not only for personal data!!

GDPR requires us to ask ourselves questions about personal data...

... but these questions are important to ask for all project data!!



Conclusion

FAIR Data, DMP, GDPR...

- If you are thinking about FAIR data, you are building your DMP
- If you're thinking about your DMP, you're in the process of setting up FAIR management.
- In any case, the DMP is a mandatory part of all projects, so you might as well do it properly.
- The GDPR is a legal formalisation designed to protect the rights of individuals, but most of the questions and points of attention raised are of interest for all types of data.



Thank you for your attention!



OpenSILEX Team - <u>http://opensilex.org/</u>

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