



# Plant Cyber-infrastructures: wheatIS & French elixir node

Hadi Quesneville

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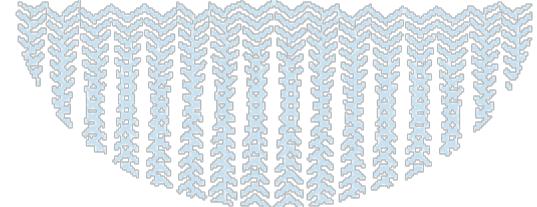
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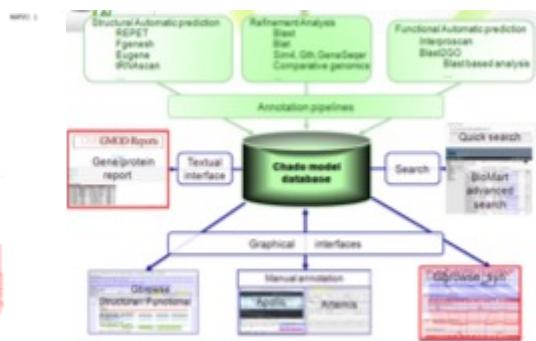
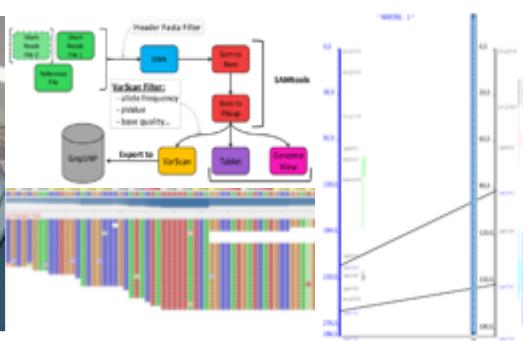
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# Plant Cyber-infrastructures: WheatIS & French Elixir node

Hadi Quesneville

Biatalent, May 29, Poznan



# What is a cyber-infrastructure



A data infrastructure

- Collect/Store/Manage
- Integrate/Visualize
- Explore/Mine
- Process

Serve a community

- Plant scientists
- Wheat research
- ...

Large scope

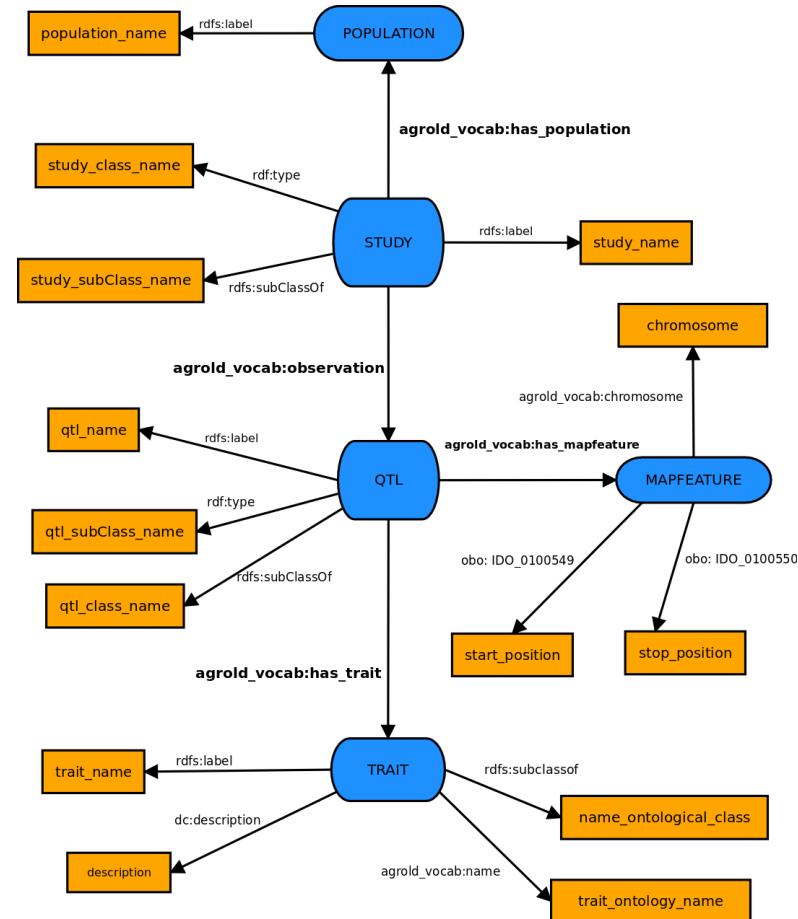
- Several institutes
- Country
- Continent
- Worldwide
- ...

# Plant scientific challenge



**Scientific challenge**  
Study of Complex interactions

*Phenotype = Genome  
x Environment  
x Management  
practices*





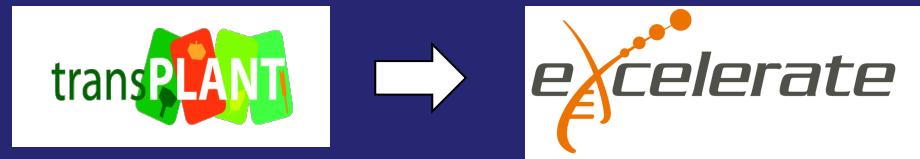
# Some cyber-infrastructure under construction



**WheatIS:** the information system of the International Wheat Initiative



**Elixir:** The European Bioinformatics infrastructure



**CyVerse:** The US cyberinfrastructure (iPlant)



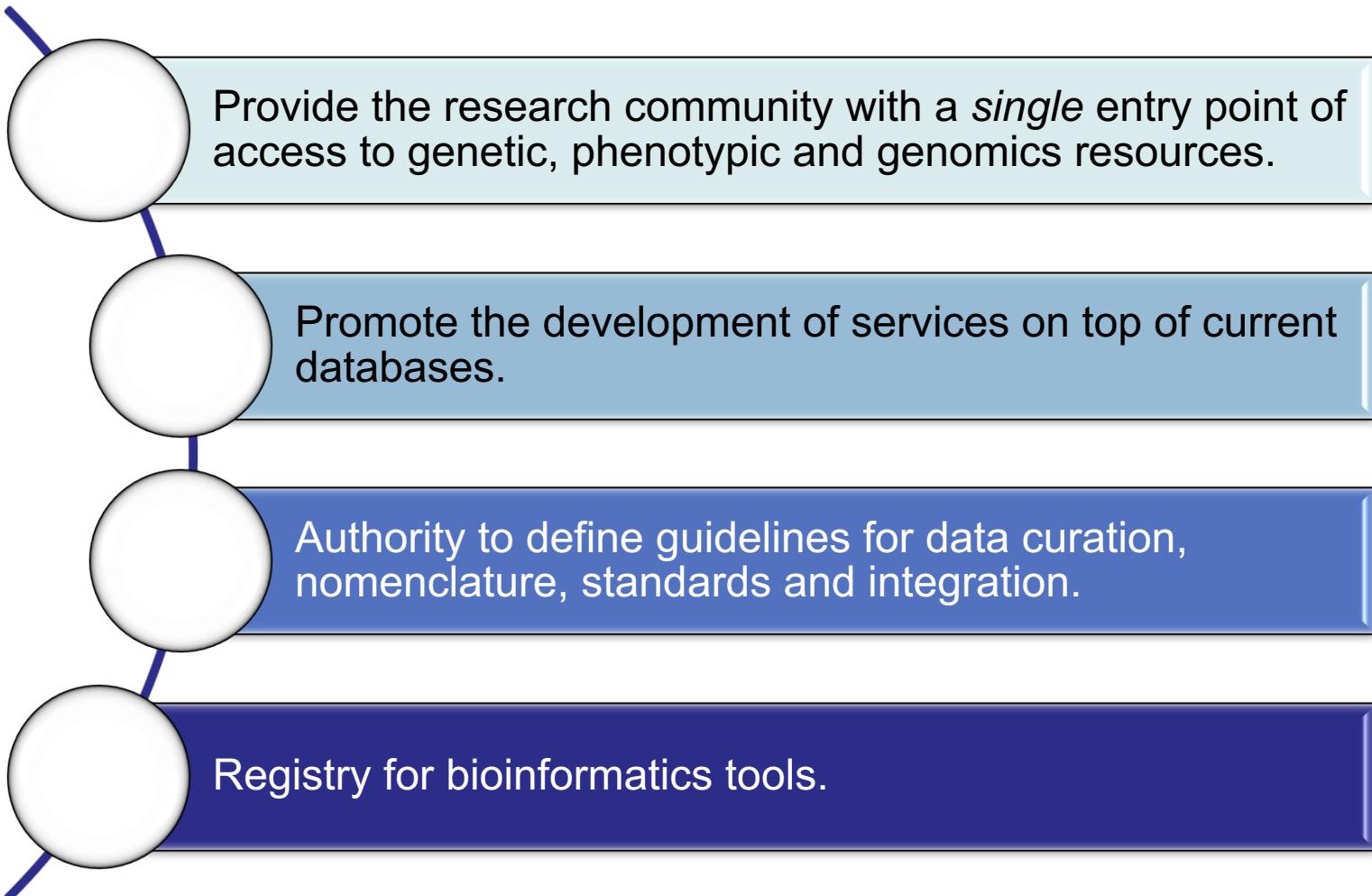
**IFB:** French Bioinformatics Institute French Elixir node



**Phenome/FPPN/EPPN:** Information system for French Plant Phenotyping Network



# Cyber-infrastructure goals

- 
- Provide the research community with a *single* entry point of access to genetic, phenotypic and genomics resources.
  - Promote the development of services on top of current databases.
  - Authority to define guidelines for data curation, nomenclature, standards and integration.
  - Registry for bioinformatics tools.



# IFB/Elixir – Plant Bioinformatics

# The French Plant bioinformatics node

(33 FTEs)



**Genetics and genomics resources  
for plants and crop parasites**  
**(INRA)**



**Genomic resource for southern  
and mediterranean plants.**  
**(CIRAD, INRA, IRD)**

## Contributors (data, tools, and expertise)



**Resources for plants,  
symbionts and pathogens**  
**(INRA,CNRS)**



**Marine biology analysis**  
**(CNRS, UPMC)**



**Arthropods for  
Agroecosystems**  
**(INRA)**

# Services



- analysis
- genomics annotation
- software hosting
- data repository
- data integration
- database design
- software engineering

A photograph of a man in a green and yellow checkered shirt and dark trousers, carrying two large, heavy bundles of harvested wheat on his shoulders. He is walking away from the camera on a narrow, paved path through a lush, green, hilly landscape. The sun is low, creating long shadows and a warm glow.

# WheatIS – An information system for the wheat international research community



# WheatIS Expert Working Group



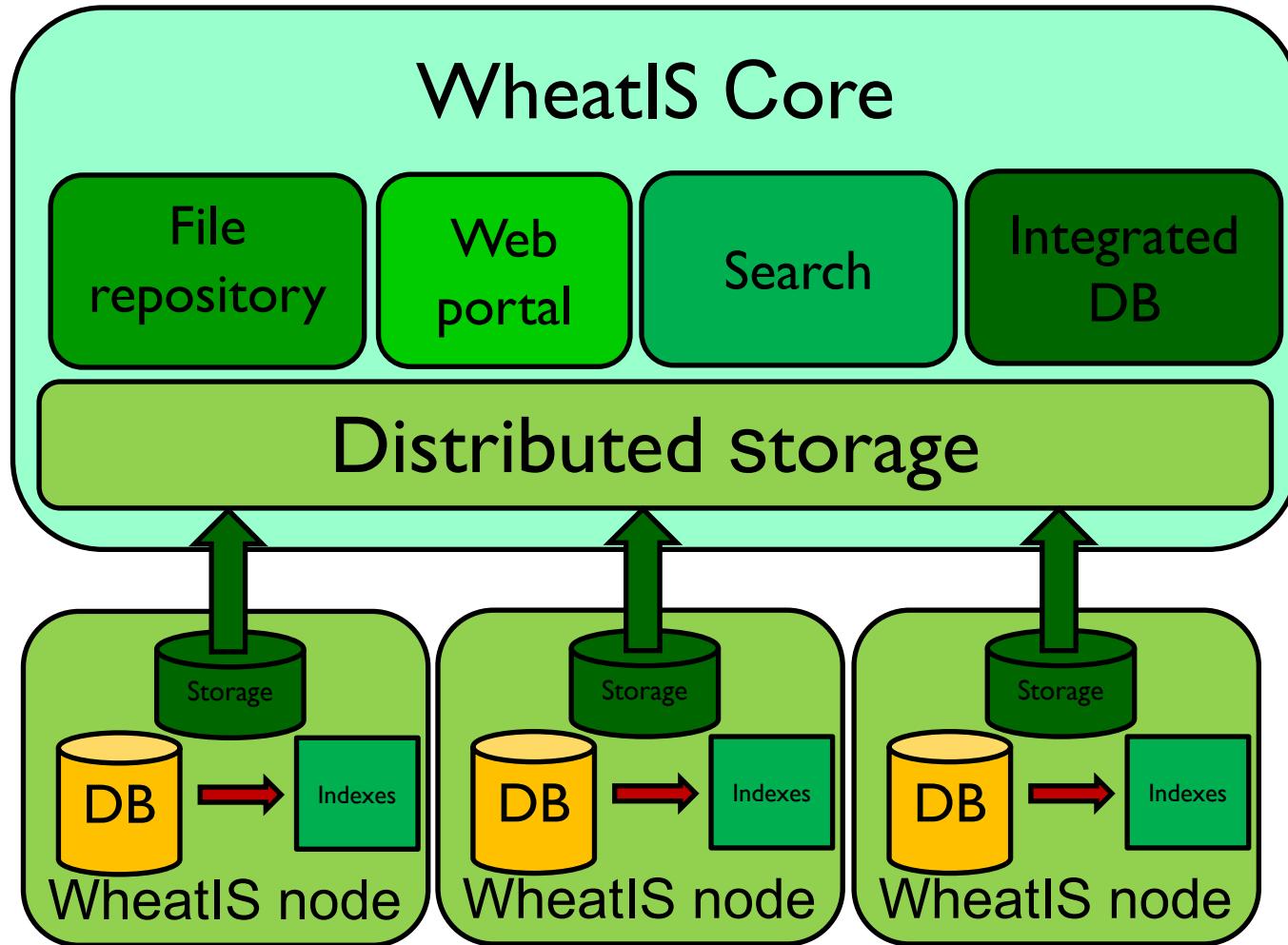
- Build projects
- Build infrastructure
- Report to the Wheat Initiative



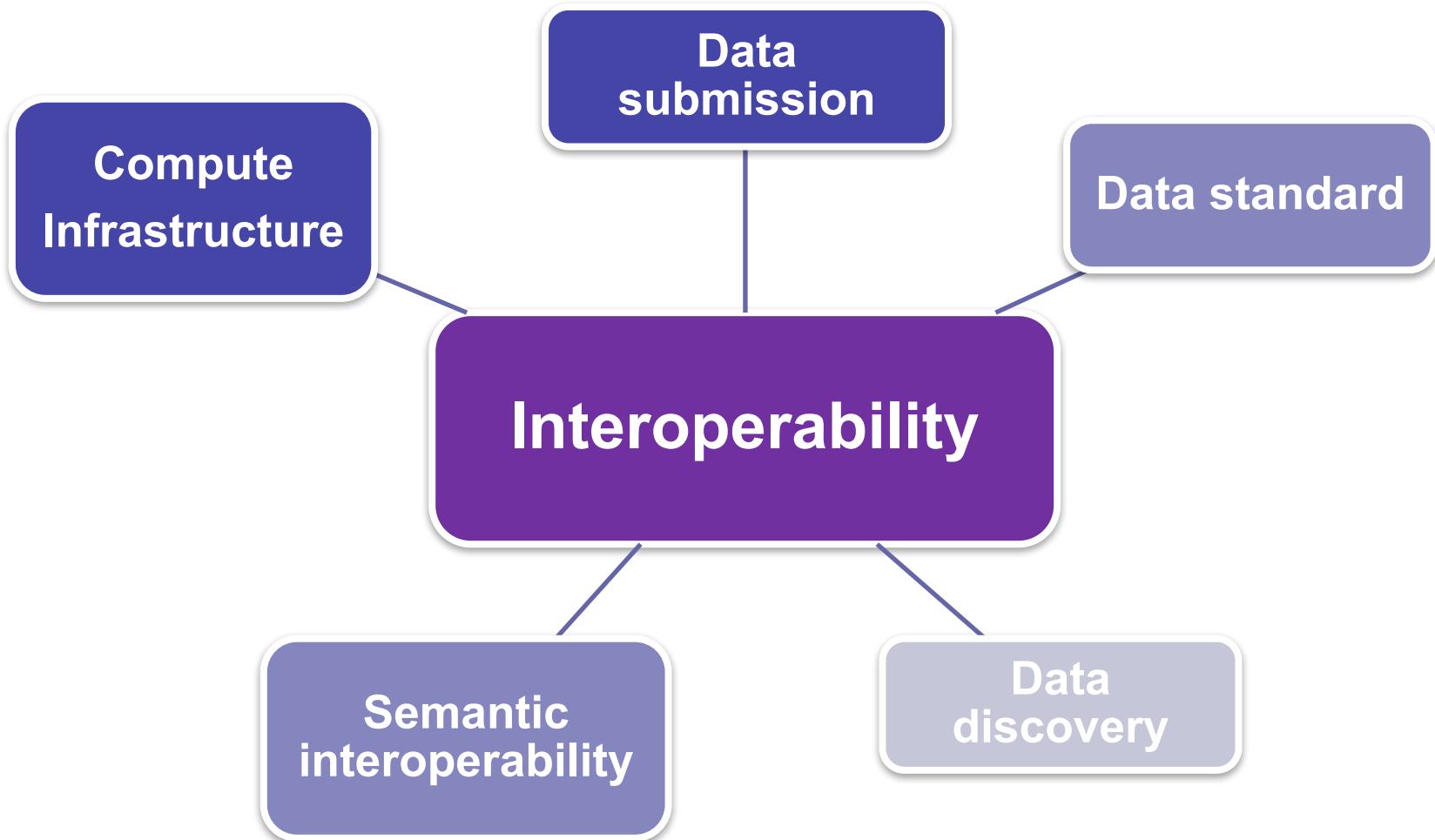
# WheatIS nodes (#12)



# WheatIS Architecture



# Cyber-infrastructures key issue



# Data must follow FAIR principles

force11.org

## To be Findable:

- F1. (meta)data are assigned a globally unique and eternally persistent identifier.
- F2. data are described with rich metadata.
- F3. (meta)data are registered or indexed in a searchable resource.
- F4. metadata specify the data identifier.

## To be Accessible:

- A1 (meta)data are retrievable by their identifier using a standardized communications protocol.
  - A1.1 the protocol is open, free, and universally implementable.
  - A1.2 the protocol allows for an authentication and authorization procedure, where necessary.
- A2 metadata are accessible, even when the data are no longer available.

## To be Interoperable:

- I1. (meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.
- I2. (meta)data use vocabularies that follow FAIR principles.
- I3. (meta)data include qualified references to other (meta)data.

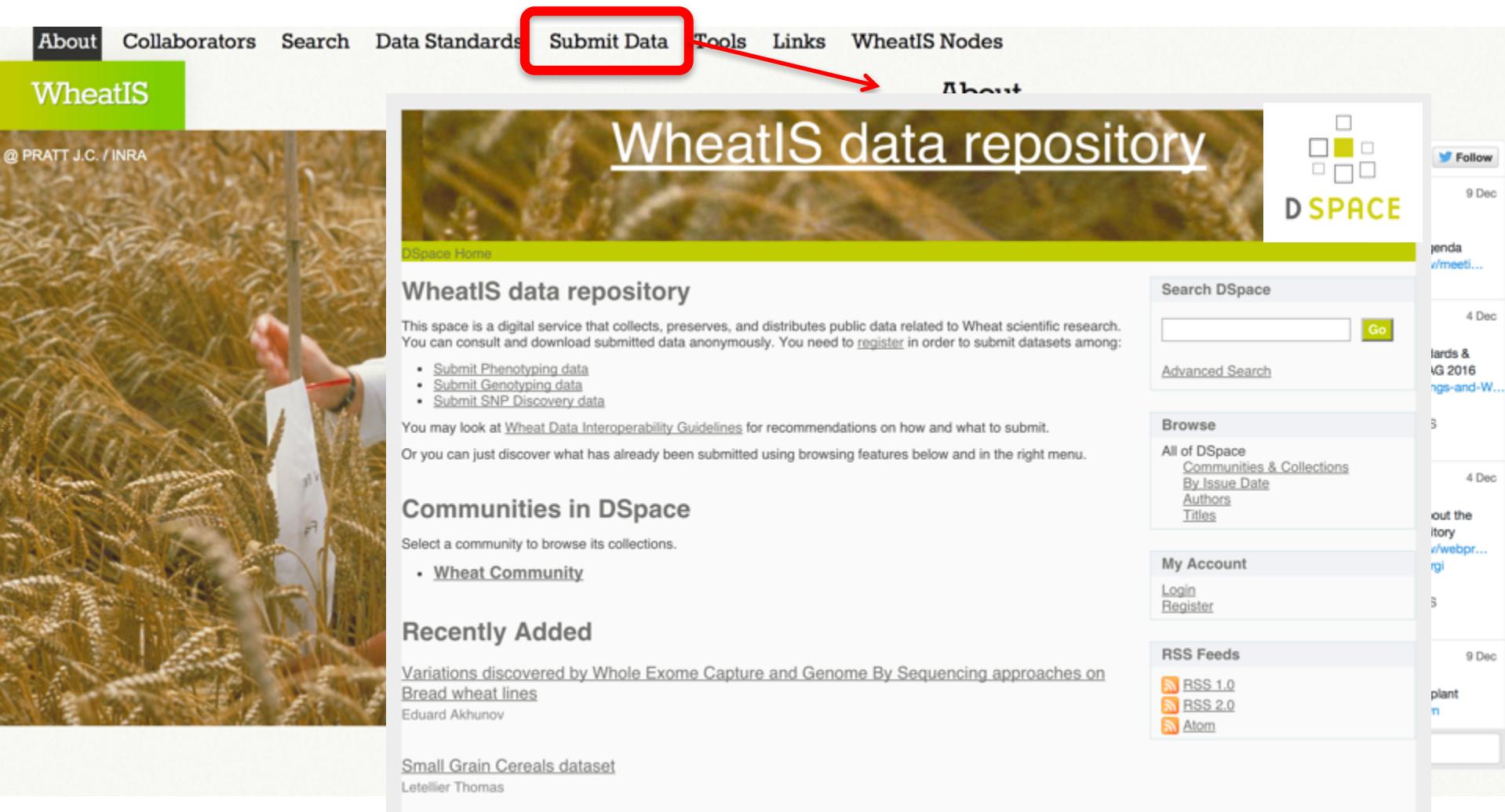
## To be Re-usable:

- R1. meta(data) have a plurality of accurate and relevant attributes.
  - R1.1. (meta)data are released with a clear and accessible data usage license.
  - R1.2. (meta)data are associated with their provenance.
  - R1.3. (meta)data meet domain-relevant community



# DATA SUBMISSION

# Data file repository



About Collaborators Search Data Standards **Submit Data** Tools Links WheatIS Nodes

## WheatIS

@ PRATT J.C. / INRA

DSpace Home

### WheatIS data repository

This space is a digital service that collects, preserves, and distributes public data related to Wheat scientific research. You can consult and download submitted data anonymously. You need to [register](#) in order to submit datasets among:

- Submit Phenotyping data
- Submit Genotyping data
- Submit SNP Discovery data

You may look at [Wheat Data Interoperability Guidelines](#) for recommendations on how and what to submit.

Or you can just discover what has already been submitted using browsing features below and in the right menu.

#### Communities in DSpace

Select a community to browse its collections.

- [Wheat Community](#)

#### Recently Added

[Variations discovered by Whole Exome Capture and Genome By Sequencing approaches on Bread wheat lines](#)  
Eduard Akhunov

[Small Grain Cereals dataset](#)  
Letellier Thomas

Search DSpace

Advanced Search

Browse

All of DSpace  
[Communities & Collections](#)  
[By Issue Date](#)  
[Authors](#)  
[Titles](#)

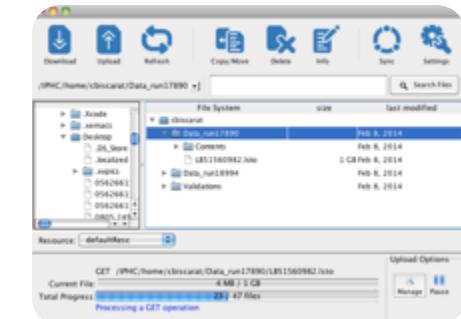
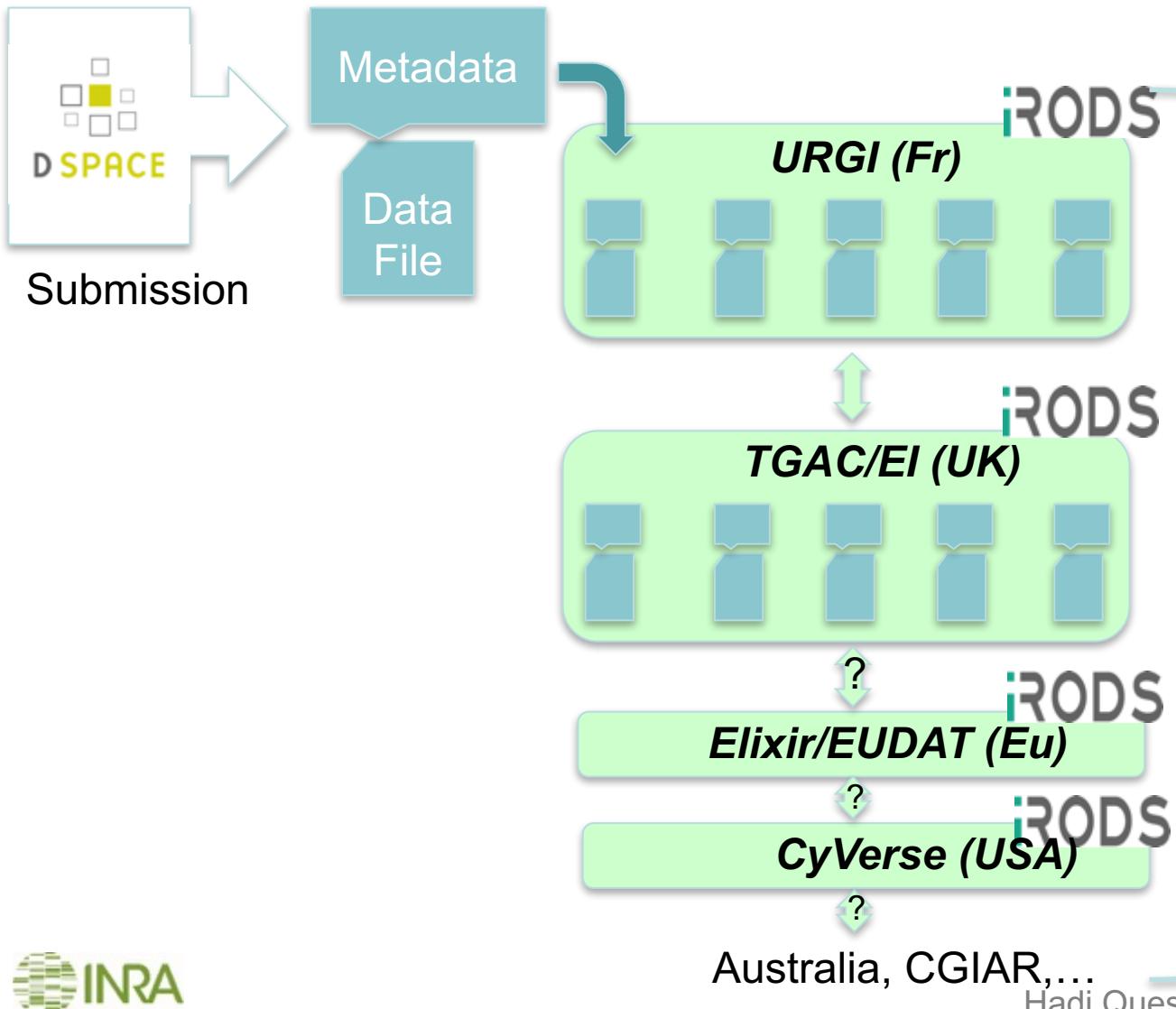
My Account

Login  
Register

RSS Feeds

 [RSS 1.0](#)  
 [RSS 2.0](#)  
 [Atom](#)

# Data workflow



*iRODS federation*



# DATA STANDARDS

## WheatIS



### Wheat Data Interoperability Guidelines

[Home](#) [Guidelines](#) [Ontologies & Vocabularies](#) [Use cases](#) [Getting involved](#) [About](#)



#### Welcome

These recommendations have been prepared by members of the [Wheat Data Interoperability Working Group](#) (WG), one of the WGs of the Research Data Alliance and the only WG of the [Agriculture Data Interoperability Interest Group](#). The group is coordinated by members of the [Wheat Initiative](#), a global initiative that aims to reinforce synergies between bread and durum wheat national and international research programmes to increase food security, nutritional value and safety while taking into account societal demands for sustainable and resilient agricultural production systems.

More specifically, the WG aims to:



PROMOTE  
the adoption of common  
standards, vocabularies and  
best practices for Wheat data  
management



FACILITATE  
access, discovery and reuse  
of wheat data



FACILITATE  
wheat data integration

#### GETTING INVOLVED



**WheatIS**





# Wheat Data Interoperability Guidelines



Home Guidelines Ontology

Phenotypes

Phenotypes are the observable characteristics of an organism between genes and the environment in which it grows. Plant phenotypes can be used in several fields, such as breeding programs and biological or agro-environmental applications. Furthermore, phenotypes are in interaction, like for instance in pretreatments have an effect on the glucose yield or in breeding affected by the number of grains and the grain weight.

This section provides standard formats that are used by the community and trials in fields and the minimum metadata required for documentation platforms.

## Welcome

These recommendations have been developed by the Working Group (WG), one of the Working Groups of the Interoperability Interest Group initiative that aims to reinforce research programmes to incorporate societal demands for sustainable development.



**PROMOTE**  
the adoption of common standards, vocabularies and best practices for Wheat data management



Guidelines

Wheat Data Interoperability guidelines

Home / Phenotypes

## Phenotypes

Phenotypes are the observable characteristics of an organism between genes and the environment in which it grows. Plant phenotypes can be used in several fields, such as breeding programs and biological or agro-environmental applications. Furthermore, phenotypes are in interaction, like for instance in pretreatments have an effect on the glucose yield or in breeding affected by the number of grains and the grain weight.

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## Recommendations

### Summary

1. Data format: use data matrices in csv, excel
2. Metadata and vocabularies: use complete metadata for all observation variables
3. Keep curated data (checked outliers)

### 1. Data formats

We recommend following minimum format principles with data least variables (trait along with method, units and scales or environments).

[ISA-Tab](#) is an implementation of this principle. It consists of or files and metadata files, the latter being used for data discovery information can be found on this dedicated page or in this preso. Genome 2015. It is currently well suited for generation by software format, phenotype specific configuration and tools are under in See the [germplasm recommendations](#) for data format regarding

### 2. Metadata and vocabularies

#### Observation variables

Observation Variables include trait and environment variables. We recommend using existing variables, listed in the vocabulary. To create new observation variables, we recommend using the [Template](#) available at [Crop Ontology](#) website. It must include a description, abbreviation, synonyms, methods, and scales) to creation and sharing. The most important field in this template remain stable and never be modified. Furthermore it must never be deprecated if needed. This way, it can be used in trials and rem

For Nursery and Trial metadata and description we recommend [Ontology](#), which describes the terms related to nurseries and trial environments, study design, etc. These metadata are actively maintained.

For biorefinery, we recommend using the [Biorefinery ontology](#) and terms associated with biomass composition and characterization area, particle size, porosity, etc.), physico-chemical pretreatment experimental processes descriptions.

#### Recommended Variable ontologies and vocabularies

- [Wheat crop ontology](#)
- [INRA Wheat Ontology \(soon publicly available\)](#)
- [Wheat Phenotype](#)
- [Biorefinery ontology](#)
- [XEO, XEML, Environment Ontology](#)

For the difference between metadata, ontologies and vocabularies

## 3. Raw data

We recommend sharing at least clean documented raw data, like plant Phenotype data lifecycle begins with acquisition, then cleaning, elaboration combines several variables, like phenological stages and elaborated/computed variables used as input for analyses softwares, and phenology can be combined to get height at flowering. Different el produced for different purposes, it is therefore important to be able to ones from raw data.

## Some popular Tools

### 1. Repositories, information systems and data tools

The Breeding Management System, [BMS](#) generates standard format for trial data in fields and uses for variables the [Crop Research Ontology](#) for experiment related metadata and trait related ontologies of the Crop makes it possible to analyze data directly using statistical tools such as R.

[GnpIS](#) is an INRA information system designed for plant and pest genetic scientists to mine genomic, phenomic and genetic data. For phenomic allows data discovery through a keyword based, google like, search engine. The latter allows [dataset building](#) for genetic or phenomic analysis. It is based on a strict identification of germplasms on variables through the [Crop Ontology](#).

The [Breeding API](#) specifies a standard interface for plant phenotype/genome providers to serve their data to crop breeding applications. It is a shared, open API, providers and data consumers who wish to participate.

For biorefinery applications, the best match pretreatment-biomass yields can be found through the [@Web platform](#). The Documents tab contains information by a kind of pretreatment (topics Bioref-XX). Data available on pretreatments used, biomass types and characterization, etc. In the future it will be possible to find the best match pretreatment-phenotype.

[iPlant collaborative](#) offers many services that allow the analysis of genomic and phenotypic data.

### 2. Data acquisition

[Field Book](#) is a simple app for taking phenotypic notes on field research. In the field has traditionally been a laborious process requiring writing by transcription. We have created Field Book to replace paper field book collection speed with greater data integrity.

## Things to follow in the future

### Candidate formats

- ped
- Bagit
- Hadoop File System : HDFS

2 Comments

Bettina Berger 27 November 2015

Sincere apologies for not taking sufficient time for a thorough assessment of this site. Just some minor points I noticed while browsing through.

I could not find a link to PATO, which I would assume is a useful tool for annotating phenotypes.

Also, there's no reference to iPlant in the US. This may be intentional, but the first phenotype dataset we were requested to make available for a publication was deposited on iPlant and more may follow in future.

[Reply](#)

Cyril Pommier 22 December 2015

Thank you for your feedback.

We have added the link to PATO on the ontology page. There is now also a quick reference to iPlant, but not very detailed since we are not direct users of this system. Feel free to send us a more detailed description, we will work on its integration.

[Reply](#)

## Leave a Reply

Your email address will not be published. Required fields are marked \*

### Comment

Name \*

Email \*

Website

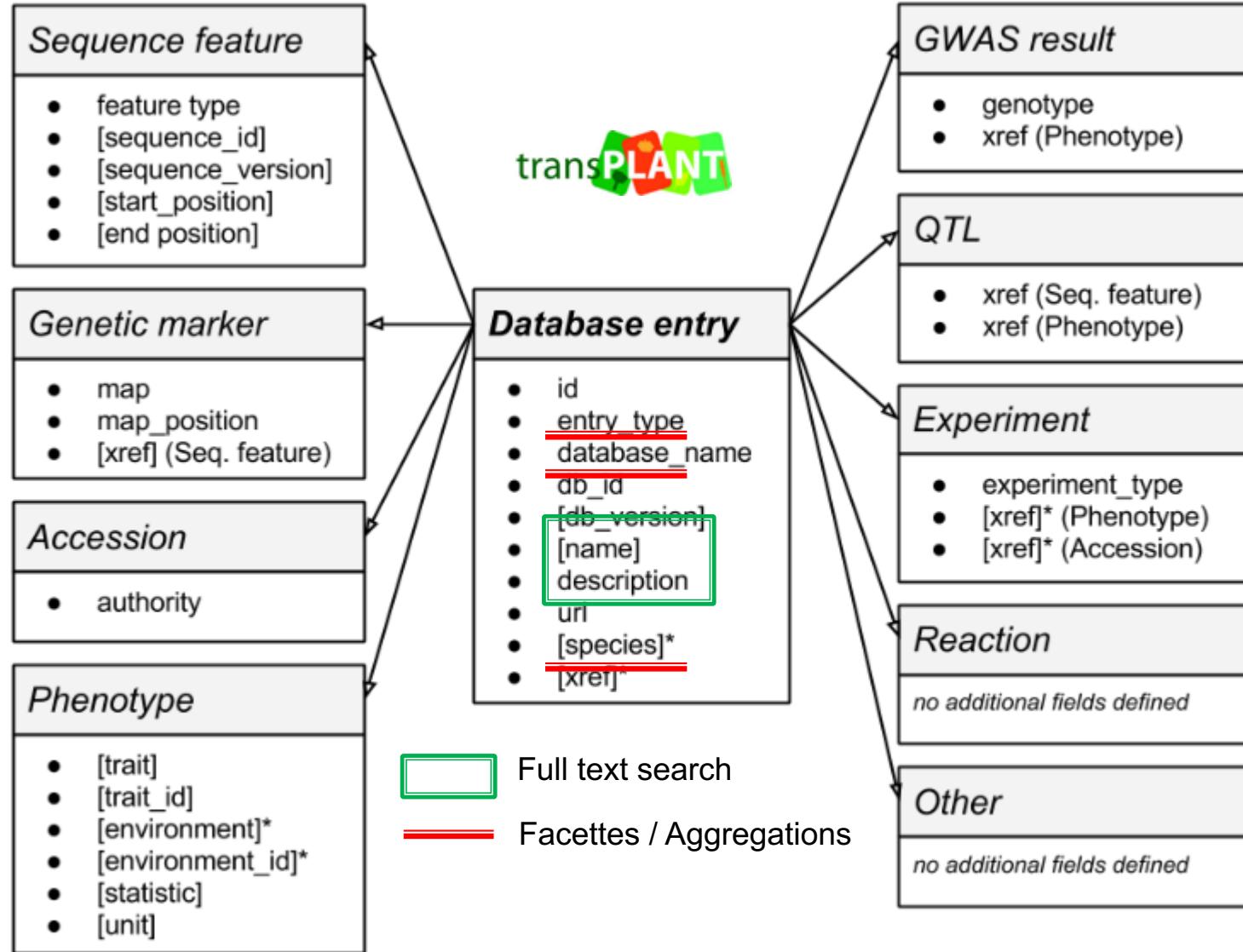
[Post Comment](#)





# DATA DISCOVERY

# Data Discovery data model





# Full text search of distributed databases



Search results for "WheatS nodes":

- transPlant-MIPS (UP):
  - CrowsNest: 13324
- transPlant-IPK (UP):
  - CR-EST: 199220
  - GBIBIS: 52978
  - MetaCrop: 355
- transPlant-EBI (UP):
  - Ensembl Plants: 218282
- UROGI (UP):
  - Gripli: 1757714
  - WheatGBMiner: 371197
  - Gripli JBrowse: 232783
  - WheatS repository: 13
- transplant-IPOFAS (UP):
  - PlantPhenoDB: 2
- T3 (UP):
  - Trifoliate Toolbox: 171159

Showing 1 to 10 of 67 entries

Search in all WheatS nodes... Examples: [Gb](#), [wmc430](#), [Triticum](#), [TRAEB3BF901000010CFD](#)

maui Quesneville

## WheatIS

[Search](#)
[About](#)
[WheatIS nodes:](#)
[transPlant-MIPS \(UP\):](#)

- CrowsNest: 13324

[transPlant-IPK \(UP\):](#)

- CR-EST: 199220
- GEBIS: 52878
- MetaCrop: 355

[transPlant-EBI \(UP\):](#)

- Ensembl Plants: 21828

[transplant-IPGPAS \(UP\):](#)

- PlantPhenoDB: 2

[T3 \(UP\):](#)

- Triticeae Toolbox: 1711

[CIMMYT \(UP\):](#)

- CIMMYT Dspace: 918
- CIMMYT dataverse: 37

[URGI \(UP\):](#)

- GnPLS: 1757714
- Wheat3BMine: 271197
- GnPLS JBrowse: 23278

## WheatIS

[Filters](#)
[Clear](#)

### Database

- TRITICEAE TOOLBOX (54)
- CR-EST (7)
- GNPIS (3)
- ENSEMBL PLANTS (1)
- GNPIS JBROWSE (1)
- PLANTPHENODB (1)

### Type

- ACCESSION (42)
- PHENOTYPE (14)
- EXPERIMENT (9)
- EXPRESSED SEQUENCE

- TAGS (7)
- SEQUENCE FEATURE (2)
- PHENOTYPE (1)
- QTL (1)
- SEQUENCE FEATURE (1)

### Species

- TRITICUM AESTIVUM (69)
- HORDEUM VULGARE (6)
- TRITICUM AESTIVUM L. (1)
- TRITICUM DURUM (1)

### Search

### About

### WheatIS nodes:

[transPlant-MIPS \(UP\):](#)

- CrowsNest: 13324

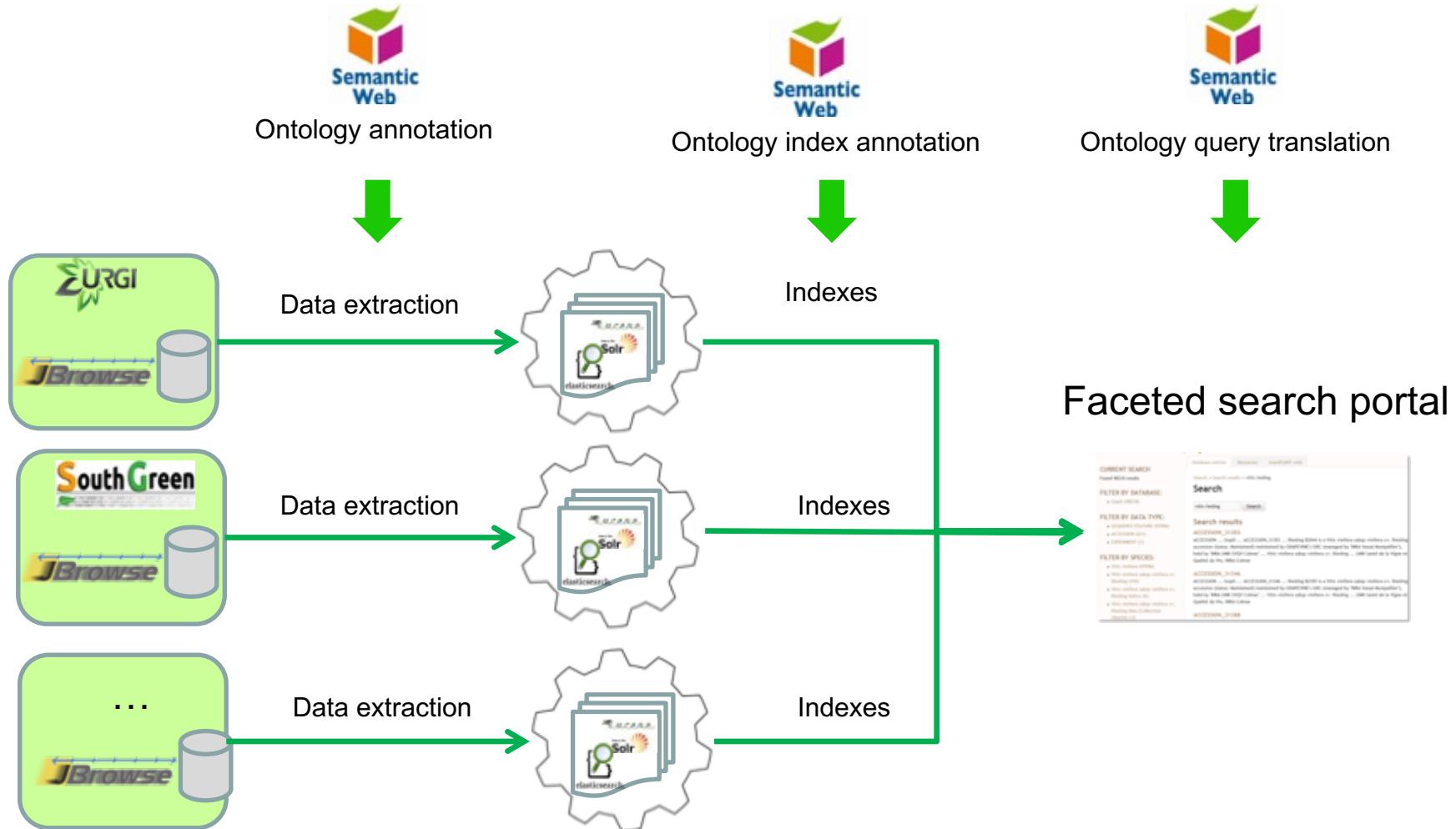
[transPlant-IPK \(UP\):](#)

- CR-EST: 199220
- GEBIS: 52878
- MetaCrop: 355

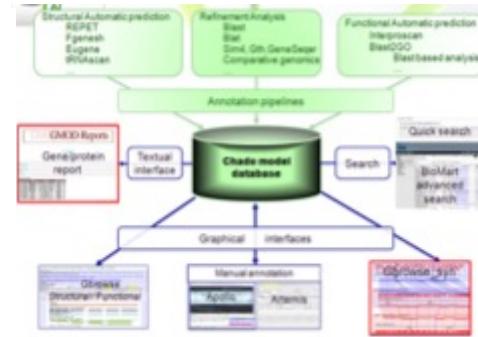
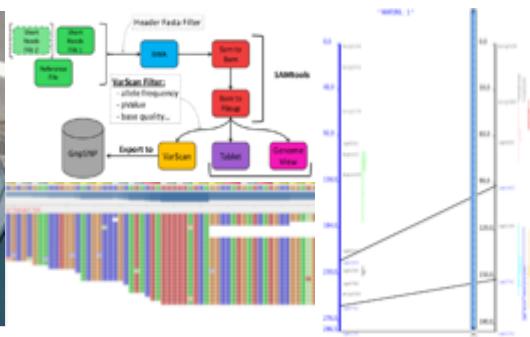


ID	Source	Type	Taxon	Description
<a href="#">Traes_5DL_E12C501B4</a>	Ensembl Plants	-	Triticum aestivum	Sequence feature, Ensembl Plants, Traes_5DL_E12C501B4, Traes_5DL_E12C501B4, Multiple inositol polyphosphate phosphatase Phylla1 [Source:UniProtKB/TrEMBL;Acc:A0FHB0], Triticum aestivum, protein_coding, 5D
<a href="#">HDP14M22T</a>	CR-EST	-	Hordeum vulgare	HDP14M22T, expressed sequence tags, CR-EST, Hordeum vulgare, gi 26248924 ref NP_754964.1  Hypothetical protein yfhB [Escherichia coli CFT073] Hypothetical protein; gi 28951047 gb AAC63447.1  Al2g37930 [Arabidopsis thal...]
<a href="#">HDP20D01w</a>	CR-EST	-	Hordeum vulgare	HDP20D01w, expressed sequence tags, CR-EST, Hordeum vulgare, gi 15604676 ref NP_221194.1  SFHB PROTEIN HOMOLOG (sfhb) [Rickettsia prowazekii str. Madrid E] SFHB ; gi 34906406 ref NP_914550.1  P0710E05.16 [Oryza sativa ...]
<a href="#">HDP20D01T</a>	CR-EST	-	Hordeum vulgare	HDP20D01T, expressed sequence tags, CR-EST, Hordeum vulgare, gi 15604676 ref NP_221194.1  SFHB PROTEIN HOMOLOG (sfhb) [Rickettsia prowazekii str. Madrid E] SFHB ; gi 34906406 ref NP_914550.1  P0710E05.16 [Oryza sativa ...]
<a href="#">HDP21C08T</a>	CR-EST	-	Hordeum vulgare	HDP21C08T, expressed sequence tags, CR-EST, Hordeum vulgare, gi 15604676 ref NP_221194.1  SFHB PROTEIN HOMOLOG (sfhb) [Rickettsia prowazekii str. Madrid E] SFHB ; gi 31979237 gb AAP68831.1  bone morphogenetic protein 1[...]
<a href="#">HDP31N10w</a>	CR-EST	-	Hordeum vulgare	HDP31N10w, expressed sequence tags, CR-EST, Hordeum vulgare, gi 15604676 ref NP_221194.1  SFHB PROTEIN HOMOLOG (sfhb) [Rickettsia prowazekii str. Madrid E] SFHB ; gi 34906406 ref NP_914550.1  P0710E05.16 [Oryza sativa ...]
<a href="#">HDP35A10T</a>	CR-EST	-	Hordeum vulgare	HDP35A10T, expressed sequence tags, CR-EST, Hordeum vulgare, gi 26248924 ref NP_754964.1  Hypothetical protein yfhB [Escherichia coli CFT073] Hypothetical protein; gi 28951047 gb AAC63447.1  Al2g37930 [Arabidopsis thal...]
<a href="#">TS034Q07u</a>	CR-EST	-	Triticum aestivum	TS034Q07u, expressed sequence tags, CR-EST, Triticum aestivum, gi 15233419 ref NP_192328.1  hypothetical protein [Arabidopsis thaliana] gi 7487460 pir  T01820 hypo; gi 15604676 ref NP_221194.1  SFHB PROTEIN HOMOLOG (sfhb)
<a href="#">HWW FHB</a>	Triticeae Toolbox	Experiment	Triticum aestivum	Experiment, Triticeae Toolbox, HWW FHB, phenotype experiment, includes trials FHB_2014_Lincoln, HWWFHB_2014_Brookings, HWWFHB_2014_Fargo, Triticum aestivum, phenotype
<a href="#">URSN_2012_BrookingsSD</a>	Triticeae Toolbox	Experiment	Triticum aestivum	Experiment, Triticeae Toolbox, URSN_2012_BrookingsSD, phenotype trial, traits=Fusarium head blight incidence, Fusarium head blight severity, Fusarium head blight disease index, visually scabby kernels URSN, descript[...]

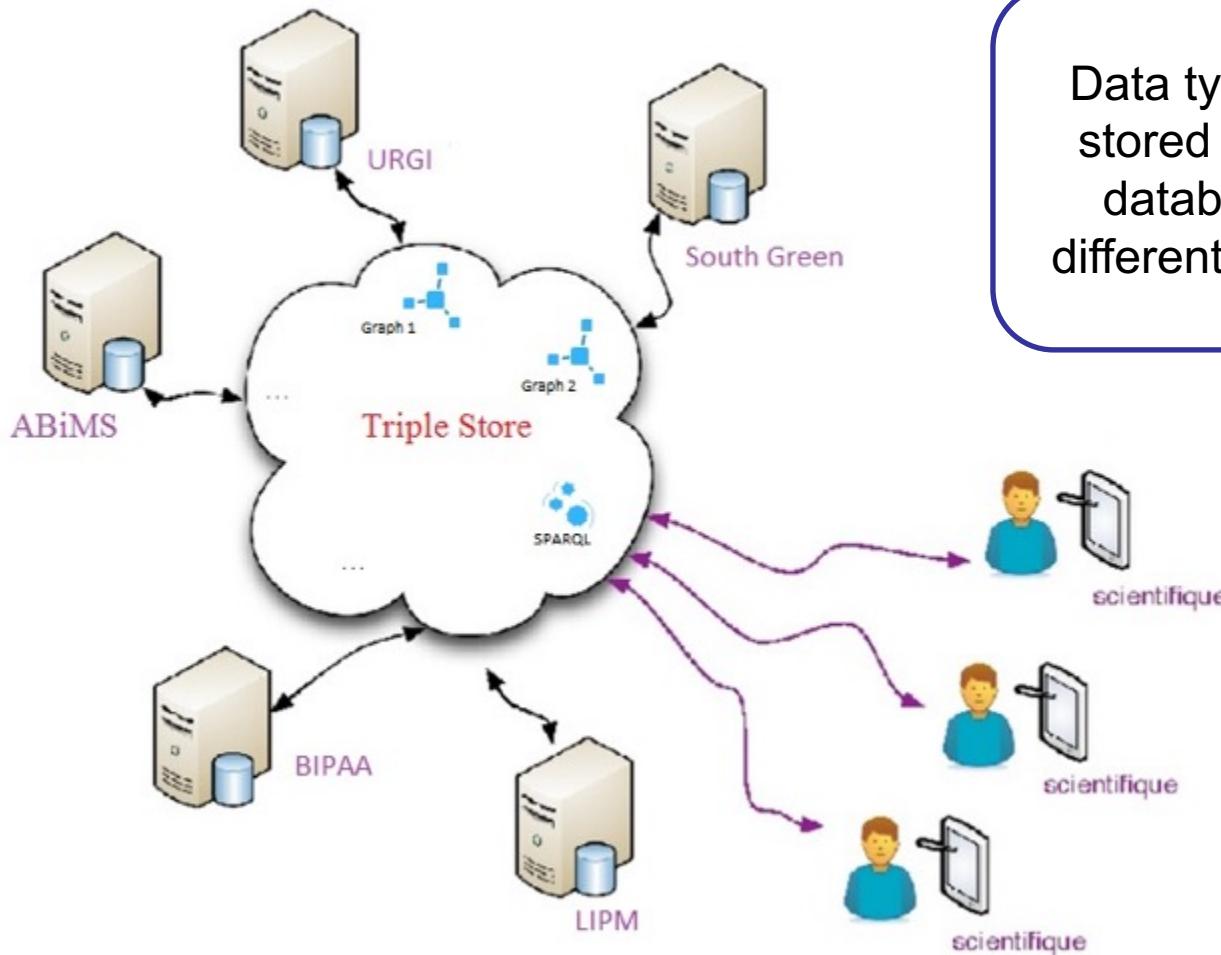
# Next for data discovery



# Semantic Interoperability

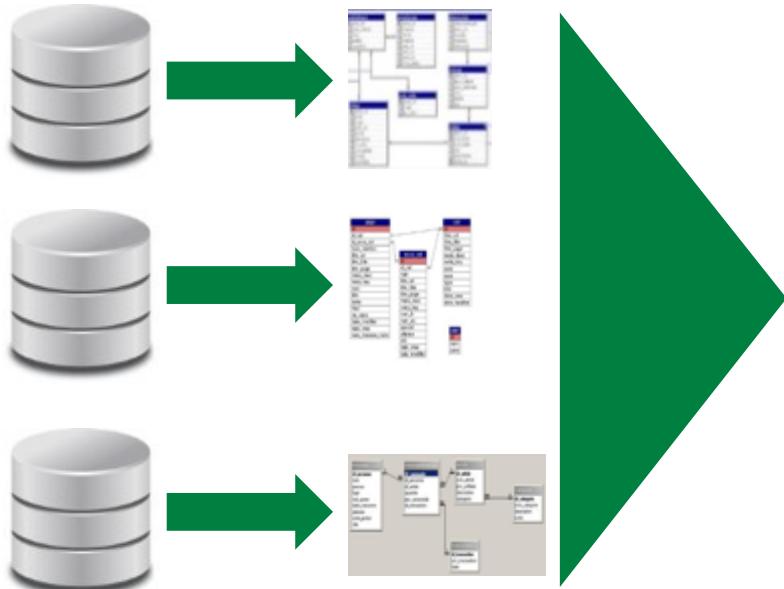


# Why a semantic interoperability



Data types can be stored in different databases with different data model

# Develop a web semantic interoperability



Ontology based annotation  
of database schemas  
(GO, PO, TO, CO, ...)

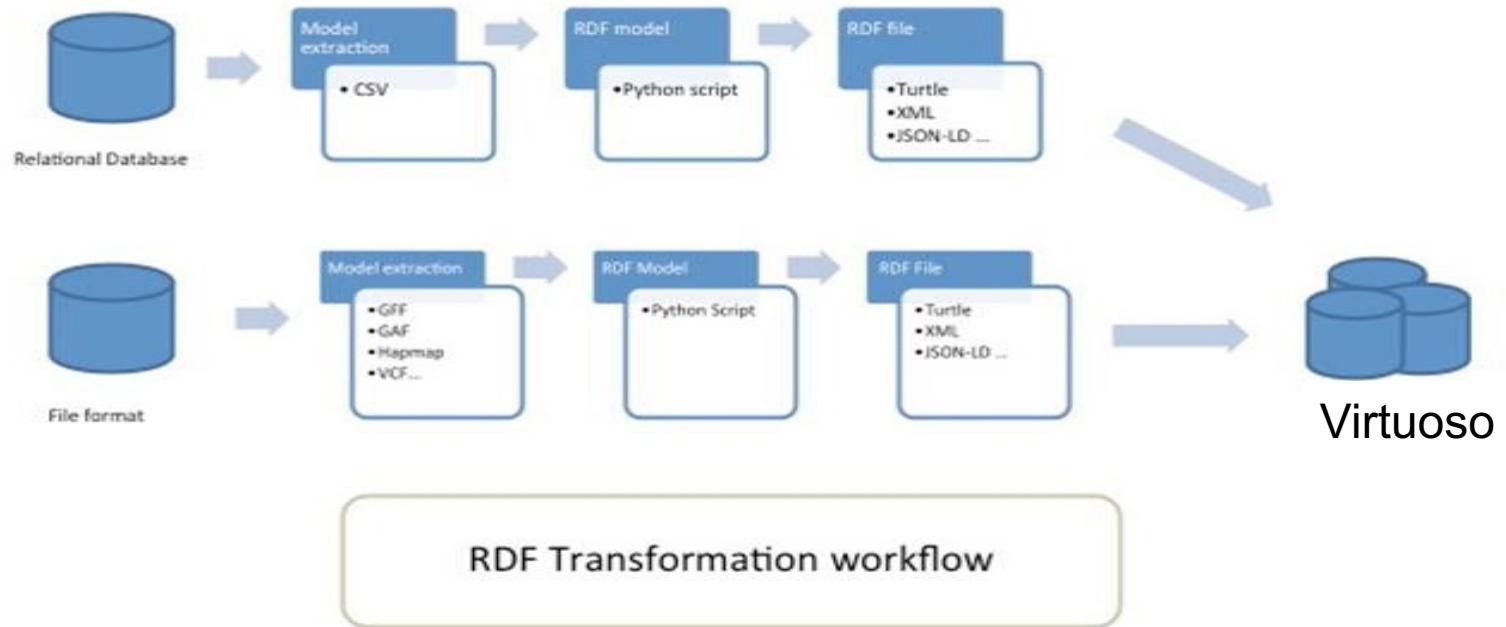
RDF modeling of the  
databases schemas

RDF triple store  
storage

Query of dispersed  
data for data  
integration through  
Semantic web services  
(SPARQL, web user  
interface)

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# Workflow ETL



- Some workflows are generic enough to be reused (i.e. GFF3 or HapMap)
- Codes available on GitHub,  
[https://github.com/SouthGreenPlatform/AgroLD.](https://github.com/SouthGreenPlatform/AgroLD)

# AgroLD portal

([www.agrold.org](http://www.agrold.org))

- **Different user profiles**
- **Provides different entry points**

## [Quick Search](#)

Search with keywords and browse AgroLD Knowledge Base

## [Advanced Search](#)

Search with keywords, browse, and get answers to some biological questions

## [Explore Relationships](#)

Search easily existing relationships between entities

## [SPARQL Query Editor](#)

Edit and submit your SPARQL Queries to the sparql endpoint of AgroLD located at  
<http://volvestre.cirad.fr:8890/sparql>

# Integrates information from:

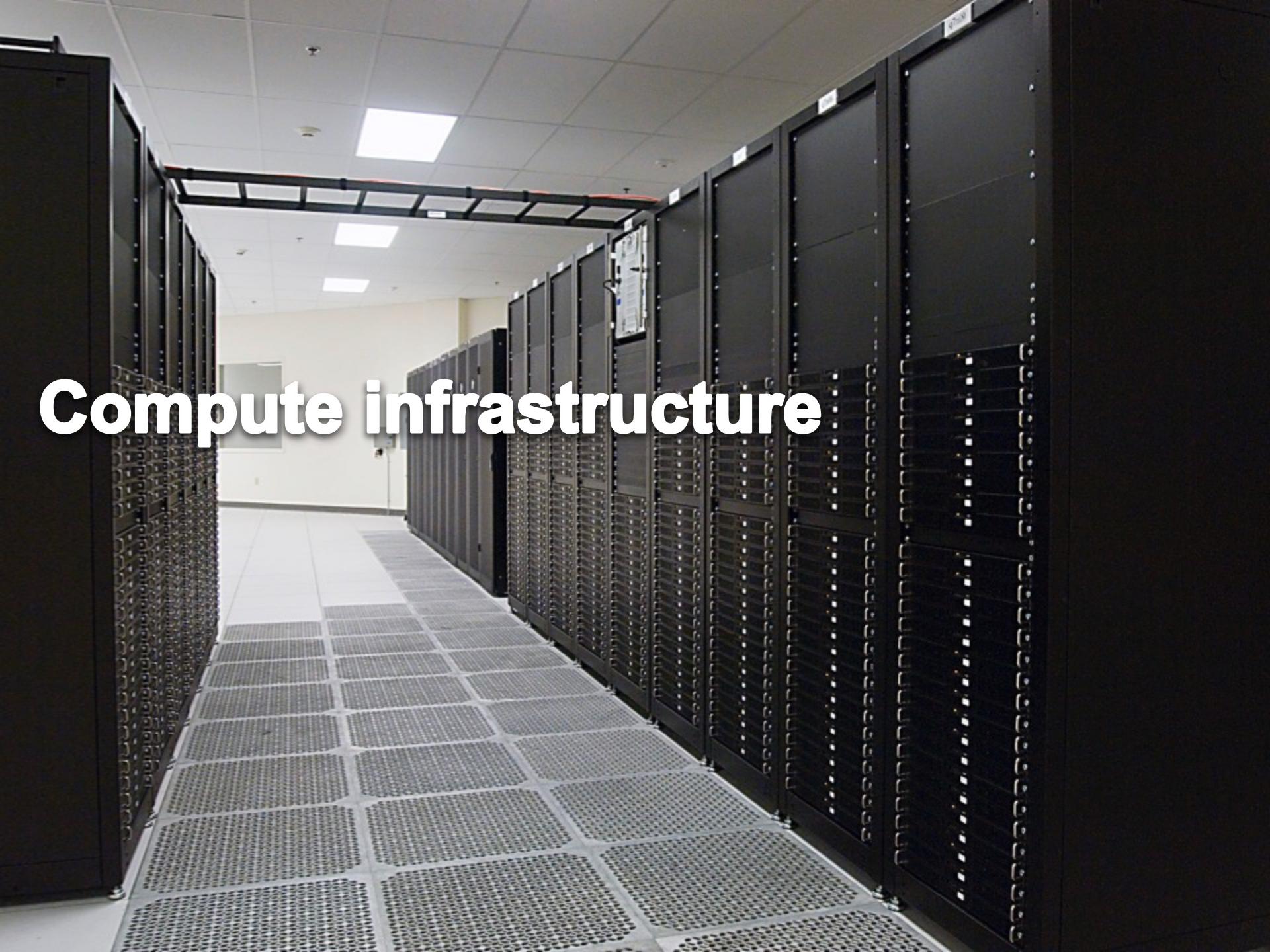
- **Ontologies:** Gene Ontology (GO), Plant Ontology (PO), Plant Trait Ontology (TO), Plant Environment Ontology (EO)...
- **Information sources:**
  - Ontology association: GOA, Gramene (TO, PO and EO)
  - Gene/Protein information: OryGenesDB, Gramene, UniProt
  - QTL information: TropGeneDB, Gramene
  - Polymorphisms: SniPlay
  - Pathway information: Gramene - Cyc
  - Phenotype information: Oryza Tag Line
  - Phylogenomic information: GreenPhyIDB

# Phenotypic data integration

- **RDF conversion from the Breeding API standard**
- **Benefit from the work of the BRAPI international consortium**
  - ◆ REST API and JSON format
  - ◆ Web Service Swagger

<https://urgi.versailles.inra.fr/ws/swagger-ui/index.html#/Phenotyping>

# Compute infrastructure



**Tools**

search tools

**Get Data**

- [Text Manipulation](#)
- [Filter and Sort](#)
- [Join, Subtract and Group](#)
- [Convert Formats](#)
- [Operate on Genomic Intervals](#)
- [FASTA manipulation](#)
- [Emboss Tools](#)

**NGS TOOLS**

- [NGS: QC and manipulation](#)
- [NGS: Mapping](#)
- [NGS: Assembly](#)
- [NGS: RNA Analysis](#)
- [NGS: SAM Tools](#)
- [NGS: Peak Calling](#)
- [Alternative splicing tools](#)
- [Picard Tools](#)
- [BEDTools](#)

**VARIANT/SNP TOOLS**

- [URGI: MAPHITS 2.0](#)
- [SnpEff tools](#)
- [Vcf utils](#)
- [VCF Tools](#)

**ANNOTATION TOOLS**

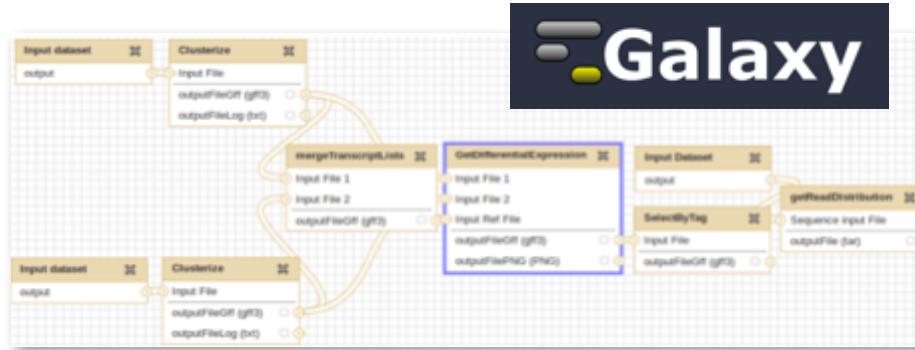
- [Gene Ontology Annotation tools](#)
- [Repeats annotation](#)

**SEQUENCE SIMILARITY TOOLS**

- [NCBI BLAST+](#)

**URGI TOOLS**

- [URGI: Get Data for grapevine](#)
- [URGI: BAC analysis](#)
- [URGI: MAPHITS - PreProcess Tools](#)
- [URGI: MAPHITS - Tools](#)
- [URGI: MAPHITS - PostProcess Tools](#)
- [URGI: MAPHITS - SNPs Chip Tools](#)
- [URGI: S-MART](#)
- [URGI: Differential expression Analysis Tools](#)
- [Tools for APLIBIO pipelines](#)



## Annotation analysis

- Gene structural and functional annotation
- Repeat detection and annotation (TE, SSR, SD)

## Structural analysis

- SNP calling, InDel detection
- Transcript assembly

## Functional analysis

- Differential expression
- ChIP-seq, BS-seq

## Genetic diversity analysis

- Population genetic statistics
- genome wide association mapping

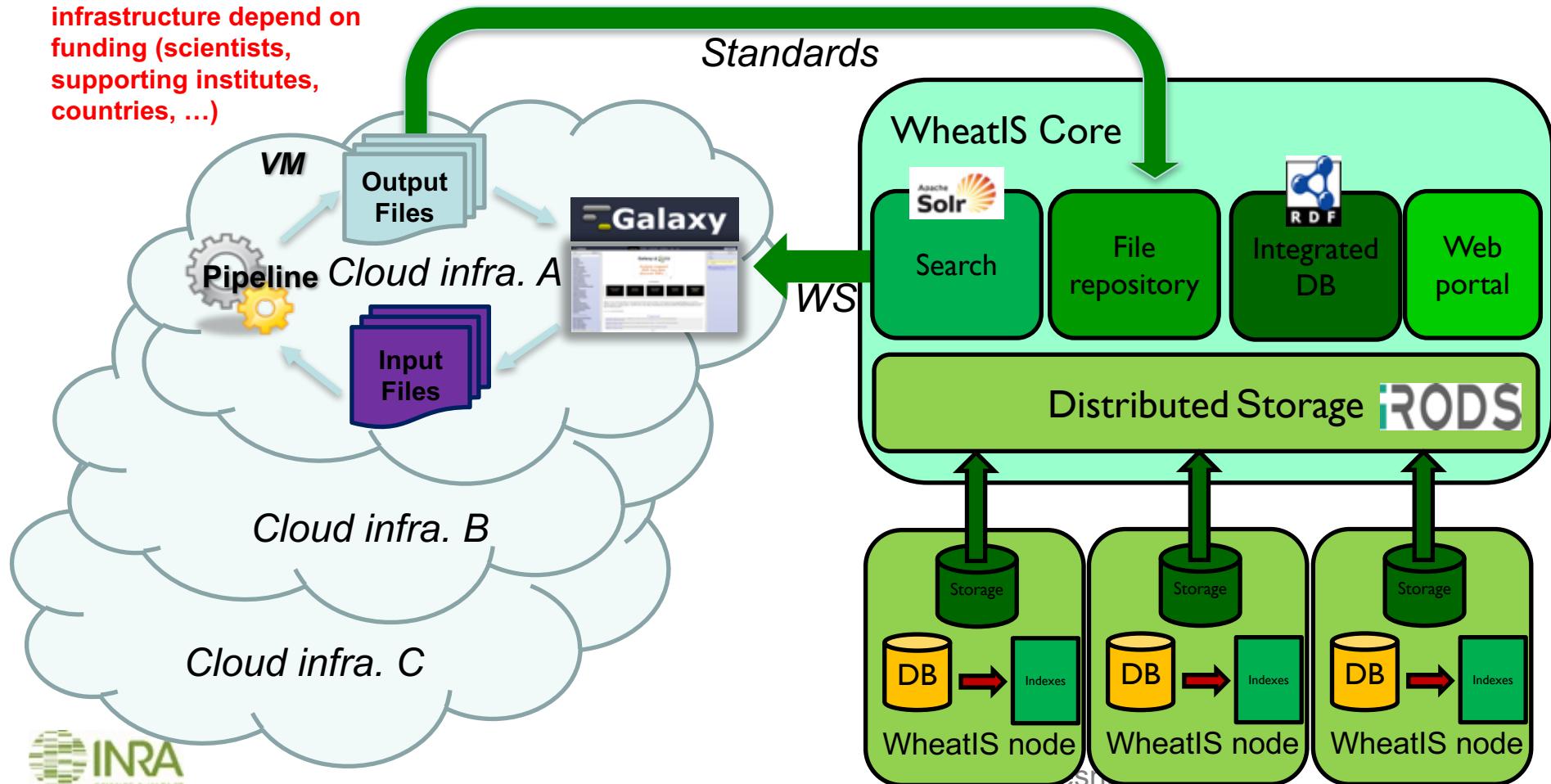
# Compute infrastructures

Several Compute infrastructure

One data infrastructure



Availability of infrastructure depend on funding (scientists, supporting institutes, countries, ...)



# A wheat use case

NGS  
data

1Gb of  
genomic  
sequence

50 Tb

16 Gb  
wheat  
genome

would need  
800 Tb

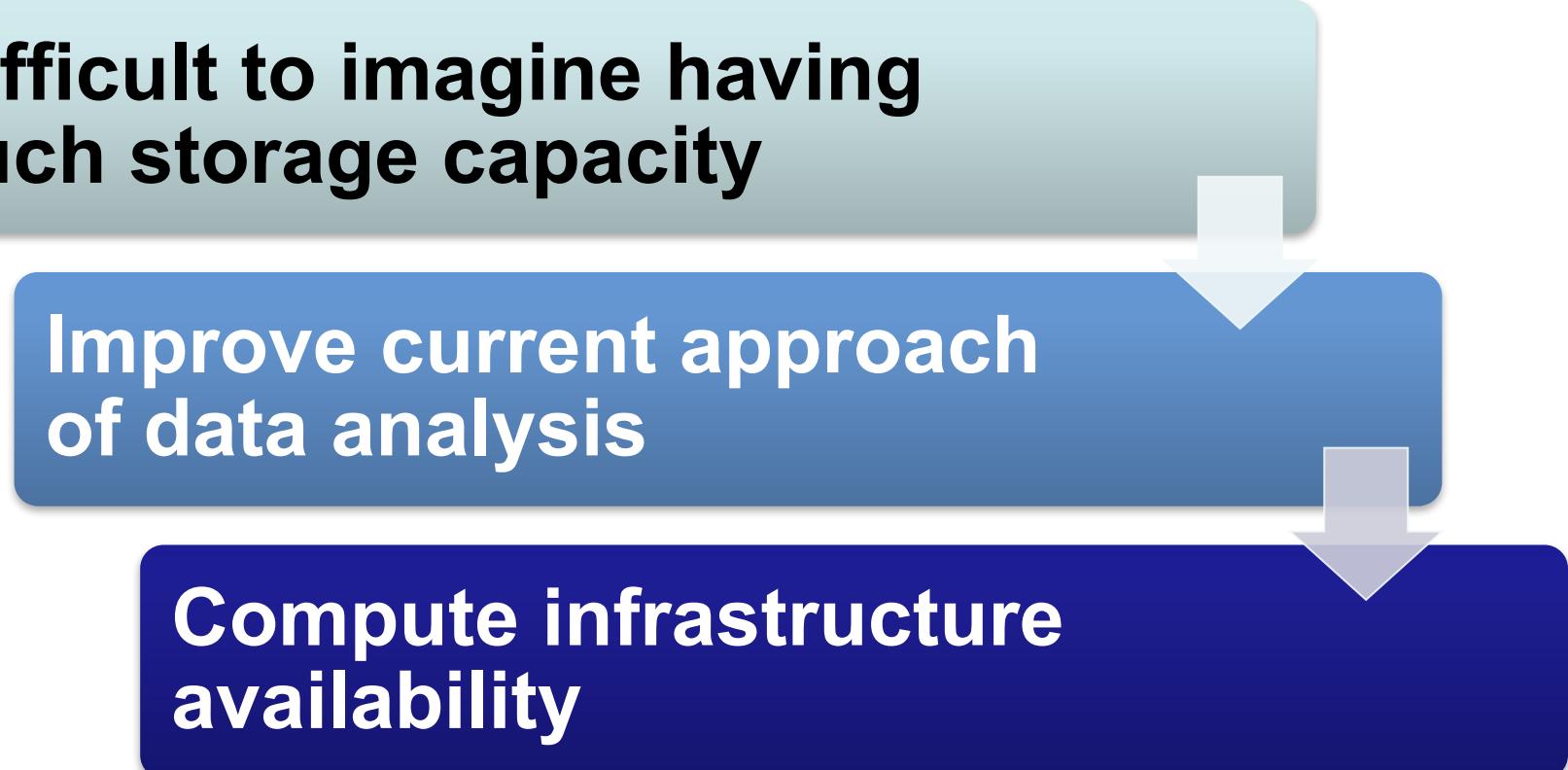
Future  
standard  
analysis

18 varieties  
(Plant J 2017  
Feb 23.)

14400 Tb =  
14 Pb ?

# Big data issues

Difficult to imagine having  
such storage capacity



Improve current approach  
of data analysis

Compute infrastructure  
availability



Metadata

« FAIR »  
repositories

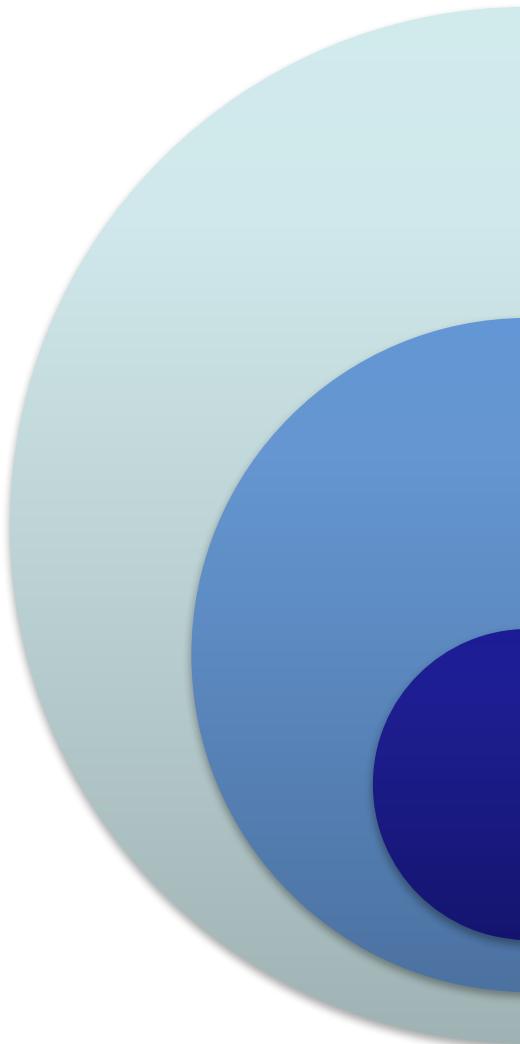


Safe data  
transfert  
protocoles

File completion validation : *MD5 checksum, ...*

Fault tolerance: *Rsync, ...*

# Efficient workflows



## Data reduction

- Noise reduction
- Fit to computing resources
- Store on adapted media: quick access vs storage capacity
- Keep only data that cannot be recomputed easily

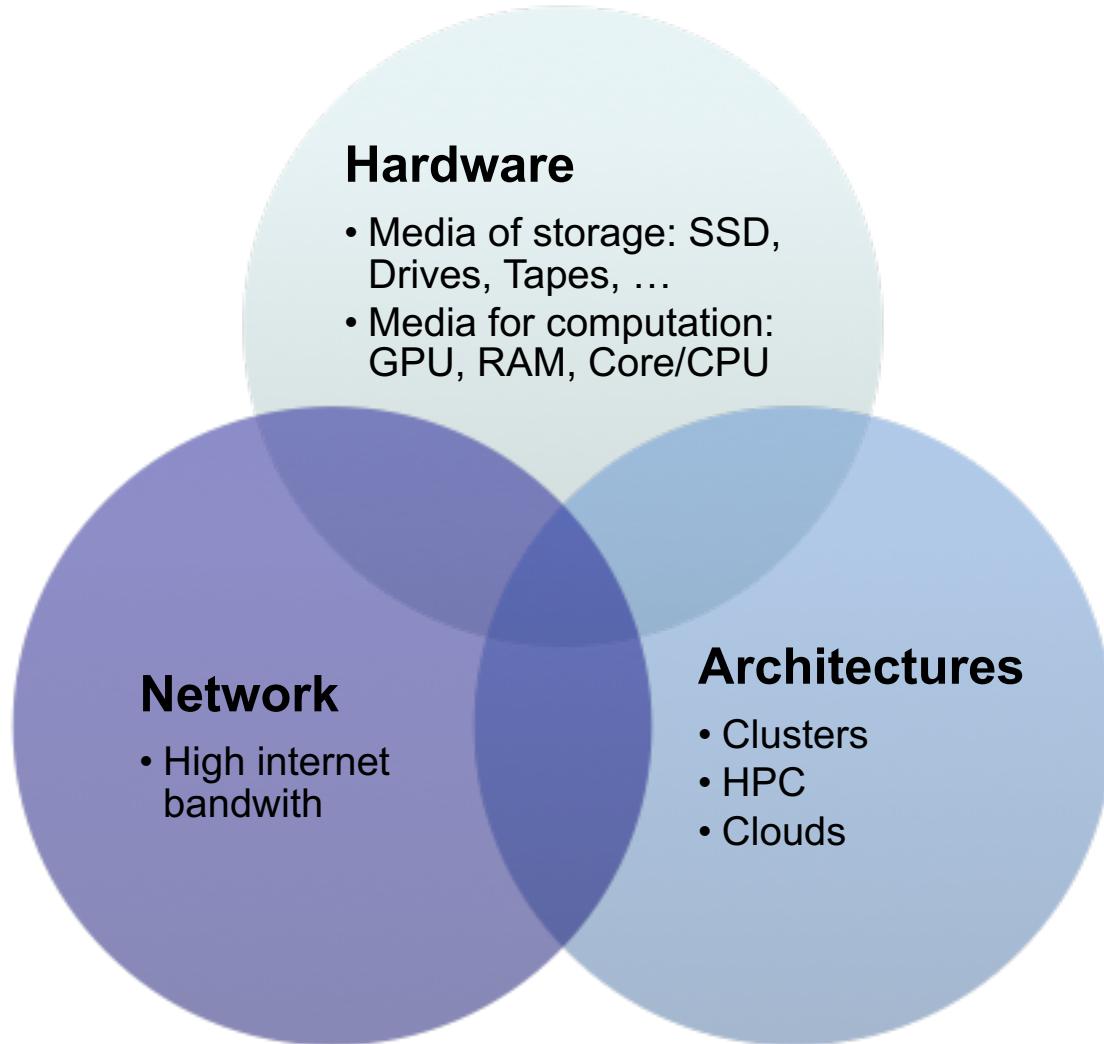
## Data dependancies

- Parallelization
- Compute time estimation

## Analysis reproducibility

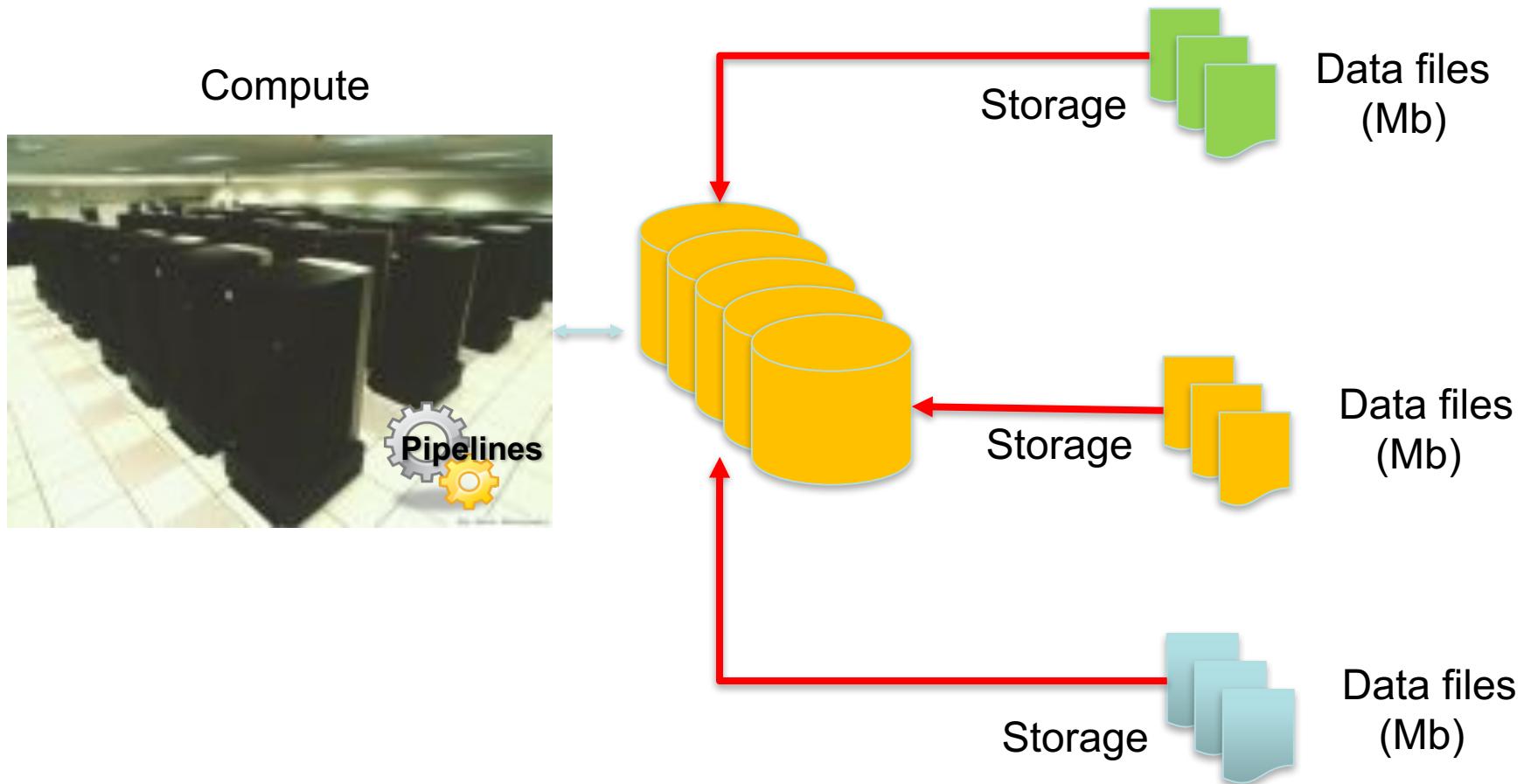
- Notebooks
- Follows workflow process
- Fault tolerant → resume from previous steps

# Efficient computer resources

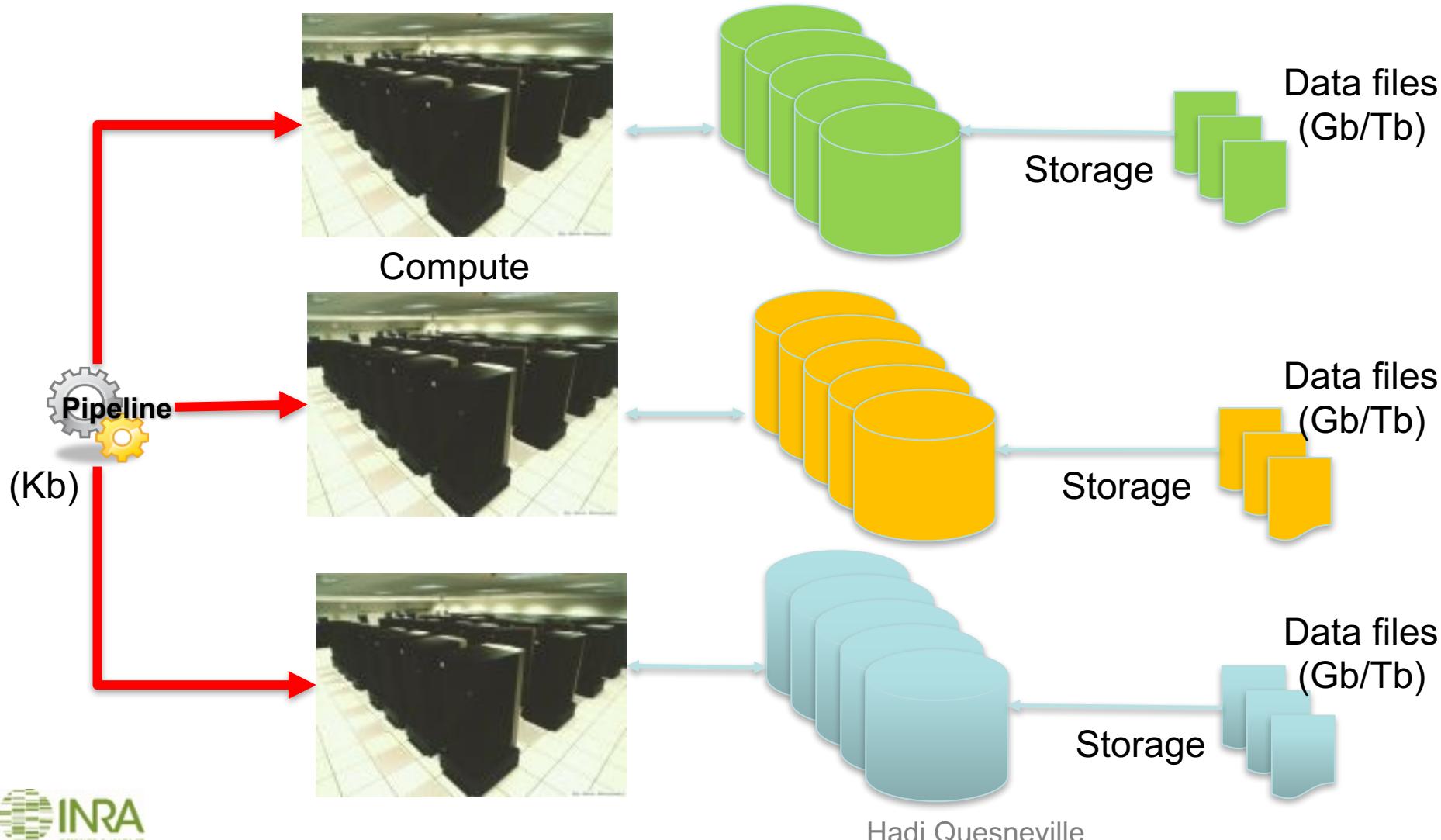


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# Today's paradigm: moving data to tools



# Paradigm shift: moving tools to data

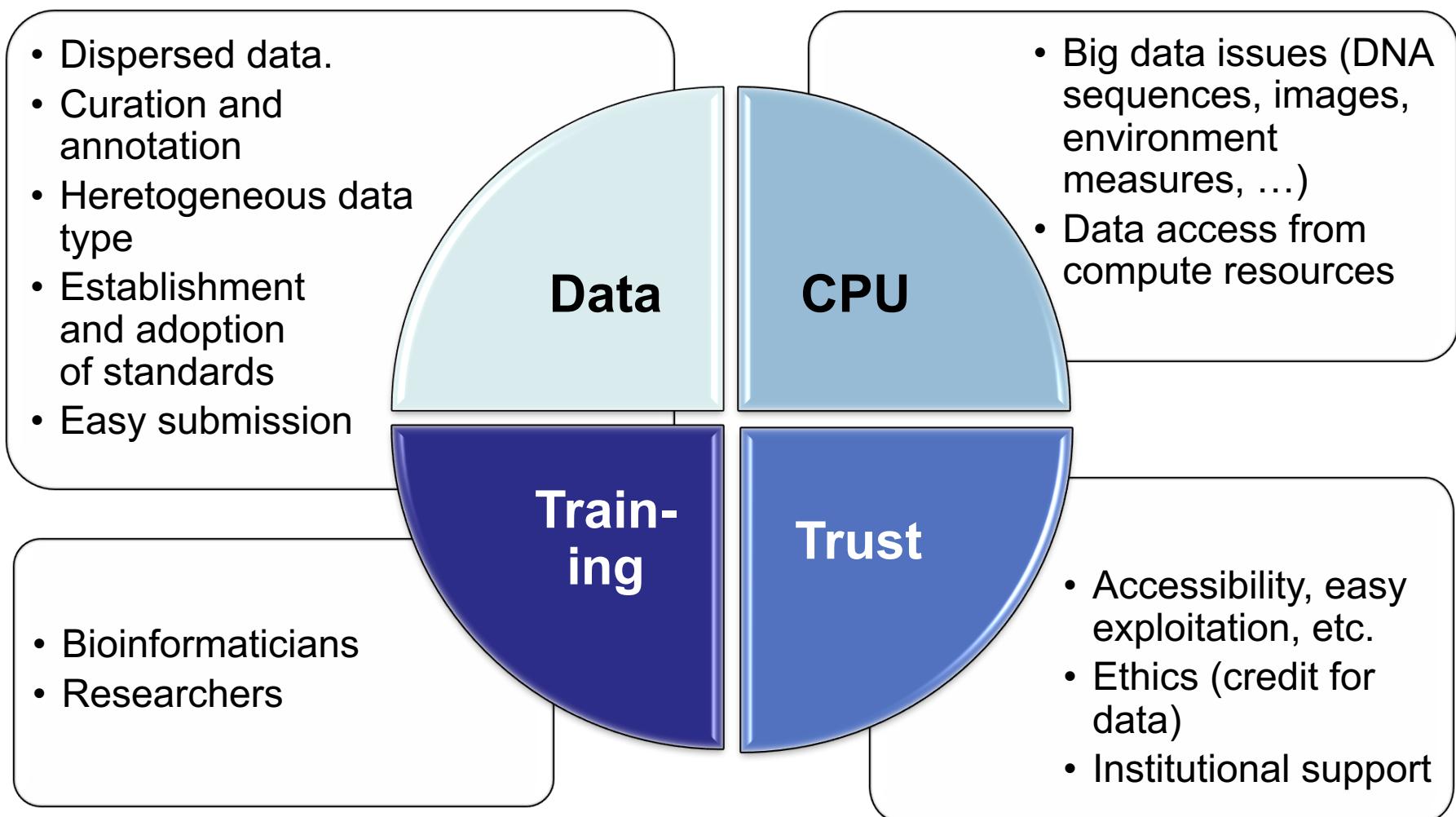


# Moving workflows

- **Moving complex workflows is challenging**
  - ◆ Hardware dependancies (Cluster)
  - ◆ OS dependancies (Unix/Windows/..., Scheduler)
  - ◆ Software dependancies
- **Technical solutions exist**
  - ◆ Virtualisation: moving an image as a file
  - ◆ Installation package: rpm, conda, ansible, puppet,...

→ Cloud infrastructure

# Conclusions: Cyber-infrastructure challenges





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