ado2019 : journée thématique sur les autorités de données

8 avr. 2019 Toulouse (France)



# FAIR principles, a new opportunity to improve the data lifecycle

**Preliminary question :** 

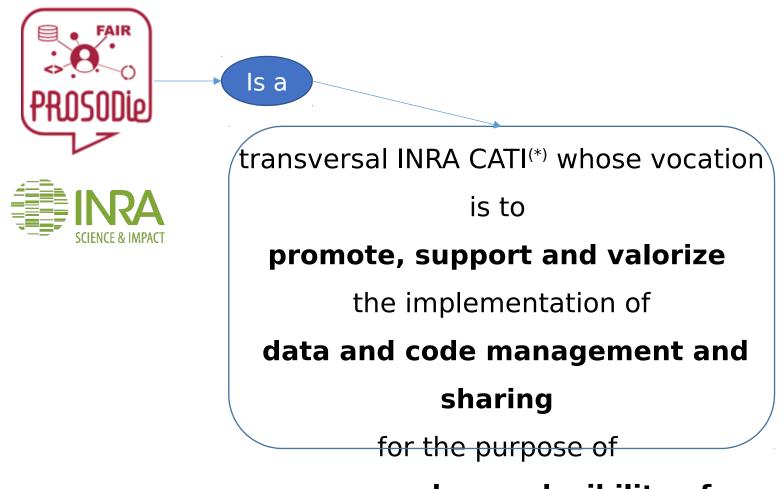
**Data Capture ?** 

## **Daniel Jacob**

INRA UMR 1332 BFP – Metabolism Group

Bordeaux Metabolome Facility



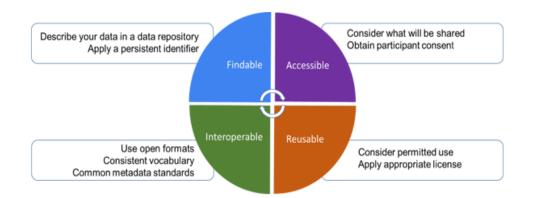


# reuse and reproducibility of

science.

(\*) Centre Automatisé de Traitement de l'Information - Automated Information Processing Center

#### THE FAIR DATA PRINCIPLES



The "FAIR" principles **define the basis** for data sharing easily to find, accessible, interoperable and reusable.

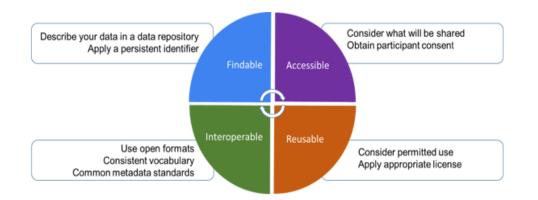
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However, it is to the <u>communities</u> to specify the actions necessary for their implementation

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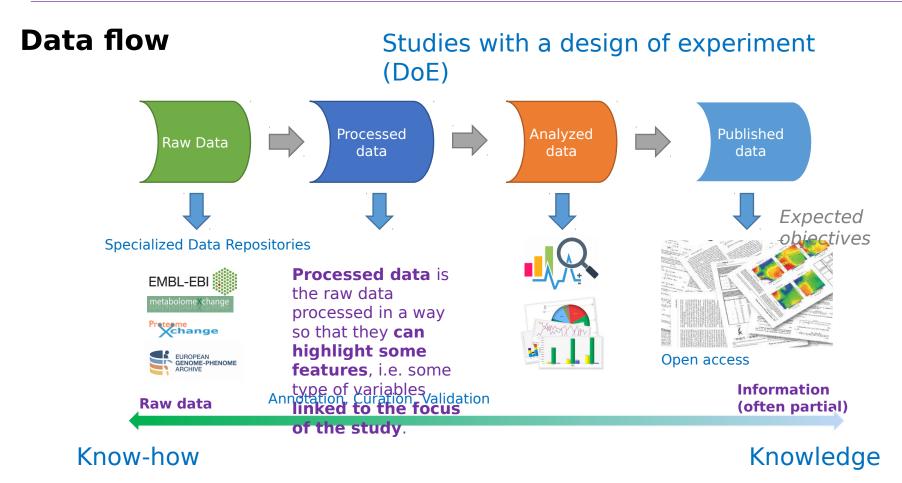


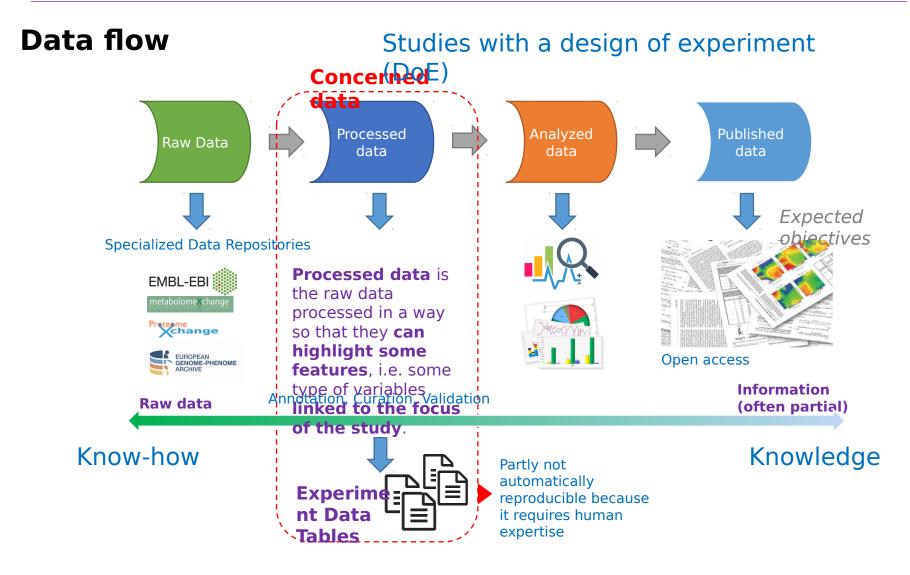
The "FAIR" principles **define the basis** for data sharing easily to find, accessible, interoperable and reusable.

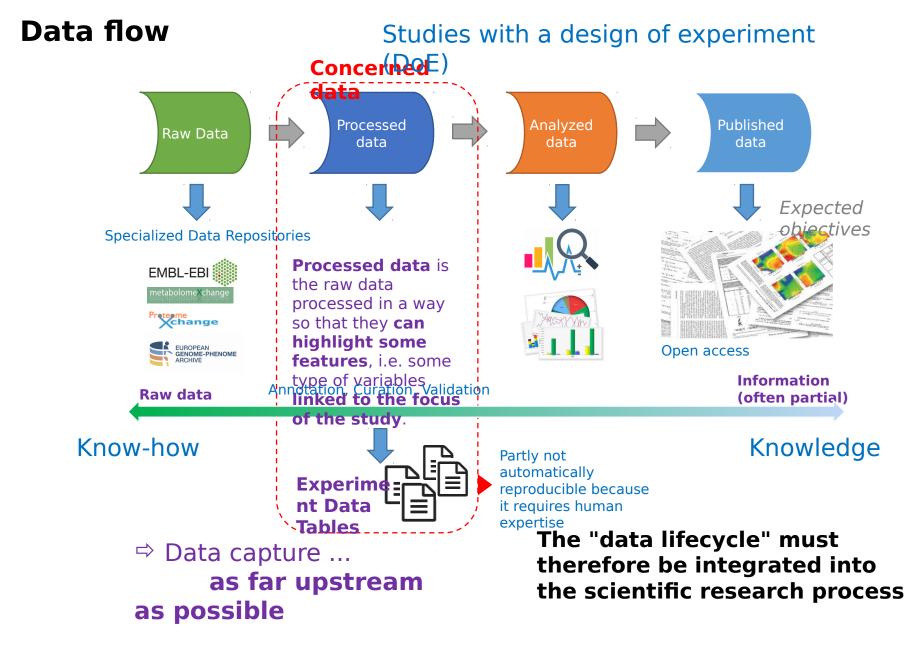
However, it is to the <u>communities</u> to specify the actions necessary for their implementation

The implementation of FAIR principles is a process that must be thought of in a progressive and <u>community-</u> <u>oriented way</u>.

It must be integrated into existing practices to ensure that they evolve without interruption and in a way that is acceptable to the various actors







Take into account users operating methods and work habits

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## Spreadsheet as a central tool

Despite all their drawbacks e.g. multiple information in a format without internal structure This does not take away any of their benefits Universal tool

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Universal tool



### **But: Repetitive and tedious**

#### tasks Gathering Data and Preparing Data

- lot of data manipulation, mainly in the form of tables,
- combine data sets according to a common field (identifiers)

## Modelisation :

- selection of subset of data then many repetitions of complex processing operations
- according to a very varied parametrization (scenarios).

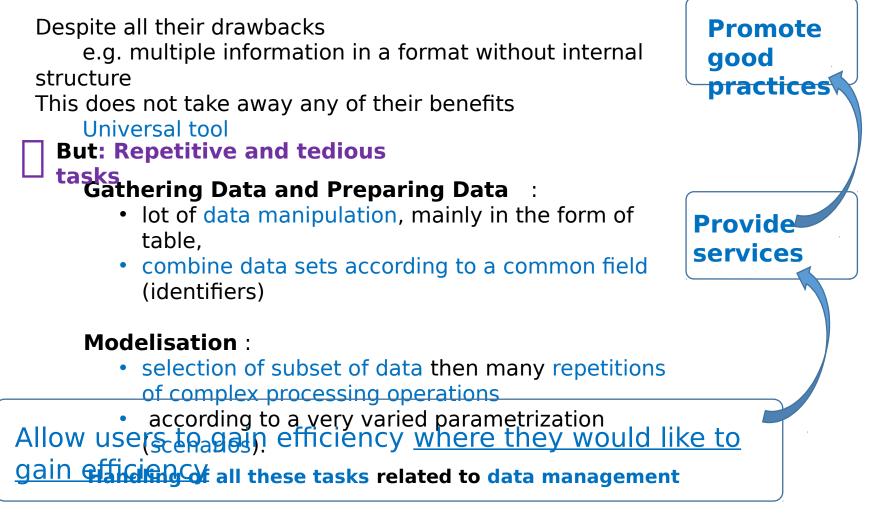
Take into account users operating methods and work habits

## Spreadsheet as a central tool

Despite all their drawbacks e.g. multiple information in a format without internal structure This does not take away any of their benefits Universal tool **But: Repetitive and tedious** tasks Gathering Data and Preparing Data lot of data manipulation, mainly in the form of **Provide** table. services combine data sets according to a common field (identifiers) Modelisation : selection of subset of data then many repetitions of complex processing operations according to a very varied parametrization
Allow users the parametrization where they would like to gain efficience all these tasks related to data management

Take into account users operating methods and work habits

## Spreadsheet as a central tool



Experiment Design (DoE)

# romote good practices









samples : Sample features

А	В	С	D	E	F	G	Н	I	J
SampleID	Treatment	DevStage	FruitAge	FruitPosition	FruitDiamete	FruitHeight	FruitFW	Rank	Truss
115	Control	FF.01	07DPA	3	11.95	10.42	0.81	Α	T7
121	Control	FF.03	22DPA	3	36.13	31.77	21.43	Α	T6
164	Control	FR.01	42DPA	2	51.09	46.85	64.05	А	T5
353	Control	FR.04	55DPA	5	48.28	43.35	66.64	Α	T5
355	Control	FR.04	55DPA	3	49.84	44.93	66.98	Α	T5
413	Control	FR.02	47DPA	1	60.48	54.23	106.13	А	T7
512	Control	FF.03	21DPA	NA	41	35.82	37.22	Α	TA
117	Control	FF.01	07DPA	3	13.44	12.39	1.14	А	T7
536	Control	FR.02	47DPA	NA	59.4	49.05	87.28	Α	TA
544	Control	FR.03	50DPA	NA	57.31	47.69	92.86	Α	TA
158	Control	FF.04	35DPA	5	58.38	49.3	92.86	Α	T5
109	Control	FF.03	22DPA	7	43.37	35.77	38.73	Α	T5
134	Control	FF.02	15DPA	3	27.89	23.8	9.88	А	T7
31	Control	FF.01	08DPA	4	NA	NA	0.48	Α	T6
179	Control	FF.03	28DPA	3	53.68	45.43	65.34	Α	T7
383	Control	FF.04	34DPA	5	47.04	41.19	48.96	А	T7
425	Control	FR.04	55DPA	2	62.74	50.27	115.3	Α	T7
520	Control	FF.03	30DPA	NA	48.86	41.52	52.94	Α	TA
419	Control	FR.03	50DPA	2	55.63	48.02	86.79	Α	T7
138	Control	FF.02	15DPA	6	27.96	22.14	9.69	Α	T7
143	Control	FF.03	29DPA	4	48.45	42.92	51.35	Α	Т6
365	Control	FR.02	47DPA	5	55.11	44.9	71.82	Α	Т6
127	Control	FF.03	27DPA	3	45.71	43.28	47.8	A	T5
188	Control	FR.01	42DPA	3	55.38	47.1	77.39	А	T6

Data

x≣ ... and related to others (data) \*\*\*\*\* 5 \star OPEN DATA identified by URIs \*\*\*\* OL RE OF UR and non-proprietary format OL RE OF RDF ... in a structured format 0. 86 999 Data on the web, open license Ø 🔤 🖬 PDF

> necessary and indispensable step towards « Linked Open Data ». Promote nonproprietary format like CSV or TSV

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# romote good practices









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134	Control	FF.02	15DPA	3	27.89	23.8	9.88	Α	Т7
31	Control	FF.01	08DPA	4	NA	NA	0.48	Α	T6
179	Control	FF.03	28DPA	3	53.68	45.43	65.34	А	Т7
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# ... and related to others (data) ... and related to others ... and related to others ... and related to

necessary and indispensable step towards « Linked Open Data ». Promote nonproprietary format like CSV or TSV

#### Data

#### Well organized data

- Each variable forms a column
- Each observation forms a line
- Each "observational entity" forms a table

# omote good practices









#### Experiment Design (DoE)

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lden	tifia	4	55DPA	:	49.84	44.93	66.98	А	T5
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536	Control	acto	ors	NA	59.4	49.05	87.28	А	ТА
544	Control	11.05	500 M	NΔ	57 31	47 69	92.86	А	ТА
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383	Control	FF.04	34DPA		5 47.04	41.19	49 04	^	т7
425	Control	FR.04	55DPA		2 62.74	50.27	1	<b>Num</b>	
520	Control	FF.03	30DPA	NA	48.86	6 41.52	5	Qual	ιατ
419	Control	FR.03	50DPA		2 55.63	48.02	86./9	А	17
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# X∄

Whatever the kind of experiment, this assumes design of а experiment (DoE) involving individuals, samples or whatever things, as the main objects of study (e.g. plants, animal, bacteria, tissues....)

This also assumes the observation Section dependent variables resulting of effects of controlled some experiment factors.

Moreover, the objects of study have usually an identifier for each of them, and the variables can be quantitative or qualitative.

> Promote nonproprietary format like CSV or TSV



#### Daniel Jacob, INRA - April

512	Lontrol	FF.03	ZIDPA	NA		41	35.82	37.22	А
117	Control			3	3	13.44	12.39	1.14	А
536	Control	acto	ors	NA		59.4	49.05	87.28	Α
544	Control	11.00	5051 M	NΔ		57 31	47 69	92.86	Α
158	Control	FF.04	35DPA	<b>.</b>				2.86	А
109	Control	FF.03	22DPA	Qu	an	τιτ	ativ	<b>es</b> 3.73	Α
134	Control	FF.02	15DPA	-		21.03	23.0	Э.88	А
31	Control	FF.01	08DPA	Z	I NA	1	NA	0.48	Α
179	Control	FF.03	28DPA	3	3	53.68	45.43	65.34	Α
383	Control	FF.04	34DPA	5	5	47.04	41.19	40 04	^
425	Control	FR.04	55DPA	2	2	62.74	50.27	1	<b>`</b>
520	Control	FF.03	30DPA	NA		48.86	41.52	5	zue
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	~	1		<u> </u>					

#### Data

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#### sample omote good practices harvesti sample seedin preparati analyses on Experiment Design (DoE) samples : Sample features D G x≣ SampleID FruitPosition FruitDiamete FruitHeight FruitFW Rank Truss reatment DevStage FruitAge T7 115 Control FF.01 07D 3 11.95 10.42 0.81 A Description of the 22D 3 21.43 A 121 Control FF.03 36.13 31.77 T6 42D A 2 51.09 46.85 64.05 A T5 164 Control FR.01 different columns within FP 01 55DP 5 48.28 66.64 A T5 43.35 66.98 A 55DP 3 49.84 44.93 T5 ldentifier 🗄 data files Shortname Description 47DPA 1 21DPA FF.03 NA 512 Control SampleID Pool of several harvests Identifie 117 Control 3 Treatment Treatment applied on plants Fac Factor tors 536 Control **DevStage** NΔ fruit development stage Factor 544 Control ...... ----158 Control FF.04 35DPA Qua FruitAge Days post-anthesis (dpa) fruit age Factor 22DPA 109 Control FF.03 FruitDiameter Fruit diameter Variable mm 15DPA 134 FF.02 Control 31 Control FF.01 08DPA 4 N FruitHeight Fruit height Variable mm 28DPA 3 179 Control FF.03 FruitFW Fruit Fresh Weight(g) Variable g 5 383 FF.04 34DPA Control Row of the invidual plant on the table 2 Rank Feature 425 Control FR.04 55DPA 520 Control FF.03 30DPA NA categories Position on the stem of the truss Truss Feature 2 419 FR.03 50DPA Control 6 9.69 A T7 138 Control FF.02 15DPA 27.96 22.14 identifier 143 Control FF.03 29DPA 48.45 42.92 51.35 A Т6 4 Metadata 5 71.82 A T6 factor 365 FR.02 47DPA 55.11 44.9 Control 127 Control FF.03 27DPA 3 45.71 43.28 47.8 A T5 qualitative 188 Control 42DPA 3 55.38 47.1 77.39 A Т6 FR.01 quantitative

#### Data

 $\Rightarrow$  Metadata : not just on the "top" linked to datasets but more deeply linked to the variables.

Promote nonproprietary format like CSV or TSV



Daniel Jacob, INRA - April

## romote good practicesinimal but relevant Metadata

#### Metadata file allowing to associate a key concept to each data subset file

	Α	В	С	D	E	F	G	Н
1	rank	obtainedFrom	subset	identifier	file	description	CV_term_id	CV_term_name
2	1	0	plants	PlanteID	plants.csv	Plant features	http://purl.obolibrary.org/obo/PO_0000003	whole plant
3	2	1	harvests	Lot	harvests.csv	Harvest features	http://purl.obolibrary.org/obo/OBI_1110046	organ harvesting
4	3	2	samples	SampleID	samples.csv	Samples features	http://purl.obolibrary.org/obo/PO_0009001	fruit
5	4	3	compounds	SampleID	compounds.csv	Compound quantifications	http://purl.obolibrary.org/obo/CHEBI_24431	chemical entity
6	5	3	enzymes	SampleID	enzymes.csv	Enzyme Features	http://purl.obolibrary.org/obo/OBI_0000427	enzyme
			·					

#### Entity $\Leftrightarrow$ Observational entity (e.g. samples, compounds, ...)

# x≣

categories

x∎

# Metadata file allowing each attribute (variable) to be annotated

	A	В	С	D	E	F	G	н
	1 subset	attribute	entry	category	type	description	CV_term_id	CV_term_name
	2 plants	PlanteID	plantid	identifier	numeric	Plant identifier	http://purl.obolibrary.org	individual organism identifier
	3 plants	Row	row	qualitative	string	Row of the invidual plant on the table	http://ncicb.nci.nih.gov/	Row
	4 plants	Plant	plant		string	Code identifier of the individual plant	http://ncicb.nci.nih.gov/	Discrete Set Coded String Data Type
	5 plants	Treatment	treatment	factor	string	Treatment applied on plants	http://www.ebi.ac.uk/ef	environmental factor
	6 plants	Genotype		qualitative	string	Genotype		
	7 harvests	Lot	lot	identifier	numeric	Pool of several harvests	http://www.ebi.ac.uk/ef	
	8 harvests	PlanteID			numeric	Plant identifier		individual organism identifier
	9 harvests	Truss		qualitative	string	Position on the stem of the truss	http://purl.obolibrary.or	stem node
	10 harvests	HarvestDate			string	Harvest date		
	11 harvests	HarvestHour			string	Harvest hour		
	12 harvests	FruitAge	age	factor	string	fruit development stage	http://purl.obolibrary.org	
	13 harvests	FruitPosition		qualitative	numeric	Poistion on the truss of the fruit	http://ncicb.nci.nih.gov/	•
	14 harvests	FruitDiameter		quantitative	numeric	Fruit diameter (mm)	http://ncicb.nci.nih.gov/	
	15 harvests	FruitHeight		quantitative	numeric	Fruit height (mm)	http://ncicb.nci.nih.gov/	
	16 harvests	FruitFW		quantitative	numeric	Fruit Fresh Weight(g)	http://ncicb.nci.nih.gov/	
	17 samples	SampleID	sampleid	identifier	numeric	Sample identifier		centrally registered identifier
	18 samples	Lot			numeric	Pool of several harvests	http://www.ebi.ac.uk/ef	sample pooling
	19 samples	NbFruit			numeric	Fruit Number per sample		
to a cried	20 samples	GellyFW		quantitative	numeric	Gelly Fred Weight(g) per sample		
ategories	21 samples 22 samples	GellyFruit BER		quantitative	numeric	Gelly per Fruit (estimated g) BER		
	231 compounds		sampleid	identifier	string numeric	Sample identifier	http://purl.obolibrary.org	centrally registered identifier
identifier	24 compounds		sampielu	factor	numeric	Day Per Anthesis	intip.//puri.obolibrary.org	centrally registered identifier
	25 compounds			quantitative	numeric	m av.extraction (g)		
factor	26 compounds			quantitative	numeric	masse MIA (g)		
au alitativa	27 compounds			quantitative	numeric	Rdt (% MIA/DW)		
🗕 qualitative 🔤	28 compounds			Mantitative	numeric	Dosage amidon (%poids/MIA)	http://purl.obolibrary.org	starch
guantitative	29 compounds			Juantitative	numeric	amidon (g/gDW)	http://purl.obolibrary.org	
	compounds	RHAMNOSE		quantitative	numeric	RHAMNOSE	http://purl.obolibrary.org	rhamnose

Attribute ⇔ Variable, Feature, ... (e.g. Plants, Fruits, Glucose, Rank, ....) Daniel Jacob, INRA - April

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	Α	В	С	D	E	F		<u> </u>	H
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3		2	1 harvests	Lot	harvests.csv	Harvest features	http://purl.obolibre	org/obo/ODI 1110046	organ harvesting
4		3	2 samples	SampleID	samples.csv	Samples features	http://purl.oboli	Ontional	fruit
5		4	3 compounds	SampleID	compounds.csv	Compound quantifications	http://purl.oboli	Optional	chemical entity
6		5	3 enzymes	SampleID	enzymes.csv	Enzyme Features	http://purl.obolipra	ary.org/obo/UBI_UUUU42/	enzyme
						L. L			

#### Entity $\Leftrightarrow$ Observational entity (e.g. samples, compounds, ...)



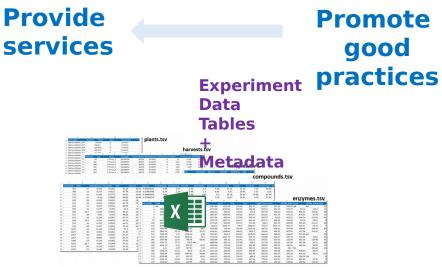
categories

x≣

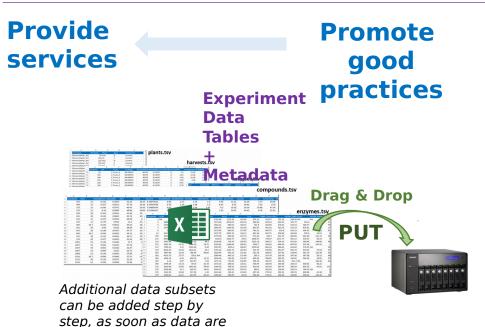
## Metadata file allowing each attribute (variable) to be annotated

	A	В	C	D	E	F .	
$\mathbf{v}$ $\mathbf{\Xi}$	1 subset	attribute	entry	category	type	description	CV_term_id CV_term_name
x≣	2 plants	PlanteID	plantid	identifier	numeric	Plant identifier	http://purl.obolibrary.org individual organism identifier
	3 plants	Row	row	qualitative	string	Row of the invidual plant on the table	http://ncicb.nci.nih.gov/x Row
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	5 plants	Treatment	treatment	factor	string	Treatment applied on plants	http://www.ebi.ac.uk/efcenvironmental factor
	6 plants	Genotype		qualitative	string	Genotype	
	7 harvests	Lot	lot	identifier	numeric	Pool of several harvests	<u>http://www.ebi.ac.uk/efc</u> sample pooling
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	10 harvests	HarvestDate			string	Harvest date	
	11 harvests	HarvestHour			string	Harvest hour	Letter and the second
	12 harvests	FruitAge	age	factor	string	fruit development stage	http://purl.obolibrary.org fruit development stage
	13 harvests	FruitPosition		qualitative	numeric	Poistion on the truss of the fruit	http://ncicb.nci.
	14 harvests	FruitDiameter		quantitative	numeric	Fruit diameter (mm)	http://ncicb.nci. Optional
	15 harvests	FruitHeight		quantitative	numeric	Fruit height (mm)	
	16 harvests	FruitFW		quantitative	numeric	Fruit Fresh Weight(g)	http://ncicb.nci.nih.gov/x Weight
	17 samples	SampleID	sampleid	identifier	numeric	Sample identifier	http://purl.obolibrary.org centrally registered identifier
	18 samples	Lot			numeric	Pool of several harvests	http://www.ebi.ac.uk/efgsample pooling
	19 samples	NbFruit			numeric	Fruit Number per sample	
	20 samples	GellyFW		quantitative	numeric	Gelly Fred Weight(g) per sample	
ategories	21 samples	GellyFruit BER		quantitative	numeric	Gelly per Fruit (estimated g) BER	
	22 samples 23 compounds		sampleid	identifier	string numeric	Sample identifier	http://purl.obolibrary.org centrally registered identifier
identifier	24 compounds	DPA	sampielu	factor	numeric	Day Per Anthesis	http://pdn.obonbrary.org/centrany/registered identifier
	25 compounds	MassBefore		quantitative	numeric	m av.extraction (g)	
factor	26 compounds			quantitative	numeric	masse MIA (g)	
qualitative	27 compounds			quantitative	numeric	Rdt (% MIA/DW)	
🗕 qualitative 🔤	28 compounds	Starch1		antitative 🔊	numeric	Dosage amidon (%poids/MIA)	http://purl.obolibrary.orgstarch
guantitative	29 compounds	Starch2		Jantitative	numeric	amidon (g/gDW)	http://purl.obolibrary.org starch
	compounds	RHAMNOSE		quantitative	numeric	RHAMNOSE	http://purl.obolibrary.org rhamnose

Attribute ⇔ Variable, Feature, ... (e.g. Plants, Fruits, Glucose, Rank, ....) Daniel Jacob, INRA - April

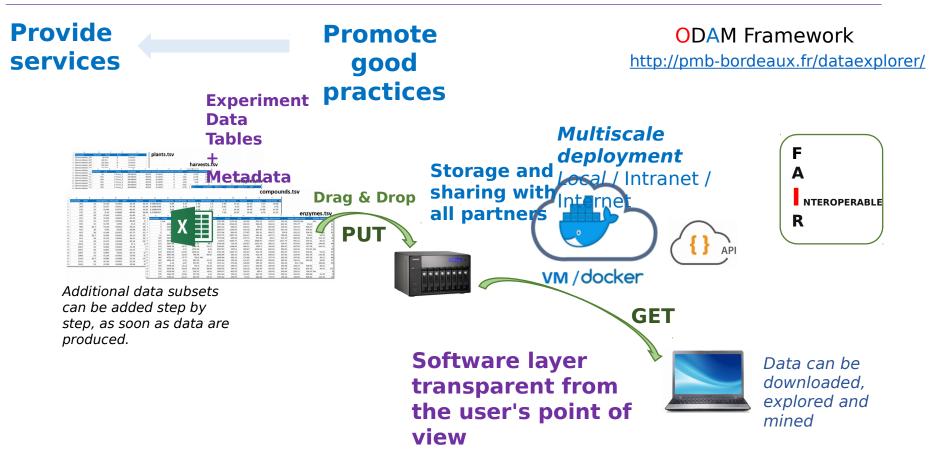


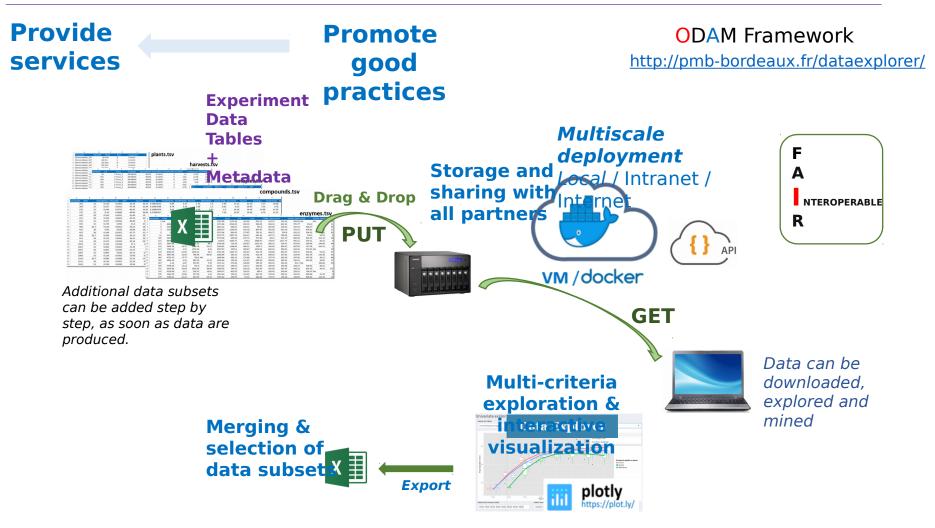
Additional data subsets can be added step by step, as soon as data are produced. ODAM Framework http://pmb-bordeaux.fr/dataexplorer/

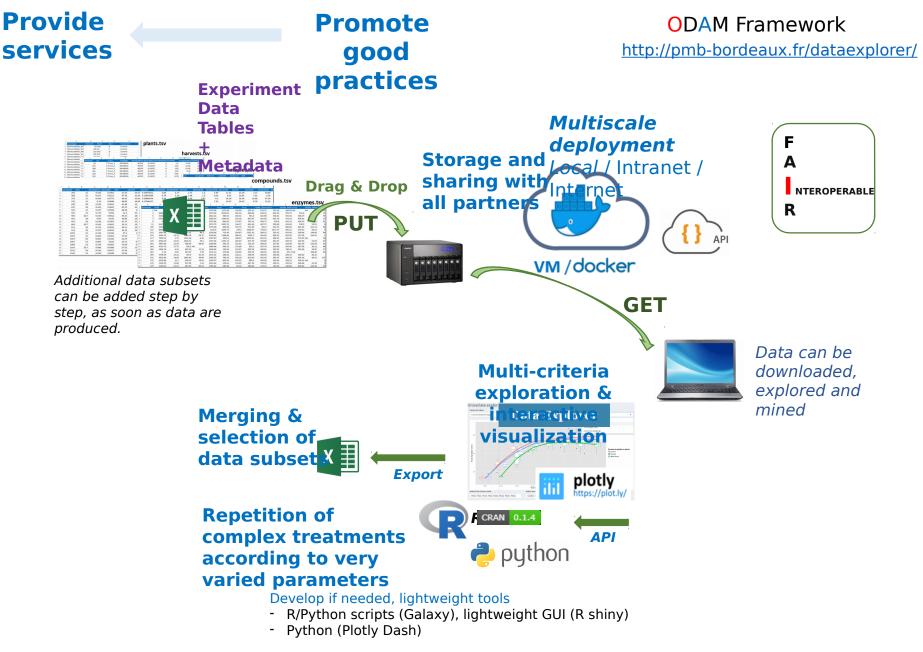


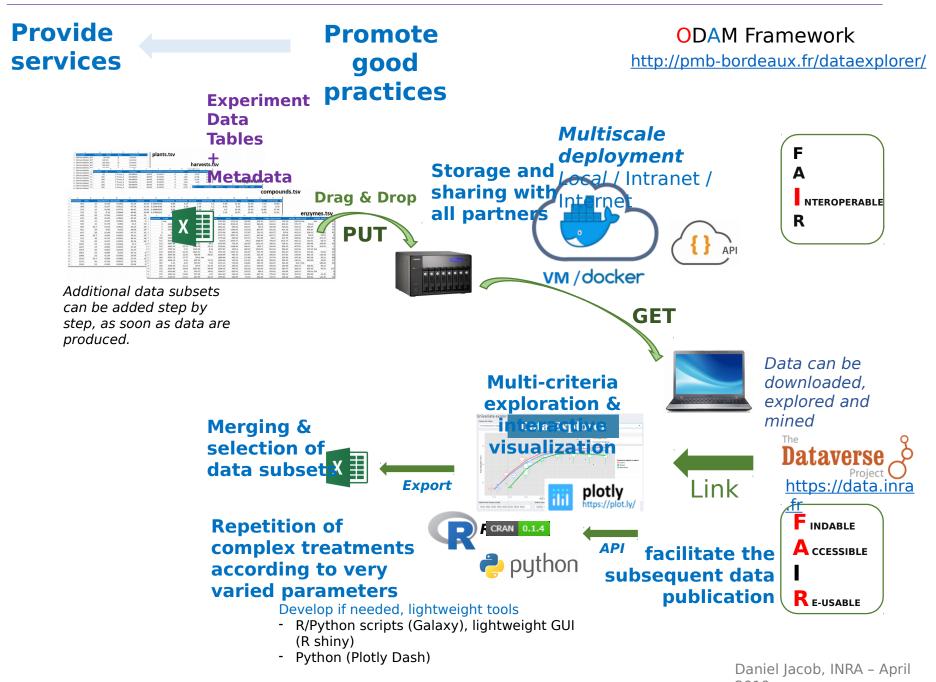
produced.

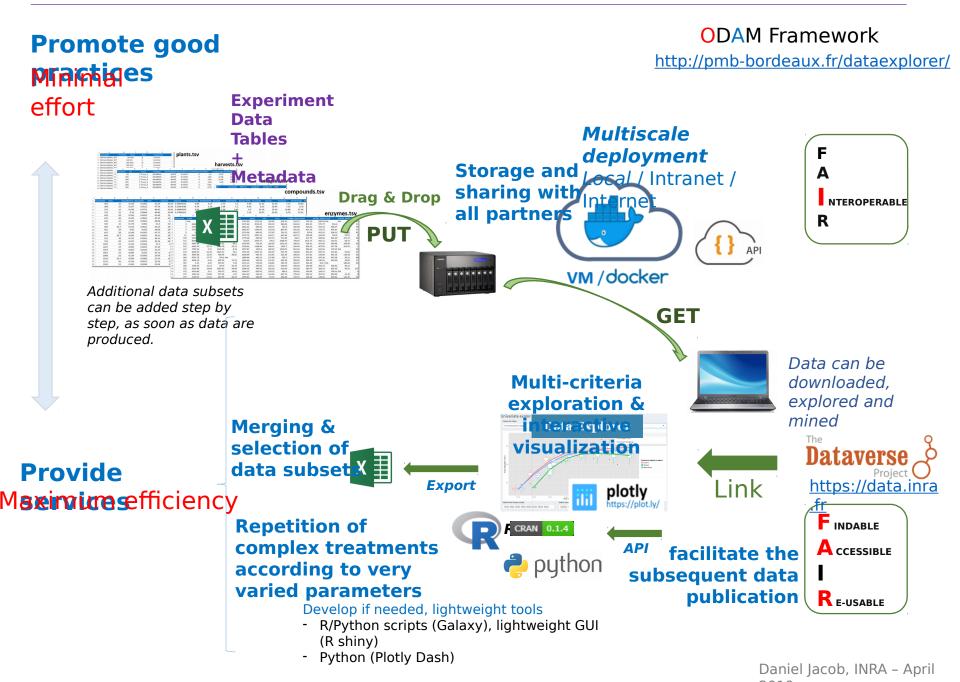
ODAM Framework http://pmb-bordeaux.fr/dataexplorer/

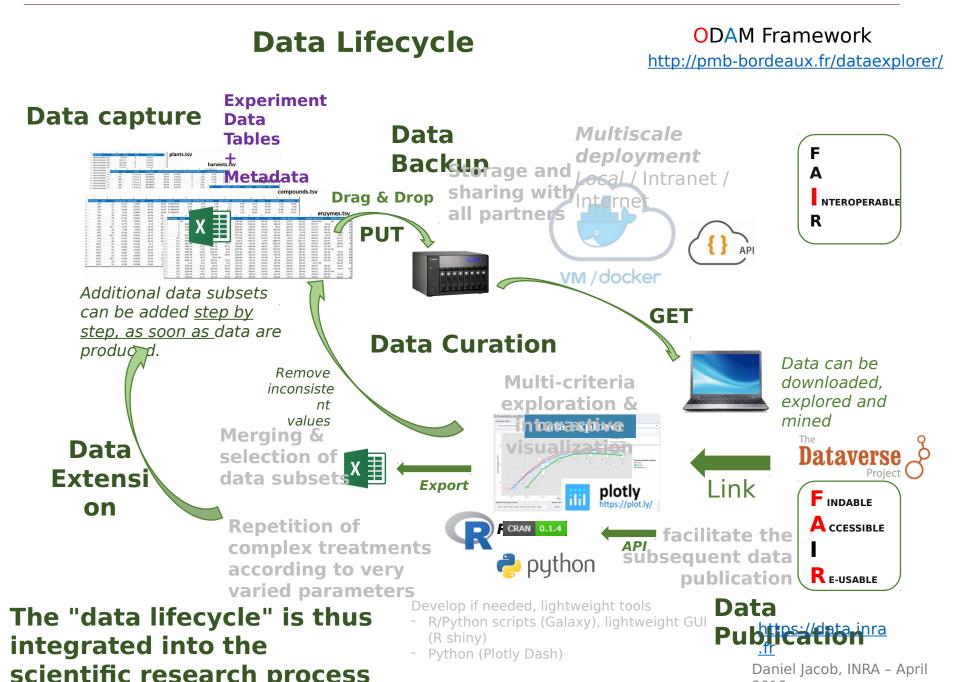


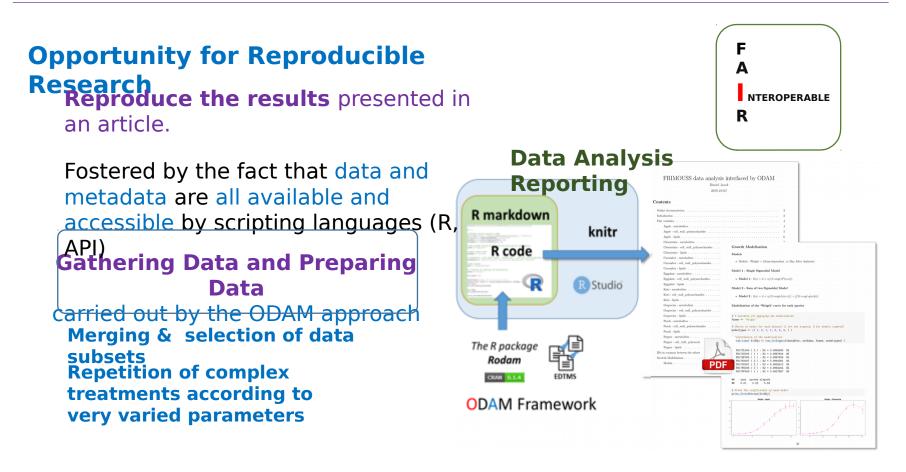


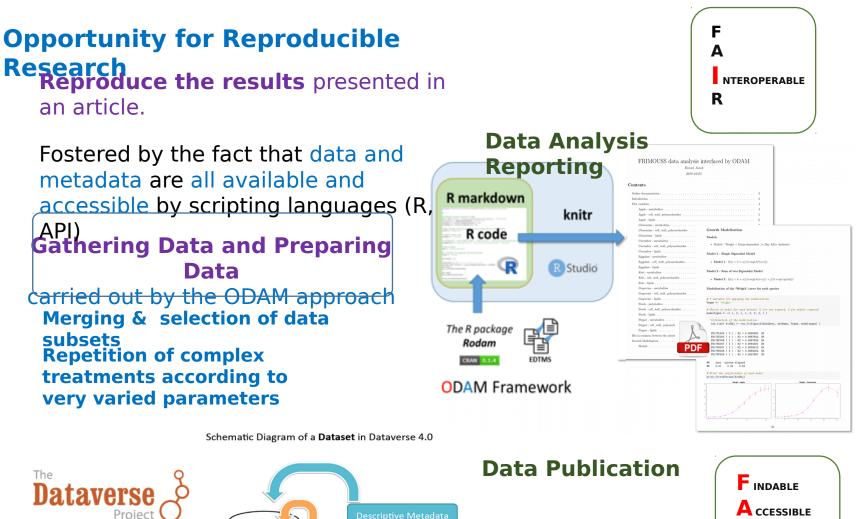




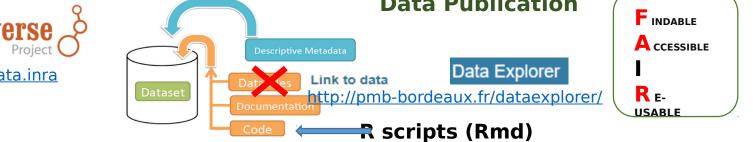








<u>https://data.inra</u> .fr



Container for your data, documentation, and code.

# **Opportunity for the Web Of Data** Metadata

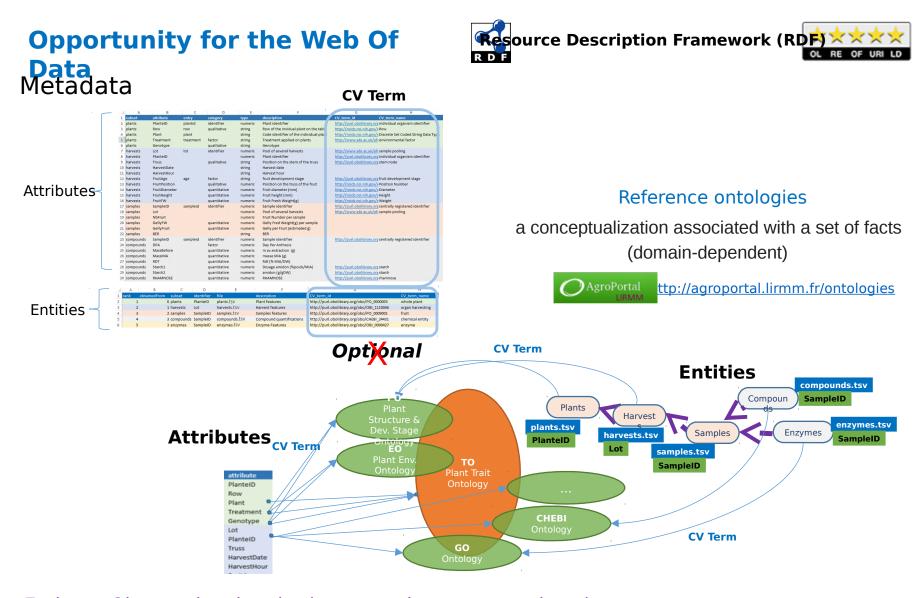


	A	В	C D	E	F	G H
	1 subset	attribute entr		type	description	CV_term_id CV_term_name
	2 plants	PlanteID plan		numeric	Plant identifier	http://purl.obolibrary.org individual organism identifier
	3 plants	Row row		string	Row of the invidual plant or	
	4 plants	Plant plan	it	string	Code identifier of the indivi	dual plant http://ncicb.nci.nih.gov/x Discrete Set Coded String Data Type
	5 plants	Treatment trea	tment factor	string	Treatment applied on plant	http://www.ebi.ac.uk/efcenvironmental factor
	6 plants	Genotype	qualitative	string	Genotype	
	7 harvests	Lot lot	identifier	numeric	Pool of several harvests	http://www.ebi.ac.uk/efcsample.pooling
	8 harvests	PlanteID		numeric	Plant identifier	http://purl.obolibrary.org individual organism identifier
	9 harvests	Truss	qualitative	string	Position on the stem of the	truss http://purl.obolibrary.org stem node
	10 harvests	HarvestDate		string	Harvest date	
	11 harvests	HarvestHour		string	Harvest hour	
	12 harvests	FruitAge age	factor	string	fruit development stage	http://purl.obolibrary.org fruit development stage
<b>. .</b>	13 harvests	FruitPosition	qualitative	numeric	Poistion on the truss of the	fruit http://ncicb.nci.nih.gov/>Position Number
Attributes	14 harvests	FruitDiameter	quantitative	numeric	Fruit diameter (mm)	http://ncicb.nci.nih.gov/>Diameter
ALLIDULES	15 harvests	FruitHeight	quantitative	numeric	Fruit height (mm)	http://ncicb.nci.nih.gov/>Height
	16 harvests	FruitFW	quantitative	numeric	Fruit Fresh Weight(g)	http://ncicb.nci.nih.gov/>Weight
	17 samples	SampleID sam	pleid identifier	numeric	Sample identifier	http://purl.obolibrary.org centrally registered identifier
	18 samples	Lot		numeric	Pool of several harvests	http://www.ebi.ac.uk/efcsample pooling
	19 samples	NbFruit		numeric	Fruit Number per sample	
	20 samples	GellyFW	quantitative	numeric	Gelly Fred Weight(g) per sa	nple
	21 samples	GellyFruit	quantitative	numeric	Gelly per Fruit (estimated g	
	22 samples	BER		string	BER	
	23 compound	s SampleID sam	pleid identifier	numeric	Sample identifier	http://purl.obolibrary.org centrally registered identifier
	24 compound	s DPA	factor	numeric	Day Per Anthesis	
	25 compound	s MassBefore	quantitative	numeric	m av.extraction (g)	
	26 compound	s MassMIA	quantitative	numeric	masse MIA (g)	
	27 compound	s RDT	quantitative	numeric	Rdt (% MIA/DW)	
	28 compound	s Starch1	quantitative	numeric	Dosage amidon (%poids/MI	A) http://purl.obolibrary.org starch
	29 compound	s Starch2	quantitative	numeric	amidon (g/gDW)	http://purl.obolibrary.org starch
	30 compound	s RHAMNOSE	quantitative	numeric	RHAMNOSE	http://purl.obolibrary.org rhamnose
	A	B C	D	E	F	G H
	1 rank ob	tainedFrom subset	identifier file		description	CV_term_id CV_term_name
	2 1	0 plants	PlanteID plants.ts	/	Plant features	http://purl.obolibrary.org/obo/PO_0000003 whole plant
Entities 🚽	3 2	1 harvests	Lot harvests.	tsv	Harvest features	http://purl.obolibrary.org/obo/OBI_1110046 organ harvesting
	4 3	2 samples	SampleID samples.	tsv	Samples features	http://purl.obolibrary.org/obo/PO 0009001 fruit
	5 4	3 compound				http://purl.obolibrary.org/obo/CHEBI 24431 chemical entity
	6 5	3 enzymes	SampleID enzymes.			http://purl.obolibrary.org/obo/OBI 0000427 enzyme
		5 chapmes	chapters.			in the second seco

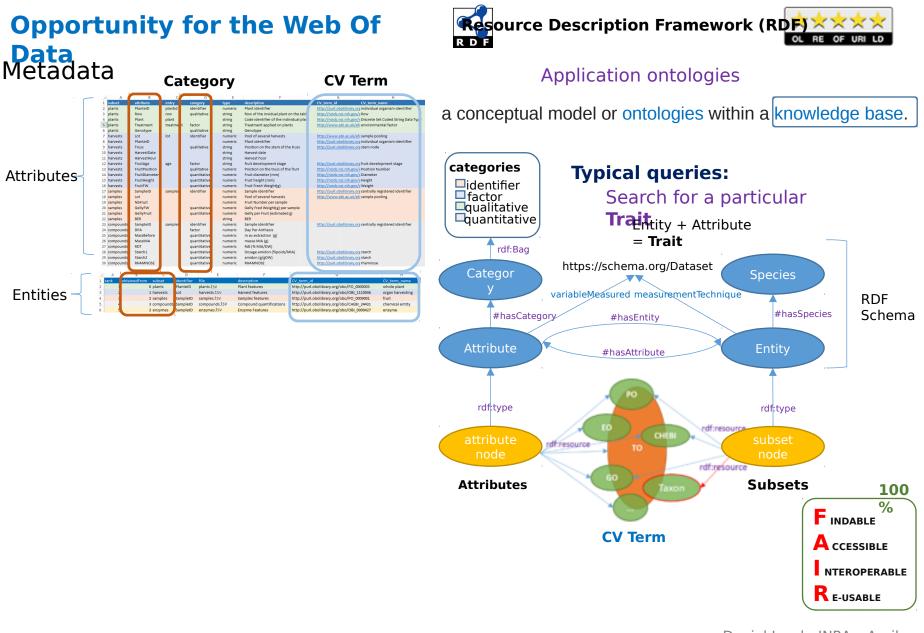


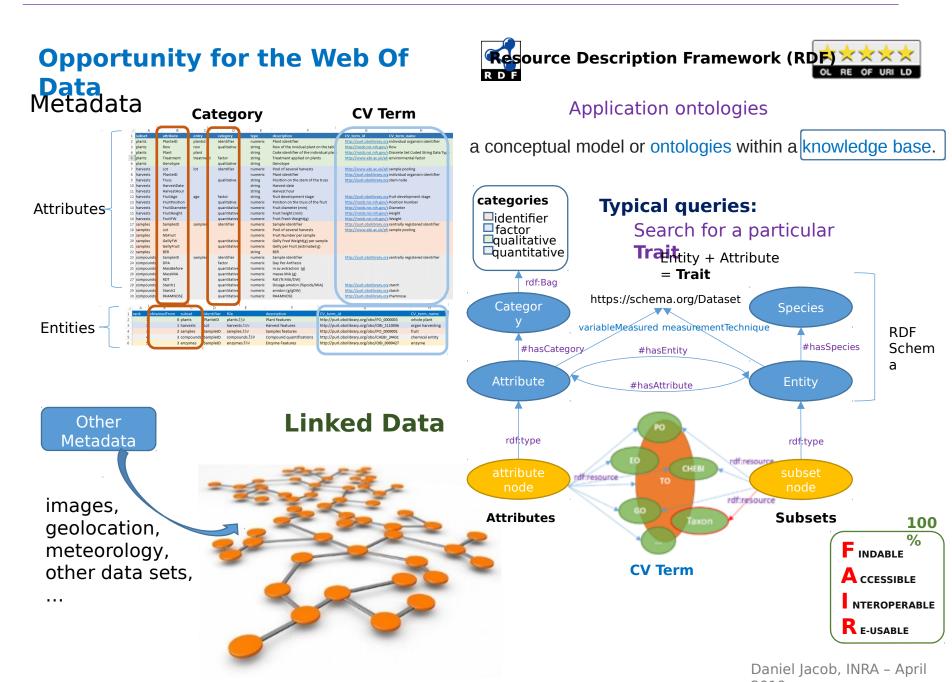
Entity  $\Leftrightarrow$  Observational entity (e.g. samples, compounds, ...) Attribute  $\Leftrightarrow$  Variable, Feature, ... (e.g. Plants, Fruits, Glucose, Rank, ....)





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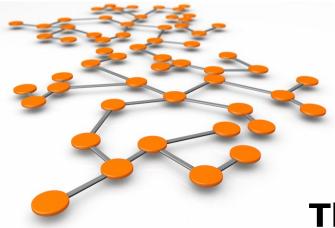
# FAIR principles

- can improve the data lifecycle by relying on technologies,
- but only if they serve the concerned communities by meeting their expectations.

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The role of a <u>data authority</u> is to translate <u>principles</u> into <u>standards</u> in agreement with the concerned <u>communities</u>



# Thank you for your attention

