Sharing massive data analysis : from provenance to linked experiment reports

Scientific workflows, provenance and linked data to the rescue

Alban Gaignard, PhD, CNRS

13 november 2018 APSEM 2018

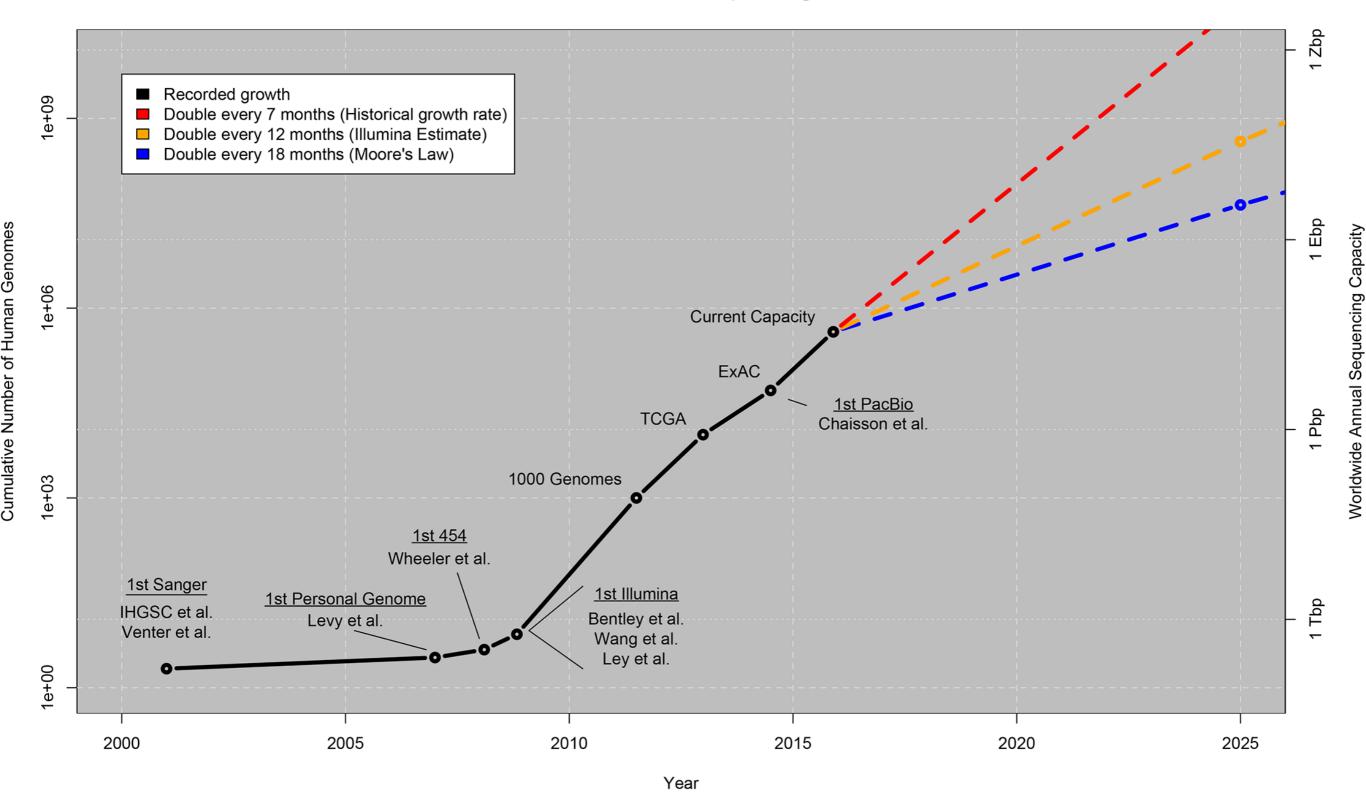




Reproducibility at the age of **massive data**

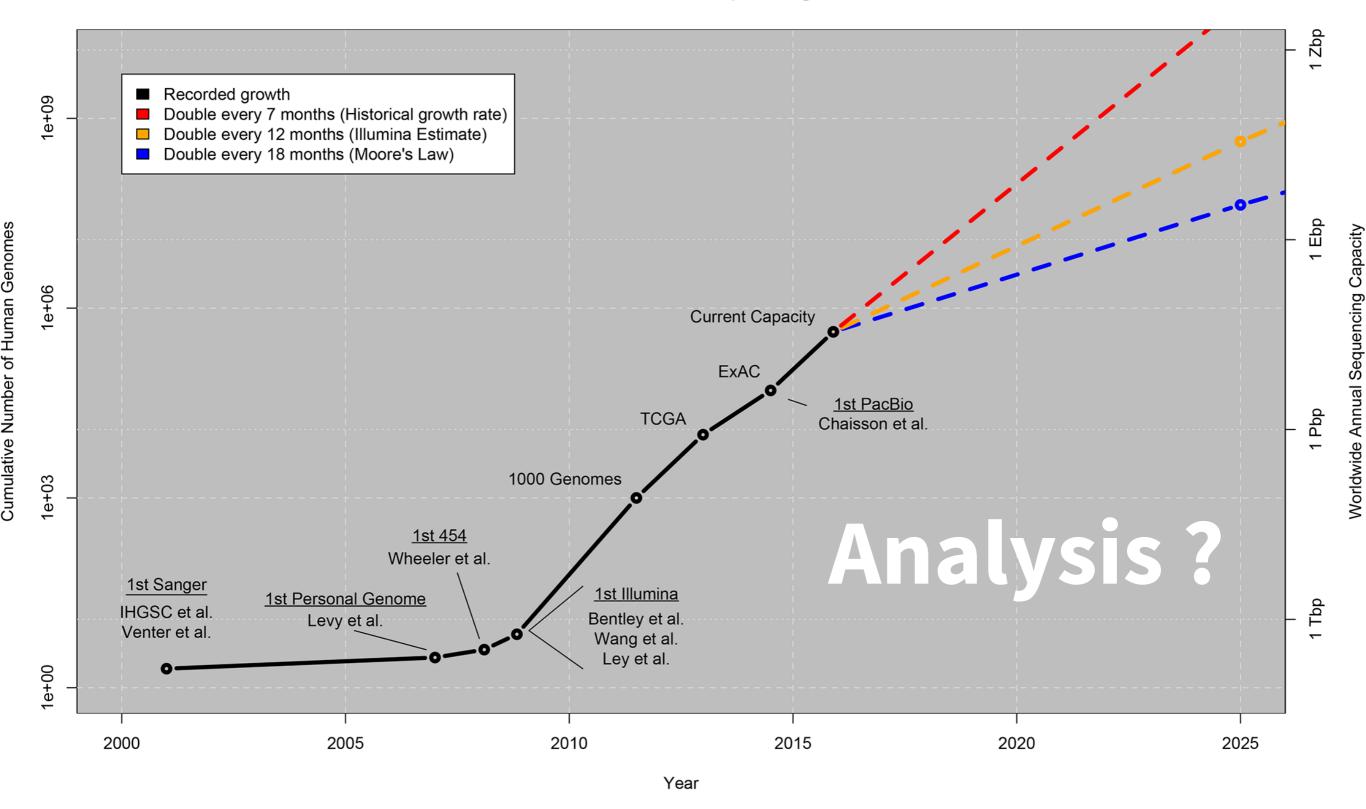
Massive life science data production

Growth of DNA Sequencing

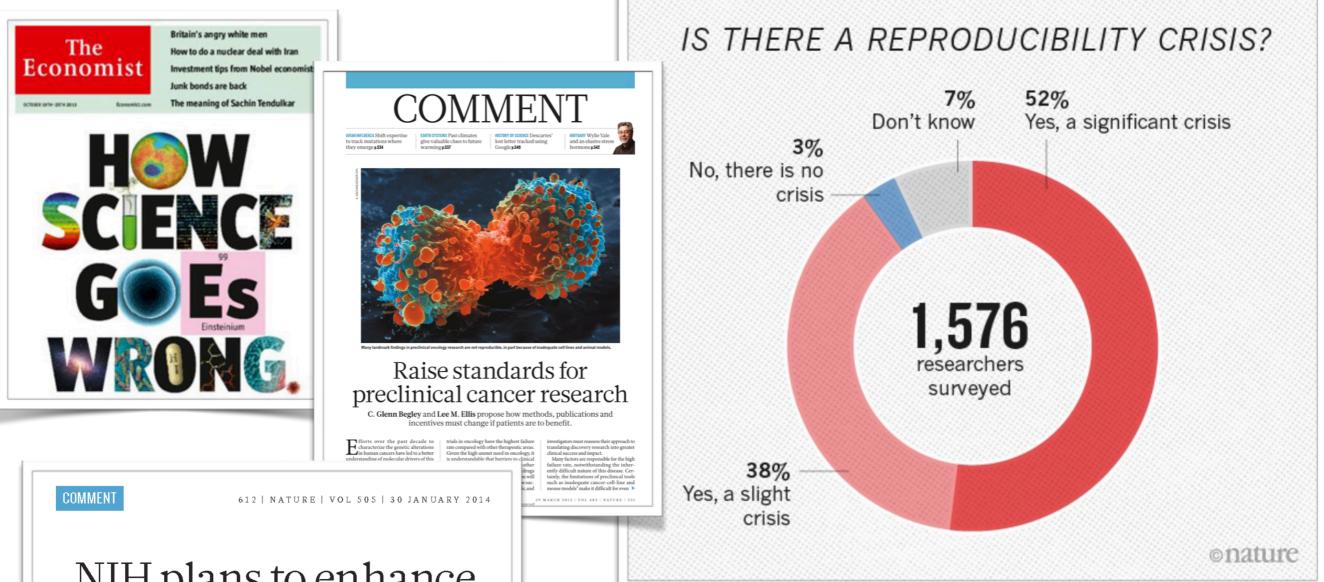


Massive life science data production

Growth of DNA Sequencing



Knowledge production



NIH plans to enhance reproducibility

Francis S. Collins and Lawrence A. Tabak discuss initiatives that the US National Institutes of Health is exploring to restore the self-correcting nature of preclinical research.

growing chorus of concern, from scientists and laypeople, contends that the complex system for ensuring the reproducibility of biomedical research is failing and is in need of restructuring^{1,2}. As leaders of the US National Institutes of Health (NIH), we share this concern and here explore some of the significant interventions that we are planning.

Science has long been regarded as 'selfcorrecting', given that it is founded on the shorter term, however, the checks and balances that once ensured scientific fidelity have been hobbled. This has compromised the ability of today's researchers to reproduce others' findings.

Let's be clear: with rare exceptions, we have no evidence to suggest that irreproducibility is about scientific misconduct. In 2011, the Office of Research Integrity of the US Department of Health and Human Services pursued only 12 such cases³. « In 2012, Amgen researchers made headlines when they declared that they had been unable to reproduce the findings in 47 of 53 'landmark' cancer papers » (doi:10.1038/nature.2016.19269)

Same experiment

Same setup

Same lab

Same experiment

Same setup

Samelab

Same experiment

Same setup

Same lab

New ideas, new experiment, some comonalities

Intracranial aneurysms : localized dilation or ballooning in cerebral blood vessels

Intracranial aneurysms : localized dilation or ballooning in cerebral blood vessels

Intracranial aneurysms : localized dilation or ballooning in cerebral blood vessels

Objective, systematic, reapatable measures?

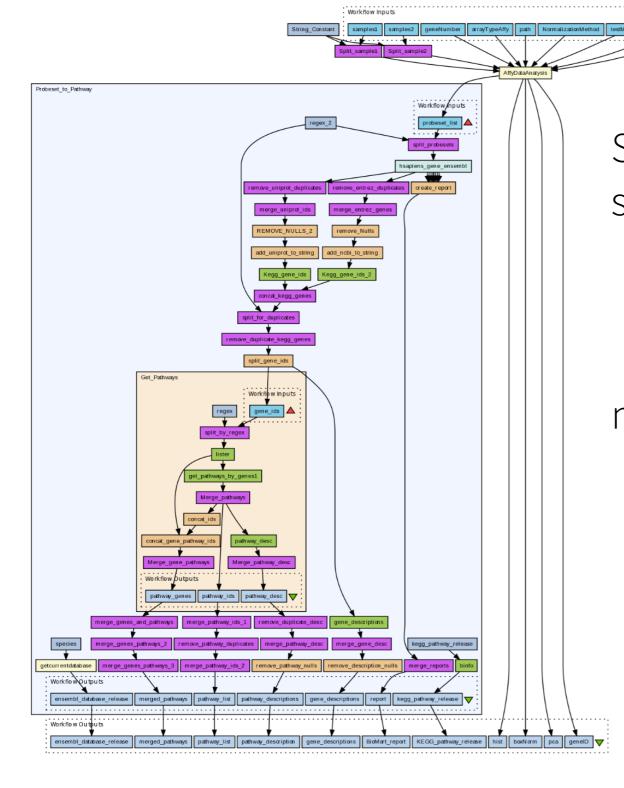
Scientific **workflows** to the rescue ...

What is a workflow ?

« Workflows provide a systematic way of describing the **methods** needed and provide the **interface** between **domain specialists** and **computing infrastructures**. »

« Workflow management systems (WMS) **perform** the complex analyses on a variety of **distributed resources** »

Malcolm Atkinson, Sandra Gesing, Johan Montagnat, Ian Taylor. **Scientific workflows: Past, present and future**. Future Generation Computer Systems, Elsevier, 2017, 75, pp.216 - 227. <10.1016/j.future.2017.05.041>





TensorFlow

Taverna



Scientific workflows to enhance **trust** in scientific results :

- → automate data analysis (at scale)
- → **abstraction** (describe/share methods)
 - → provenance (~transparency)

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		ed workflow framew		ata analysis.			
	h-level languag						
-		or data pipelines.					
		utility for managing	builds and compl	ex workflows.			
		vork with web monit					
 Bistro - Lib 	rary to build an	d execute typed sci	entific workflows.				
 Bpipe - Too 	l for running ar	d managing bioinfo	rmatics pipelines.				
 Briefly - Py 	thon Meta-prog	gramming Library fo	r Job Flow Control				
Cluster Flor	v - Command-I	ine tool which uses	common cluster n	anagers to run bio	oinformatics (pipelines.	
Clusterjob	Automated re	producibility, and ha	ssle-free submiss	on of computation	al jobs to clu	isters.	
 Compss - F 	Programming m	odel for distributed	infrastructures.				
 Conan2 - L 	ight-weight wo	rkflow management	application.				
 Consecutio 	n - A Python pi	peline abstraction i	nspired by Apache	Storm topologies.			
 Cosmos - F 	ython library fo	or massively parallel	workflows.				
Cromwell -	Workflow Mana	agement System ge	ared towards scier	tific workflows fro	m the Broad	Institute.	
		ctional workflow lar		ork, implemented	in Erlang.		
-		ised job scheduler i					
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		arallel computing lib					
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Provenance : a way to **reuse** produced & analysed data

Definition: Oxford dictionnary

« The beginning of something's existence; something's origin. »

Definition: Computer Science

« Provenance information describes the **origins** and the **history of data in its life cycle**. »

« Today, data is often made available on the Internet with **no centralized control over its integrity**: data is constantly being created, copied, moved around, and combined indiscriminately. Because information sources (or different parts of a single large source) may vary widely in terms of quality, it is essential to provide **provenance** and other context information which can **help end users** judge whether query results are **trustworthy**. »

James Cheney, Laura Chiticariu, and Wang-Chiew Tan. 2009. **Provenance in Databases: Why, How, and Where**. Found. Trends databases 1, 4 (April 2009), 379-474. DOI=http:// dx.doi.org/10.1561/1900000006

Representing provenance



PROV-O: The PROV Ontology

W3C Recommendation 30 April 2013

This version:

http://www.w3.org/TR/2013/REC-prov-o-20130430/

Latest published version:

http://www.w3.org/TR/prov-o/

Implementation report:

http://www.w3.org/TR/2013/NOTE-prov-implementations-20130430/

Previous version:

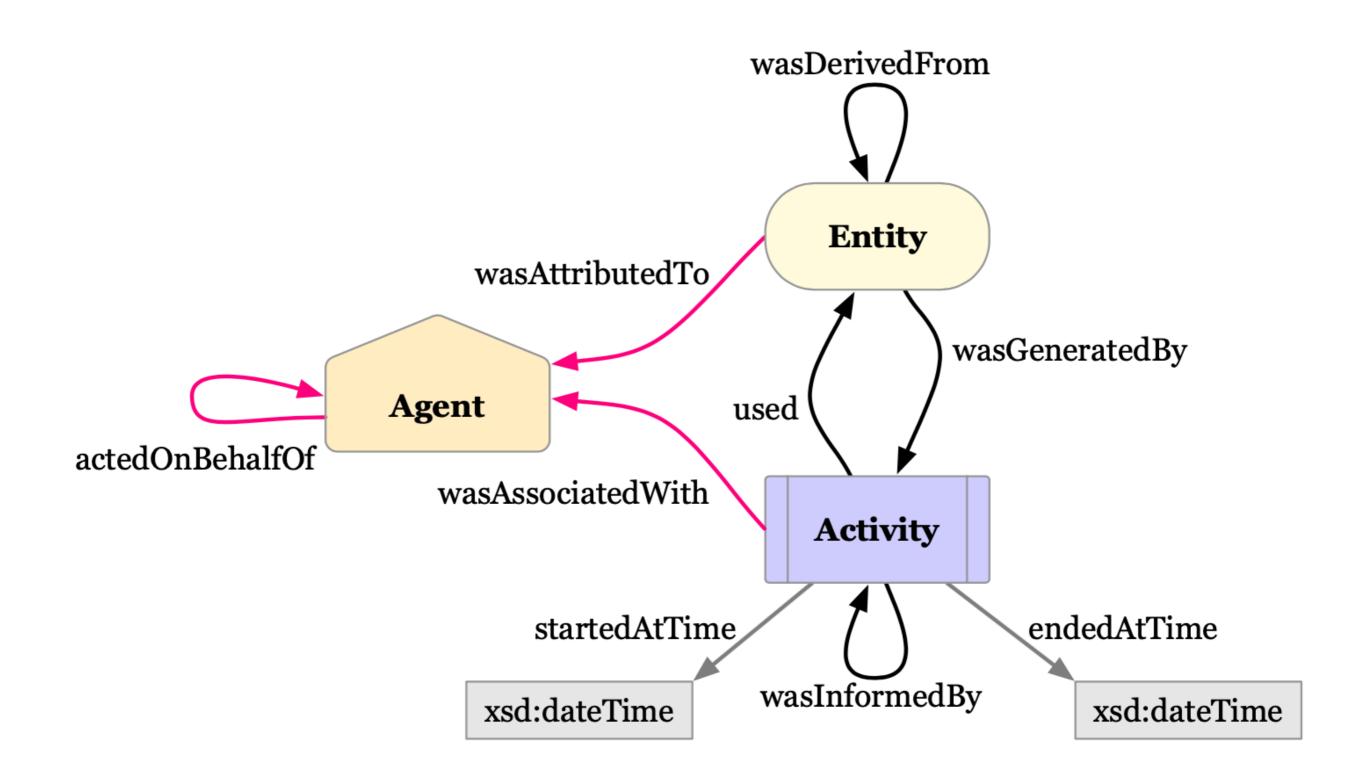
http://www.w3.org/TR/2013/PR-prov-o-20130312/

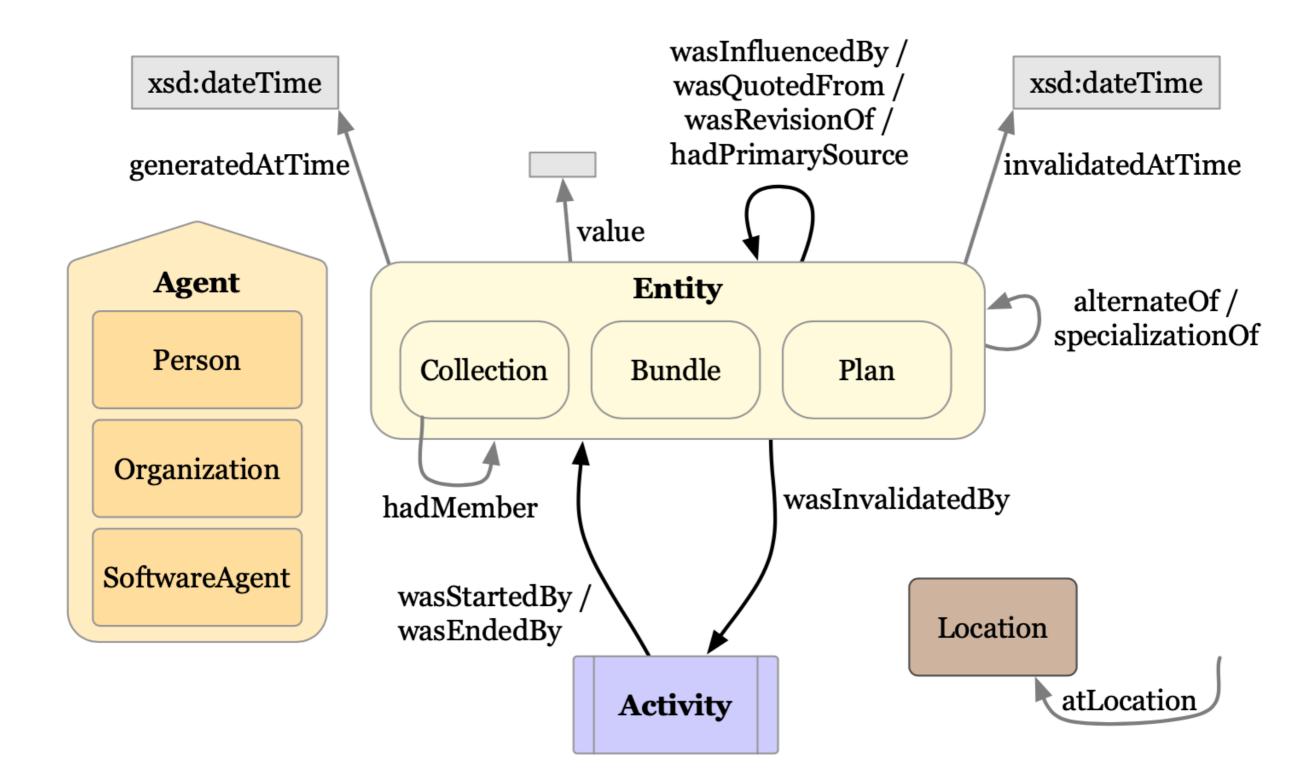
Editors:

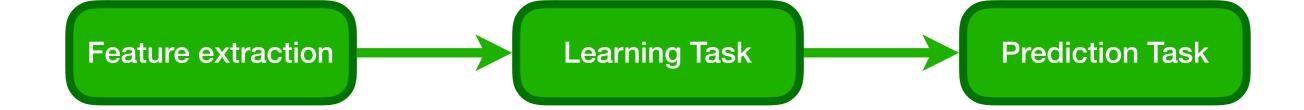
<u>Timothy Lebo</u>, Rensselaer Polytechnic Institute, USA <u>Satya Sahoo</u>, Case Western Reserve University, USA <u>Deborah McGuinness</u>, Rensselaer Polytechnic Institute, USA

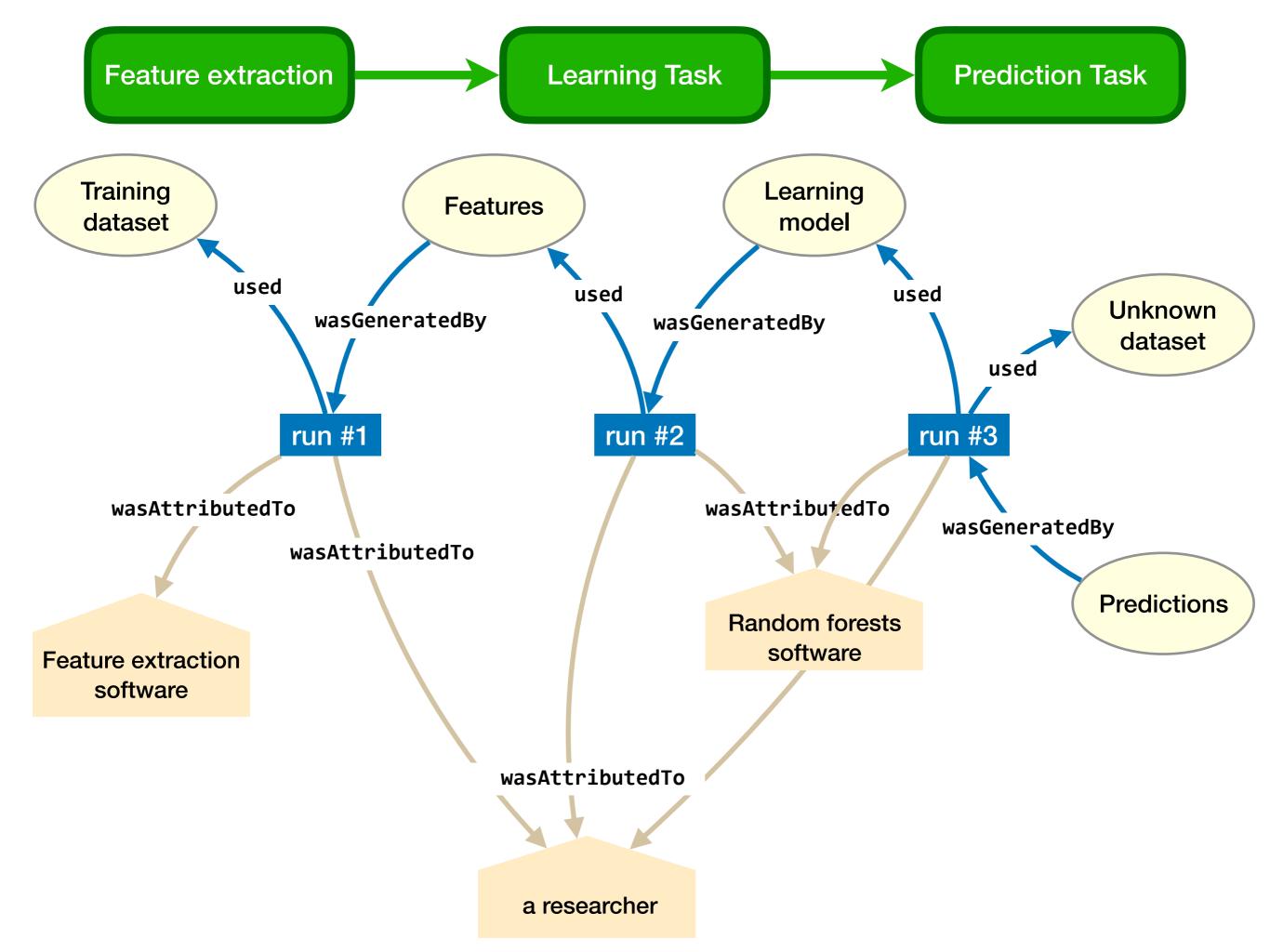
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Reasoning with provenance



Constraints of the PROV Data Model

W3C Recommendation 30 April 2013

This version:

http://www.w3.org/TR/2013/REC-prov-constraints-20130430/

Latest published version:

http://www.w3.org/TR/prov-constraints/

Test suite:

http://dvcs.w3.org/hg/prov/raw-file/default/testcases/process.html

Implementation report:

http://www.w3.org/TR/2013/NOTE-prov-implementations-20130430/

Previous version:

http://www.w3.org/TR/2013/PR-prov-constraints-20130312/ (color-coded diff)

Editors:

<u>James Cheney</u>, University of Edinburgh <u>Paolo Missier</u>, Newcastle University <u>Luc Moreau</u>, University of Southampton

Author:

Tom De Nies, iMinds - Ghent University

Please refer to the errata for this document, which may include some normative corrections.

The English version of this specification is the only normative version. Non-normative translations may also be available.

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5.3 Derivations

Derivations with explicit activity, generation, and usage admit the following inference:

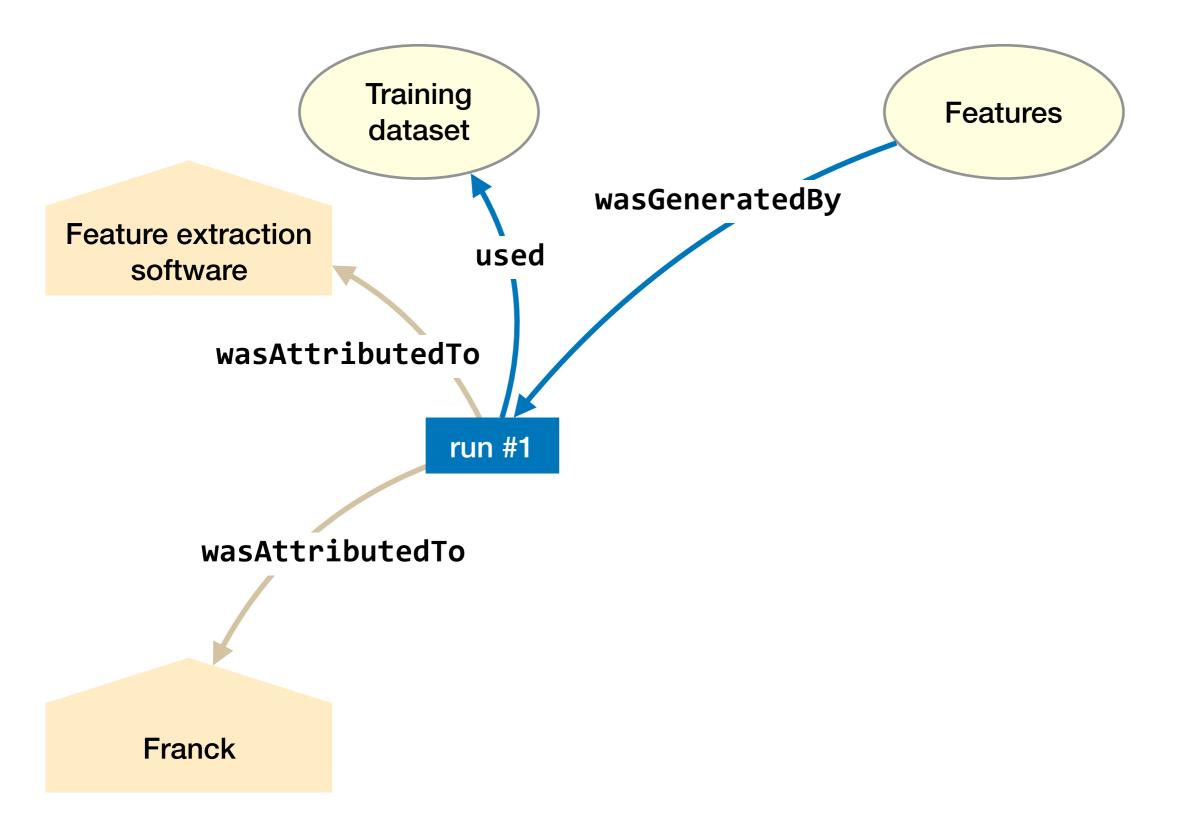
Inference 11 (derivation-generation-use-inference)

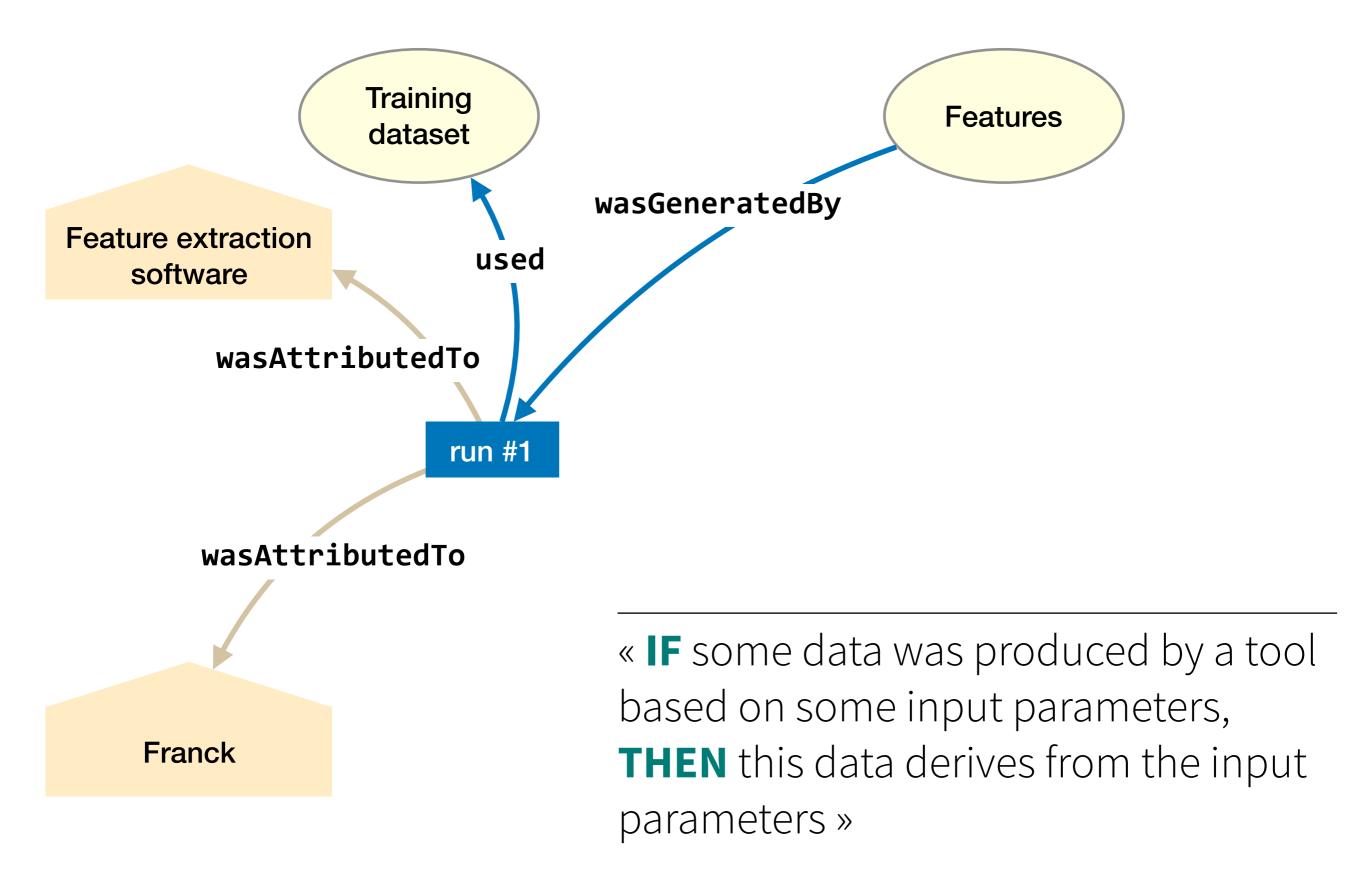
In this inference, none of a, gen2 or use1 can be placeholders -.

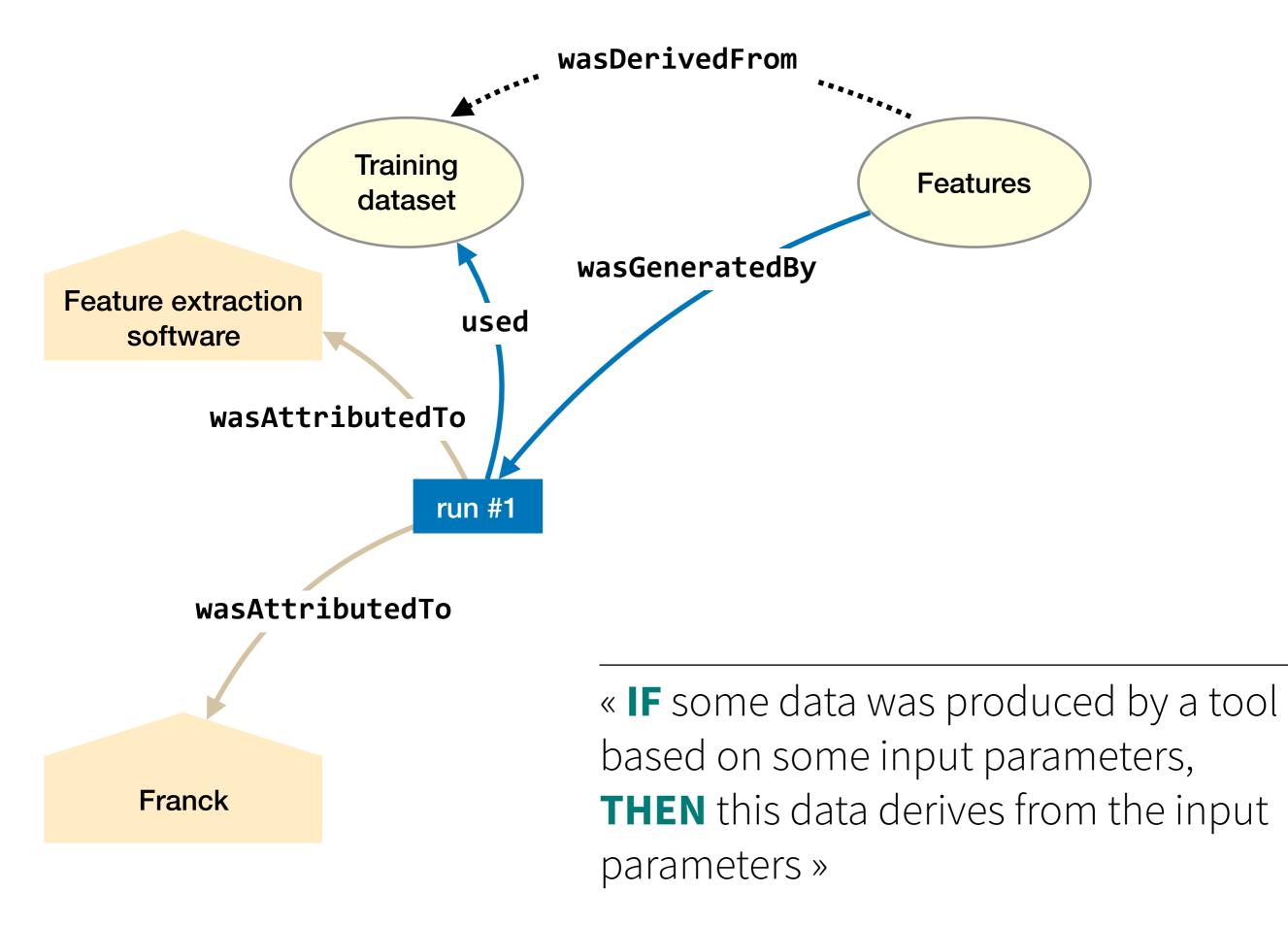
IF wasDerivedFrom(_id; e2,e1,a,gen2,use1,_attrs), THEN there exists _t1 and _t2 such that used(use1; a,e1,_t1,[]) and wasGeneratedBy(gen2; e2,a,_t2,[]).

Inference 15 (influence-inference)

- 1. IF wasGeneratedBy(id; e,a,_t,attrs) THEN wasInfluencedBy(id; e, a, attrs).
- 2. IF used(id; a,e,_t,attrs) THEN wasInfluencedBy(id; a, e, attrs).
- 3. IF wasInformedBy(id; a2,a1,attrs) THEN wasInfluencedBy(id; a2, a1, attrs).
- 4. IF wasStartedBy(id; a2,e,_a1,_t,attrs) THEN wasInfluencedBy(id; a2, e, attrs).
- 5. IF wasEndedBy(id; a2,e,_a1,_t,attrs) THEN wasInfluencedBy(id; a2, e, attrs).
- 6. IF wasInvalidatedBy(id; e,a,_t,attrs) THEN wasInfluencedBy(id; e, a, attrs).
- 7. IF wasDerivedFrom(id; e2, e1, _a, _g, _u, attrs) THEN wasInfluencedBy(id; e2, e1, attrs). Here, _a, _g, _u MAY be placeholders -.
- 8. IF wasAttributedTo(id; e,ag,attrs) THEN wasInfluencedBy(id; e, ag, attrs).
- 9. IF wasAssociatedWith(id; a,ag,_pl,attrs) THEN wasInfluencedBy(id; a, ag, attrs). Here, _pl MAY be a placeholder -.
- 10. IF actedOnBehalfOf(id; ag2,ag1,_a,attrs) THEN wasInfluencedBy(id; ag2, ag1, attrs).







PROV, how-to record/query ?

Writing PROV statements

<samples sample1="" sample1.hapcaller.g.vcf="" vcf=""></samples>	
a prov:Entity;	
<pre>prov:wasGeneratedBy <http: <#haplotypecaller="" prov:wasattributedto="" snakemake-provenance#activity-945311db-8f46-440d-="">;</http:></pre>	-ad05-e8c93832006e>;
<pre>rdfs:label "Samples/Sample1/VCF/Sample1.hapcaller.g.vcf"; crypto:sha512</pre>	
"28df1599bd0053ac08ce195db5750cf5c5f3a05597695449a2acee49b72245aee290bbc3f9f	fcbe0f3f43b8c07156a175a424a25f2de5
3c326906340081d1c7b"^^xsd:string ;	
<pre>prov:wasDerivedFrom <bed capture.extended1000.bed=""> ;</bed></pre>	
<pre>prov:wasDerivedFrom <samples bam="" sample1="" sample1.final.bam=""> ;</samples></pre>	
<pre>prov:wasDerivedFrom ;</pre>	
<pre>prov:wasDerivedFrom <gatkpresent.txt> ;</gatkpresent.txt></pre>	
<pre>prov:wasDerivedFrom ;</pre>	
<pre>prov:wasDerivedFrom ;</pre>	
<pre>prov:wasDerivedFrom <samples bam="" sample1="" sample1.final.bai=""> ;</samples></pre>	

Writing PROV statements

<http://snakemake-provenance#activity-945311db-8f46-440d-ad05-e8c93832006e> a prov:Activity ; rdfs:comment """ gatk -Djava.io.tmpdir=Samples/Sample1/VCF -XX:ParallelGCThreads=5 -Xmx3g -T HaplotypeCaller -R ../testdata/human_g1k_v37.chr22.fasta -variant_index_type LINEAR --emitRefConfidence GVCF -stand_call_conf 30.0 -variant_index_parameter 128000 -nct 1 -rf ReadLength -minRead 0 -maxRead 10000 -S SILENT -L:capture,BED BED/capture.extended1000.bed -ISamples/Sample1/BAM/Sample1.final.bam --dbsnp:dbsnp,VCF ../testdata/dbsnp_138.b37.chr22.recode.vcf.gz -0Samples/Sample1/VCF/Sample1.hapcaller.g.vcf prov:wasAssociatedWith <#haplotypeCaller> ; prov:startedAtTime "2018-04-04T16:19:57.054054"^^xsd:dateTime; prov:endedAtTime "2018-04-04T16:19:57.054076"^^xsd:dateTime; prov:used <BED/capture.extended1000.bed> ; prov:used <Samples/Sample1/BAM/Sample1.final.bam> ; prov:used <../testdata/dbsnp_138.b37.chr22.recode.vcf.gz> ; prov:used <gatkPresent.txt> ; prov:used <../testdata/human_g1k_v37.chr22.fasta> ; prov:used <../testdata/human_g1k_v37.chr22.dict> ; prov:used <Samples/Sample1/BAM/Sample1.final.bai> ;

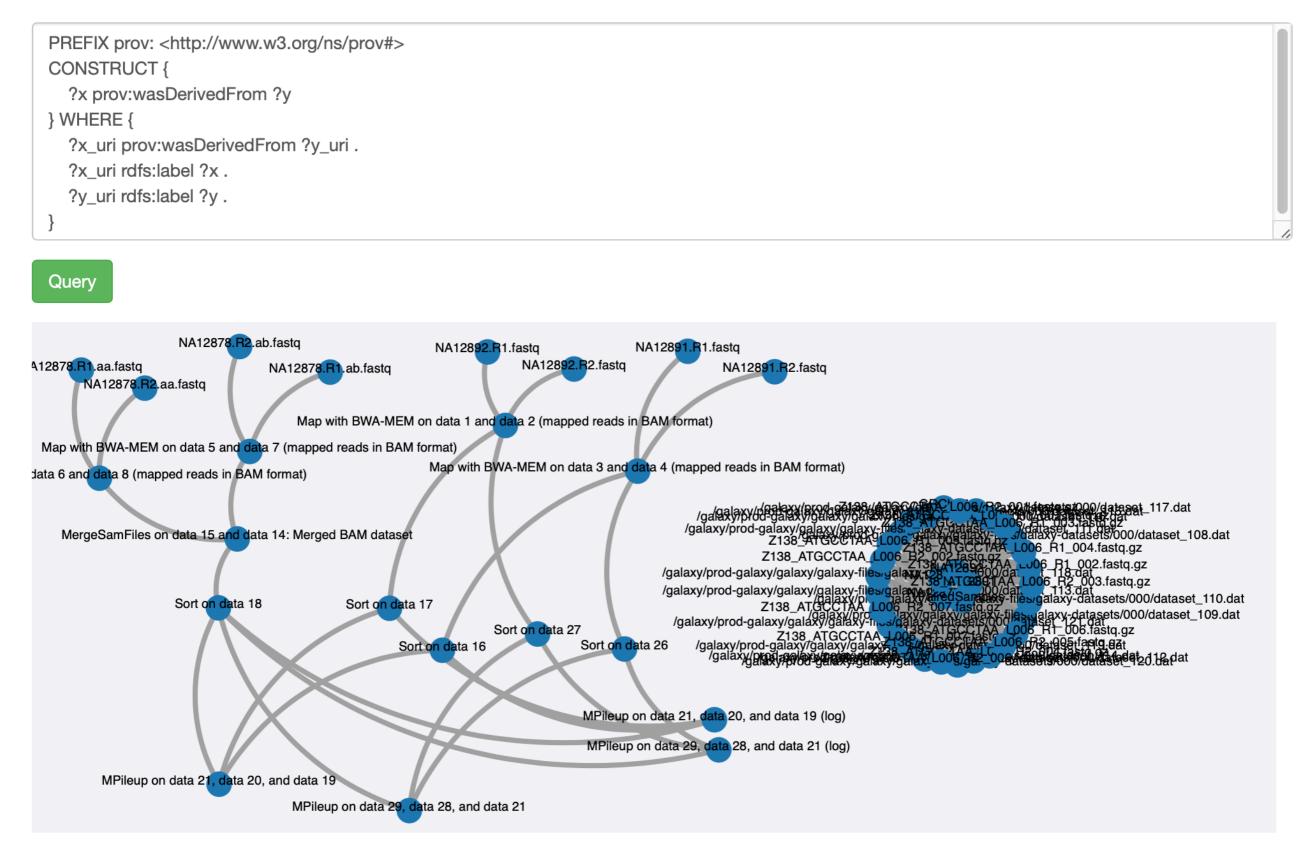
Querying PROV graphs

CONSTRUCT {?x ?p ?y} WHERE {?x ?p ?y}

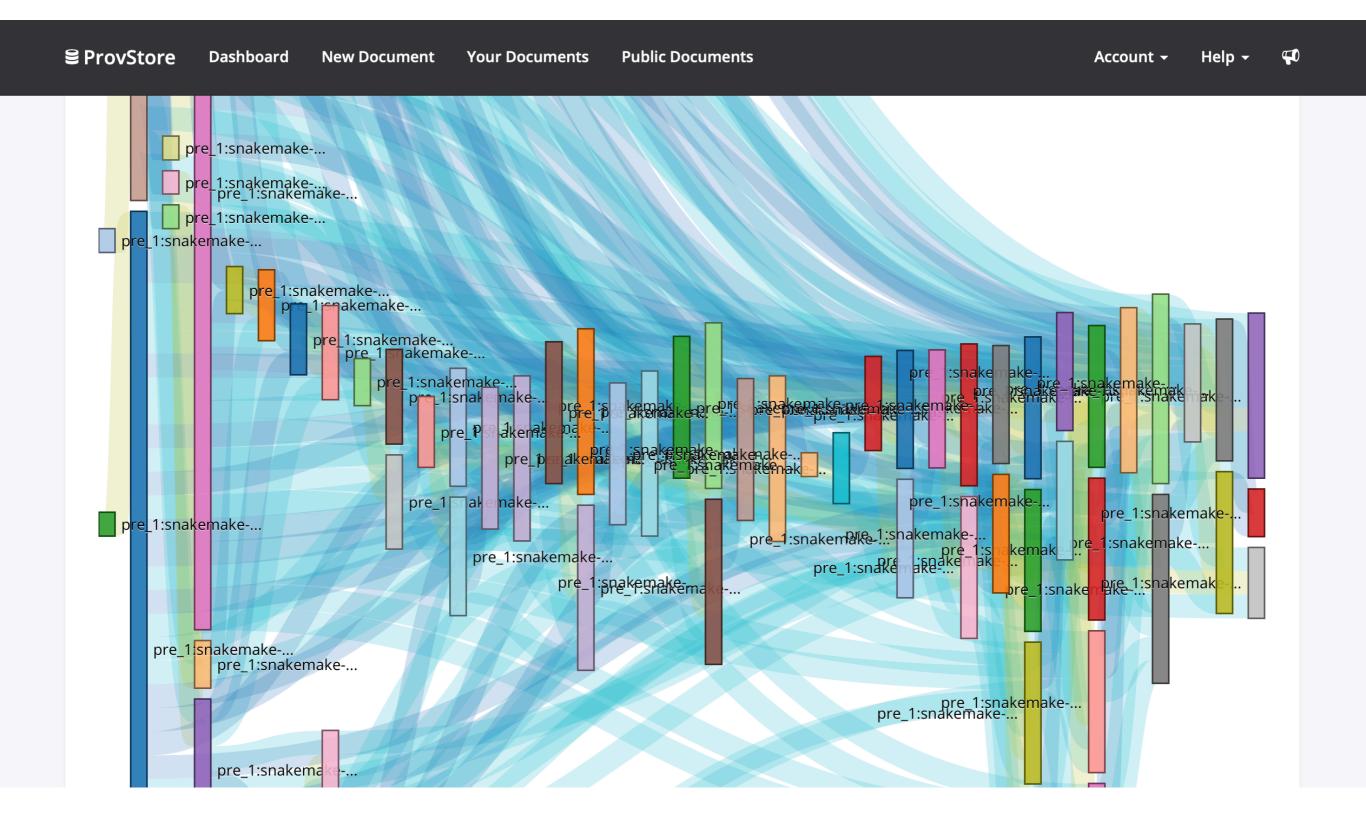
Query

NA12878.R1.ab.fastq 12878.R1.aa.fastq NA12878.R2.aa.fastq 2016-0t_JT15:10:23.522526 2016-06-28T08:19:29.354904 2016-06-28T08:19:33.81717 BAN 2992. HZ HAS ON BAN 92. R16 28 29T15:11:58.223705 /galaxy/prod-galaxy/galaxy/galaxy/galaxy-file 2842 8628108:19:28.041412 /galaxy/prod-galaxy/galaxy/prod-galaxy/galax 016-06-28T08:19:28 100107 28 108:19:19.7040 Z138_ATGCCTAA_L006_R1_005.fastq.gz Z138_ATGCCTAA_L006_R3_007/leastm.gta /galaxy/prod-galaxy/galaxy/galaxy/files/galaxy-da___ts/__dataset_119 06b42b7a99da 2016-06-30 09:50 3265 8579:28.106 g#d167#24979480688968aac1 /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datasets/000/da 2016-06-30209:509:286928:20.94 /galaxy/prod-galaxy/galaxy/galaxy/galaxy/galaxy/atasets/000/datasett110/da RedeOf 2016-06-29T15:10:48.879585 /galaxy/prod-galaxy/galaxy 773c7f Z138_ATGCCTAA_L006_R2_0089 Symetrid#12c6d0a46sbagatepros#Aethid#47b9a56c1 2016-06-30T09:56:12.234 http://fr.symetric#toolshed.g2.bx.psu. os/devteam/tophat2/tophat2 a chara 2 (mapped reads in BAM format) 2016-06-30109:55:39.095104 NA12892-09T16:51:51,906052fr.svr **14**5018 NA1287 on data 3 and data 4 (mapped reads in BAM format) 78a1 _____ ca98ch14b16-30T09:56:51.33563 PairedSamples http://ft.sy/ne NA128 12878.R1. http://froumage 03708989999006308109:54508.629929 2016-06-29T15:132016403-B0T09:56:43.91290 5c242fcfa290e0 /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datasets/000/dataset_108pdatr.syme 3018506199915:12:5319396130T09:56:54.47672 Z138_ATGCCTAA_L006_R1_004.fastq.gzttp://intsy Z138_ATGCATGCCTAA_L006_R1_004.fastq.gzttp://intsy Sort on data 27 2016-06-29 T15:12:55.663322 /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datas 000/dataset 114.dat /galaxy/prod-galaxy/galaxy 2016-06-29T15:12:35.8677 tastets/000/dataset_115.dat GCCTAA_LOOM://t2s00@fastqcotshed.g2.bx.psu.edu/repos/degtorn date of n date

Querying PROV graphs

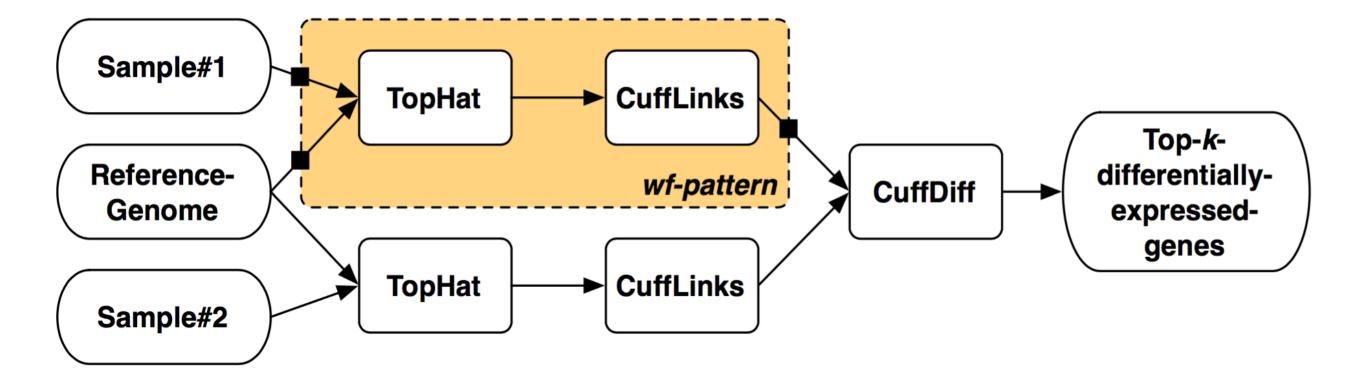


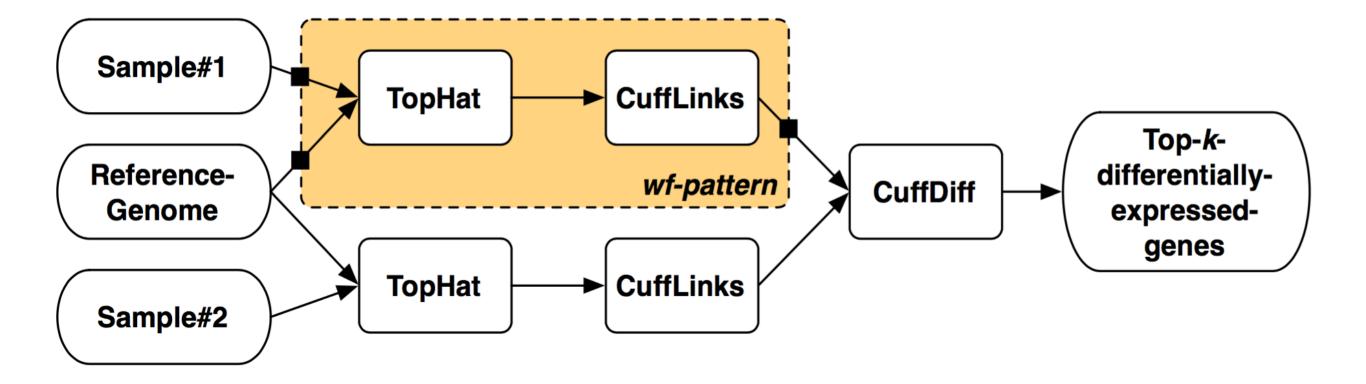
PROV store



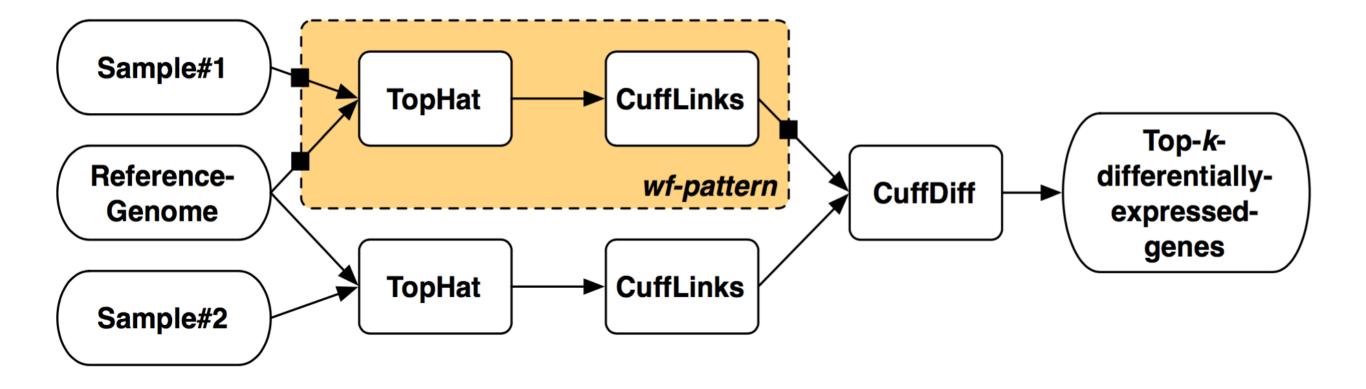
Still open issues ...

Reuse instead of re-execution ?



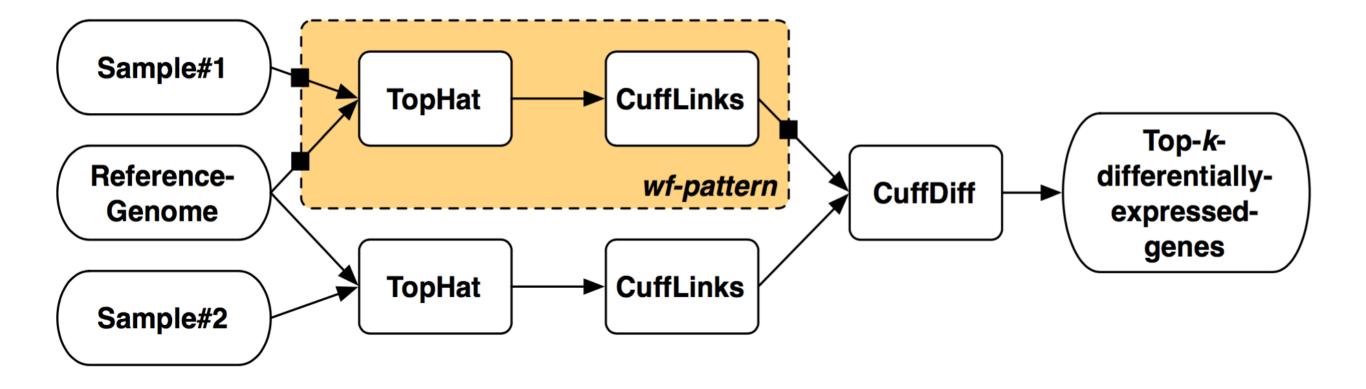


Compute and storage intensive



TopHat	1 sample	300 samples
Input data	2 x 17 Gb	10.2 Tb
1-core CPU	170 hours	5.9 years
32-cores CPU	32 hours	14 months
Output data	12 Gb	3.6 Tb

Compute and storage intensive



TopHat	1 sample	300 samples
Input data	2 x 17 Gb	10.2 Tb
1-core CPU	170 hours	5.9 years
32-cores CPU	32 hours	14 months
Output data	12 Gb	3.6 Tb

Compute and storage intensive

Avoid duplicated storage / computing

Is provenance enough for reuse?

- 11 a prov:Bundle, prov:Entity;
- 12 prov:wasAttributedTo <#galaxy2prov>;
- 13 prov:generatedAtTime "2016-04-14T18:18:37.000409"^^xsd:dateTime;
- 14
- 15
- 16 <#72486b583fe152f0>
- 17 a prov:Activity ;
- 18 prov:wasAssociatedWith <#catl> ;
- 19 prov:startedAtTime "2015-12-15T12:54:50.749845"^^xsd:dateTime;
- 20 prov.ended&+Time "2015_12_15T12.55.57.016799"^^xsd.dateTime.

Visualise

bolat on 45W 13 Store isosafriant/3_R2.fastq / L004: H2_005:fasto.gz / L004: H2_005:fasto.gz / L004: H2_005:fasto.gz / L004: H2_005:fasto.gz / Jaxy/grod-galaxy-files/galaxy-datasets/001/dataset_1467.dat / Jaxy/grod-galaxy-files/galaxy-datasets/001/dataset_1467.dat / Jaxy/grod-galaxy-files/galaxy-datasets/001/dataset_1467.dat / JopHat on 45WT2 : epites/Unctionsepted_hits / Jaxy/grod-galaxy/galaxy-files/galaxy-datasets/001/dataset_1062.dat / JopHat on 45WT2 : epites/Unctionsepted_hits / Jaxy/galaxy/galaxy/galaxy-files/galaxy-datasets/001/dataset_1062.dat / JopHat on 45WT2 : epites/Unctionsepted_hits / Jaxy/galaxy/galaxy/galaxy-files/galaxy-datasets/001/dataset_10/4.dat / JopHat on 45WT2 : epites/Unctionsepted_hits / Jaxy/galaxy/galaxy/galaxy-files/galaxy-datasets/001/dataset_10/4.dat / JopHat on 45WT2 : epites/Unctionsepted_hits / JopHat on 45WT2 : epites/galaxy-files/galaxy-datasets/001/dataset_11/4.dat / JopHat on 45WT2 : epites/galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat / JopHat on 45WT2 : epites/galaxy/galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat / JopH TopHat on 45WT3 : insertions LOCHER LOOZINE 004 fasta.dz /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datasets/00 /galaxy/prod-galaxy/galaxy/galaxy/galaxy-files/galaxy-datas 6VGWT3 ATGTCA L004 R1 004.fastq.gz auxy ties/galaxy-datasets/001/dataset_1176.dat Cufflinks or CLEWALKSIGHTS STATE OF STORESSION 1 : splitigitasotionaxy-files/galaxy-datasets/001/dataset_1177.dat Cuttinking Cutting oression appened Ryly and on data 43 and data 12713 Ballara mass of Cufflinks on 45 Wuff: as the produce of provident of the produce of the second SQA Es/ochos axophes/ealaw T2: asers/0004/dataset 1173.dat Willes/galater 1: accepted dataset_1167.dat B1 002 feta 97 atasets/001/dataset_1094.dau axy/prod-galaxy TopHat on 6WT3 : accepted 1093.dat Manand data dataset 1089.dat datasetg 9784, dat datasets/001/dataset_1088.dat Cuffmerge on data .go92.dat /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datasets/001/dataset_1450.dat http://fr.symetric#toolshed.g2.bs.psu.edu/repos /galaxy/prod-galaxy/galaxy/galaxy/galaxy/galaxy-files/galaxy-datasets/ /galaxy/prod-galaxy/gal LOGRES Galage data gis/001/dataset_1120.dat Ane version 1001/dataset 1104 dat 901 43 4 901 dataset_1056.dat a ov that a souther so 1076.dat STAN EBS A

Is provenance enough for reuse?

- 11 a prov:Bundle, prov:Entity;
- 12 prov:wasAttributedTo <#galaxy2prov>;
- 13 prov:generatedAtTime "2016-04-14T18:18:37.000409"^^xsd:dateTime;
- 14
- 15
- 16 <#72486b583fe152f0>
- 17 a prov:Activity ;
- 18 prov:wasAssociatedWith <#catl> ;
- 19 prov:startedAtTime "2015-12-15T12:54:50.749845"^^xsd:dateTime;
- 20 prov.endedatrime "2015_12_15#12.55.57.016799"^^xsd.dateTime.

Too fine-grained

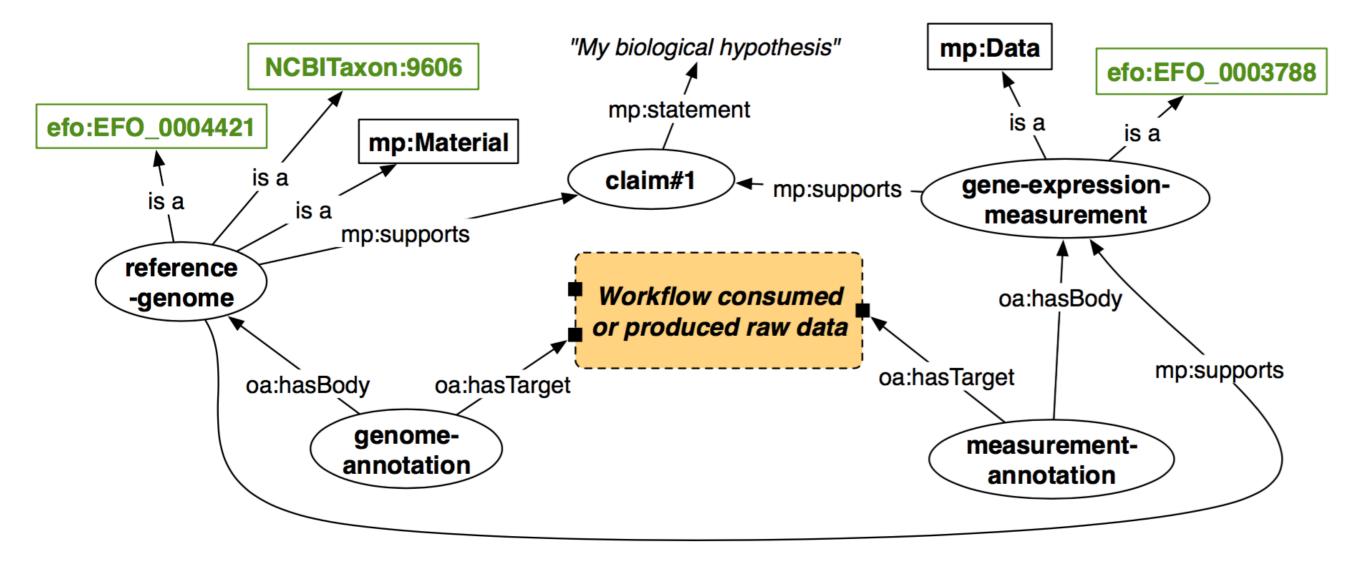
No domain concepts

Visualise

alaxy/galaxy/mes/galaxy/mes/galaxy/mes/galaxy/galaxy/mes/galaxy/galaxy/mes/gala ophat on 45W 13 actions April 73_R2.fastq TopHat on 45WT3 : insertions /galaxy-files/galaxy-datasets/001/dataset_1468.dat Logalazy/galaxy/galaxy/galaxy/galaxy/galaxy/galaxy/galaxy/galaxy/galaxy/galaxy/galaxy-datasets/001/dataset_1468.dat /galaxy/prod-galaxy/galaxy-files/galaxy-datasets/001/dataset_1467.dat TopHat on 45WT2 : files/galaxy-files/galaxy-datasets/001/dataset_1467.dat TopHat on 45WT2 : files/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/prod-galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/prod-galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/prod-galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/prod-galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/prod-galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/prod-galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/prod-galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/prod-galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datasets/001/dataset_11/4.dat /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datasets/00 /galaxy/prod-galaxy/galaxy/galaxy/galaxy-files/galaxy-datas GWT3_ATGTCA_L004_R1_004.fastq.gz es/galaxy-datasets/001/dataset_1176.dat ieilasotoataxy-files/galaxy-datasets/001/dataset_1177.dat nd data 1278 data a mans o SQA 6s/galas Cufflinks on 45 WWT: as a fight or the reader the second s PalaWT2: asersaded 40 attaset 1173.dat topHat 8 a WT1 tasets (001/dataset_1167.dat stav97atasets/001/dataset_1094.dau TopHat on 6WT3 : accepted f 1089.dat 43819 10784, dat assets/001/dataset_1088.dat Cuffmerge on data .gz)92.dat /galaxy/prod-galaxy/galaxy/galaxy-files/galaxy-datasets/001/dataset_14 http://fr.symetric#toolshed LOOKE TGaller tattes gis/001/dataset_1120.dat Logar Logar States 1104 dat 1128.dat /galaxy/prod-galaxy/galaxy/galaxy/galaxy/ /galaxy/pgatagologataxy/gataxy/gataxy/jataxy/jataxy/gataxy 001 4334 Con (001/dataset_1056.dat DOGCASSIELSOD Tasta aset 1077.dat A George And A George And A George And A Content of A Con AR CIGO

Human & machine-tractable report needed !

Annotated paper's "**Material & Methods**" with links to **some** workflow artifacts (algorithms, data).



Problem statement & objectives

Problem statement

Scientific workflows produce massive raw results. Their publication into curated query-able linked data repositories requires lot of time and expertise.

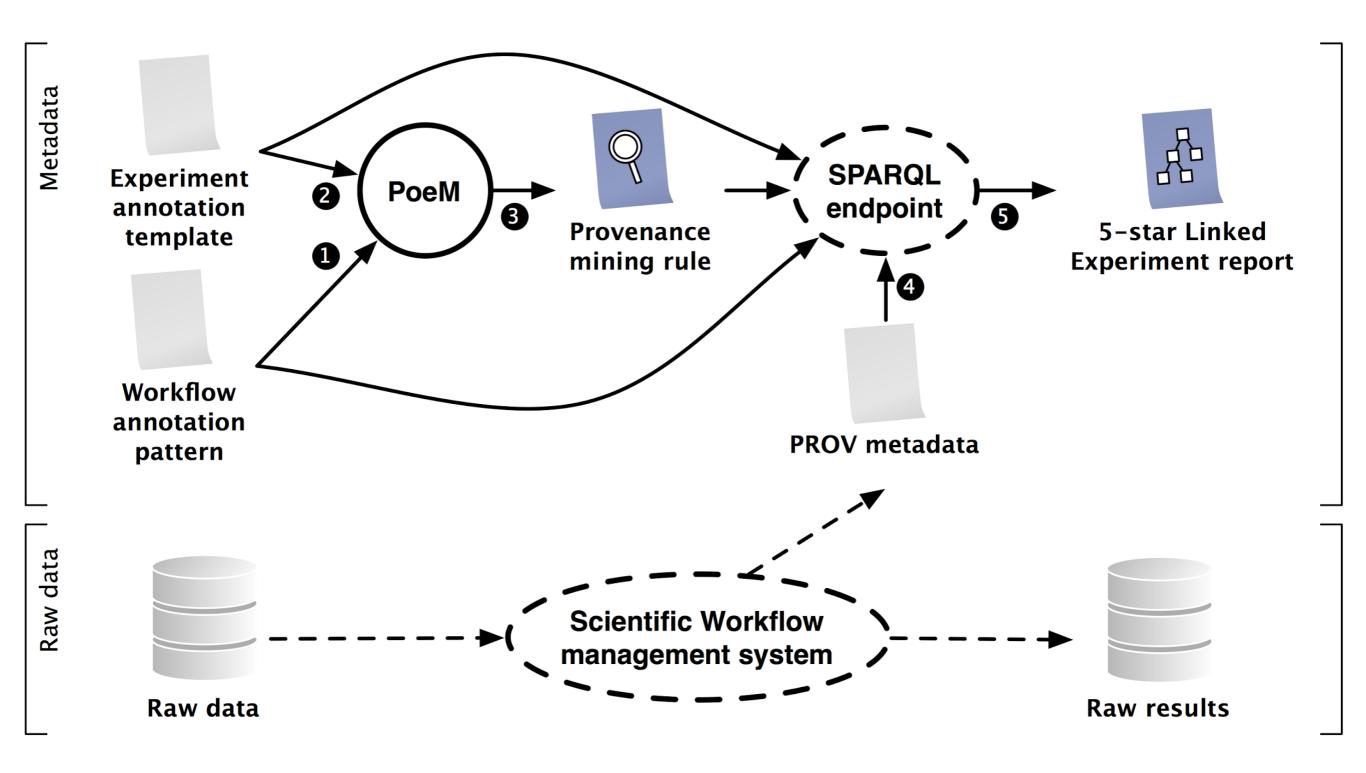
Can we exploit provenance traces to ease the publication of scientific results as Linked Data ?

Objectives

(1)Leverage annotated workflow patterns to generate **provenance mining rules**.

(2)Refine provenance traces into **linked experiment reports**.

Approach



A. Gaignard, H. Skaf-Molli, A. Bihouée: From Scientific Workflow Patterns to 5-star Linked Open Data. 8th USENIX Workshop on the Theory and Practice of Provenance, TaPP 2016.

PoeM: generating PrOvEnance Mining rules ③

Input : W : Workflow annotated pattern ①, S_1 : First step of W, S_2 : Last step of W,

 \overline{A} : Annotation template **@**.

Output: *Rule*: Provenance mining rule.

```
begin
1
       IN_{S1} \leftarrow getInputs(S_1)
2
                                                                              SPARQL Property Path
       OUT_{S2} \leftarrow getOutputs(S_2)
3
                                                                           SPARQL Basic graph pattern
4
       provGraph \leftarrow genDataLineage(OUT_{S2}, IN_{S1})
5
       reportGraph \leftarrow bindReportTargets(provGraph, A)
6
7
                                                                             SPARQL Construct query
       Rule \leftarrow \underbrace{provGraph.edge_1 \land \dots \land provGraph.edge_N}_{G_1}
8
                                      reportGraph
```

Demo

poem.univ-nantes.fr

C

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PoeM: Provenance Mining for scientific linked data publishing

Contact : Alban Gaignard, Hala Skaf, Audrey Bihouee, {firstname.lastname}@univ-nantes.fr.

For demonstration purpose only.

This web page illustrates our semi-automated approach for mining provenance traces and assembling linked experiment reports. PoeM generates Semantic Web rules from (i) annotated workflow patterns, (ii) domain-specific annotations, and (iii) provenance traces of a workflow run. The rules finally match provenance subgraphs and produce linked experiment reports.

We illustrate our approach in the context of an RNAseq bioinformatics workflow .

This work reuses existing linked open vocabularies, namely PROV-O, P-PLAN, Micropublications Ontology, Experimental Factors Ontology, and EDAM.

This demo is supported by the Corese Semantic Web factory, Apache Jena, D3.js, Codemirror.js and Twitter Bootstrap.

Show input annotations	Show provenance trace	Show generated rule	Show resulting report

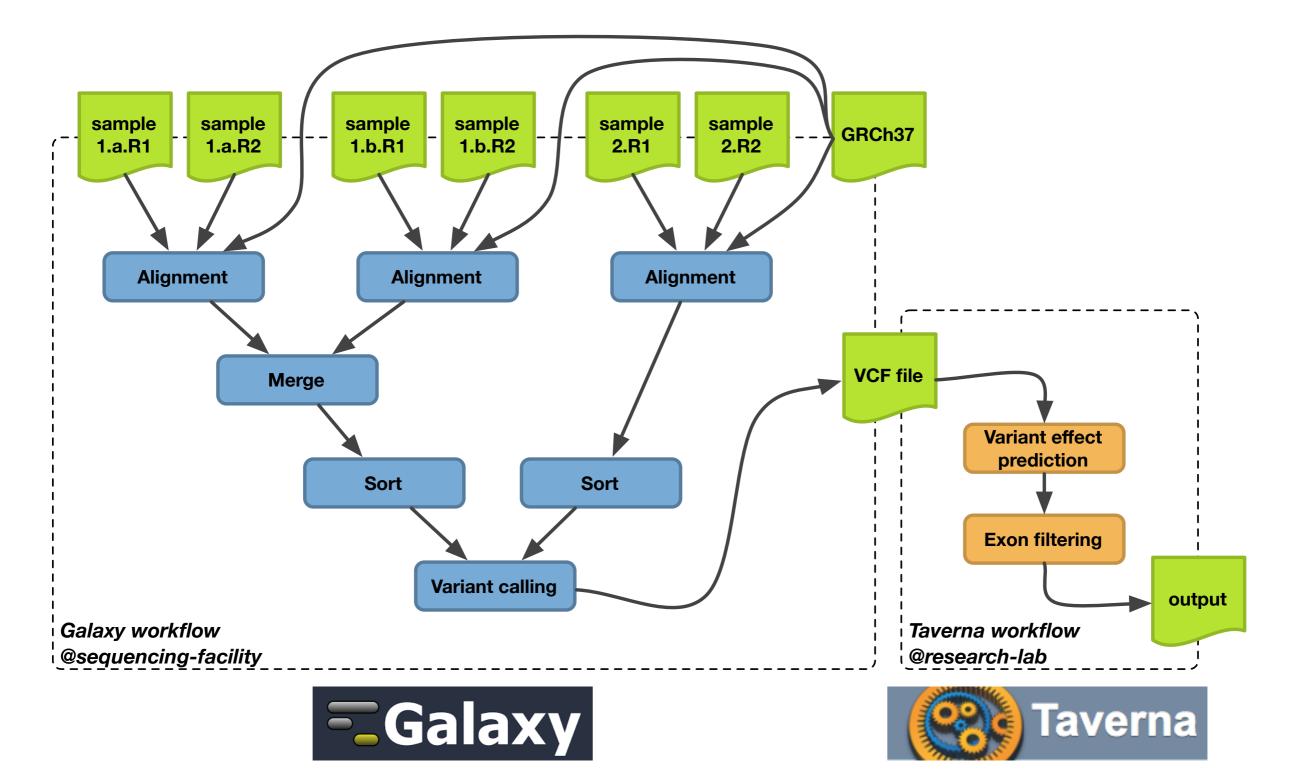
Resulting linked experiment report

1	<pre>@prefix void: <http: ns="" rdfs.org="" void#=""> .</http:></pre>	
2	<pre>@prefix mp: <http: mp="" purl.org=""></http:> .</pre>	
3	<pre>@prefix edam: <http: edamontology.org=""></http:> .</pre>	
4	<pre>@prefix sym: <http: fr.symetric="" vocab#=""> .</http:></pre>	
5	<pre>@prefix xsd: <http: 2001="" www.w3.org="" xmlschema#=""> .</http:></pre>	
6	<pre>@prefix rdfs: <http: 01="" 2000="" rdf-schema#="" www.w3.org=""> .</http:></pre>	Ì
7	<pre>@prefix p-plan: <http: net="" p-plan#="" purl.org=""> .</http:></pre>	
8	<pre>@prefix efo: <http: efo="" www.ebi.ac.uk=""></http:> .</pre>	
9	<pre>@prefix ncbitaxon: <http: ncbitaxon="" obo="" owl="" purl.org=""> .</http:></pre>	
10	<pre>@prefix oa: <http: ns="" oa#="" www.w3.org=""> .</http:></pre>	

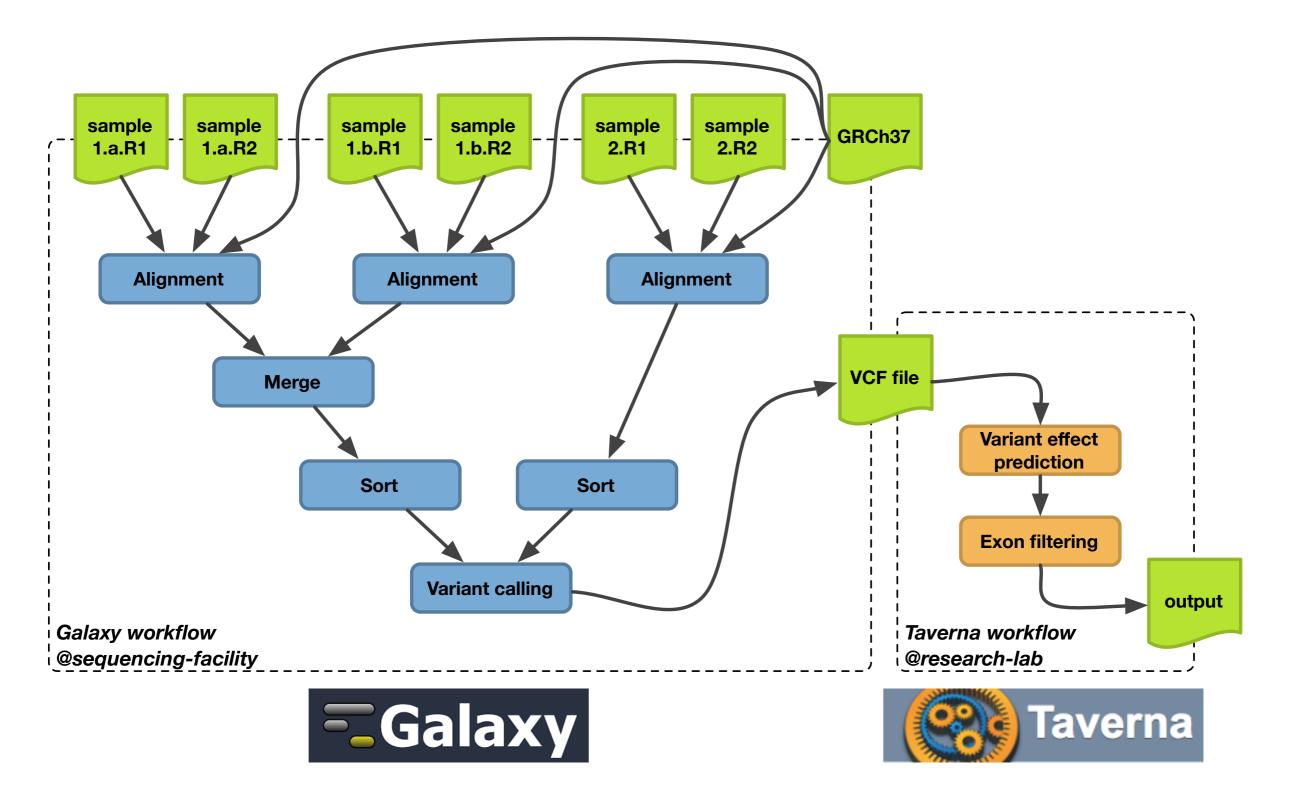
Provenance in **multi-site** studies ?

Multi-site studies → ≠ workflow engines !

Multi-site studies → ≠ workflow engines !

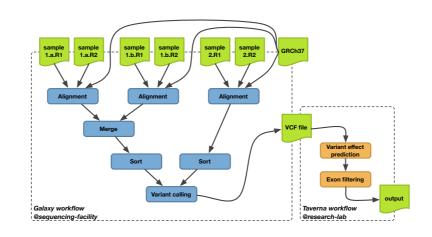


Multi-site studies → ≠ workflow engines !



Scattered provenance capture ?

Provenance issues



« Which alignment algorithm was used when predicting these effects ? »

« A new version of a reference genome is available, which genome was used when predicting these phenotypes ? »

Need for an overall tracking of provenance over both Galaxy and Taverna workflows !

Provenance « heterogeneity »

Galaxy PROV predicates	counts
prov:wasDerivedFrom	118
rdf:type	76
rdfs:label	62
prov:used	61
prov:wasAttributedTo	34
prov:wasGeneratedBy	33
prov:endedAtTime	26
prov:startedAtTime	26
prov:wasAssociatedWith	26
prov:generatedAtTime	1

Taverna PROV predicates	counts
rdf:type	54
rdfs:label	13
prov:atTime	8
wfprov:describedByParameter	6
rdfs:comment	6
prov:hadRole	6
prov:activity	5
dcterms:hasPart	4
prov:agent	4
prov:endedAtTime	4
prov:hadPlan	4
prov:qualifiedAssociation	4
prov:qualifiedEnd	4
prov:qualifiedStart	4
prov:startedAtTime	4
prov:wasAssociatedWith	4
tavernaprov:content	3
wfprov:usedInput	3
wfprov:wasEnactedBy	3
wfprov:wasOutputFrom	3

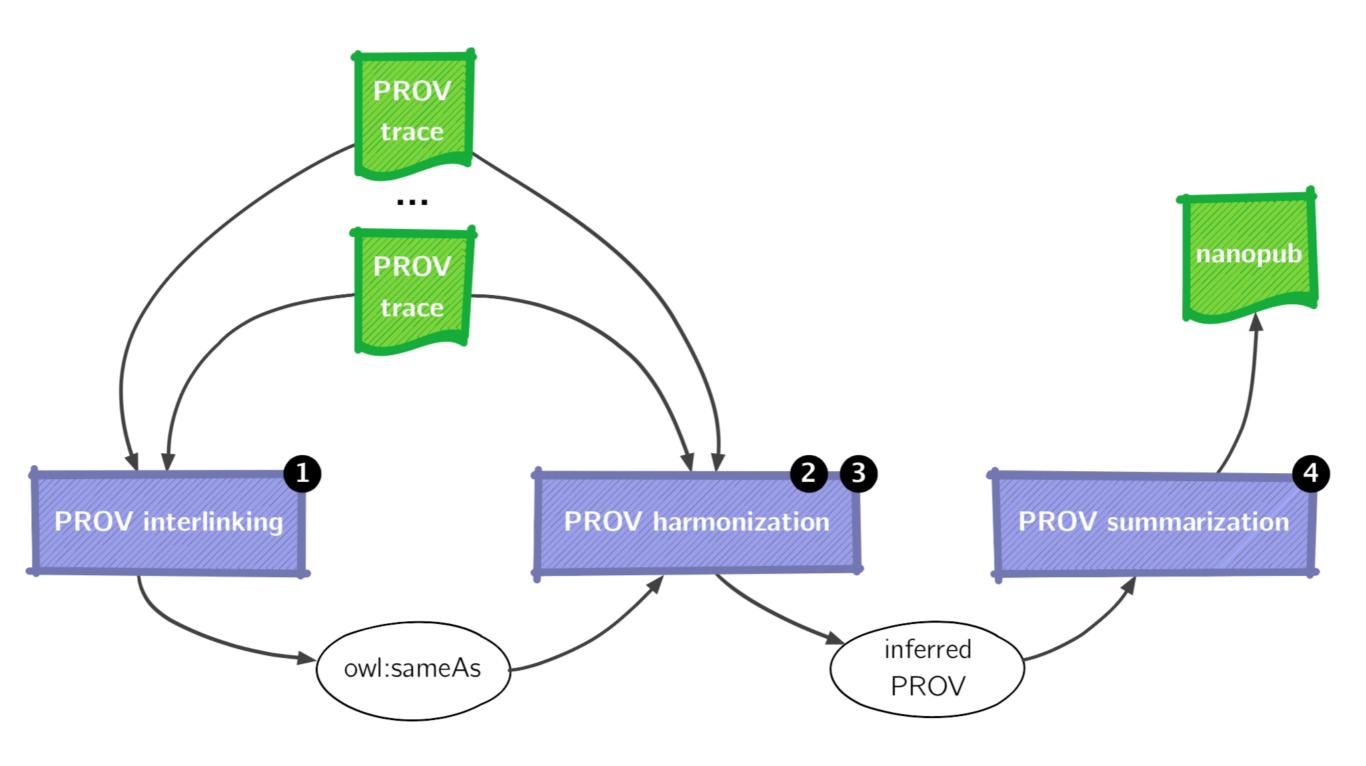
Provenance « heterogeneity »

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prov:startedAtTime	26
prov:wasAssociatedWith	26
prov:generatedAtTime	1

How to reconcile these provenance traces ?

Taverna PROV predicates	counts
rdf:type	54
rdfs:label	13
prov:atTime	8
wfprov:describedByParameter	6
rdfs:comment	6
prov:hadRole	6
prov:activity	5
dcterms:hasPart	4
prov:agent	4
prov:endedAtTime	4
prov:hadPlan	4
prov:qualifiedAssociation	4
prov:qualifiedEnd	4
prov:qualifiedStart	4
prov:startedAtTime	4
prov:wasAssociatedWith	4
tavernaprov:content	3
wfprov:usedInput	3
wfprov:wasEnactedBy	3
wfprov:wasOutputFrom	3

Approach

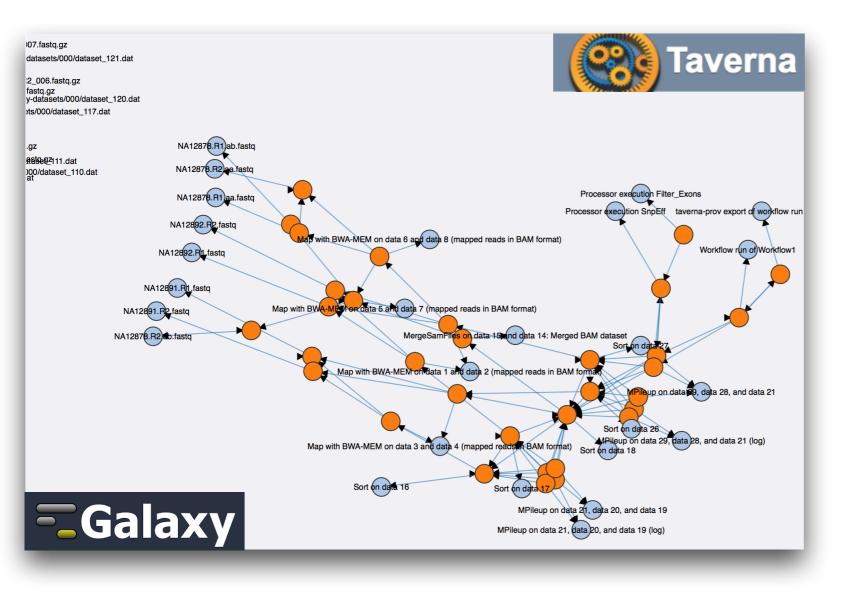


A. Gaignard, K. Belhajjame, H. Skaf-Molli. SHARP: Harmonizing and Bridging Cross-Workflow Provenance. The Semantic Web: ESWC 2017 Satellite Events Portorož, Slovenia, May 28 – June 1, 2017, Revised Selected Papers, 2017

Results

https://github.com/albangaignard/sharp-prov-toolbox

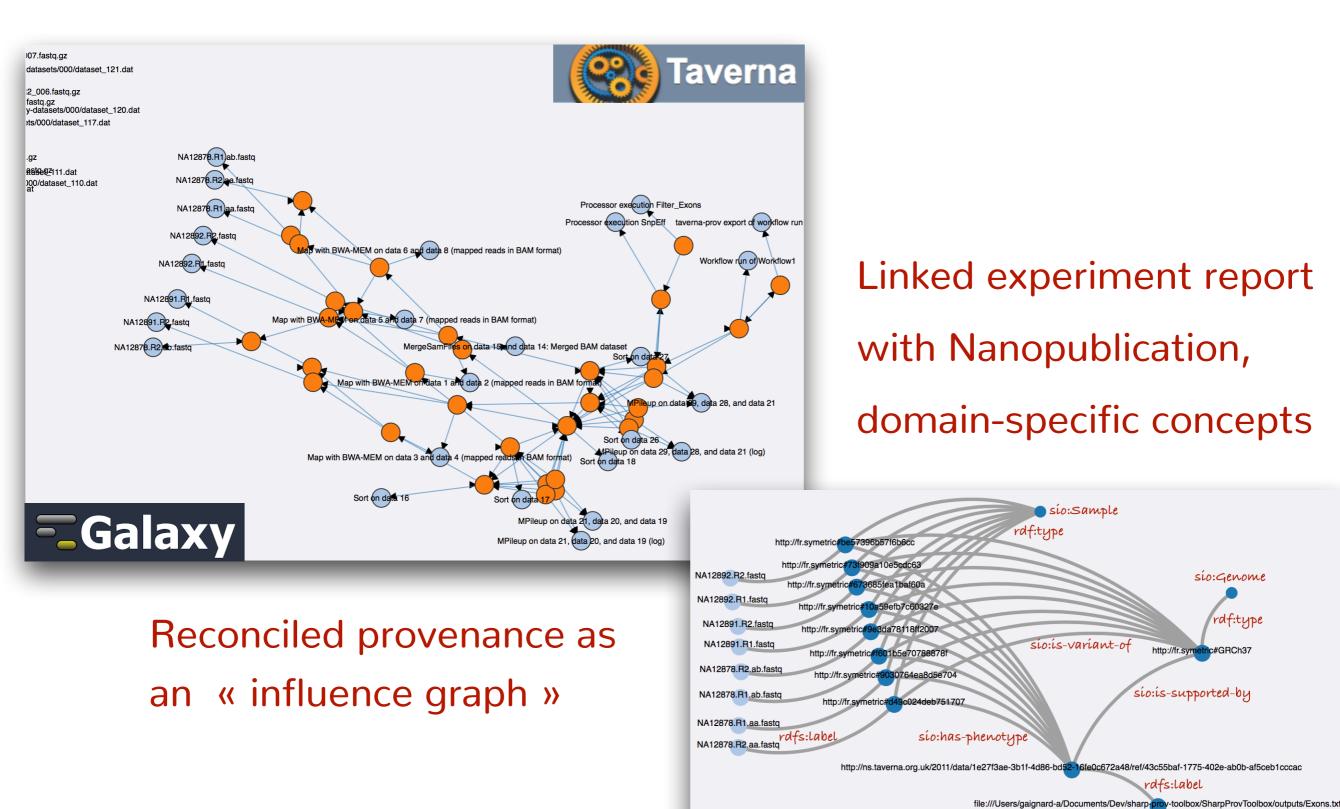
Results



Reconciled provenance as an « influence graph »

https://github.com/albangaignard/sharp-prov-toolbox

Results



https://github.com/albangaignard/sharp-prov-toolbox



Take home message & perspectives

- Scientific Workflows → automation, abstraction, provenance
- Standards for **provenance representation** and **reasoning**
- Better handle **multi-site studies** (ESWC'17 satelite event paper)
- Linked experiment reports = **contextualized** and **summarized** provenance (TaPP'16 paper)
- Distributed data analysis → Distributed provenance, reasoning ?
- Learning patterns in provenance graphs?
- **Predicting domain-specific annotation** for workflow results?

Acknowledgments



Audrey Bihouée, Institut du Thorax, BiRD Bioinformatics facility, University of Nantes



Hala Skaf-Molli, LS2N, University of Nantes GDR MaDICS action ReproVirtuFlow



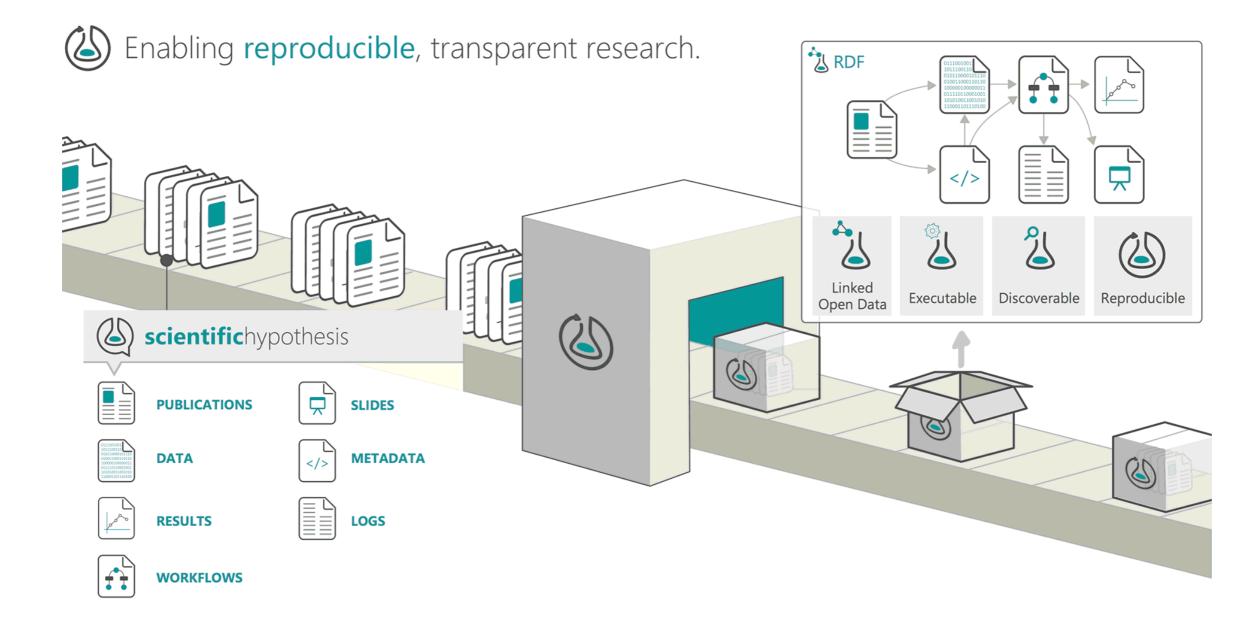
Khalid Belhajjame, LAMSADE, University of Paris-Dauphine, PSL





Backup slides

Research Objects



Sean Bechhofer, Iain Buchan, David De Roure, Paolo Missier, John Ainsworth, Jiten Bhagat, Phillip Couch, Don Cruickshank, Mark Delderfield, Ian Dunlop, Matthew Gamble, Danius Michaelides, Stuart Owen, David Newman, Shoaib Sufi, Carole Goble (2013) **Why Linked Data is Not Enough for Scientists**, Future Generation Computer Systems **29**(2), February 2013, Pages 599-611, ISSN 0167-739X, https://doi.org/10.1016/j.future.2011.08.004

Khalid Belhajjame, Jun Zhao, Daniel Garijo, Matthew Gamble, Kristina Hettne, Raul Palma, Eleni Mina, Oscar Corcho, José Manuel Gómez-Pérez, Sean Bechhofer, Graham Klyne, Carole Goble (2015) **Using a suite of ontologies for preserving workflow-centric research objects**, Web Semantics: Science, Services and Agents on the World Wide Web, https://doi.org/10.1016/j.websem.2015.01.003

schema.org Action

Action

Canonical URL: http://schema.org/Action

Thing > Action

An action performed by a direct agent and indirect participants upon a direct object. Optionally happens at a location with the help of an inanimate instrument. The execution of the action may produce a result. Specific action sub-type documentation specifies the exact expectation of each argument/role.

See also blog post and Actions overview document.

Usage: Between 100 and 1000 domains

[more...]

Property	Expected Type	Description
Properties from Action		
actionStatus	ActionStatusType	Indicates the current disposition of the Action.
agent	Organization or Person	The direct performer or driver of the action (animate or inanimate). e.g. <i>John</i> wrote a book.
endTime	<u>DateTime</u>	The endTime of something. For a reserved event or service (e.g. FoodEstablishmentReservation), the time that it is expected to end. For actions that span a period of time, when the action was performed. e.g. John wrote a book from January to <i>December</i> .
		Note that Event uses startDate/endDate instead of startTime/endTime, even when describing dates with times. This situation may be clarified in future revisions.

error	Thing	For failed actions, more information on the cause of the failure.
instrument	Thing	The object that helped the agent perform the action. e.g. John wrote a book with <i>a pen</i> .
location	Place or PostalAddress or Text	The location of for example where the event is happening, an organization is located, or where an action takes place.
object	<u>Thing</u>	The object upon which the action is carried out, whose state is kept intact or changed. Also known as the semantic roles patient, affected or undergoer (which change their state) or theme (which doesn't). e.g. John read <i>a book</i> .
participant	Organization or Person	Other co-agents that participated in the action indirectly. e.g. John wrote a book with <i>Steve</i> .
result	Thing	The result produced in the action. e.g. John wrote <i>a book</i> .
startTime	<u>DateTime</u>	The startTime of something. For a reserved event or service (e.g. FoodEstablishmentReservation), the time that it is expected to start. For actions that span a period of time, when the action was performed. e.g. John wrote a book from <i>January</i> to December. Note that Event uses startDate/endDate instead of startTime/endTime, even when describing dates with times. This situation may be clarified in future revisions.
target	EntryPoint	Indicates a target EntryPoint for an Action.