An Approach for Scientific Workflows Provenance Data Publication on the Semantic Web

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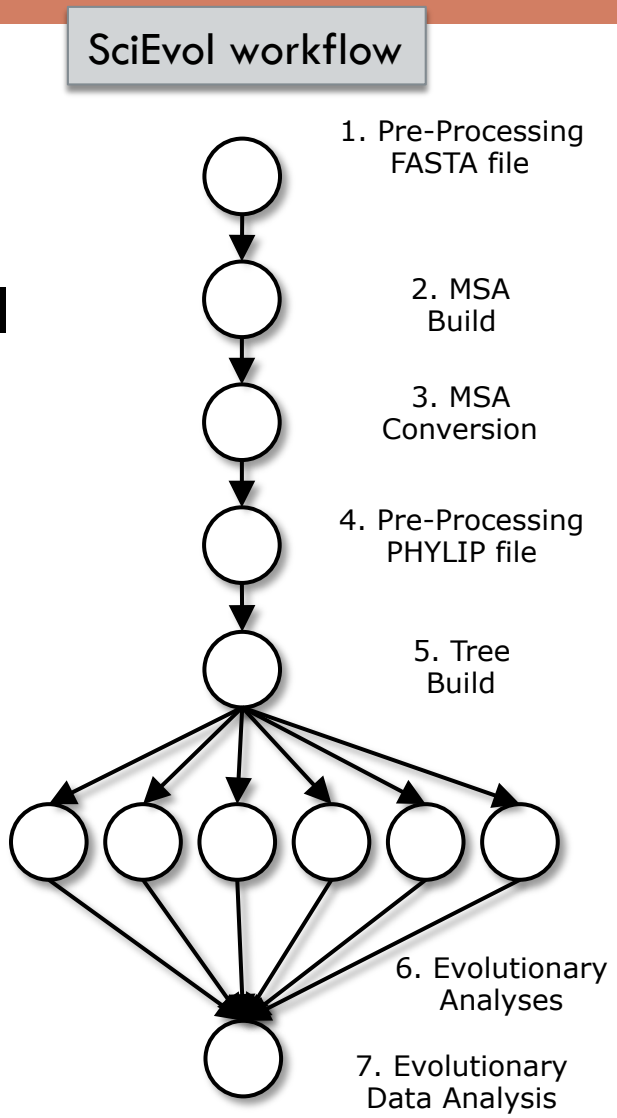
Agenda

- Introduction
- Publication Methodology on the Semantic Web
- Our approach for data publication
  - PROV-O-Wf
- Case Study
- Conclusion and Future Works

Computational simulations in large-scale

- Validation of a scientific hypothesis
- Chaining of scientific programs
- Processing of complex computational models

- Scientific Workflow Management Systems (SWfMS)
  - They allow to model, execute and monitor computational simulations by the abstraction of scientific workflows



Workflow Provenance Data

- They enable the reproduction of computational simulations
  - Data about workflow composition and execution
  - Information about the flow of data between programs

- Limitations
  - They can be stored with some access restrictions (e.g., private databases)
  - Usage of unstructured files
    - Limited query capabilities
    - Without a standard for organizing data

Workflow Provenance Data

Publication process of provenance data can enhance analysis

- Sharing of provenance data
- Validation of scientific hypothesis
- Analysis based on the history of the execution of computational simulations

Semantic Web

- An extension of the Web through standards by the World Wide Web Consortium (W3C)
  - They recommend data formats that facilitate data interchange on the Web
  - e.g., Resource Description Framework (RDF)
    - A standard model for data interchange on the web

- **Semantic Database Management Systems (DBMS)** allow to:
  - Run structured queries
  - Publish on the Web
  - Facilitate interoperability
  - e.g., OpenLink Virtuoso, Jena TDB

5-star Open Data

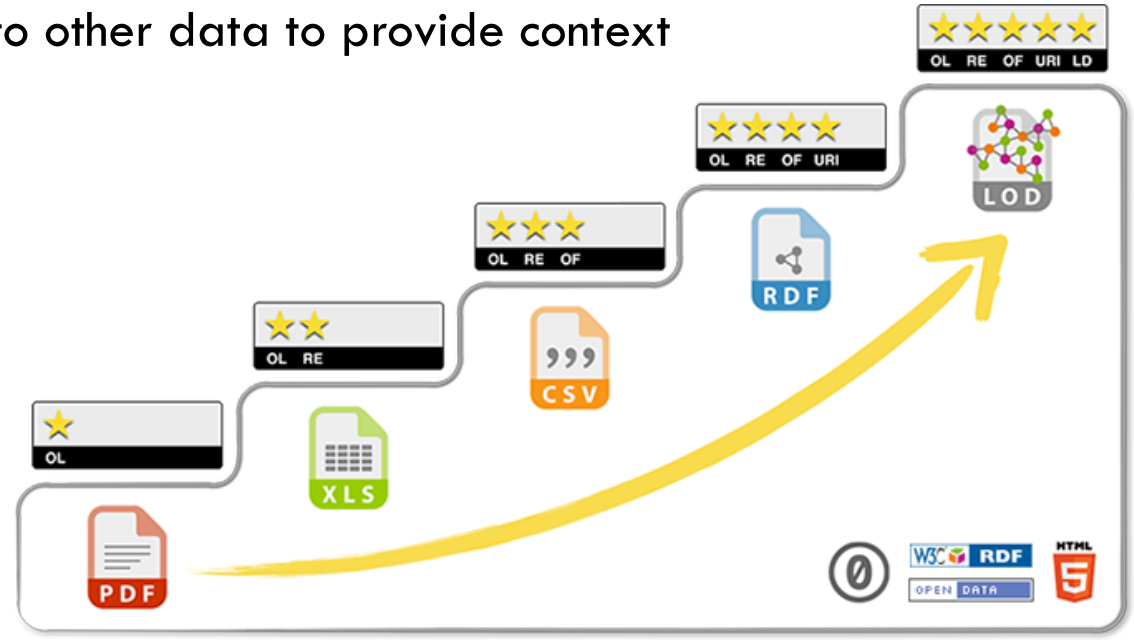
1 star → Make your data available on the web

2 stars → Make it available in a structured way

3 stars → Make it available in a non-proprietary open format

4 stars → Use URIs to denote things, so that people can point at your stuff

5 stars → Link your data to other data to provide context

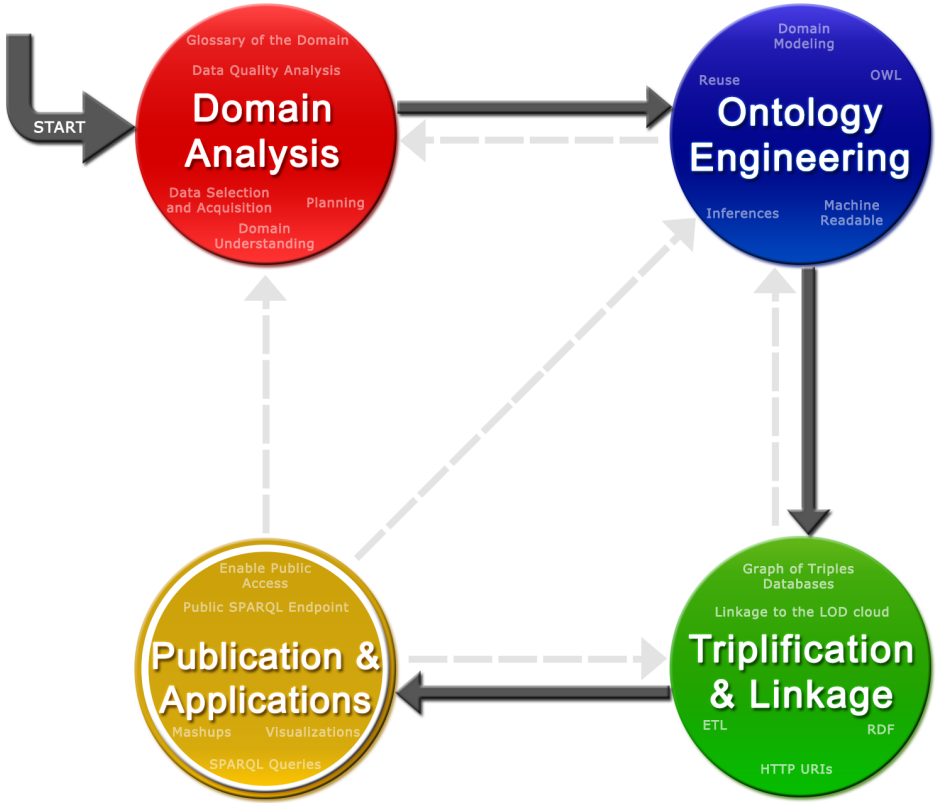


Extracted from 5-star Open Data (http://5stardata.info)

Our approach for data publication in scientific workflow scenario

- Adoption of Semantic Web technologies
  - To publish workflows provenance data on Web in a structured, standardized, open and interoperable manner
- Development of an ontology for representing the main concepts in a scientific workflow scenario
  - PROV-O-Wf
- Case study based on a bioinformatics workflow
  - SciEvol workflow

Publication Methodology on the Semantic Web



Souza, R., Cottrell, L., White, B., Campos, M. L. and Mattoso, M. (2014) "Linked Open Data Publication Strategies: Application in Networking Performance Measurement Data", In: 2nd ASE International Conference on Big Data Science and Computing, Stanford, CA, USA.

Domain Analysis

- Domain analysis based on the scenario of computational simulations
  - Execution of large-scale scientific workflows on HPC environments
- Provenance data should also be gathered during workflow execution
  - We experimented on a SWfMS that gathers fine-grained provenance data in order to present domain-specific data

Ontology engineering

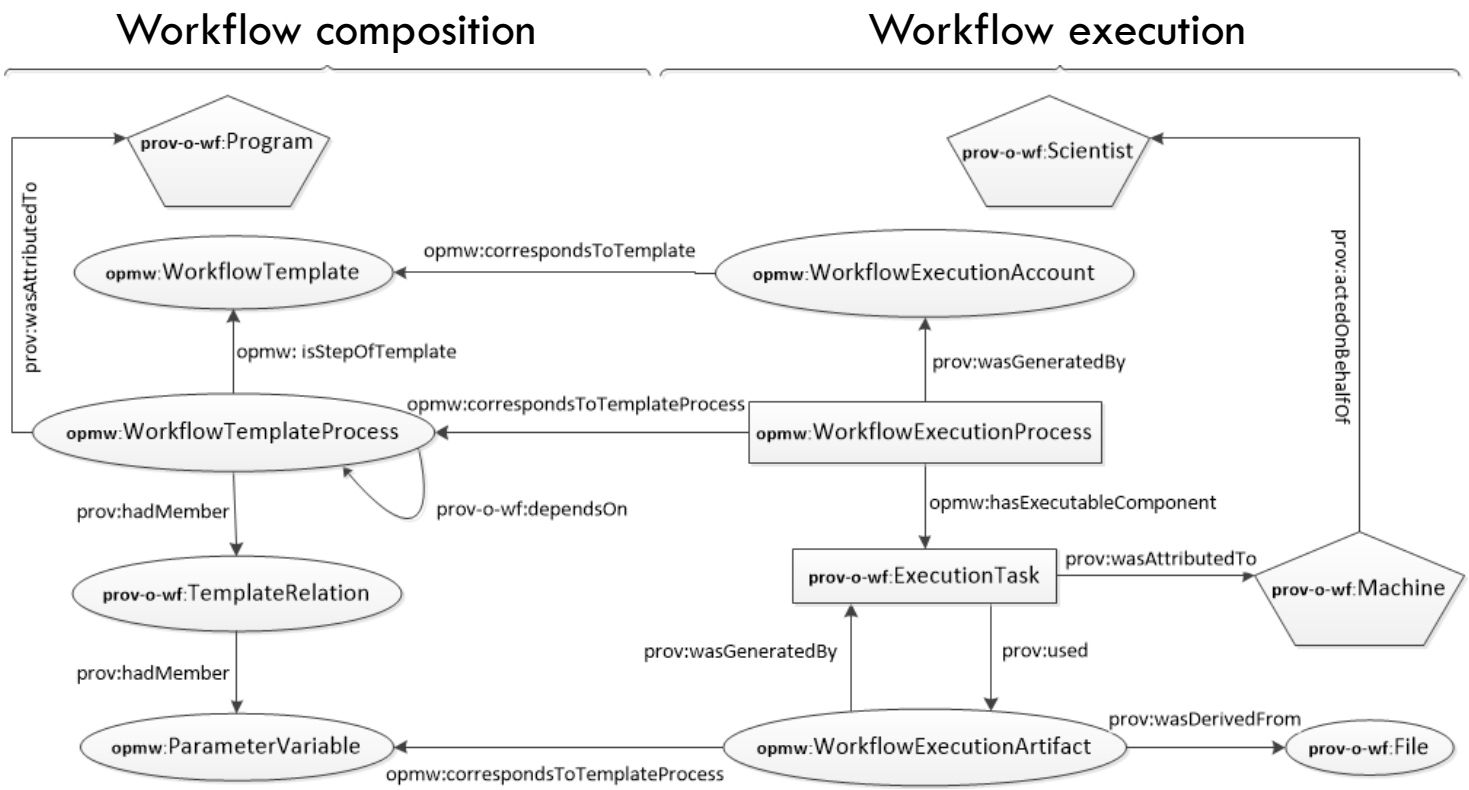
- Ontology reuse as an important characteristic
  - IntelLeo ontology
  - SGWfC Taverna → MyGrid

  } They were not used

  - PROV-O and OPMW
    - They are W3C recommendations and independent of the domain
- Data model for representing fine-grained provenance data
  - PROV-Wf

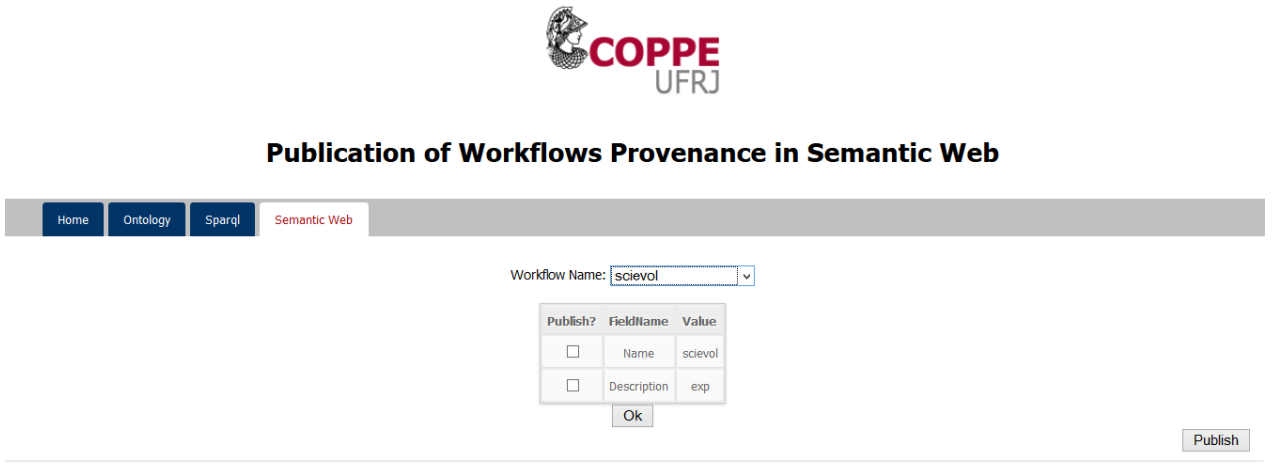
PROV-O-Wf

- PROV-O was used as a meta-model to the ontology
- Reuse of PROV-Wf for representing provenance data



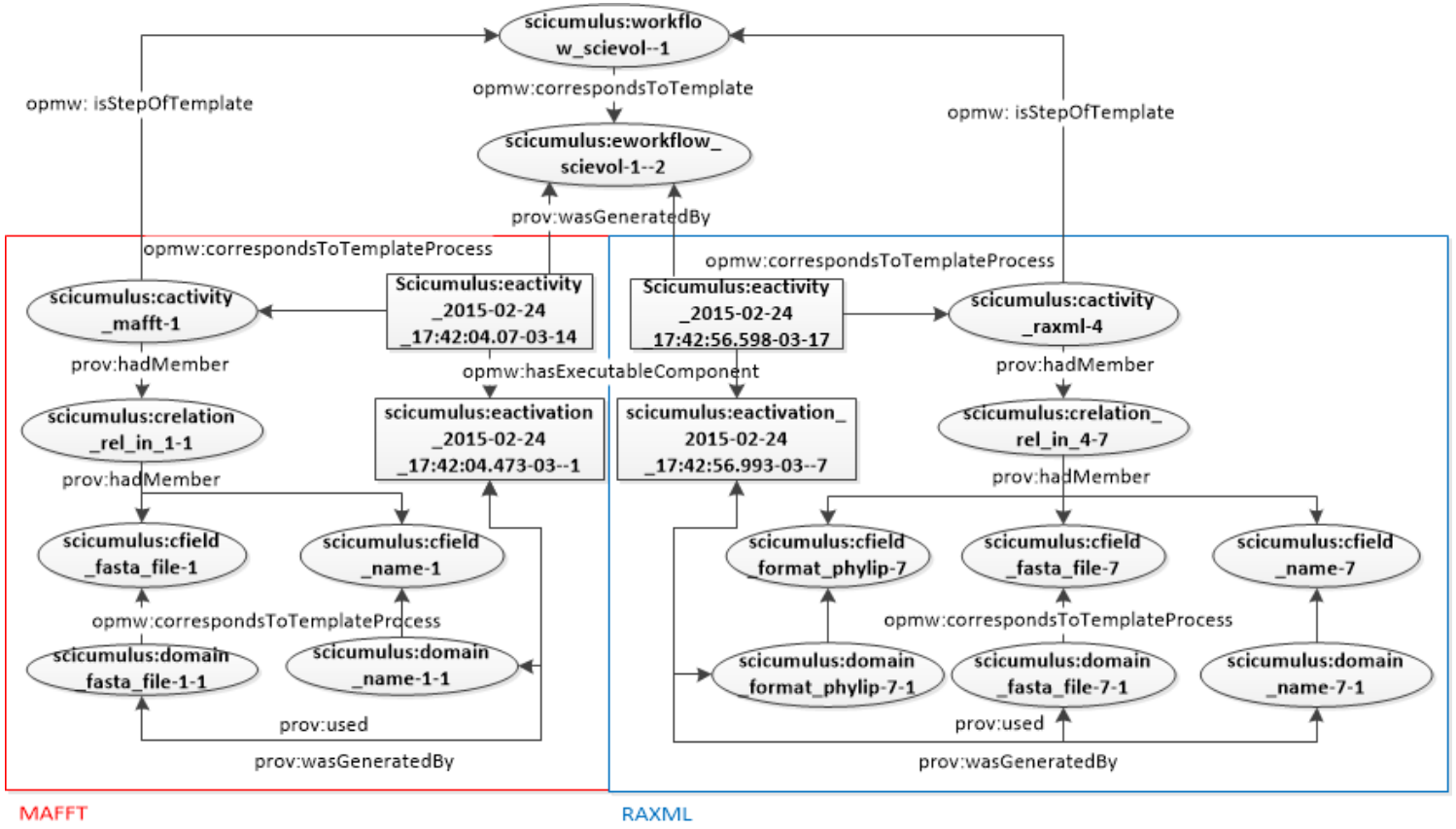
Triplification and Publication

- Generation of RDF triples following the ontology PROV-O-Wf
  - ETL operations
  - Extracting data from the SWfMS's provenance database
- Web interface
  - User defines which provenance data will be published
  - Visualization of published data



Case study

- SciEvol workflow executed using SciCumulus SWfMS
- Object-Relational DBMS: Open Link Virtuoso



Conclusion and Future works

- We developed an ontology for data publication
  - PROV-O-Wf
  - Reuse of standard ontologies
  - Representation of fine-grained provenance data on the SW
  - Independent of scientific domain and SWfMS

- Future works
  - Provide relationships with data already published on the cloud of Linked Open Data (LOD)

Thank you!

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