BIOINFORMATICS LABORATORY

Provenance Manager: PROV-man

an Implementation of the PROV Standard

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BioLab group meeting

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Outlines

- Motivation
- State-of-the-art
- PROV-man
  - The Approach, the data model, the API
- Usage examples

Motivation for Provenance

- Discoveries in modern science involve:
  - large amount of data, many people, varied tools, etc.
- Good scientific practice dictates that findings should be:
  - Traceable and reproducible
- Data provenance tracking approaches can play a major role in addressing many of these challenges.

Data provenance proposes ways to capture, manage, and use of provenance information.

State-of-the-Art

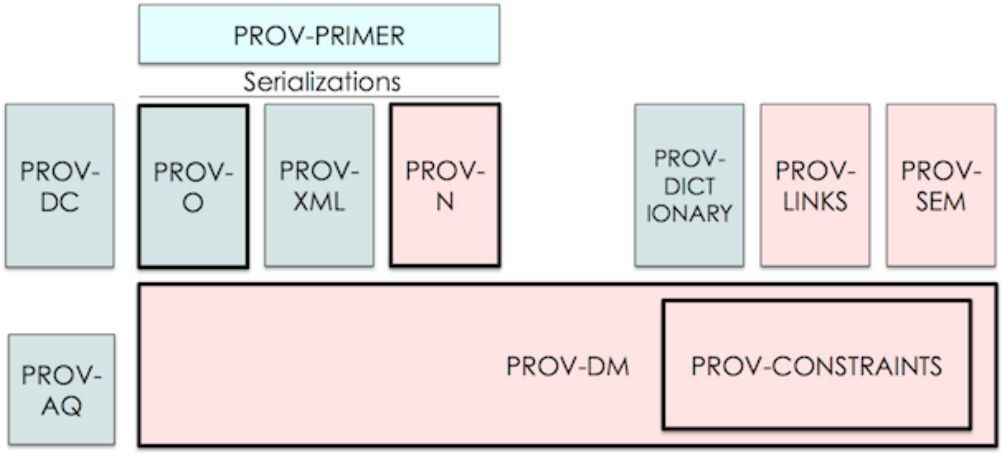
- Origin
  - from the French *provenir*, "to come from“,
  - originally mostly used for works of art,
  - currently, used in a wide range of fields, including archaeology, paleontology, archives, manuscripts, printed books, and ***e-science***

In this presentation, we refer to Provenance in e-science as *data provenance*

State-of-the-art

- Early efforts
  - < 1990: unstructured logs and temp files,
  - since 90's: information systems (e.g. DICOM, LIMS, ELN)
  - 2000+: data provenance become more prominent
  - 2007: *Open Provenance Model* (OPM)
  - 2013: PROV

Today: PROV



- Few implementations
  - Application specific
- PROV-man
  - Open/generic framework

PROV-man: The Approach

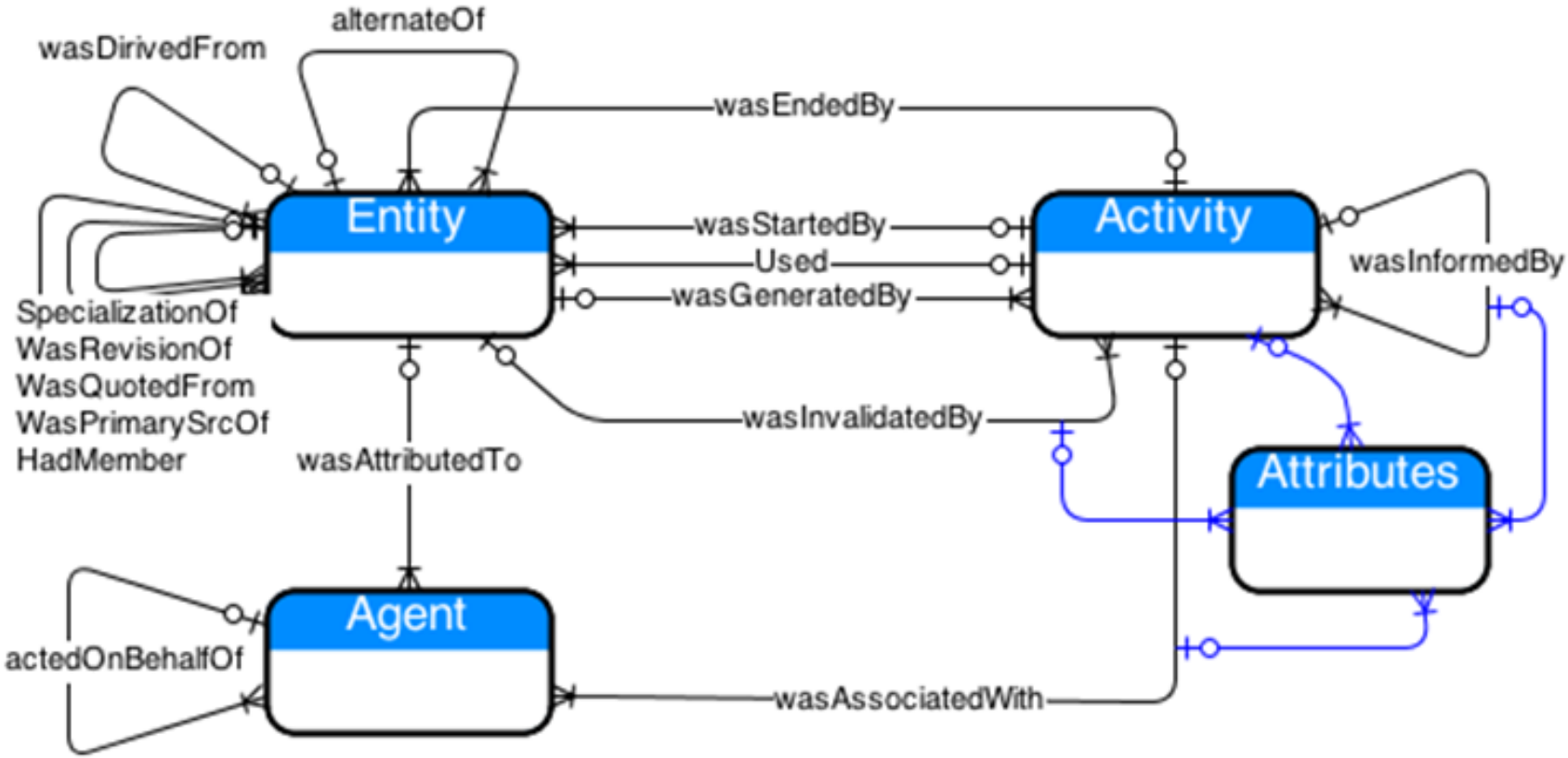
- *PROV-man* design requirements:
  - permanent storage of provenance data and approaches for optimization,
  - Easy access to provenance data
  - Support utilities for data sharing
  - Easy deployment of the framework in various use cases

- *PROV-man* framework consist of:
  - Database implementing PROV-DM
  - Application Programming Interface (API)

PROV-DM: The Data Model

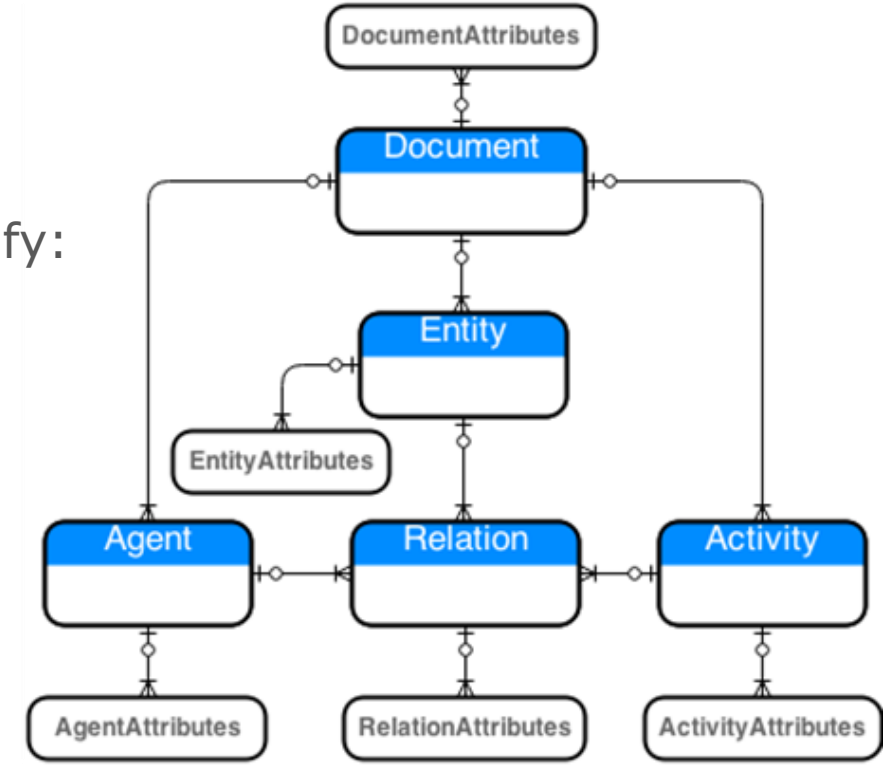
- *PROV* Data Model consists of:
  - *Core data types* (***Entity***, ***Activity***, and ***Agent***);
  - A set of ***Relations*** between the core data types;
  - A set of ***Attributes*** that could be defined for each of the core data types and Relations,
  - A ***Document*** grouping all the above.

PROV-DM: The Data Model



PROV-man: The Data Model

- *PROV-man* data model of:
  - Optimized data model
  - Relational DBMS (MySQL)
  - XML-configuration file to specify:
    - the underlying database,
    - connection parameters, and
    - tuning parameters

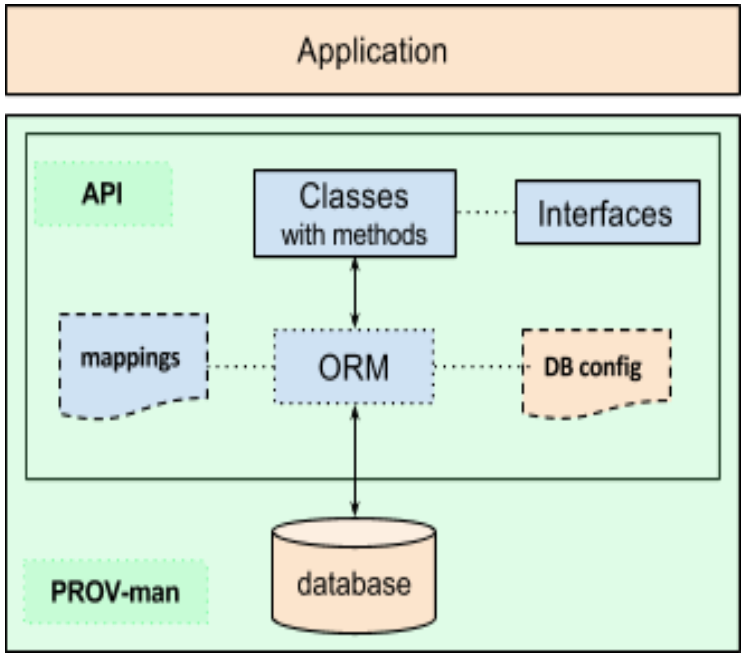


PROV-man: The API

PROV-man API provides an interface for the management of provenance data that preserves the semantics and richness defined by PROV and makes the PROV-man data model transparent to the user.

PROV-man: The API

- *PROV-man* open architecture provides:
  - *classes with methods* to manipulate provenance data;
  - *interfaces* implementing utility functions;
  - *back-end database* that serves as a main repository for storing provenance data;
  - *Object-relational mapping*.



PROV-man: The API

- *PROV-man* Classes:
  - Implements the *SET* and *GET* methods for PROV concepts;
  - *PROVmanFactory* provides a set of additional methods to create provenance data, using a human readable notation;

PROV-man: The API

- *PROV-man* Classes:
  - Implements the *SET* and *GET* methods for PROV concepts;
  - *PROVmanFactory* provides a set of additional methods to create provenance data, using a human readable notation;
- *PROV-man* Interfaces:
  - implements utility functions for data sharing and interoperation:
    - ***toDB****(document)*
    - ***toXML****(document)*
    - ***toProvN****(document)*,
    - ***toOWL2****(document),*
    - ***toGraphviz****(document),*
    - ***toGraph****(document, format).*

Example 1: on-line newspaper article

- presented in PROV-PRIMER:
  - publishes an article with a **chart** about crime statistics
  - based on data, with values **composed** by geographical regions.
  - The data uses different namespace prefixes to identify the its source (e.g. **exb**, **exn**, **exc**, and **exg**)

PROV-man: Example (1/3)

```
public static Document createSample() {
    ProvmanFactory provFactory = new ProvmanFactory();
    Collection<Entity> entities = new ArrayList<Entity>();
    Collection<Agent> agents = new ArrayList<Agent>();
    Collection<Activity> activities = new ArrayList<Activity>();
    Collection<Relation> relations = new ArrayList<Relation>();
    Document document = new Document();
    // Entities
    Entity e2 = new Entity();    e2.setId("exg:dataSet1");
    Entity e3 = new Entity();    e3.setId("exc:regionList1");
    Entity e4 = new Entity();    e4.setId("exc:composition1");
    Entity e5 = new Entity();    e5.setId("exc:chart1");
    entities.add(e2);  entities.add(e3);
    entities.add(e4);  entities.add(e5);
    // Activities
    Activity act1 = new Activity();  act1.setId("exc:compose1");
    ActivityAttributes act1Attr = new ActivityAttributes();
    act1Attr.setKey("Status");   act1Attr.setValue("Done");
    act1.getAttributes().add(act1Attr);
    activities.add(act1);
    Activity act2 = new Activity();  act2.setId("exc:illustrate1");
    ActivityAttributes act2Attr = new ActivityAttributes();
    act2Attr.setKey("Status");   act2Attr.setValue("Ongoing");
    act2.getAttributes().add(act2Attr);
    activities.add(act2);
    // Agents
    Agent agent1 = new Agent(); agent1.setId("exc:derek");
    provFactory.addAgentAttributes(agent1, "prov:type", "Person");
    provFactory.addAgentAttributes(agent1, "foaf:givenName", "Derek");
    provFactory.addAgentAttributes(agent1, "foaf:mbox", "derek@example.org");
    agents.add(agent1);
```

PROV-man: Example (2/3)

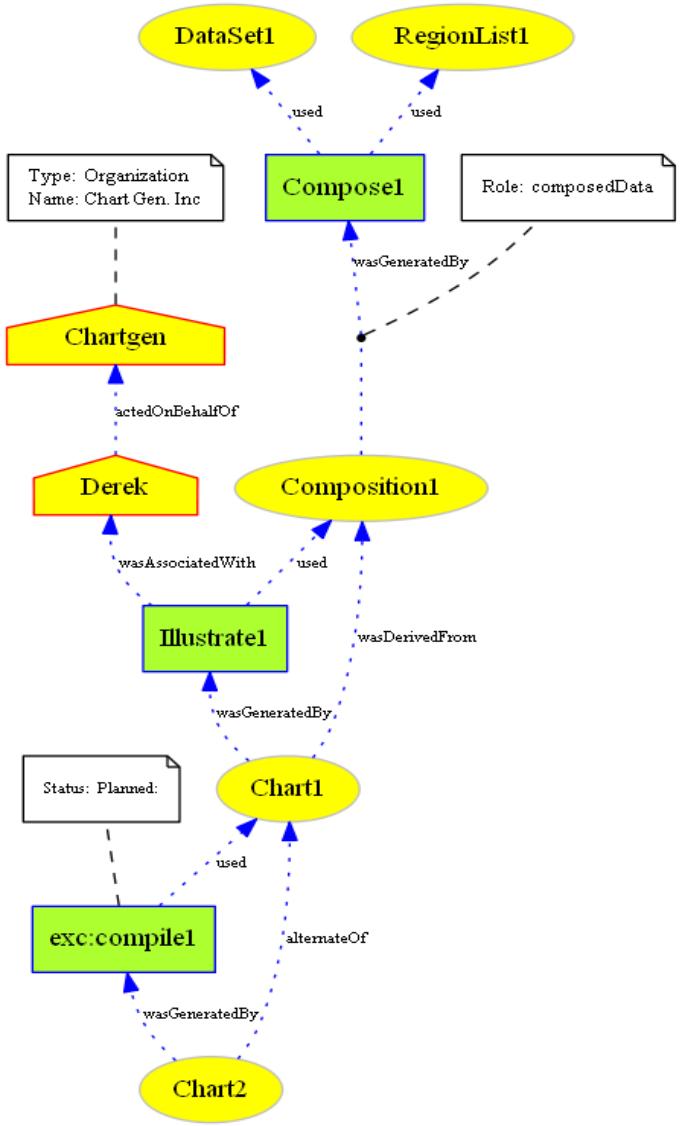
```
    Agent agent2 = new Agent(); agent2.setId("exc:chartgen");
    provFactory.addAgentAttributes(agent2, "prov:type", "Organization");
    AgentAttributes agAttr = new AgentAttributes();
    agAttr.setKey("foaf:Name");     agAttr.setValue("Chart Gen. Inc");
    agent2.getAttributes().add(agAttr);
    agents.add(agent2);
    // relationships
    WasAssociatedWith waw1 = new WasAssociatedWith();
    waw1.setId("waw1"); waw1.setActivity(act2); waw1.setAgent(agent1); waw1.setPlan(e2);
    relations.add(waw1);
    ActedOnBehalfOf abo1 = provFactory.newActedOnBehalfOf("abo1", agent1, agent2);
    relations.add(abo1);
    WasAttributedTo wat1 = provFactory.newWasAttributedTo("wat1", e5, agent1);
    relations.add(wat1);
    Used used1 = provFactory.newUsed("used1", act1, e2, "prov:role", "exc:dataToCompose");
    relations.add(used1);
    Used used2 = provFactory.newUsed("used2", act1, e3, "prov:role", "exc:regionsToAggregateBy");
    relations.add(used2);
    WasGeneratedBy wgb1 = provFactory.newWasGeneratedBy("wgb1", e4, act1, "prov:role", "exc:composedData");
    relations.add(wgb1);
    Used used3 = provFactory.newUsed("used3", act2, e4);
    relations.add(used3);
    WasGeneratedBy wgb2 = provFactory.newWasGeneratedBy("wgb2", e5, act2);
    relations.add(wgb2);
    WasDerivedFrom wdf1 = provFactory.newWasDerivedFrom("wdf2", e5, e4, "prov:type", "prov:Revision");
    relations.add(wdf1);

    document = provFactory.newProvGraph("provenance of an online newspaper article",
            activities, entities, agents, relations);

    return document;
}
```

PROV-man: Example (3/3)

```
public static void main(String args[]) {
    ProvmanPersistence PROVman = ProvmanPersistence.instance();
    PROVman.init();
    Document doc = PROVman.createSample();
    PROVman.toDB(doc);
    PROVman.toGraph(doc, "png");
}
```



Using PROV-man

- To use the PROV-man framework, please take the following steps:
  - Download PROV-man
  - Create DB
  - Deploy and test the API library
  - Define mapping Application -> PROV concepts
  - Integrate into Application

PROV-man: Download

- Download the PROV-man API form sourceforge:
  - http://sourceforge.net/projects/provman/?source=directory

- Releases
- Support
- Documentation
  - http://www.bioinformaticslaboratory.nl/twiki/bin/view/EBioScience/PROVMan

PROV-man: Create DB

- Create the PROV-man database using the PROV-man DDL script:
  - src/resources/PROV-man.ddl
- Update the database configuration file
  - src/resources/hibernate.cfg.xml

```
<?xml version="1.0" encoding="UTF-8"?>
<!DOCTYPE hibernate-configuration PUBLIC "-//Hibernate/Hibernate Configuration DTD 3.0//EN" "http
<hibernate-configuration>
  <session-factory>
    <!-- Database connection settings -->
      <property name="hibernate.connection.driver_class">com.mysql.jdbc.Driver</property>
      <property name="hibernate.connection.url">jdbc:mysql://localhost:3306/provman</property>
      <property name="hibernate.connection.username">compNSG</property>
      <property name="hibernate.connection.password">NSG!@comp#</property>
    <!-- JDBC connection pool (use the built-in) -->
    <property name="hibernate.c3p0.min_size">5</property>
    <property name="hibernate.c3p0.max_size">20</property>
    <property name="hibernate.c3p0.timeout">1800</property>
    <property name="hibernate.c3p0.max_statements">50</property>
    <!--<property name="connection.pool_size">1</property>-->
    <!-- SQL dialect -->
    <property name="dialect">org.hibernate.dialect.MySQL5InnoDBDialect</property>
    <!-- Enable Hibernate's automatic session context management -->
    <property name="current_session_context_class">thread</property>
    <!-- Disable the second-level cache  -->
    <property name="cache.provider_class">org.hibernate.cache.NoCacheProvider</property>
    <property name="hibernate.cache.use_second_level_cache">false</property>
    <!-- Echo all executed SQL to stdout -->
    <!--<property name="show_sql">true</property>-->
    <!-- Drop and re-create the database schema on startup -->
    <!--property name="hbm2ddl.auto">update</property>
    <property name="hbm2ddl.import">removefk.sql</property-->
    <mapping resource="provman.hbm.xml"/>
  </session-factory>
</hibernate-configuration>
```

```
<property name="hibernate.connection.url">jdbc:mysql://localhost:3306/provman</property>
<property name="hibernate.connection.username">UserName</property>
<property name="hibernate.connection.password">Password</property>
```

PROV-man: Deploy and Test

- Create a simple Java program that executes

```
public static void main(String args[]) {
    ProvmanPersistence PROVman = ProvmanPersistence.instance();
    PROVman.init();
    Document doc = PROVman.createSample();
    PROVman.toDB(doc);
    PROVman.toGraph(doc, "png");
}
```

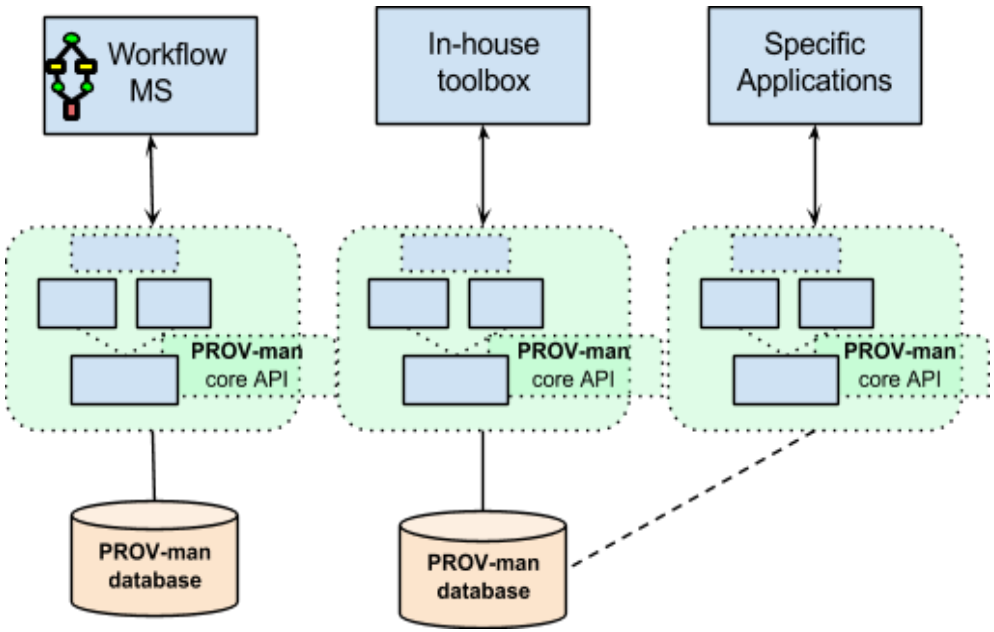
PROV-man: Define mapping

- Define the mapping between application and PROV concepts
- Decide on what data to collect and to which depth

PROV concept	***workflow counterpart***
Document	Workflow execution (experiment)
Entity	- Input data - output result
Agent	- Users of the platform - Organization - Data analysis tool
Activity	jobs executed
Relation	Input/output relationship
Attributes (all) - Document - Entity - Agent - Activity - Relation	Metadata for all above - Experiment attributes - Input/output data attributes - Agent attributes - Jobs attributes - Relationships attributes

PROV-man: Integration

- Alternatives:
  - ***Integrate*** into the implementation of the Java application.
  - ***Data collector*** as an external software module using logs, database, etc.
  - ***Extract*** the provenance data directly from the application's database
  - Combine the above

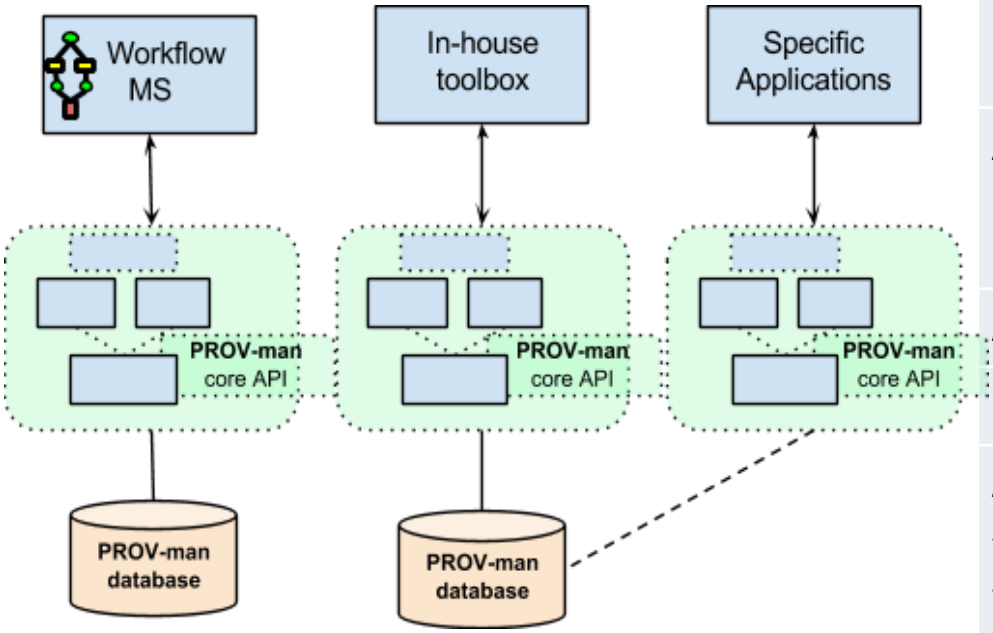


Example:
Provenance for the Neuroscience Gateway

- Major part of the data retrieved for the Neuroscience database (catalogue):
  - information about executed workflows, their jobs, status, input data and output results.
- Detailed information about each executed job parsed from the log files on the grid:
  - start time, end time, computing node, operating system on the computing node, etc.)

- Collector automatically triggered

Implementation



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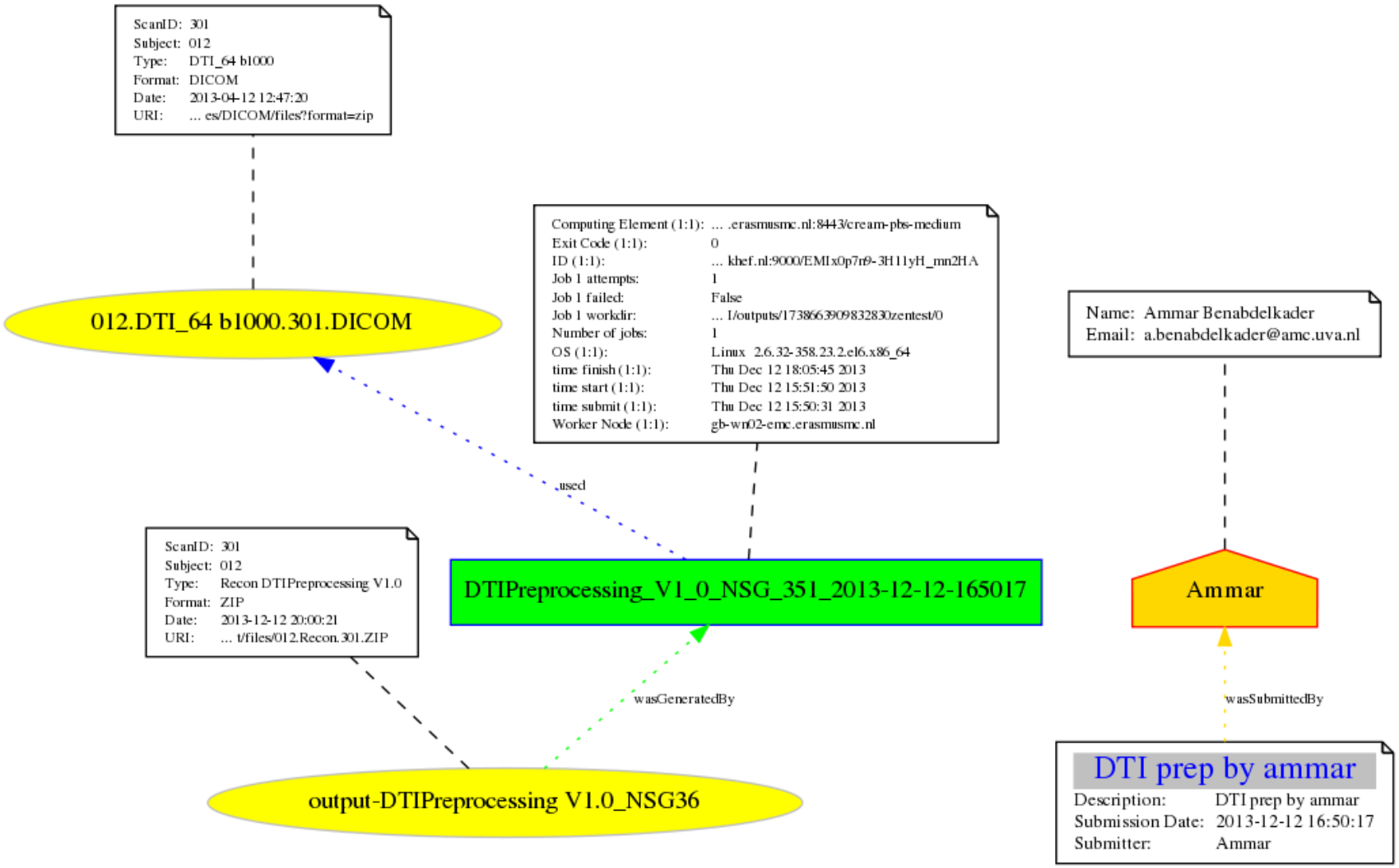
Provenance of DTI Preprocessing workflow execution

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PROV-man: your gain?

- *Developers*:
  - Reduce development time;
  - Enhance and facilitate the utilization of the standardization
  - Customize format according to user preferences and requirements

- *Users (scientists)*:
  - Provenance data for their experiments (out of the box)
    - Validated, repeated, shared, trusted, proven experiments
  - Interoperability

Thanks!

Links

- PROV-man: http://www.bioinformaticslaboratory.nl/twiki/bin/view/EBioScience/PROVMan
- PROV-Primer: http://www.w3.org/TR/2013/NOTE-prov-primer-20130430/
- PROV-DM: http://www.w3.org/TR/2013/REC-prov-dm-20130430/
- PROV-O: http://www.w3.org/TR/2013/REC-prov-o-20130430/
- PROV-N: http://www.w3.org/TR/2013/NOTE-prov-sem-20130430/
- Resource Description Framework (RDF): http://www.w3.org/TR/rdf-mt/
- Graphviz - Graph Visualization Software: www.graphviz.org

Discussion / Questions