Preserving Scientific Processes from Design to Publications

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Overview

- Preservation of research
- Process preservation
- Process Context model to describe processes
- Use Case example: music classification experiment
- Conclusions

Preservation of Research

- Long-term access to research publications desired
  - Storage, understandability of data format sufficiently addressed today

- Today’s research often based on experiments
  - Huge amounts of data (Big Data, Fourth Paradigm)
  - Often complex steps of preprocessing, transformation and analysis
  - Verification, Comparability, Repeatability, …
- Publication is often only the last step in the research process – preservation needs to go beyond the document

Preservation of Research

- Comparability: often tackled through benchmark environments, using a standard data set and evaluation measure (campaigns such as TREC, CLEF, MIREX, …)
- Repeatability: Documentation of experiment environment, publication of source code developed, …
- Complexity of processes: can be tackled by using (scientific) workflow engines such (Taverna, Kepler, …)
  - Allow exact definition of steps executed, configuration employed, data input and output, …
  - Facilitates repeatability

Preservation of Research

- Some aspects beyond the control of workflow engines
  - Computing environment outside the engine
    - Hardware, operating system, software packages installed can all have an effect on the results
    - Changes might occur without initiative and notification to the researcher (e.g. software updates)
  - Use of external services becoming more popular
    - Web services providing specialised computation, e.g. frequently used in the Bio-informatics domain
    - May become unavailable, change their interface, behaviour, …

Process Preservation

- Preserving repeatability of processes emerging topic in Digital Preservation Research (e.g. projects TIMBUS, Workflows4ever, …)
- Goal: allow re-execution of the complete process at a later stage, when e.g. changes in the technology render the original process obsolete

Process Preservation Challenges

- What needs to be captured at ingest?
  - Need to go beyond single files (and their metadata)
  - Up to complete computer systems, including additional documents needed to understand & operate process

- How do these digital objects need to be described?
  - Need to characterise several aspects of the process
  - From a top-level: organisational parameters
  - Down to technical description of systems, including hardware, operating systems, software, third-party libraries and services.

Process Preservation Challenges

- Which preservation actions are applicable?
  - Combination of several different preservation actions, such as migration of specifications and documents, code migration/cross-compilation, or emulation of hardware or software utilised in the process.

- How can a preserved process be verified and evaluated?
  - Need to ensure that the execution of the (modified) process at a later stage is equivalent to the original process

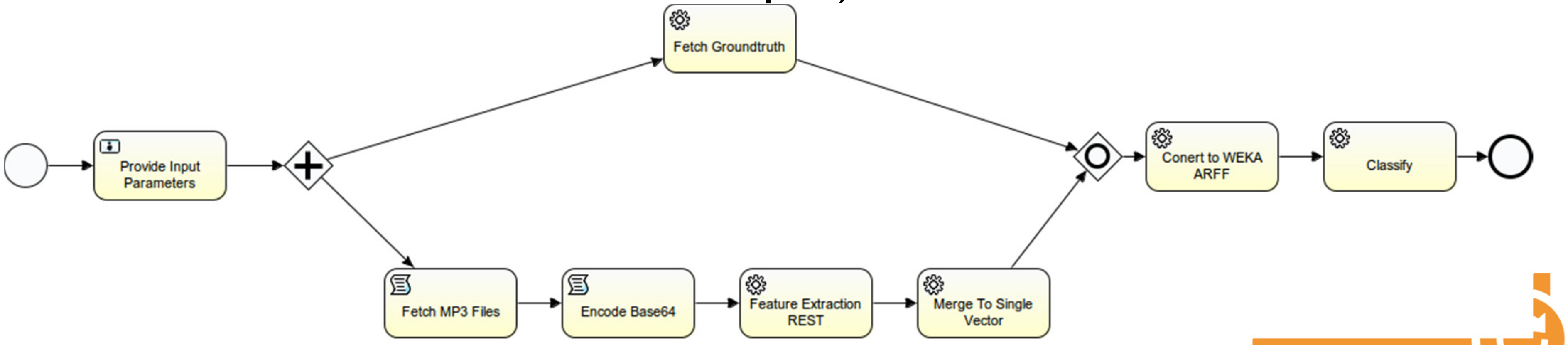
Example: Music Classification

- Scientific experiment from the machine learning/information retrieval domain

- Classification of music into predefined set of genres
- Learns a machine-learning model from given training data (i.e. data with manually assigned class/genre)
- Predicts genre for previously unseen data
- Useful e.g. for online music store, recommendation services, etc.

Example: Music Classification

- Input:
  - Music (e.g. MP3 format)
  - Ground truth/gold standard
- Output: Classification of music, e.g. into genres
- Intermediate steps
  - Extract numeric description (features) from music
  - Format conversions (feature extractor output to classification software input)



Music Classification: Aspects

- Software environment including configuration (machine learning software, operating system)
- External services: feature extraction, ground truth, …
- Hardware (e.g. computation on GPUs)
- Licenses & access keys
- Experiment parameters
- Input data, intermediate data created in the process
- …

Process Context Model

- Allows to systematically capture aspects of processes which are essential for preservation and re-execution

- Model in the form of an Ontology
  - Elements organised in a hierarchy
  - Models relations between elements (e.g. dependencies)

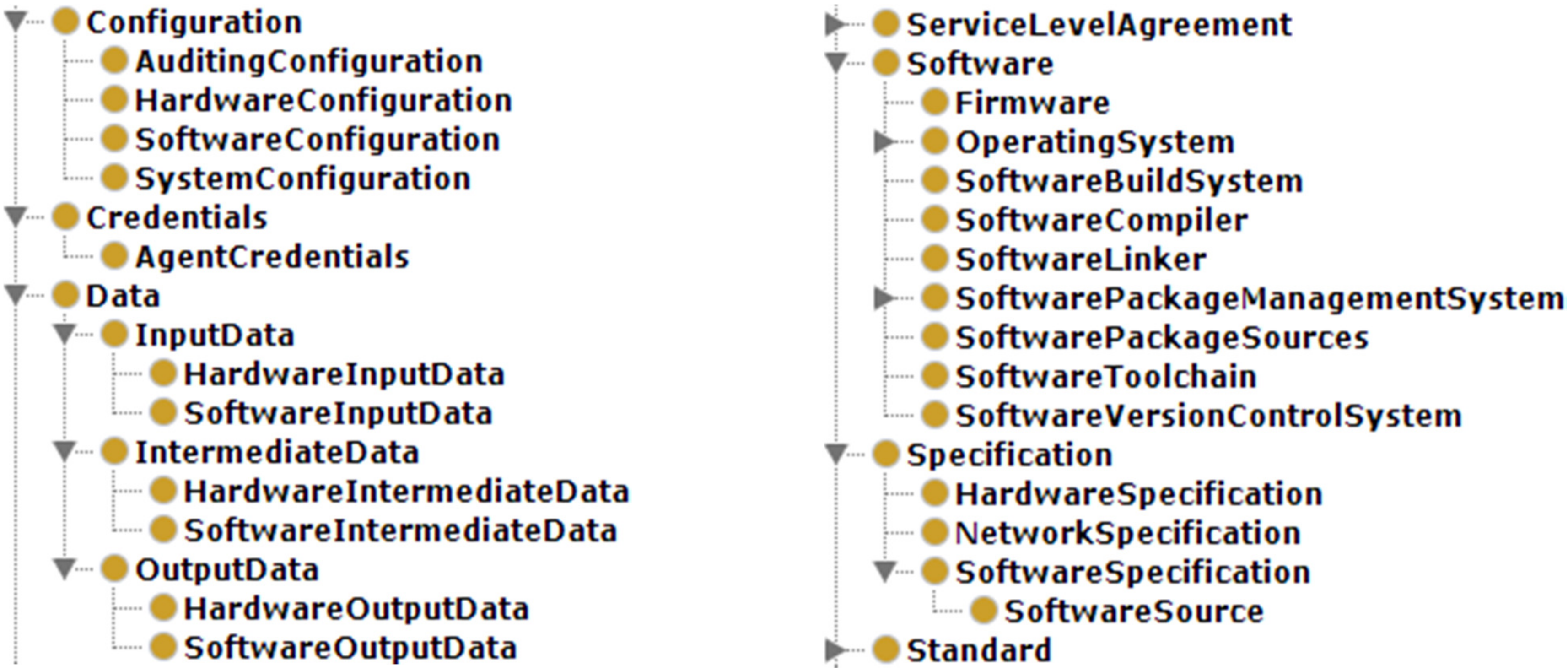
- Captures aspects diverse aspects such
  - Organisations, people, roles, legal requirements, …
  - Software, hardware, external systems, …

Process Context Model

- Similar to Representation Information Networks, but extended to capture process context

- Derived via top-down and bottom-up approach
  - Used enterprise frameworks such as ZACHMAN
  - Used existing taxonomies, such as PREMIS
  - Derived from scenarios developed by project partners
    - Intellectual property rights, data analysis, software escrow, multimedia services, …

Process Context Model



- Configuration
  - AuditingConfiguration
  - HardwareConfiguration
  - SoftwareConfiguration
  - SystemConfiguration
- Credentials
  - AgentCredentials
- Data
  - InputData
    - HardwareInputData
    - SoftwareInputData
  - IntermediateData
    - HardwareIntermediateData
    - SoftwareIntermediateData
  - OutputData
    - HardwareOutputData
    - SoftwareOutputData
- ServiceLevelAgreement
- Software
  - Firmware
  - OperatingSystem
  - SoftwareBuildSystem
  - SoftwareCompiler
  - SoftwareLinker
  - SoftwarePackageManagementSystem
  - SoftwarePackageSources
  - SoftwareToolchain
  - SoftwareVersionControlSystem
- Specification
  - HardwareSpecification
  - NetworkSpecification
  - SoftwareSpecification
    - SoftwareSource
- Standard

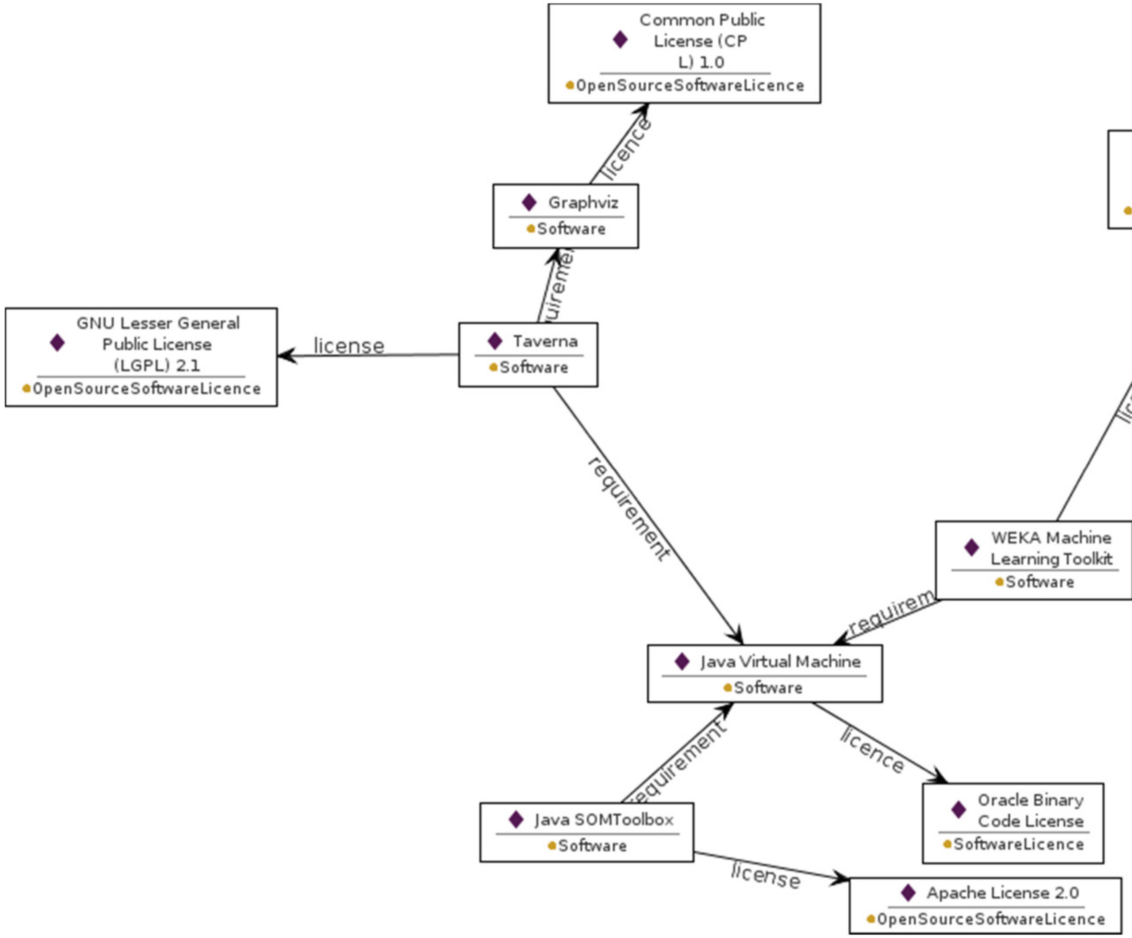
Process Context Model

- For a specific process to be preserved, an instance of this model is created
  - Creating individuals relevant to the process
  - Instance depends on nature of the process – e.g. technical focus in music classification example

- Semi-automatic approach
  - Capturing tools provide some aspects automatically
  - Knowledge from experts (e.g. process owners) needs to be added manually

Music Classification: Context Model

- Software setup can be automatically detected in OS with software packages (e.g. Linux); allows detection of licenses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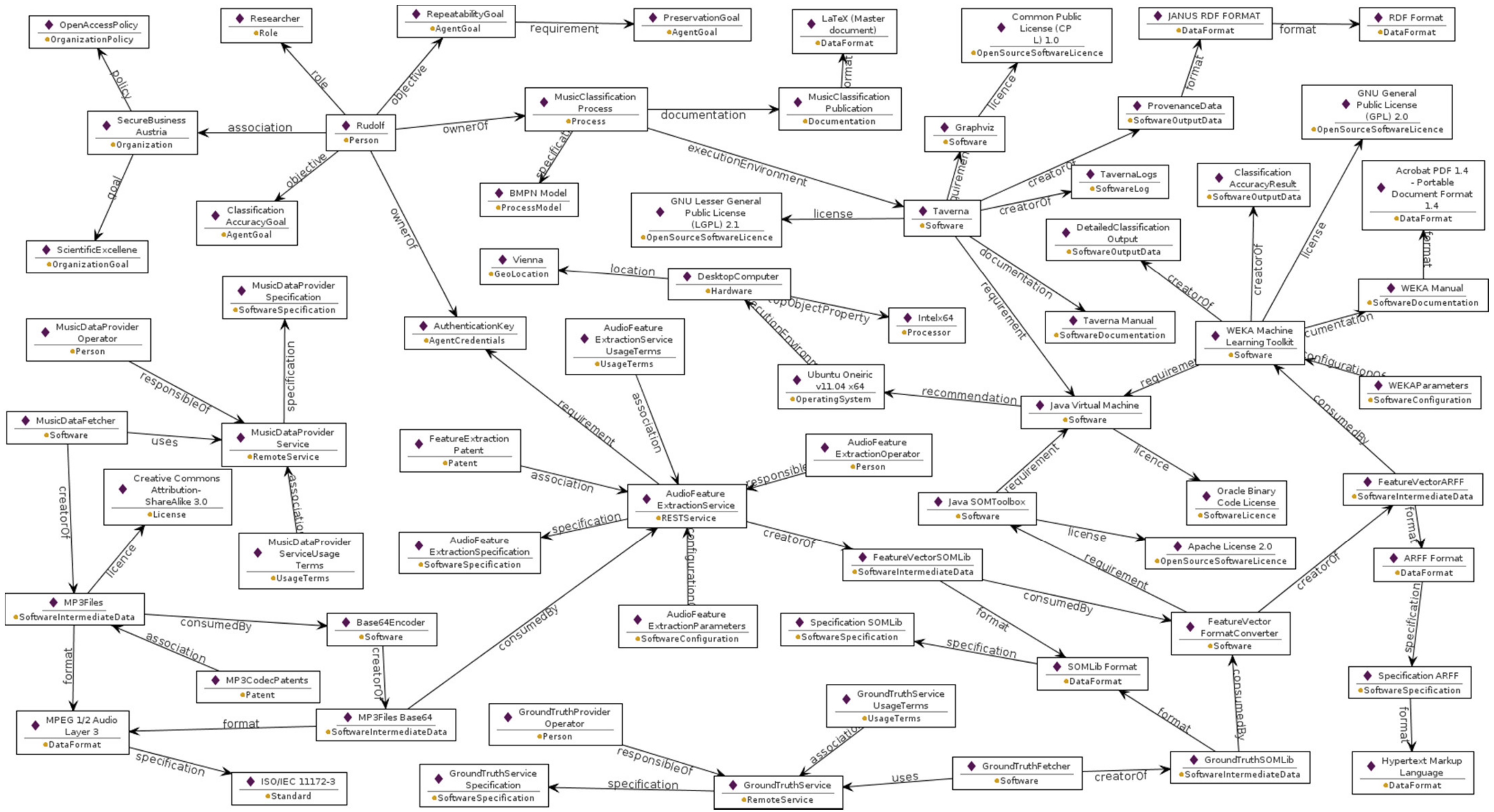
Music Classification: Context Model



Preservation Actions

- Early stage of research
- Likely a combination of existing approaches
  - Documents needed in the process can be migrated or viewed via emulation software
  - Software and hardware can be emulated
  - External services are difficult
    - Simulation via mock-up services, for deterministic cases

  - Virtualisation to allow archival of modified systems

Validation and Verification

- Need to verify that the process execution is the same as before
- Need to define points of measurement as *significant properties* that can be compared
  - Causal relationships and information flow as significant property
- Music classification example: significant properties are the input and output data, as well as the data exchanged between intermediate steps
  - Captured in workflow systems as *provenance data*
    - Capturing more difficult in less formalised executions

Validation and Verification

- External services and third party libraries: how to detect changes?
  - Monitoring necessary, via watch service

Soccer/flickr

- Comparison of intermediate results in previously recorded executions and current executions

Conclusion

- Challenges of preserving scientific processes
  - More than just the publication
  - Complex service orchestration
  - Complex software environment; libraries, external services, …
- Context model to capture and describe processes
- Preservation actions: combination of existing approaches
- Later verification and re-execution is a crucial task
  - Capturing is not enough, validation is required

Thank you for your attention!

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