Validation of E-Science Experiments using a Provenance-based Approach

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Overview

- E-Science experiment validation
- Bioinformatics scenario
- Provenance-based validation architecture
- Evaluation results

E-Science Experiments

- Large scale computations for conducting scientific research
- Multiple distributed services on the Grid
- Workflow validation
  - Part of the scientific process
  - Verify correctness of their own experiments
  - Review correctness of their peers' work

Static Validation

- Operates on workflow source code
- Checks if workflow satisfies some properties before it is run
- Examples
  - type inference, escape analysis, concurrency analysis, graph-based partitioning
- Workflow script may not be accessible or may be expressed in a language not supported by analysis tool

Dynamic Validation

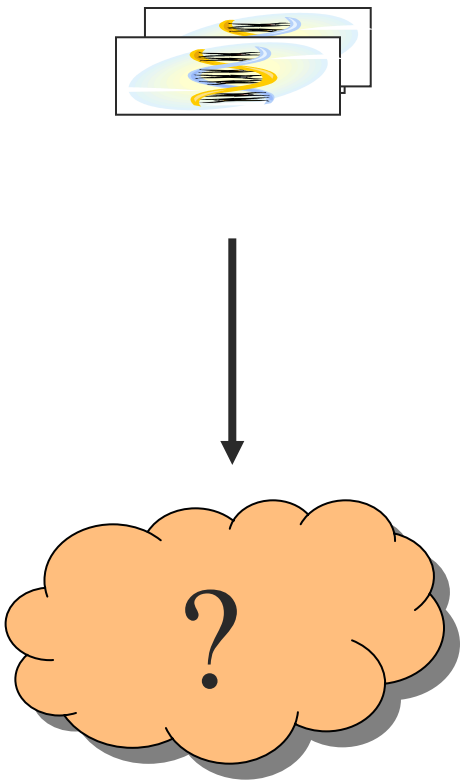
- Verifies data values satisfy constraints during execution
  - interface matching, runtime type checking
- Cannot assume services will perform validation
- Interfaces may be under-specified
  - In bioinformatics, biological sequences commonly specified as strings in interfaces

Provenance-based Validation

- Allows for validation of experiments after execution
- Third parties may want to verify that the results obtained were computed correctly according to some criteria
- These criteria may not be known when the experiment was designed or run
- Important because science progresses (and models evolve!)

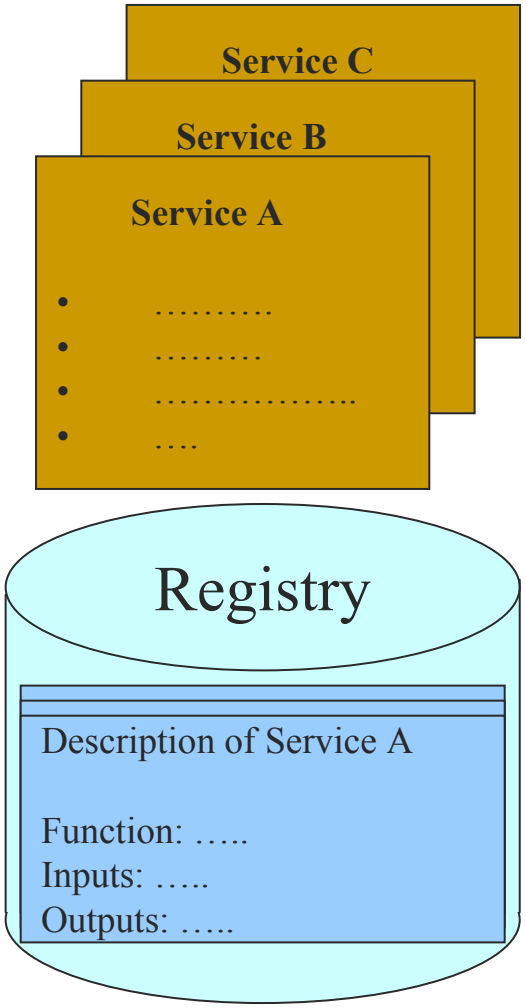
Bioinformatics Scenario

- A biologist has a set of proteins, for each of which he/she wishes to determine a particular biological property



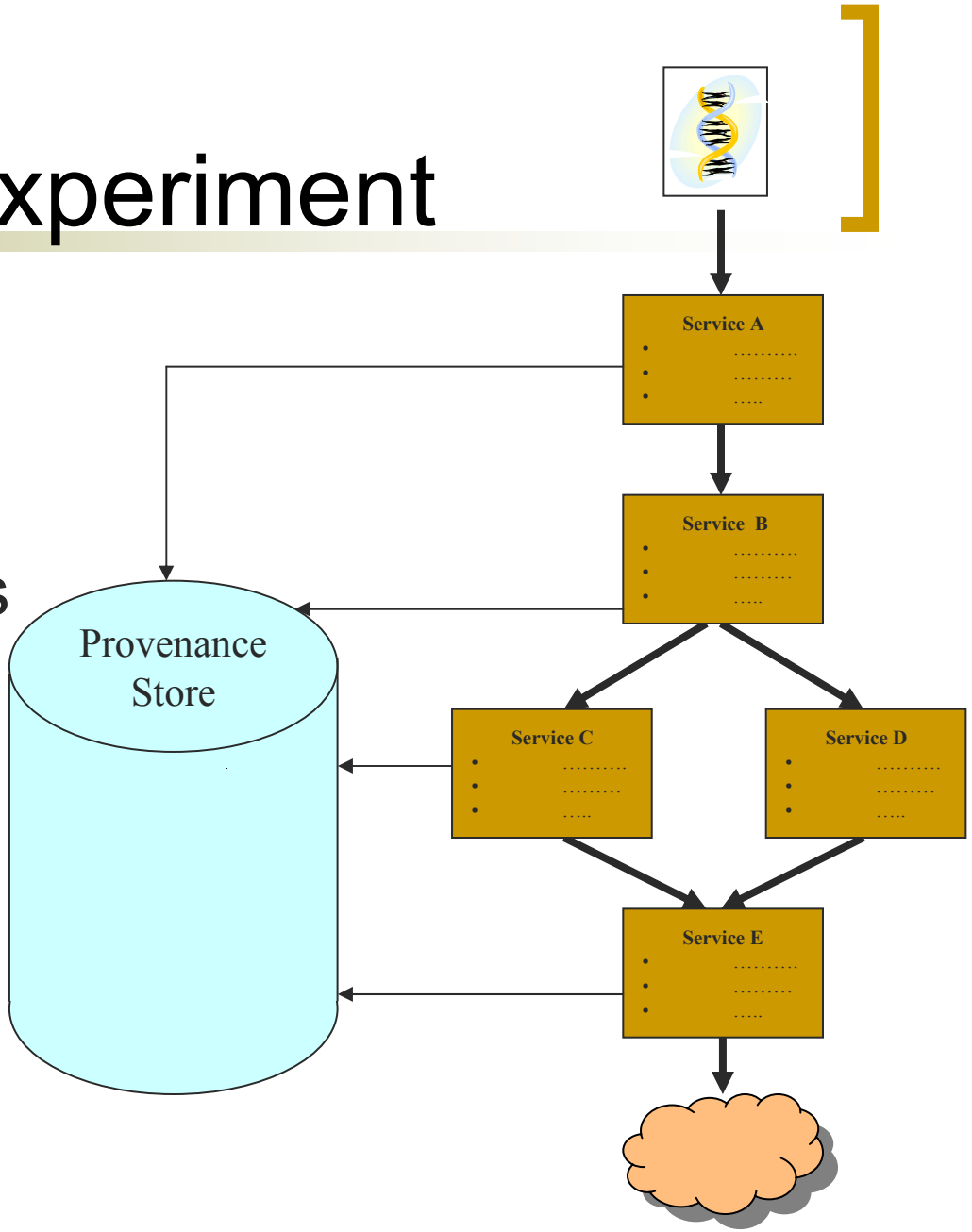
Experiment Services

- Design experiment (abstract plan)
- For each step in the plan, decide on the concrete *service* to use
- Each service may be designed by the biologist or adopted from the work of another biologist
- For each service there is a *description* of that service stating:
  - what the service does
  - what type of data it analyses (its *inputs*) and
  - what type of results it produces (its *outputs*)
- All the descriptions are stored in a *registry*



Performing Experiment

- Performs experiment
- Details of experimental process documented in a *provenance store*
- Each service documenting its own execution



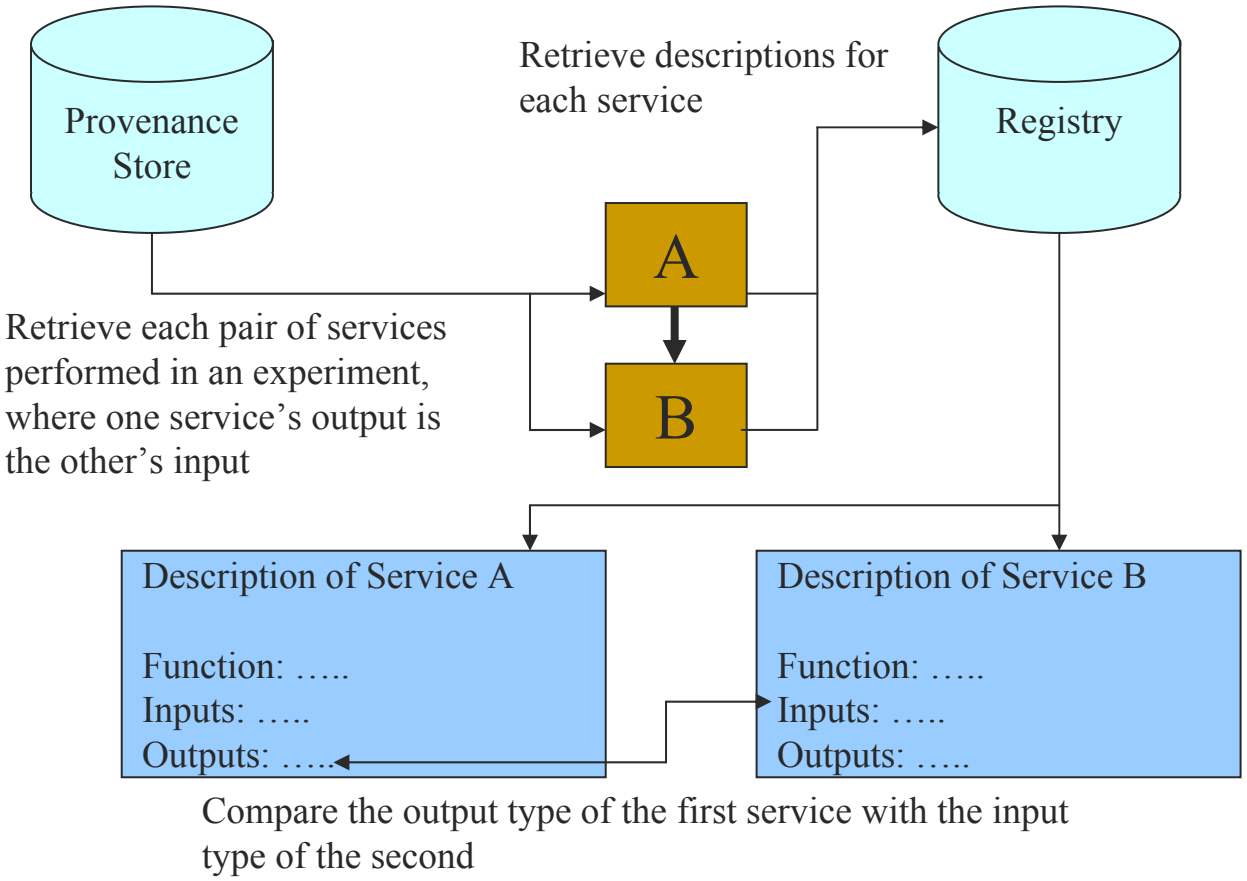
Questions

1. Did I perform each service on the type of data that the service was intended to analyse?
   - Were the inputs and outputs of each activity compatible?
2. Did the services I used actually fulfil my high level plan?

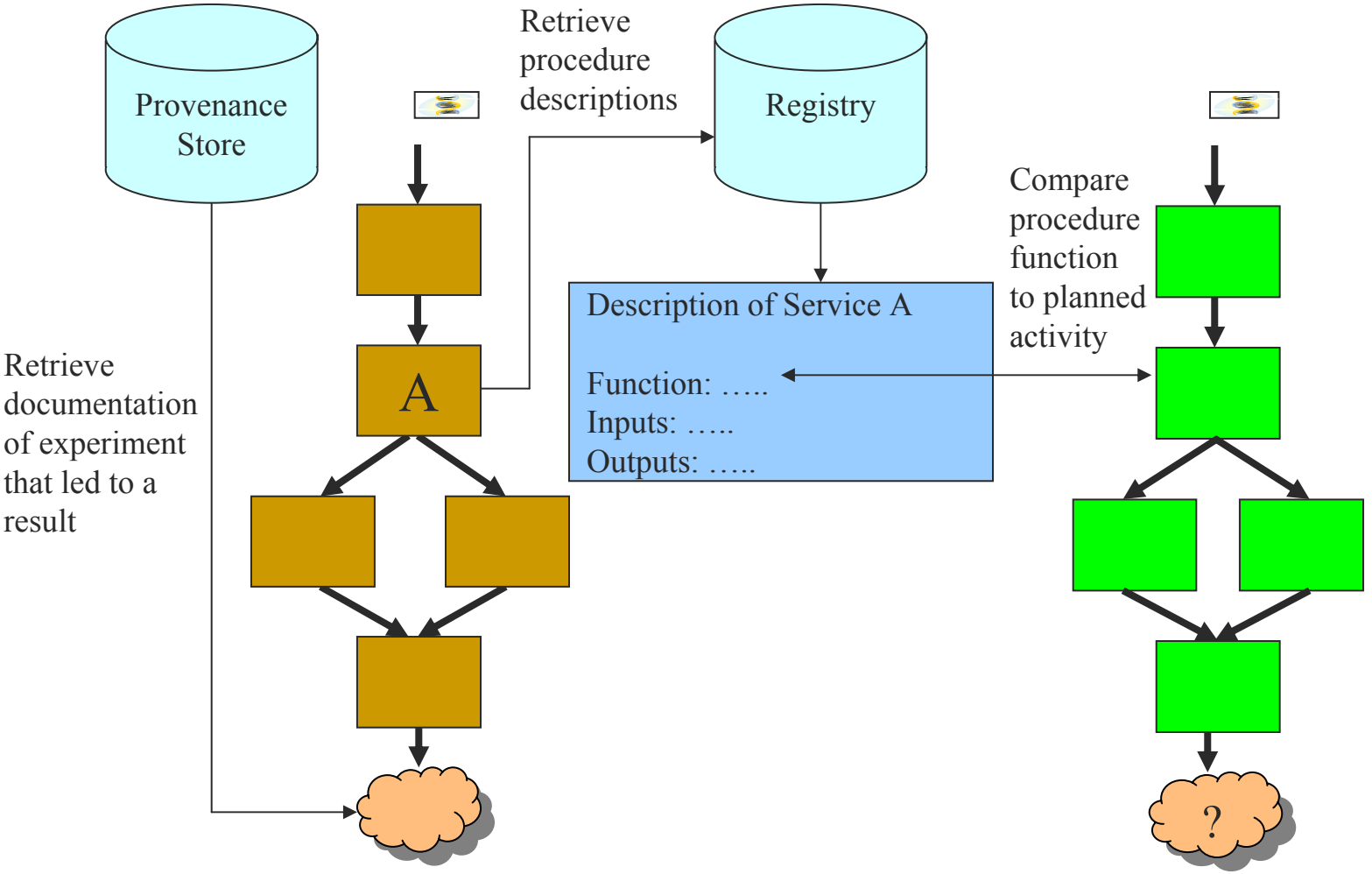
Answering the Questions

- Using the documentation in the Provenance Store, we can reconstruct the process that led to each result
- Along with the high level plan and the descriptions in the registry we have all the information required to answer the questions

Q1: Were the inputs and outputs compatible?

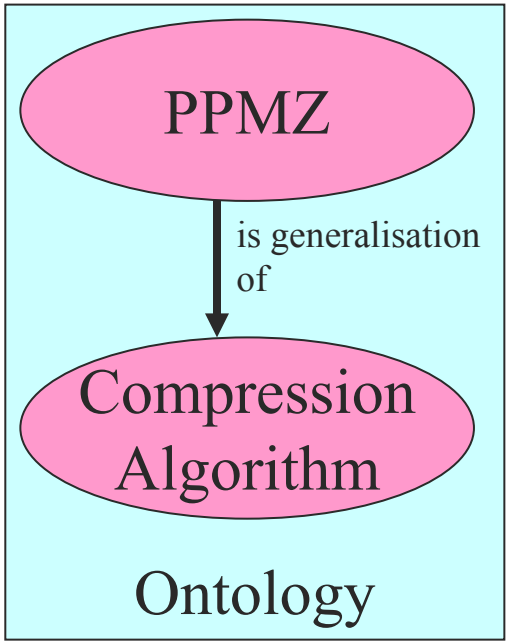


Q2: Did the experiment follow the plan?

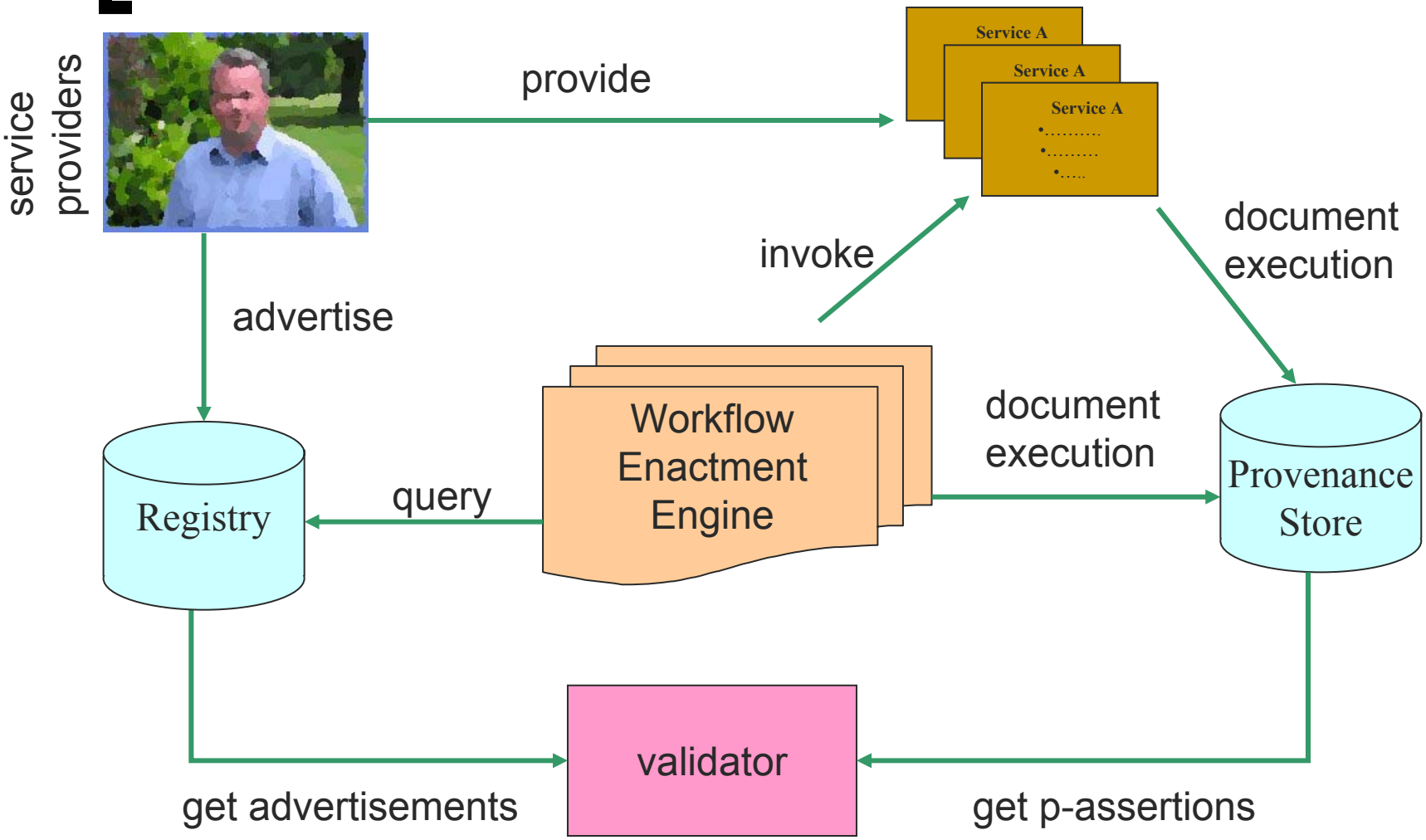


Ontological Reasoning

- High-level activity may be described in a more general way than the service which performs it
- Also, one service's input may be a generalisation of the preceding service's output
- Therefore, exact matching of types may produce a false negative: the biologist will wrongly be told the experiment was invalid
- By using an *ontology,* describing how types are related, we can reason about types and determine whether they are truly compatible



Architecture



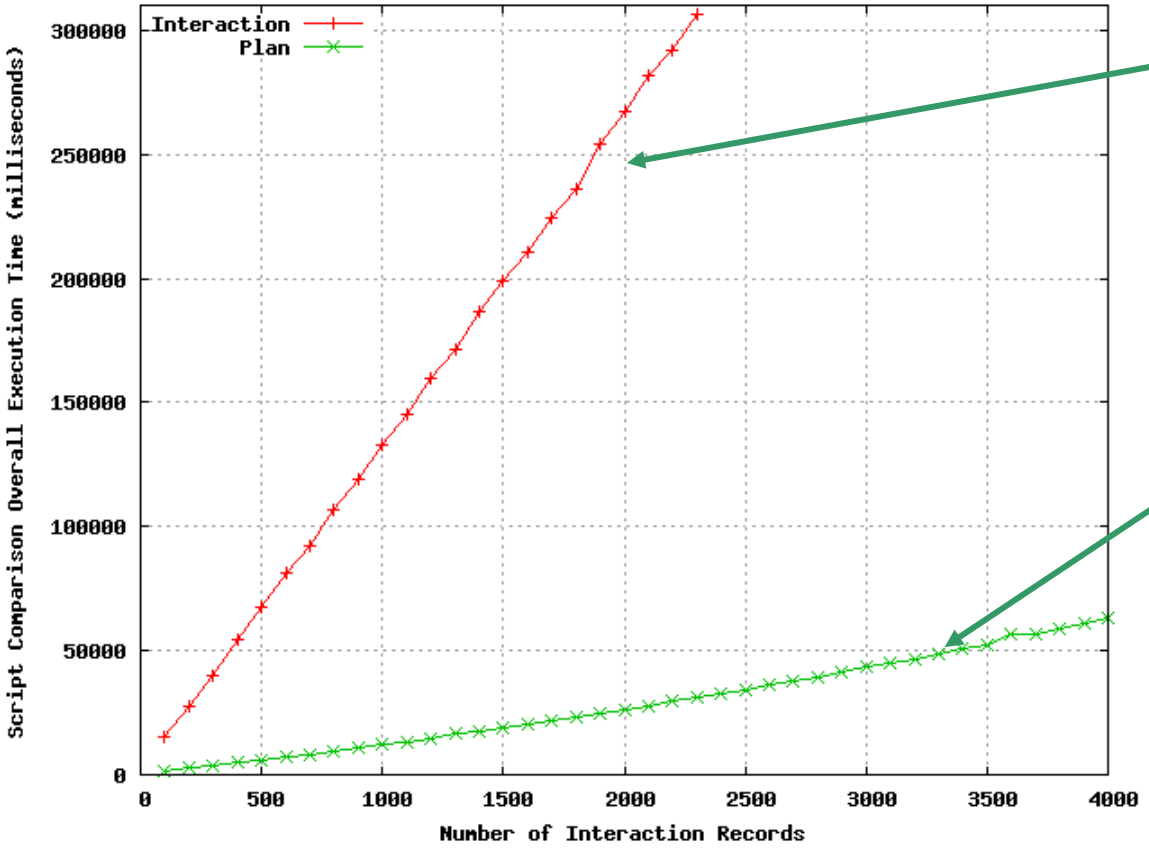
Testing

- Workflow - protein compressibility
- Provenance store – PASOA (pasoa.org)
- Registry – Grimoires (grimoires.org)
- Validator – Java, Jena 2.1
- Ontology in OWL, based on myGrid bioinformatics ontology

Performance Evaluation

- Potentially, large number of experiments are performed
- Evaluate if our approach can scale with the size of the provenance store
- Time to validate an experiment with increasing number of experiments recorded

Performance



input/output type validation

plan validation

Summary

- Provenance-based validation of workflow executions
  - Validation of experiments after execution
    - Previously unknown criteria
    - Third party validation
- Tested with a sample bioinformatics experiment
- Evaluation shows framework scales well with increasing data store size