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WSSP41

Enhancing Research with Provenance Management for HPC and AI Systems

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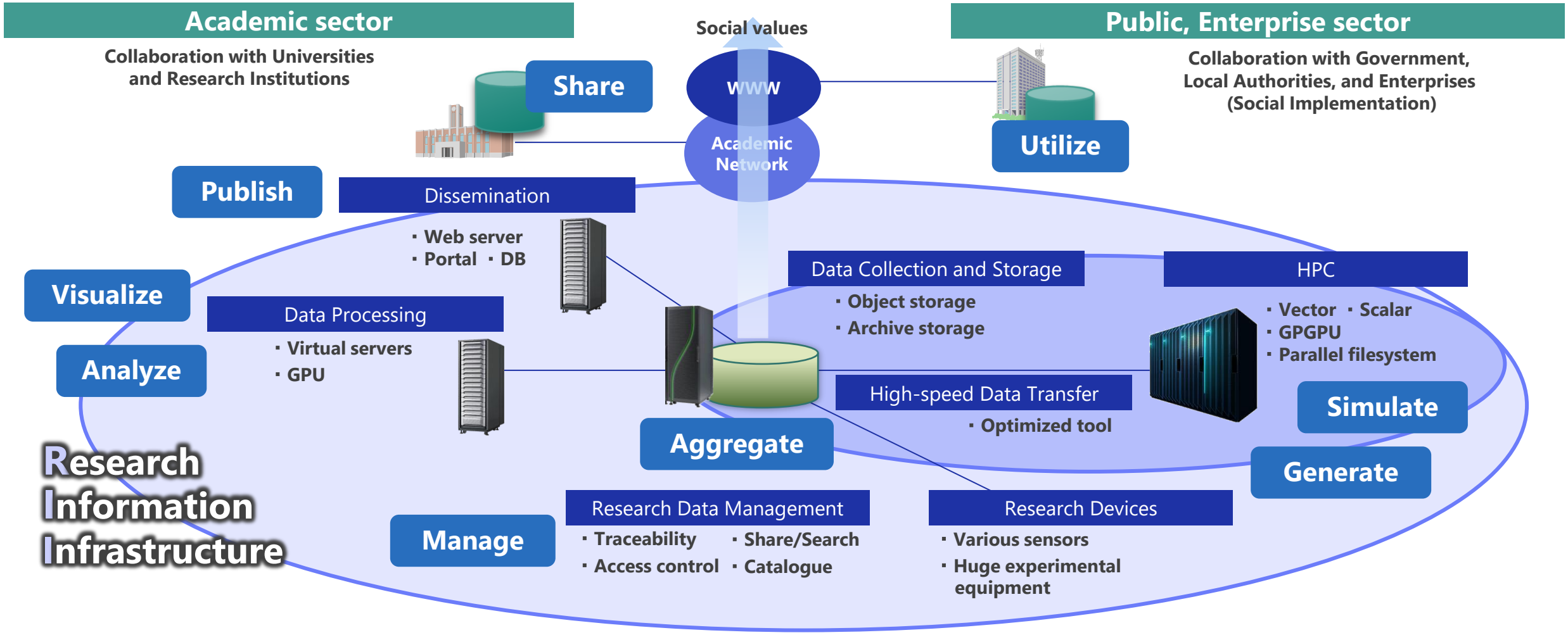
Agenda

1. Overview of Research Information Infrastructure (RII)

2. Data Provenance System for HPC (DPS4HPC)
   - Workflow Overview
   - Contribution to Reproducibility
   - System Overview
   - Management GUI
   - System Configuration
   - Performance Evaluation

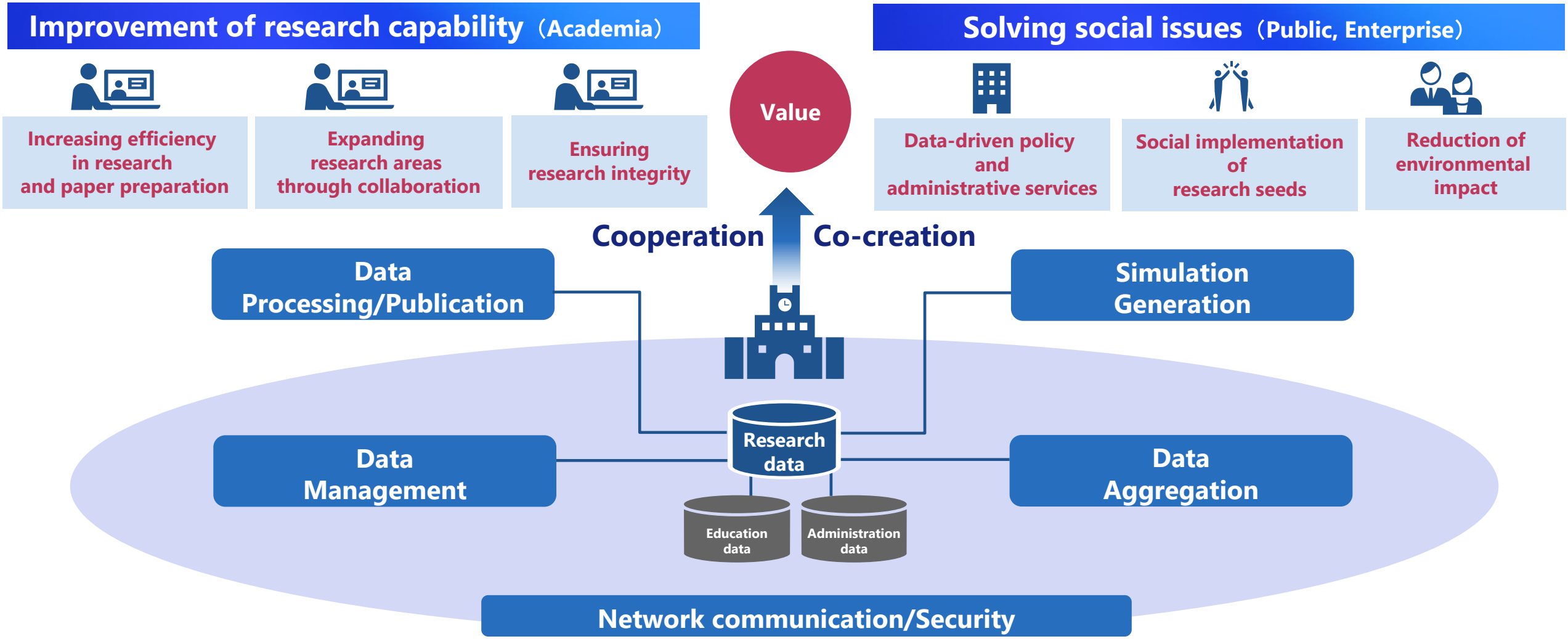
Overview of RII (Research Information Infrastructure)

- NEC provides, through total integration, a system for aggregating and utilizing large volumes of data generated by HPC and various research devices.

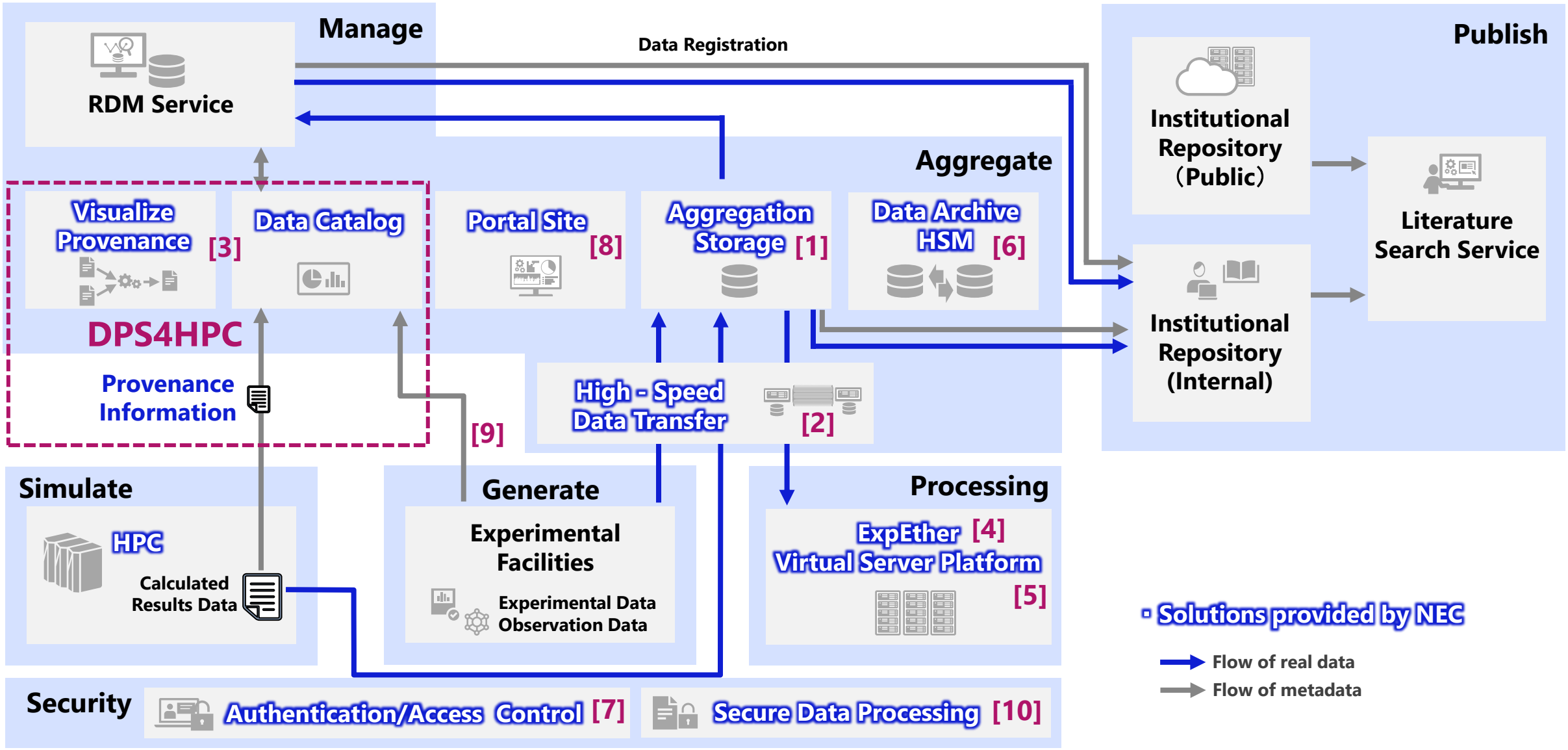


Value Provided by RII

■ NEC provides value to academic and research institutions, Improving their research capability, with RII.



Data Lifecycle and RII Solution Portfolio

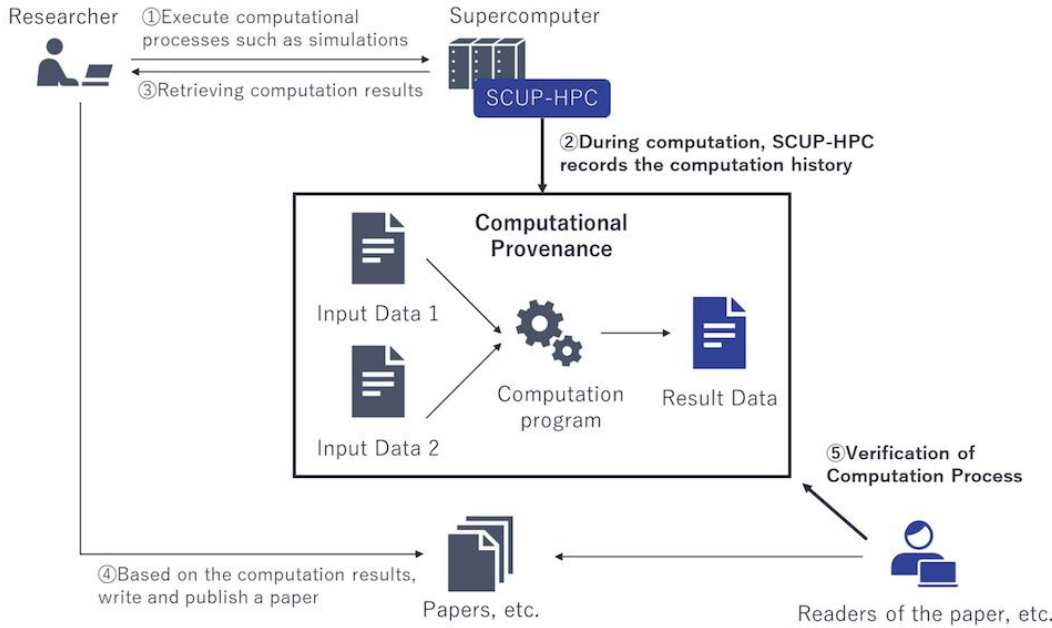


Operation Start of NEW OCTOPUS at Osaka Uni. with DPS4HPC

- We issued a press release about new OCTOPUS, short for “Osaka university Compute and sTOrage Platform Urging open Science”

Our second-generation OCTOPUS offers approximately 1.5 times the performance of the first-generation OCTOPUS and is built with a new provenance management system named SCUP-HPC ((System for Constructing and Utilizing Provenance on High-Performance Computing System)

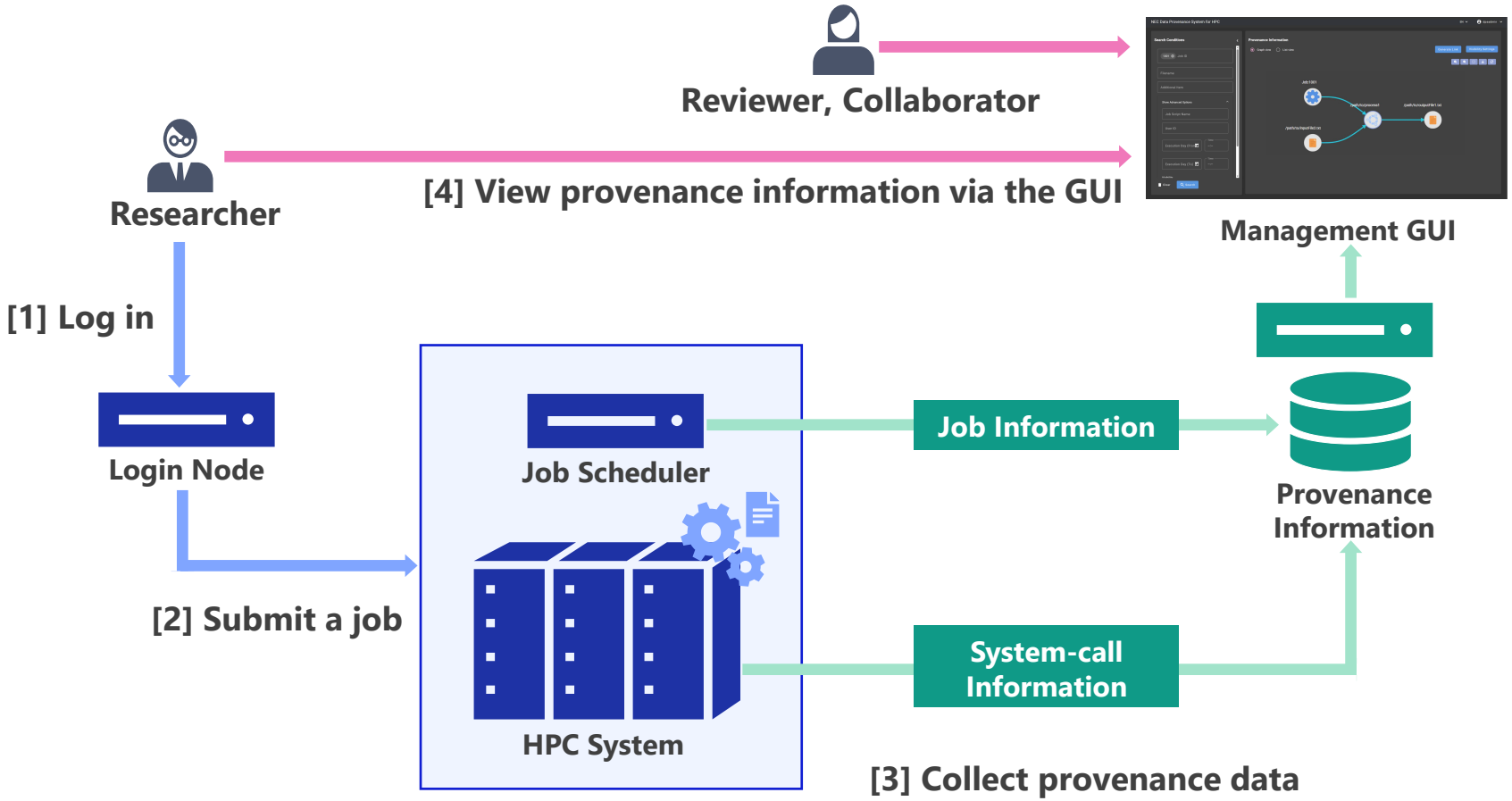
This SCUP-HPC allows researchers to record, manage and visualize computational provenance which contains the information on how data is accessed by what kind of program and what kind of data is genetated. As the result, a new scientific computing concept named “Scientific Computing Unifying Provenance – High Performance Computing” is realized on supercomputing system and is expected to improve researchers’ and scientists’ productivity of academic research using computer simulation and AI learning.



https://www.ais.cmc.osaka-u.ac.jp/date/en/press-release-octopus2/

Workflow Overview

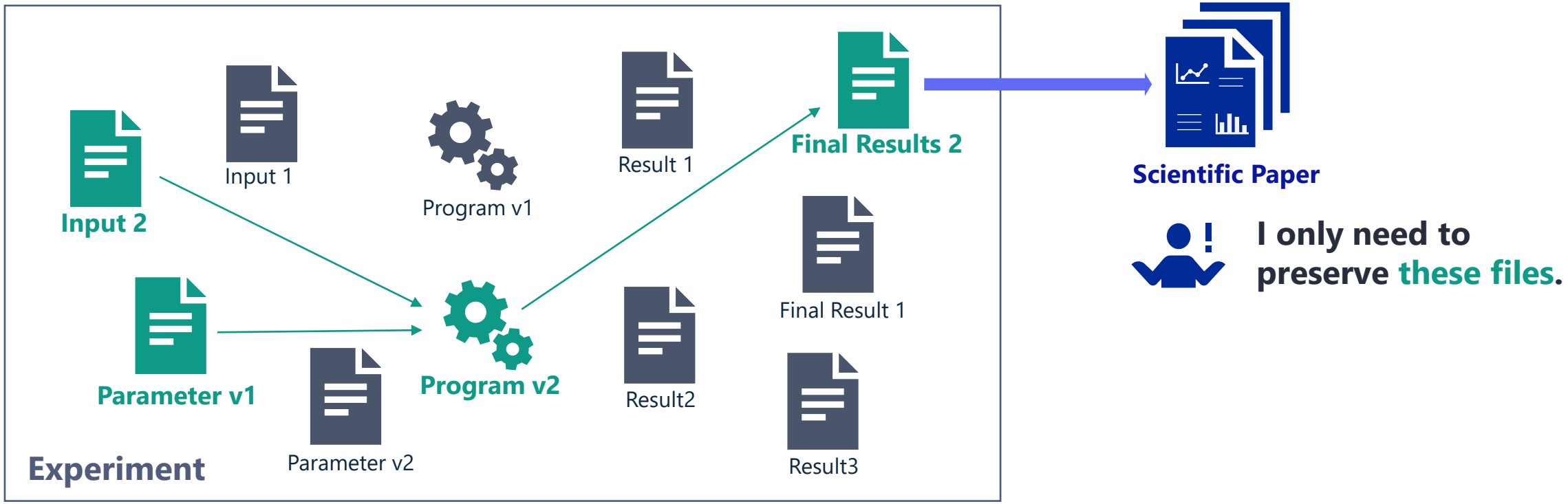
- Automatically records the provenance and metadata of a file generated in an HPC system
  — just by executing jobs as usual — without modifying the user's assets such as programs and scripts.



Contribution to Reproducibility 1

Identify research data and programs that should be preserved.

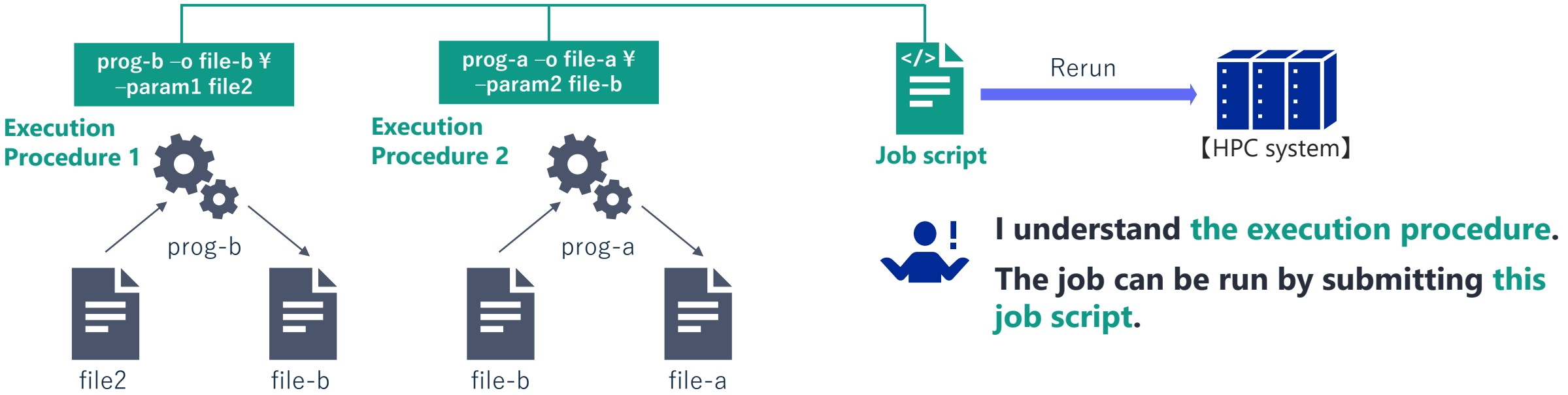
- In research, repeated experiments with modified programs and parameters often generate many similar files.
- Provenance shows which programs and input data were used to generate the final files.
- Helps identify and preserve only the truly necessary data.



Contribution to Reproducibility 2

Clarify the procedure for reproducing the experiment.

- To reproduce the experiment, in addition to the files and programs used, it is necessary to know how the program was executed.
  - The execution procedure of programs
  - Command-line options provided to the program
  - Job scripts used to run the program

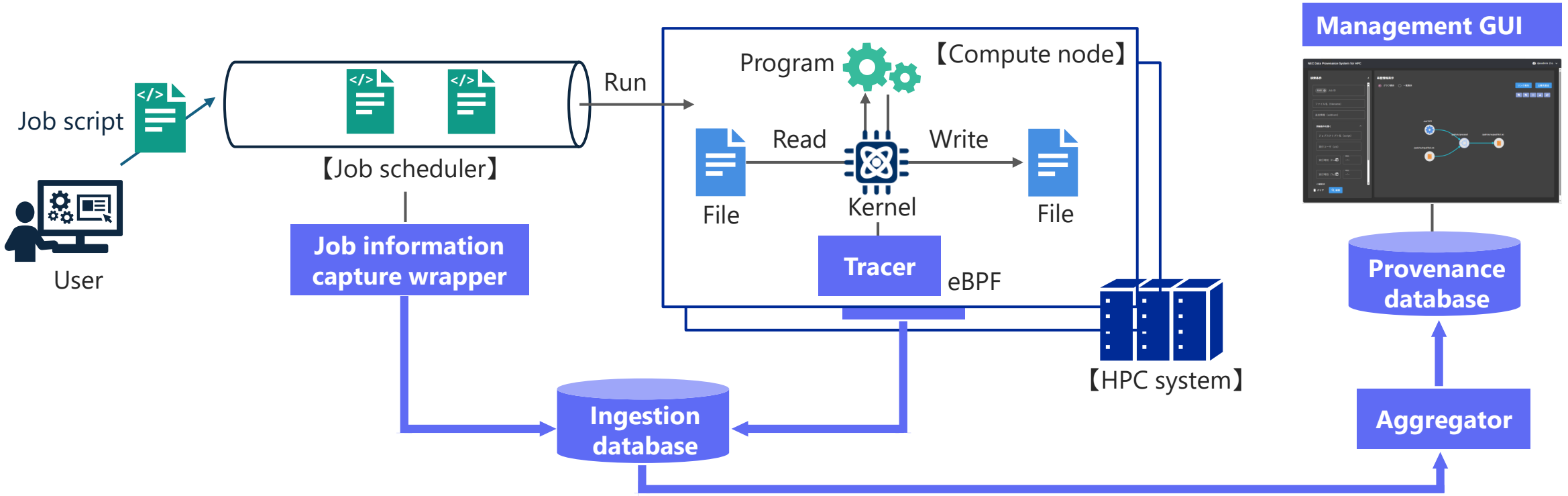


I understand the execution procedure.

The job can be run by submitting this job script.

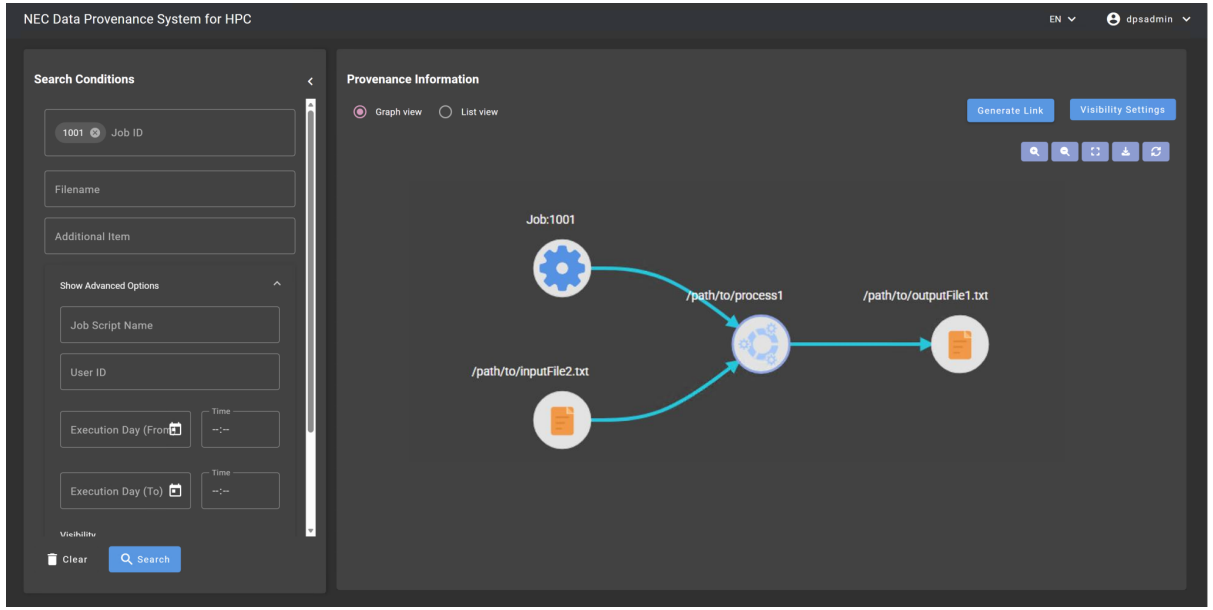
System Overview

- Capture system call invocations by applications in the Linux kernel of HPC system nodes using eBPF.
  - Information on which application read or wrote which files
  - Metadata of the accessed files
- Capture job-related information from the job scheduler.
- Build provenance by integrating the data captured above.

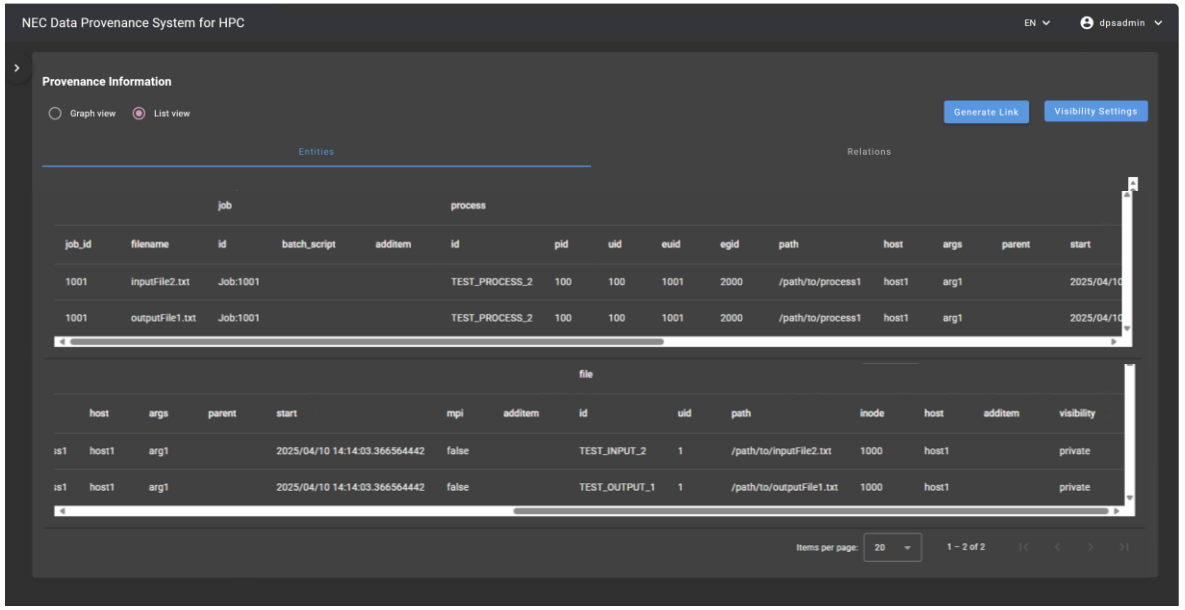


Management GUI

- Users can use the web-based management GUI to browse file input-process-output relationships and view associated metadata.
- Users can search using various criteria such as Job ID, filename, user ID, or execution time, view detailed information in a list, and visualize the results as an intuitive graph.



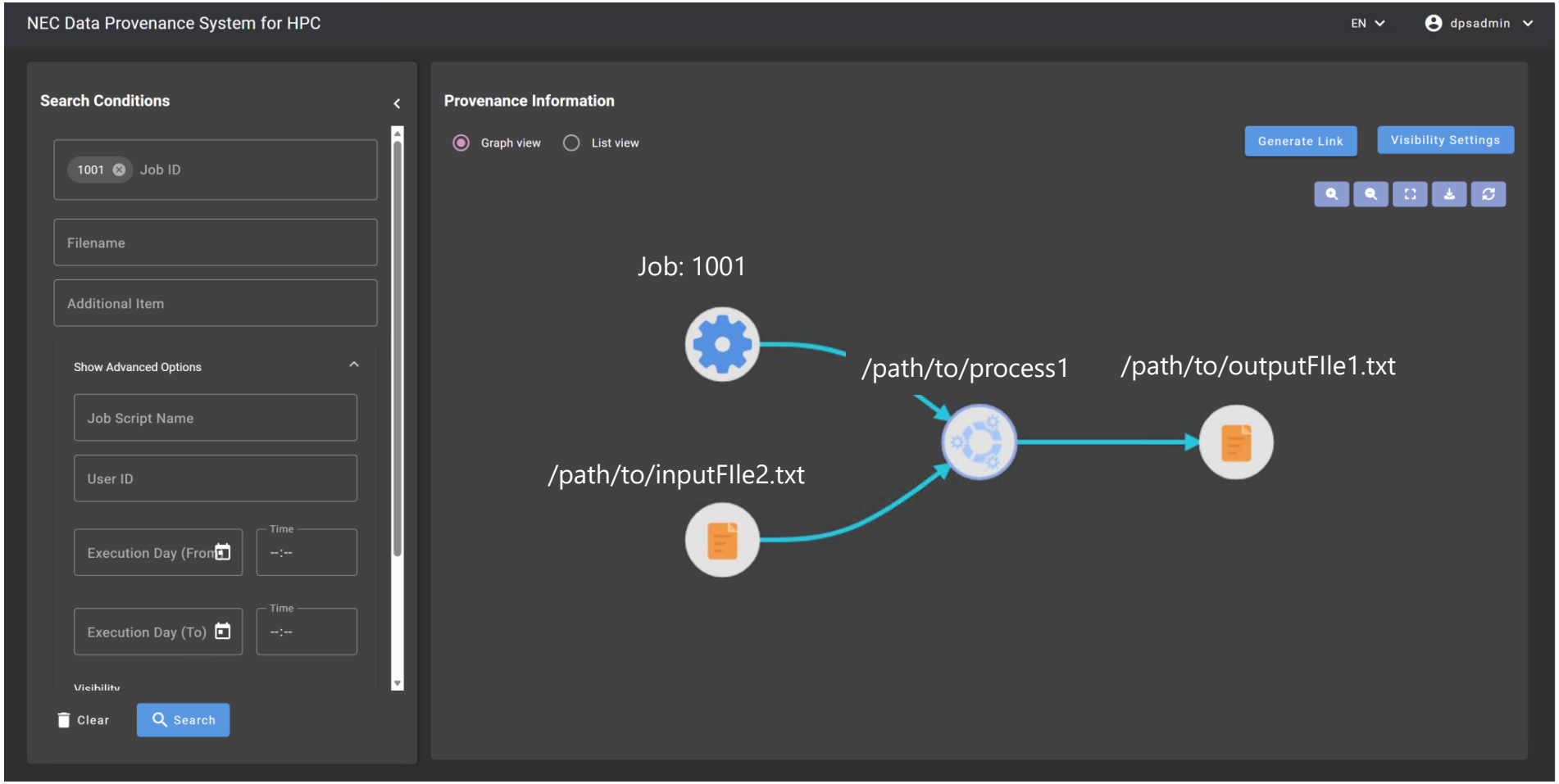
File Provenance Visualization



Provenance Information Details

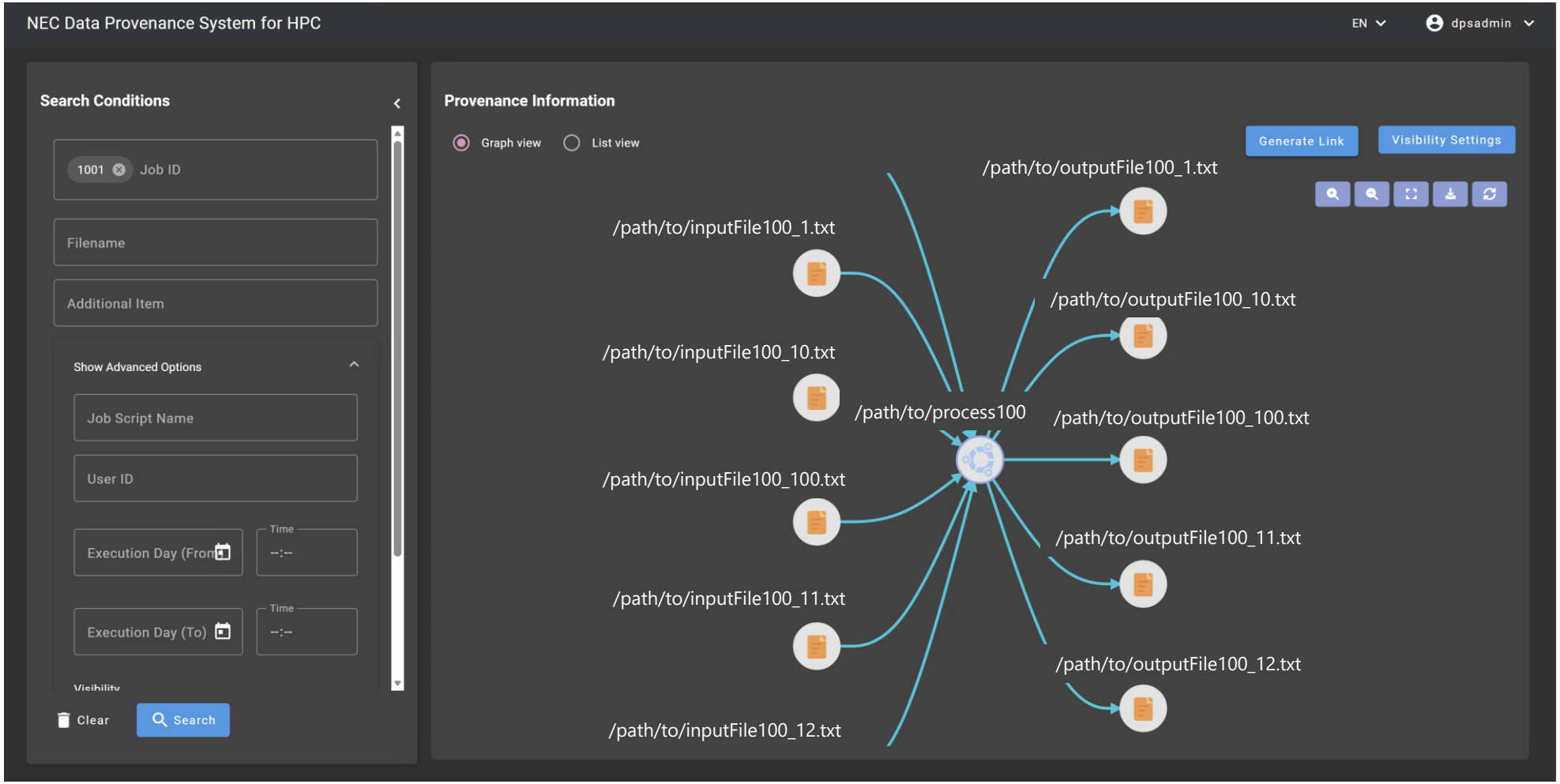
Management GUI (Graph Mode)

- Automatically captured entities and relations—visualized as circles and arrows—form a provenance graph of HPC workflows at the Job ID level

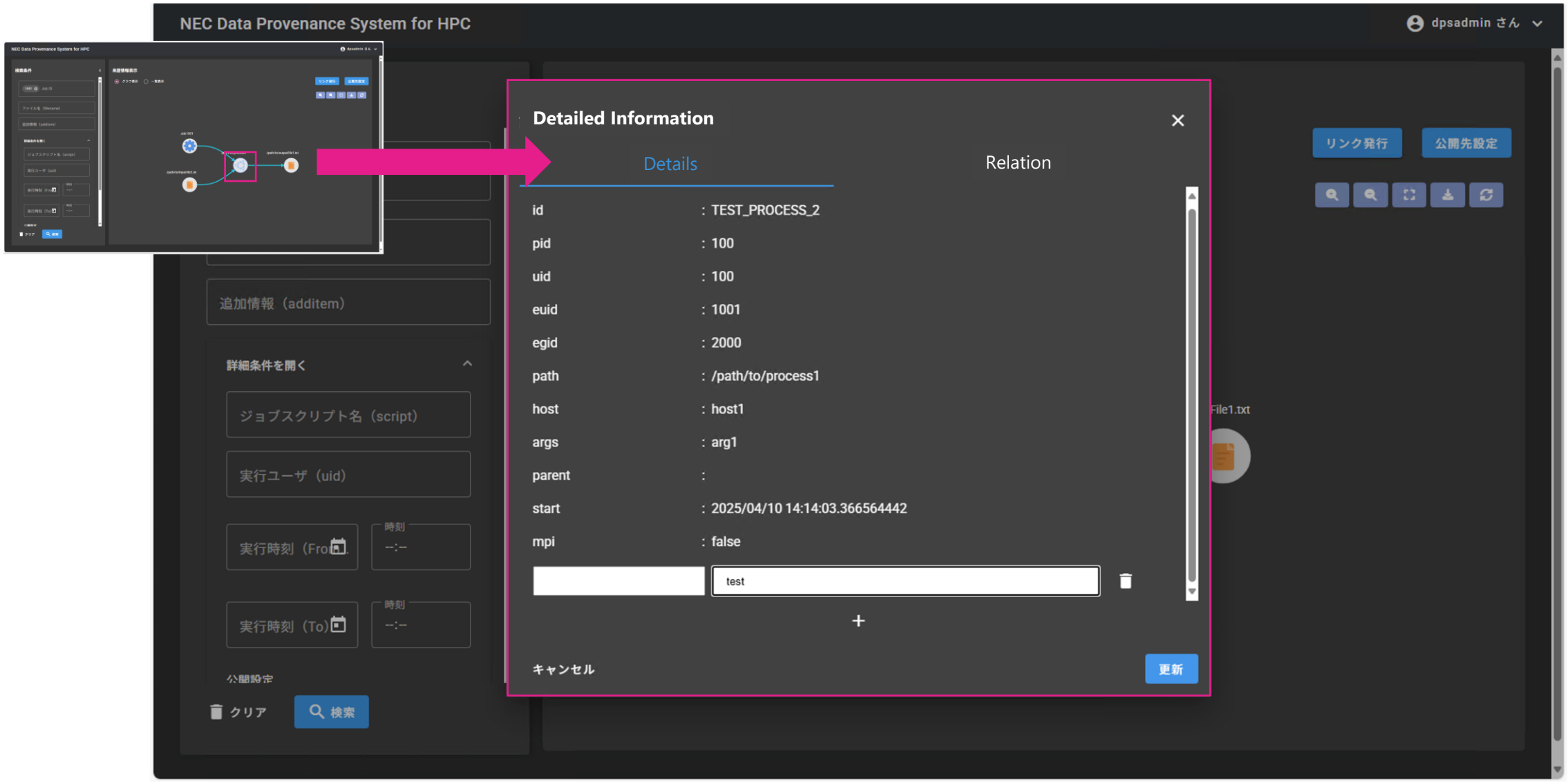


Management GUI (Graph Mode)

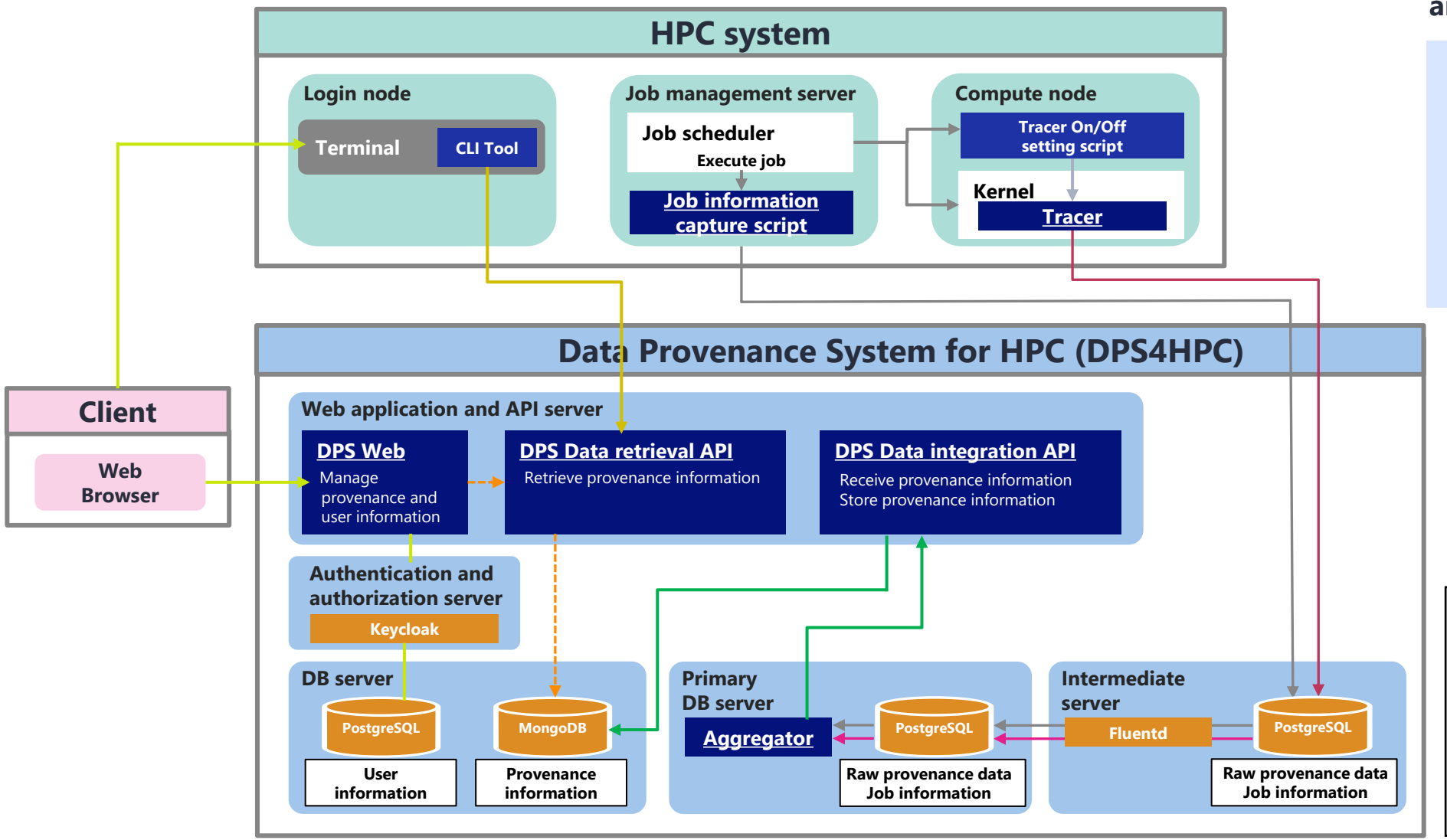
- Even for complex computational processes that handle multiple files, DPS4HPC can capture complete provenance information and visualize it.



Management GUI (Metadata Details)



System Configuration Diagram



The following software components are provided as NEC products.

- **Job scheduler wrapper**
- **Tracer**
- **DPS Web**
- **DPS Data retrieval API**
- **DPS Data integration API**
- **Aggregator**

Legend

- Server of HPC system
- Server of DPS4HPC
- Software of DPS4HPC (NEC's product)
- Software of DPS4HPC (open source)
- Job information
- Raw provenance data
- Provenance information
- Retrieve information by Web server
- Others (Browser, Authentication, etc.)

System Components and Required Specifications

Servers	Specs	Key Components	Roles
HPC System			
Login node	-	CLI Tool	
Job management server	-	Job Scheduler （NQSV / Slurm / (PBSpro) Wrapper	Capture job-related information
Compute nodes	-	Tracer	Capture system call invocations and file metadata
Authentication and authorization	-	e.g., Keycloak	Integrate with LDAP, SSO
Data Provenance System for HPC (Virtual server is acceptable)			
Intermediate server（xn）*	12 cores / 24 GB	PostgreSQL, Fluentd	Receive initial input from the Tracer and the job scheduler （Raw provenance data）
Primary DB server（x1）	12 cores / 24 GB	PostgreSQL, Aggregator	Construct provenance information from the above inputs
Web application and API server（x1）	4 cores / 8 GB	Python, Component-Based UI DPS Web　DPS Data retrieval API DPS Data integration API	Transfer the provenance information between the DB servers Retrieve and visualize the provenance information (via CLI and Web-UI) Manage user information
Provenance DB server（x1）	12 cores / 24 GB	PostgreSQL, MongoDB	Store the provenance and user information

* One server is required per 256 compute nodes, if the number of compute nodes exceeds 256 nodes.

Performance Evaluation

- Evaluation was conducted using using six representative HPC / AI applications
  - Comparison of the impact on application performance with and without provenance construction
  - Execution time increases by about 1%-3%, but within acceptable range
  - No significant changes in resource usage such as CPU, memory, and network

Application	Execution time (s) w/o Tracing	w/ Tracing	Increase		Memory Usage Increase (MB)	Network Usage (MB)	#Records
AlphaFold	7494.76	7600.74	105.98	1.41%	190	23	102 562
Bridge++	506.67	511.71	5.05	1.00%	161	16	37 757
BT-IO	57.90	59.11	1.21	2.08%	200	1	6204
PyTorch	472.66	483.59	10.93	2.31%	205	13	48 609
Quantum ESPRESSO	168.86	171.86	3.00	1.78%	159	7	22 029
TensorFlow	735.11	755.98	20.87	2.84%	221	35	65 616

- AlphaFold : Protein structure prediction using deep learning
- Bridge++ : Lattice QCD simulation for particle physics
- BT-IO : NAS Parallel Benchmark for storage performance
- PyTorch : Deep learning training framework
- Quantum ESPRESSO : First-principles materials science simulation (DFT)
- TensorFlow : Deep learning framework

IEEE Access 2025, Namiki et al.
SCUP-HPC: System for Constructing and Utilizing Provenance on High-Performance Computing Systems

PoC Idea

Target Outcome

- The provenance of data (calculation results) generated by the HPC system can be visualized and understood.
- The obtained provenance information enables the following:

Expected Benefits and Use Cases

- **1: Researchers retrieve the provenance before writing a paper and use it as supporting data for the publication.**
- **2: Reviewers of a paper refer to the provenance to verify its accuracy.**
- **3: Intellectual property staff submit the provenance as supporting material when filing a patent.**
- **4: Researchers use the provenance when transferring a project to another researcher or collaborating with others.**
- **5: Research administrators refer to the provenance to confirm that no tampering has occurred.**
- **6: When a problem is discovered in data processing, the provenance is used to check how the process was executed.**

PoC Configuration

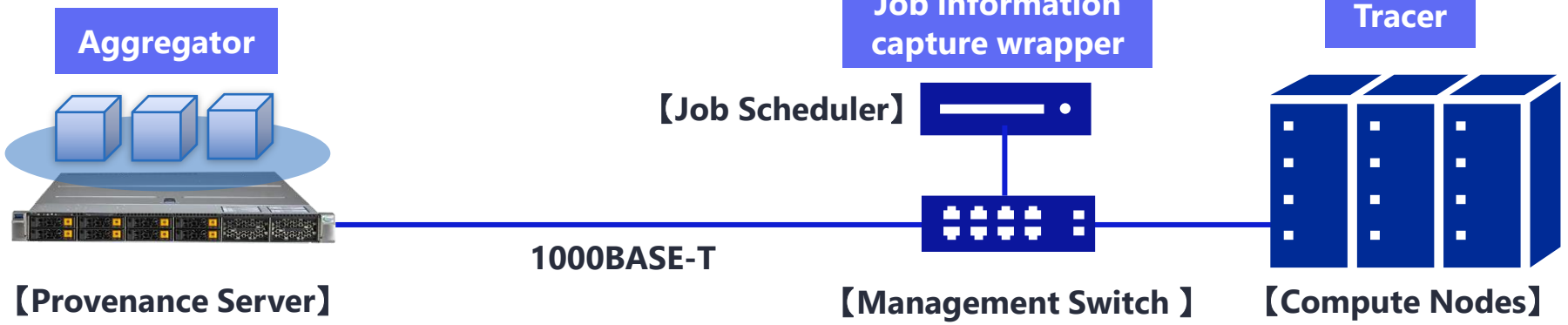
Deployment Plan

- Install Tracers on several to several dozen selected compute nodes of the existing HPC system
- Apply the wrapper to the job scheduler to capture job information
- Set up one evaluation Provenance server (VMs: Web & API Server, Primary DB Server, Provenance DB Server)

Testing Plan

- Test-run various actual jobs and verify the obtained provenance information
- Discuss possible use cases of the provenance information together, and consider incorporating your feedback into future product updates

- Virtual Servers -
・Web & API Server
・Primary DB Server
・Provenance DB Server



Conclusions

- NEC contributes to enhancing research capabilities by providing solutions that support the RII framework.
- We understand that many academic and research institutions are facing various challenges in research data management and the growing number of new computing users.
- DPS4HPC automatically visualizes the relationships between processes executed on HPC systems and their input/output data, contributing to the accountability and reproducibility of computational experiments.
- We would be happy to support you in addressing your specific research data management challenges through a PoC or collaborative research.

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