

WSSP41

# Enhancing Research with Provenance Management for HPC and AI Systems

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# Agenda

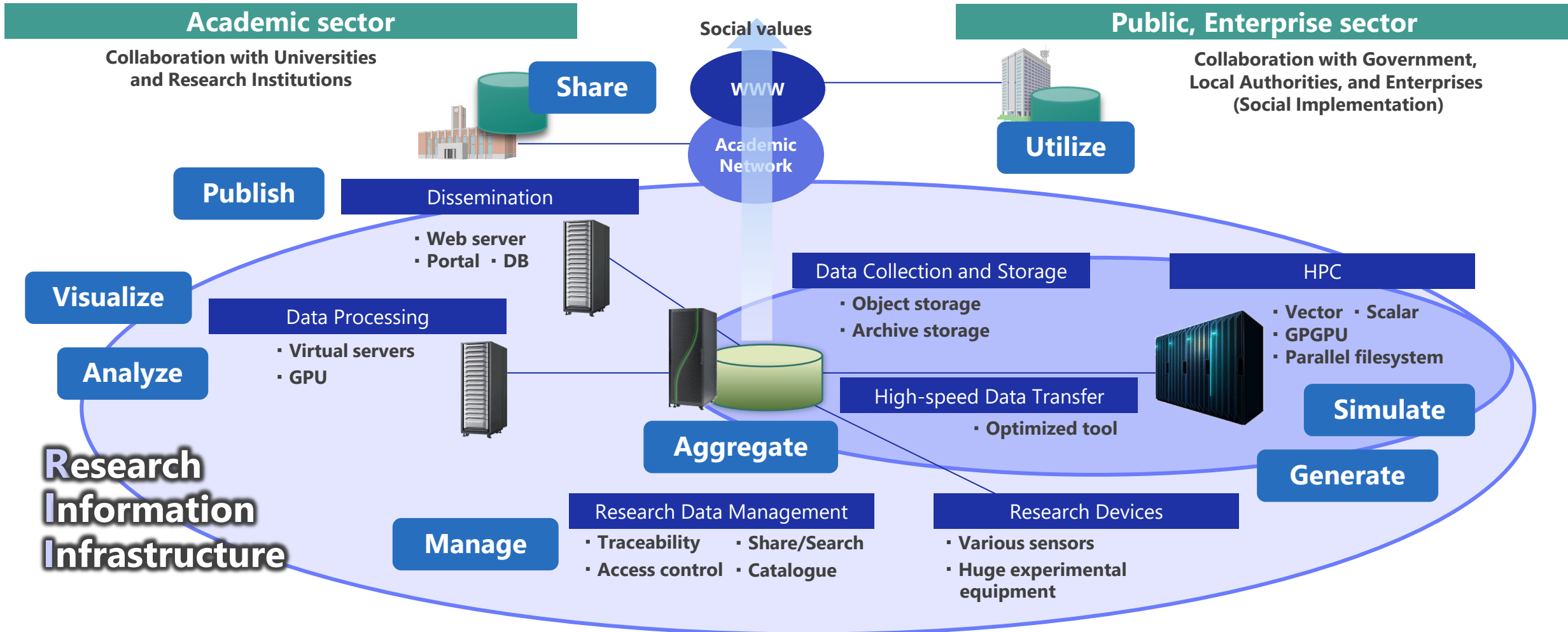
## 1. Overview of Research Information Infrastructure (RII)

## 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.

## Improvement of research capability (Academia)



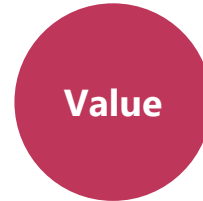
Increasing efficiency in research and paper preparation



Expanding research areas through collaboration



Ensuring research integrity



Value

## Solving social issues (Public, Enterprise)



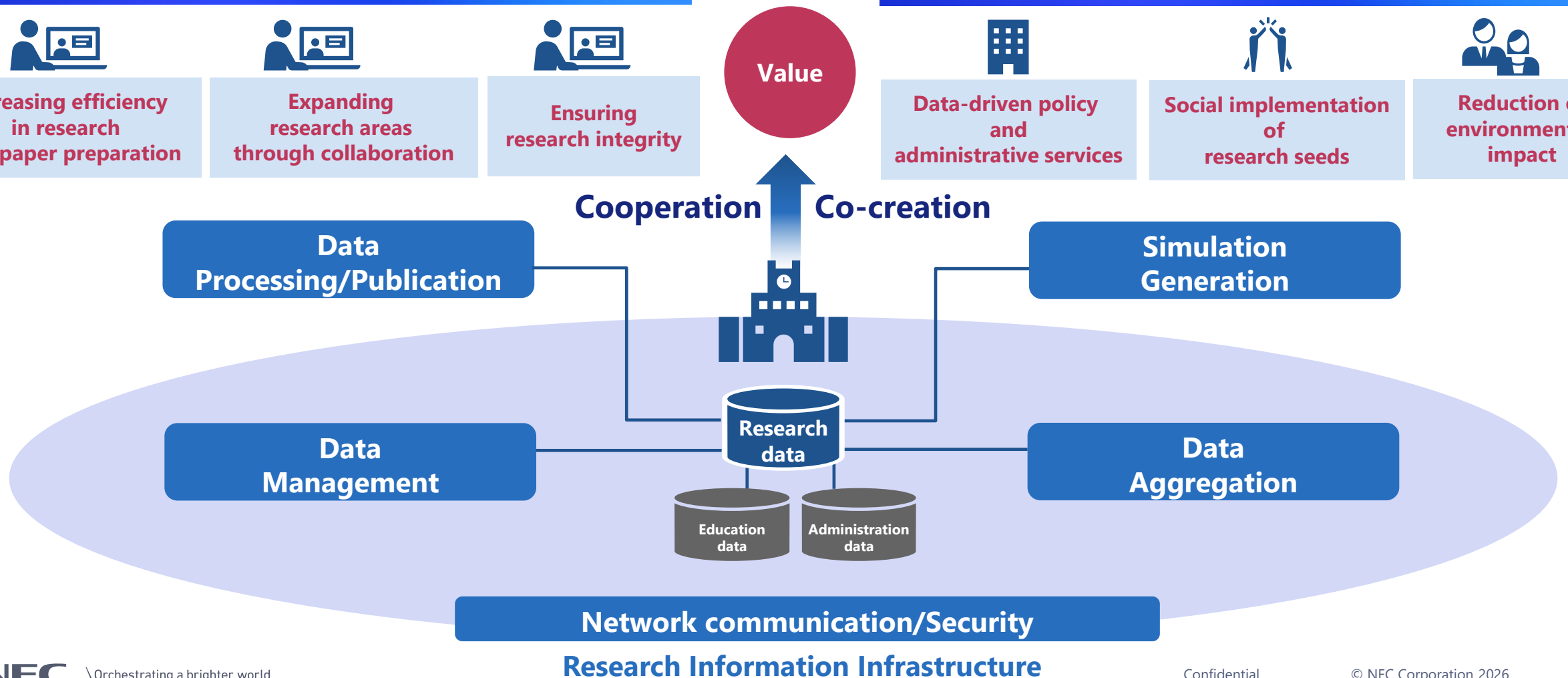
Data-driven policy and administrative services



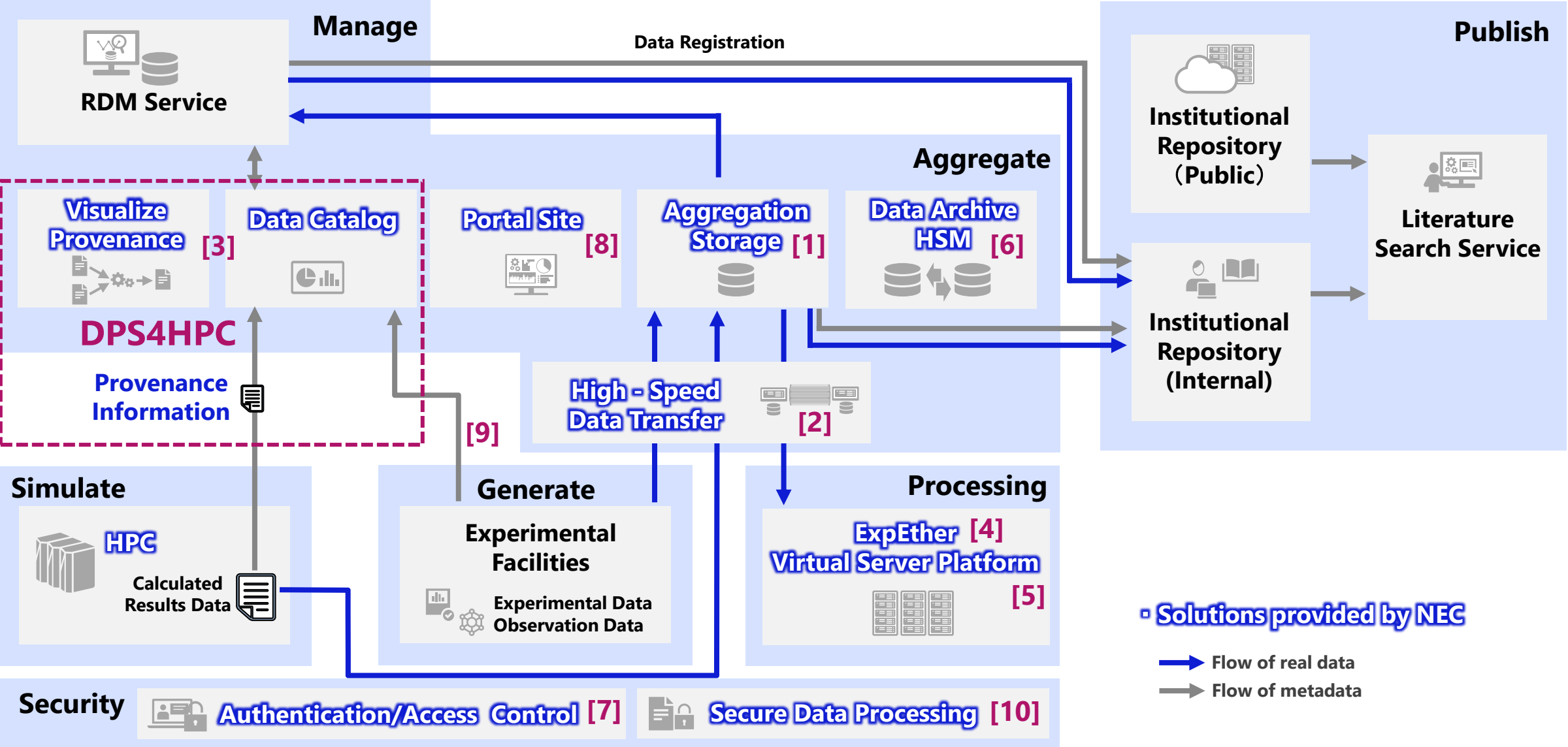
Social implementation of research seeds



Reduction of environmental impact



# Data Lifecycle and RII Solution Portfolio

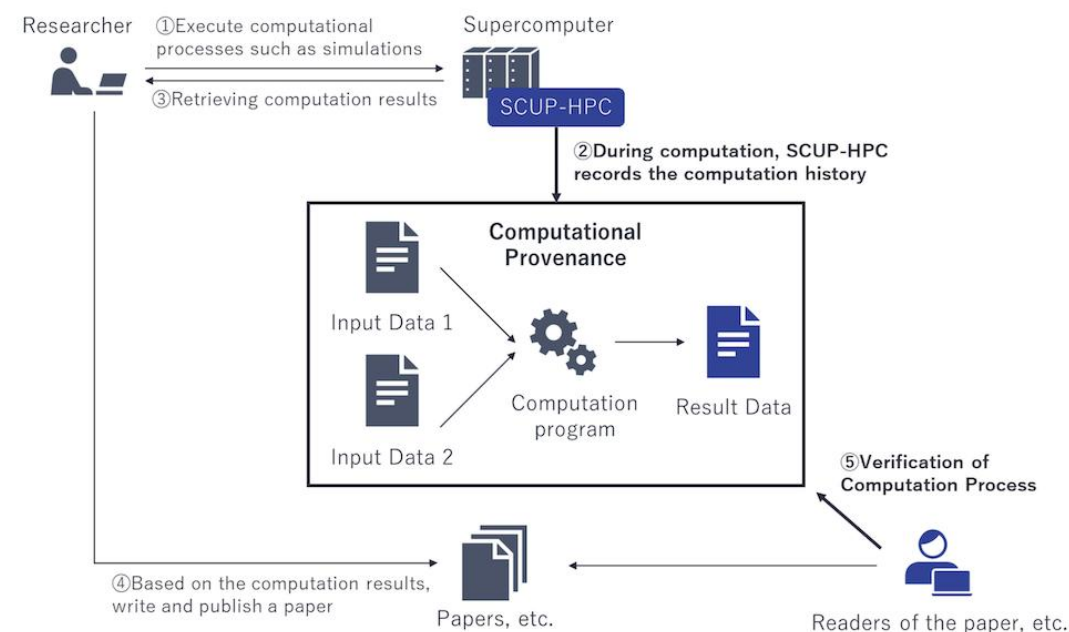


# Operation Start of NEW OCTOPUS at Osaka Uni. with DPS4HPC

■ 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)

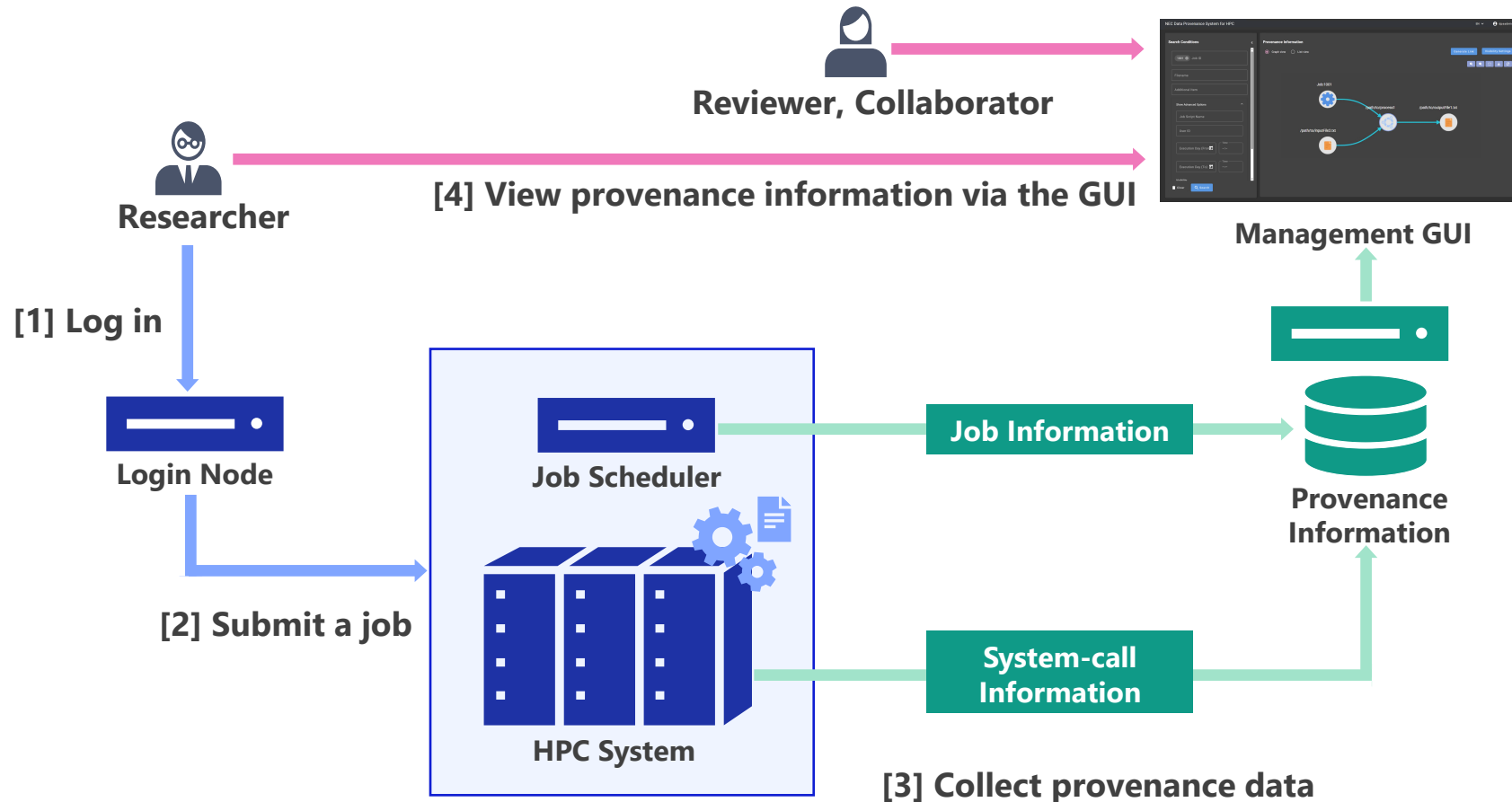
This SCUP-HPC allows researchers to record, manage and visualize computational provenance which contains the information on how data is accessed by what kind of program and what kind of data is generated. As the result, a new scientific computing concept named “Scientific Computing Unifying Provenance – 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

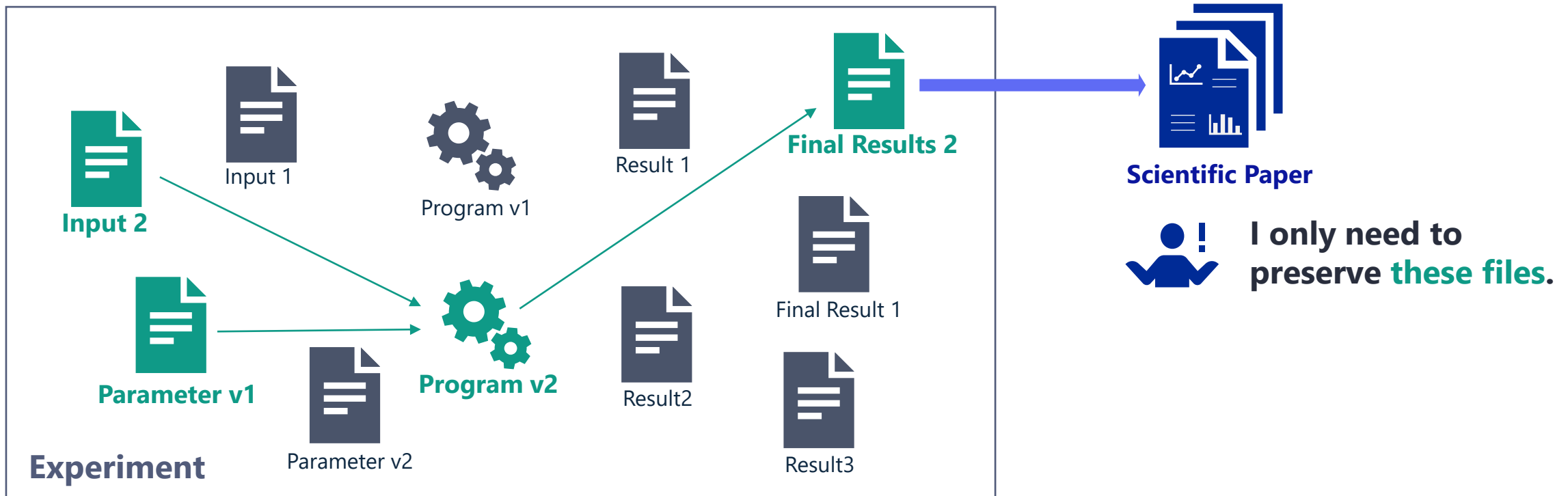
- Automatically records the provenance and metadata of a file generated in an HPC system — just by executing jobs as usual — without modifying the user's assets such as programs and scripts.



# Contribution to Reproducibility 1

## Identify research data and programs that should be preserved.

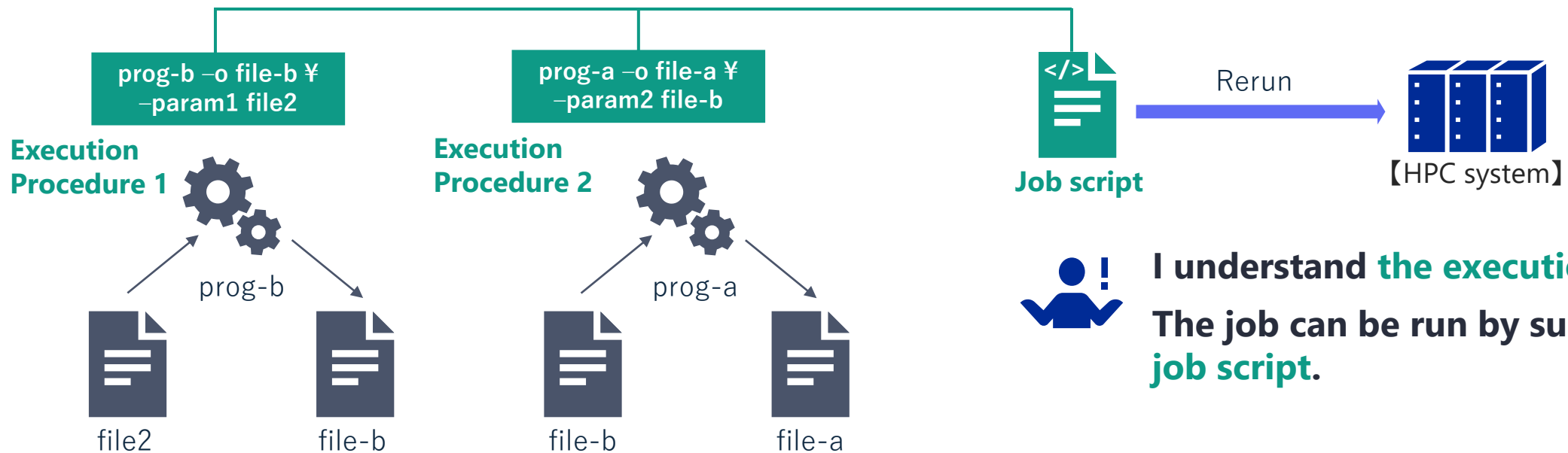
- In research, repeated experiments with modified programs and parameters often generate many similar files.
- Provenance shows which programs and input data were used to generate the final files.
- Helps identify and preserve only the truly necessary data.



# Contribution to Reproducibility 2

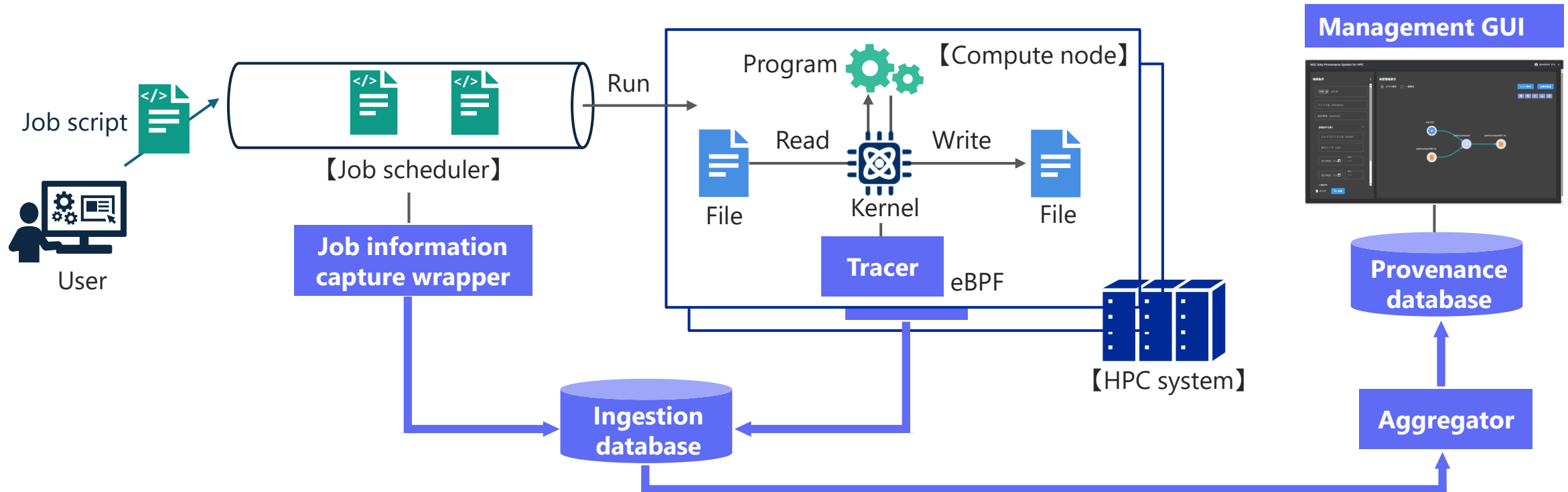
## Clarify the procedure for reproducing the experiment.

- 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



# 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.

NEC Data Provenance System for HPC

Search Conditions

1001 Job ID

Filename

Additional Item

Show Advanced Options

Job Script Name

User ID

Execution Day (From) Time

Execution Day (To) Time

Visibility

Clear Search

Provenance Information

Graph view List view

Generate Link Visibility Settings

Job:1001

/path/to/inputFile2.txt

/path/to/process1

/path/to/outputFile1.txt

**File Provenance Visualization**

NEC Data Provenance System for HPC

Provenance Information

Graph view List view

Generate Link Visibility Settings

Entities Relations

job				process									
job_id	filename	id	additem	id	pid	uid	euid	egid	path	host	args	parent	start
1001	inputFile2.txt	Job:1001		TEST_PROCESS_2	100	100	1001	2000	/path/to/process1	host1	arg1		2025/04/10
1001	outputFile1.txt	Job:1001		TEST_PROCESS_2	100	100	1001	2000	/path/to/process1	host1	arg1		2025/04/10

file												
host	args	parent	start	mpi	additem	id	uid	path	inode	host	additem	visibility
is1	host1	arg1	2025/04/10 14:14:03.366564442	false		TEST_INPUT_2	1	/path/to/inputFile2.txt	1000	host1		private
is1	host1	arg1	2025/04/10 14:14:03.366564442	false		TEST_OUTPUT_1	1	/path/to/outputFile1.txt	1000	host1		private

Items per page: 20 1 - 2 of 2

**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

The screenshot displays the NEC Data Provenance System for HPC Management GUI in Graph Mode. The interface is divided into two main sections: Search Conditions and Provenance Information.

**Search Conditions:** This section includes a search bar with the value "1001" and "Job ID" selected. Below it are input fields for "Filename" and "Additional Item". A "Show Advanced Options" toggle is visible, followed by input fields for "Job Script Name" and "User ID". There are also two date range pickers for "Execution Day (From)" and "Execution Day (To)", each with a "Time" dropdown set to "--:--". At the bottom, there are "Clear" and "Search" buttons.

**Provenance Information:** This section shows the provenance graph for Job: 1001. It includes a "Graph view" radio button (selected) and a "List view" radio button. There are buttons for "Generate Link" and "Visibility Settings". Below these are icons for search, zoom, pan, download, and refresh. The graph itself shows a central node (a gear icon) representing a process. It has two incoming arrows: one from a gear icon labeled "/path/to/process1" and one from a document icon labeled "/path/to/inputFile2.txt". It has one outgoing arrow to a document icon labeled "/path/to/outputFile1.txt".

# Management GUI (Graph Mode)

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

The screenshot displays the NEC Data Provenance System for HPC Management GUI in Graph Mode. The interface is divided into two main sections: Search Conditions and Provenance Information.

**Search Conditions:** This section includes a search bar with the value "1001" and "Job ID" selected. Below it are fields for "Filename" and "Additional Item". A "Show Advanced Options" section is expanded, showing fields for "Job Script Name", "User ID", "Execution Day (From)" with a time field "--:--", and "Execution Day (To)" with a time field "--:--". At the bottom, there are "Clear" and "Search" buttons.

**Provenance Information:** This section shows a graph view of the provenance information. The graph is centered around a process node labeled "/path/to/process100". It has several input files pointing to it: "/path/to/inputFile100\_1.txt", "/path/to/inputFile100\_10.txt", "/path/to/inputFile100\_100.txt", "/path/to/inputFile100\_11.txt", and "/path/to/inputFile100\_12.txt". From the process node, several output files are generated: "/path/to/outputFile100\_1.txt", "/path/to/outputFile100\_10.txt", "/path/to/outputFile100\_100.txt", "/path/to/outputFile100\_11.txt", and "/path/to/outputFile100\_12.txt". The graph is interactive, with buttons for "Generate Link", "Visibility Settings", and search icons.

# Management GUI (Metadata Details)

The screenshot displays the NEC Data Provenance System for HPC Management GUI. A modal window titled "Detailed Information" is open, showing the following metadata details:

Field	Value
id	TEST_PROCESS_2
pid	100
uid	100
eid	1001
egid	2000
path	/path/to/process1
host	host1
args	arg1
parent	
start	2025/04/10 14:14:03.366564442
mpi	false

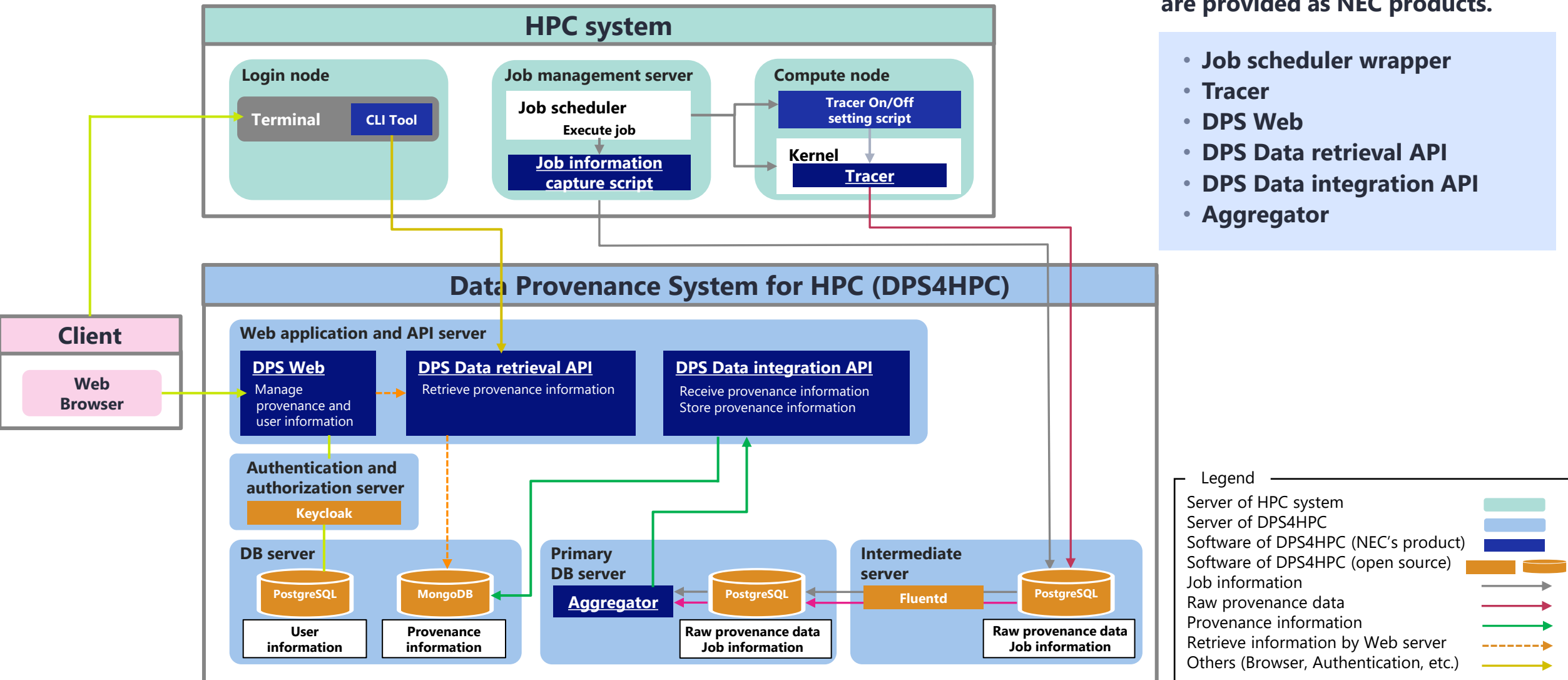
Below the table, there is a search input field containing the text "test" and a "更新" (Update) button. The modal also includes a "キャンセル" (Cancel) button at the bottom left.

The background interface shows a job execution flow diagram with a pink arrow pointing from a job node to the "Detailed Information" modal. The main interface includes sections for "追加情報 (additem)", "詳細条件を開く" (Expand detailed conditions), and "公開設定" (Public settings).

# 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



# System Components and Required Specifications

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

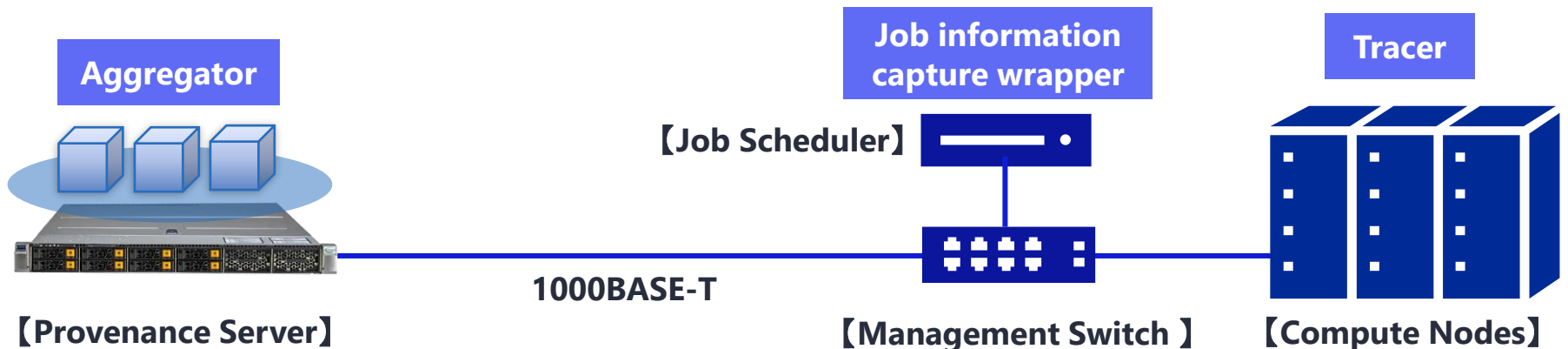
## Deployment Plan

- 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.

**NEC**

\Orchestrating a brighter world