EuroHPC Joint Undertaking

Federation Platform

https://my-eurohpc.eu

EFP Workflows

Martin Golasowski (IT4Innovations, VSB - TU Ostrava)

26th October 2026

VSB TECHNICAL UNIVERSITY OF OSTRAVA | IT4INNOVATIONS NATIONAL SUPERCOMPUTING CENTER

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Agenda

1. EuroHPC Federation Platform introduction
2. EFP Workflows overview
3. Demo with custom jobscript with GROMACS, MPI and EESSI
4. Complex workflows overview
5. Q&A Session

The EuroHPC Federation Platform (EFP)

"A one-stop-shop for accessing and utilizing EuroHPC systems and services"

A platform and federation framework which provides **a streamlined, single point of onboarding** and via which user can **access all systems and services** available to them in the EuroHPC ecosystem.

Direct access | Interactive interfaces | Programmatic APIs | Unified software stack

EuroHPC Joint Undertaking

Federation Platform

EFP Main Features



Federated identity and Single-Sign-On (SSO)

Users utilize the same login and identity (e.g. granted via their home institution or national identity provider) to authenticate to all services and systems. Process for onboarding Industry.



Resource allocation, management and monitoring across systems

Users can view and manage their allocations and project members across all systems using a single interface.



Interactive web-based usage

with e.g., remote desktop, command line, AI training monitoring and Jupiter notebooks. Ability to launch batch jobs and browse files on the supercomputers.



Federated software catalogue

providing a pre-installed pseudo-uniform software stack on all systems. Advanced discoverability features for available software.



Advanced workflows and data transfer

Workflow execution and data transfers across systems, along with smart scheduling capabilities and high-level graphical interfaces for creating and managing workflows.



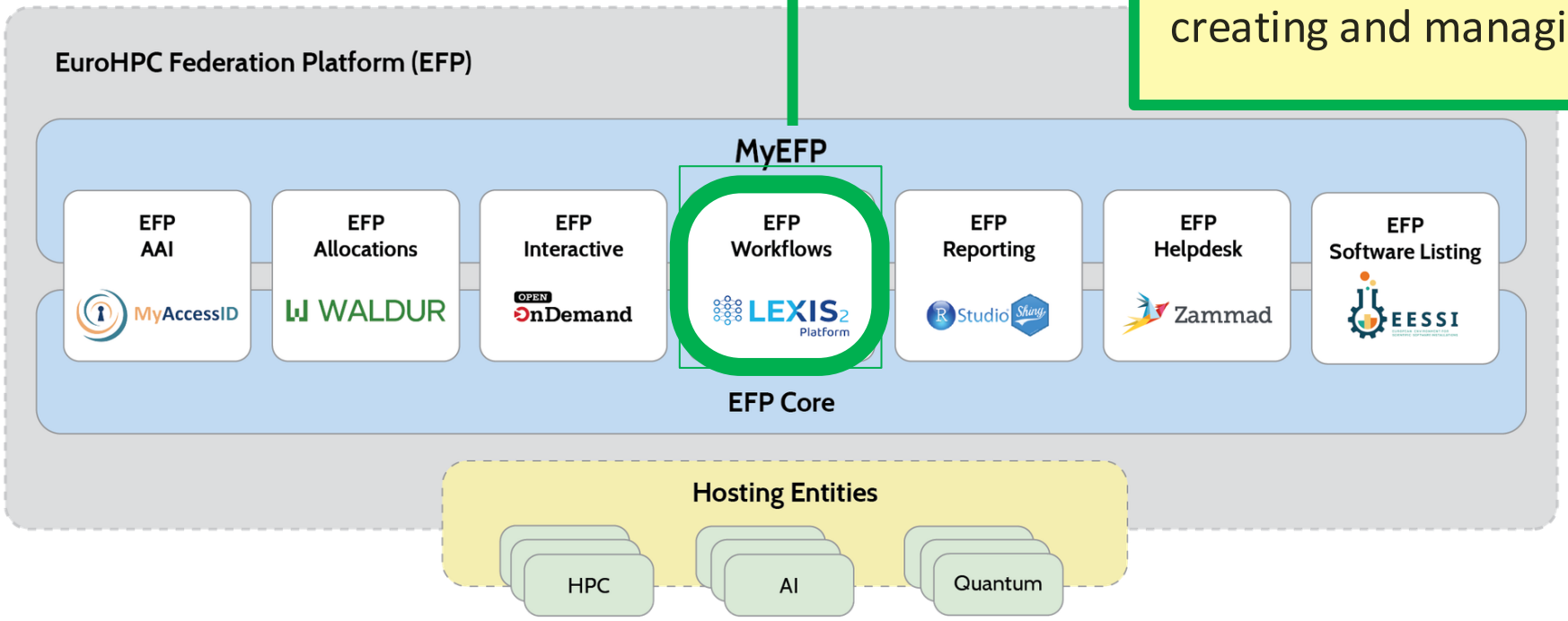
Direct access utilizing SSH certificates

Short lived certificates which are obtained via a login flow with Multi-Factor Authentication (MFA) for increased security.

EFP Architecture

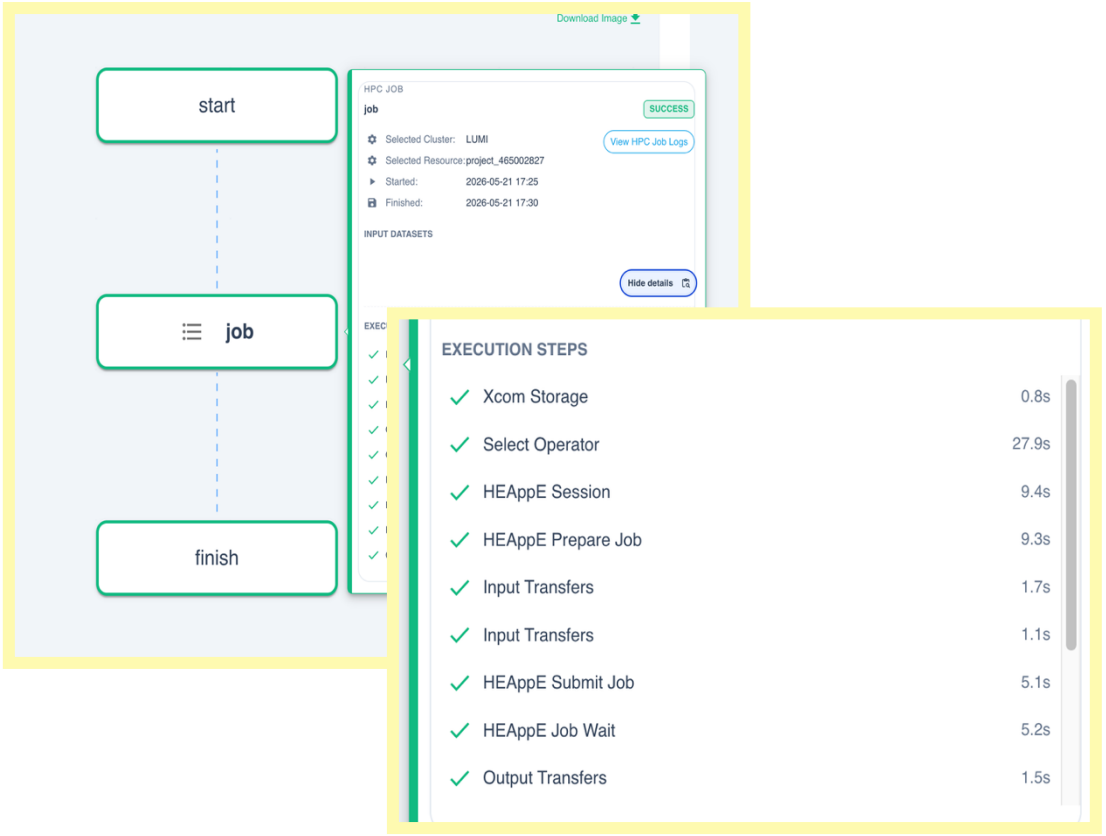
Advanced workflows and data transfer

Workflow execution and data transfers across systems, along with smart scheduling capabilities and high-level graphical interfaces for creating and managing workflows.



EFP Workflows – a way for Easy and Safe Supercomputing

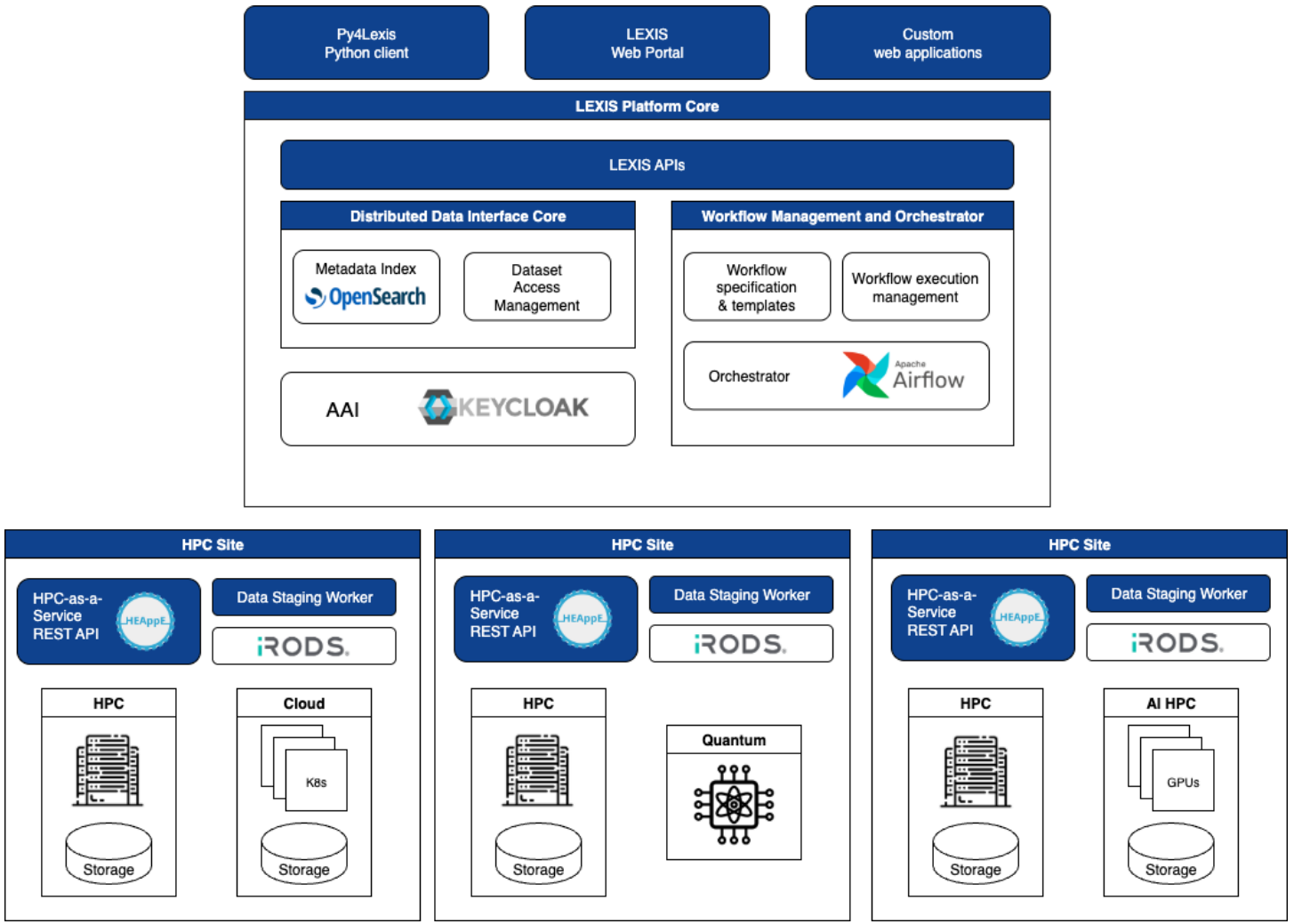
- Run your **job scripts, containers** or use a **local workflow** (e.g. CWL, HyperQueue) from a web interface
- Use **your EuroHPC allocations** across multiple systems from a single place
- **Automated data staging** to job's execution directory and straightforward dataset management
- Define and run **custom workflows** across multiple systems using **visual workflow builder** and **YAML syntax**
- Python **CLI** and **API** access included



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www.lexis.tech

LEXIS 2 Platform

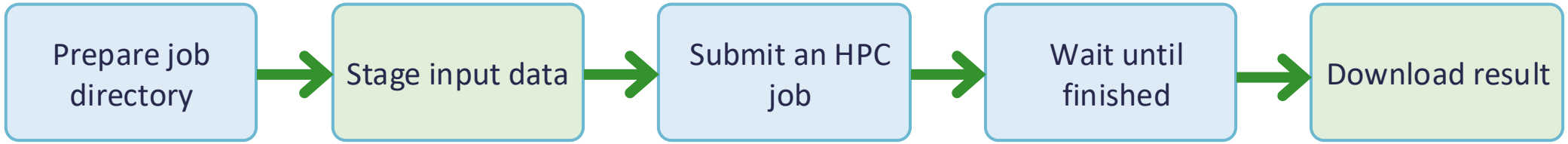
The LEXIS Platform in context of the EFP Workflows



- **Hiding** of technical and **operational differences** across systems
- **HPC & Cloud** service providers, Data providers
- Unified & distributed **workflow & data management**
- Connected to the **EFP Allocations**
- Workflow tasks can use the **EESSI modules** as part of the EFP Federated Software Catalog (e.g. GROMACS)
- **Connected to federated Authentication & Authorization** Infrastructure (MyAccessID)
- **Smart Scheduling capabilities** will be available in the next EFP release

How to run a simple HPC workflow

1. Upload your input data
2. Create your jobscript or upload a container
3. Create workflow
4. Run it
5. View results and logs

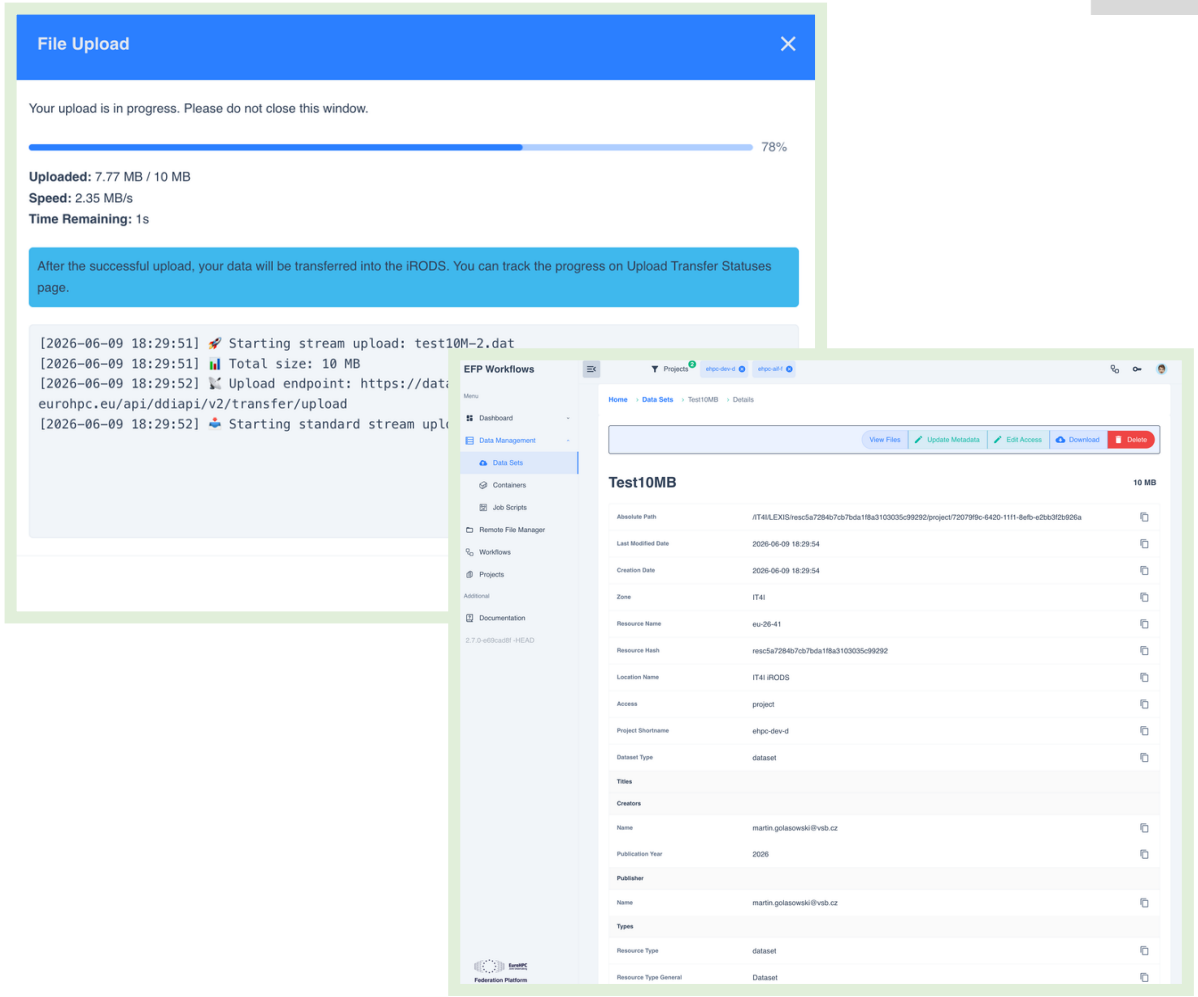


Simple HPC workflow steps

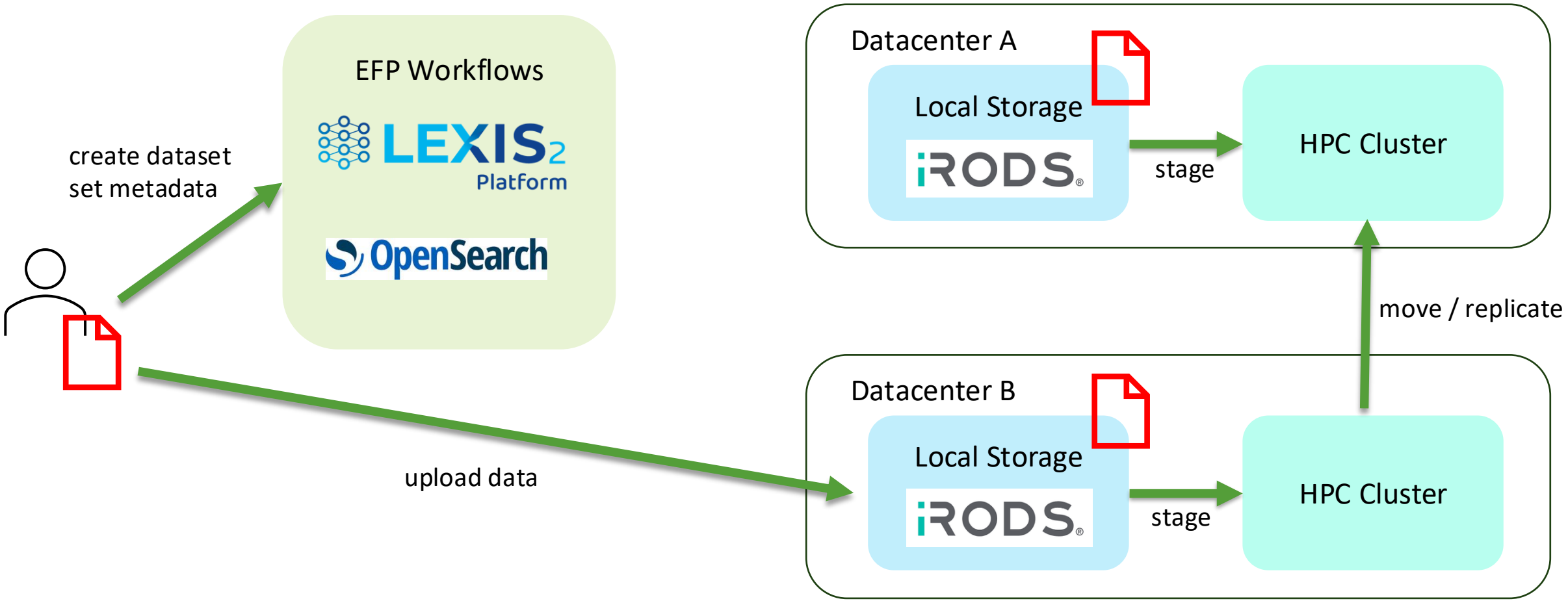
Data management in EFP Workflows

- **Datasets with metadata**
  - **Stored in object storage at the target site**
  - **Centralised metadata index**
- **File management on HPC clusters**
  - **Directly manage files on scratch**
- **HTTP/2 Upload / Download via**
  - **Web browser**
  - **Python CLI**
- **Automated data staging in workflows**
- **Access as part of compute time allocation,**

  quota differs per center
  - **Bulk copy between allocations and systems**



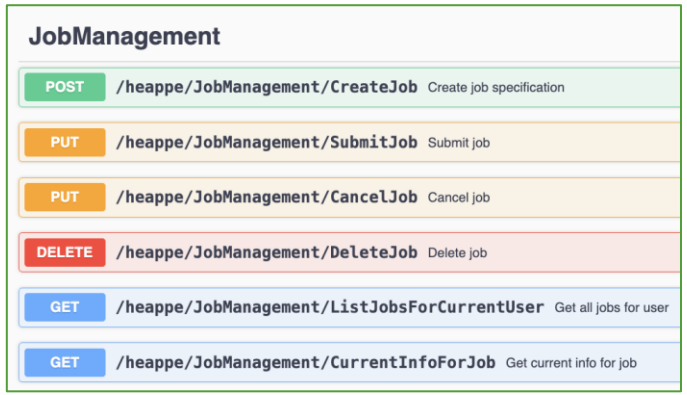
Where is my data?



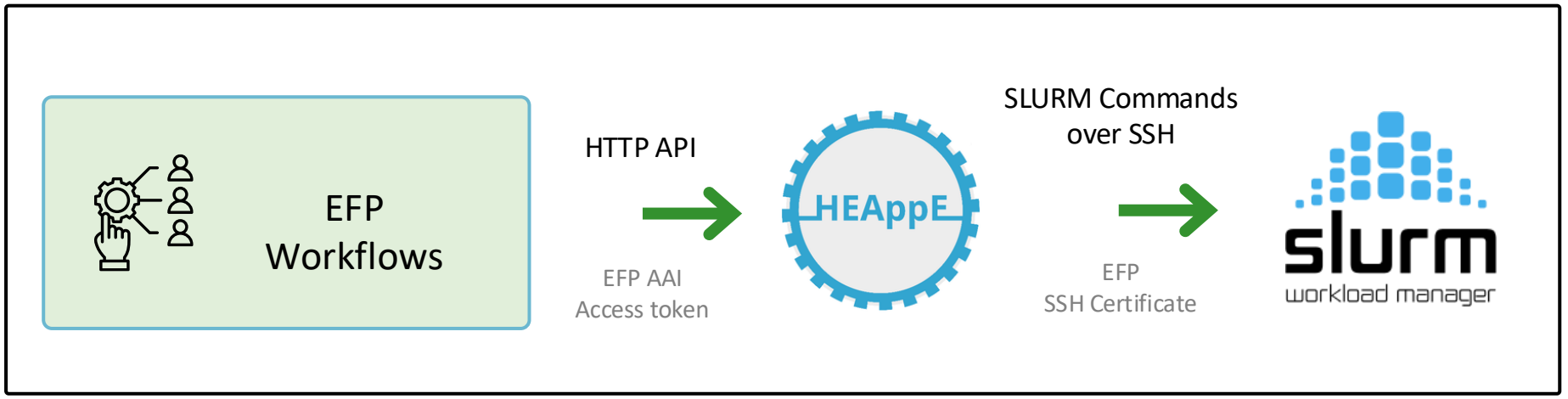
Job Management in EFP Workflows with HEAppE

High-End Application Execution Middleware (HEAppE)

- Unified HTTP API across HPC sites connected to common EFP AAI
- Abstraction of job lifecycle (prepare, execute, monitor, clean-up)
- Templated job scripts - command templates
- Job logs and audit trail never leaves the target site infrastructure
- Works only in user space - non-intrusive integration with HPC sites

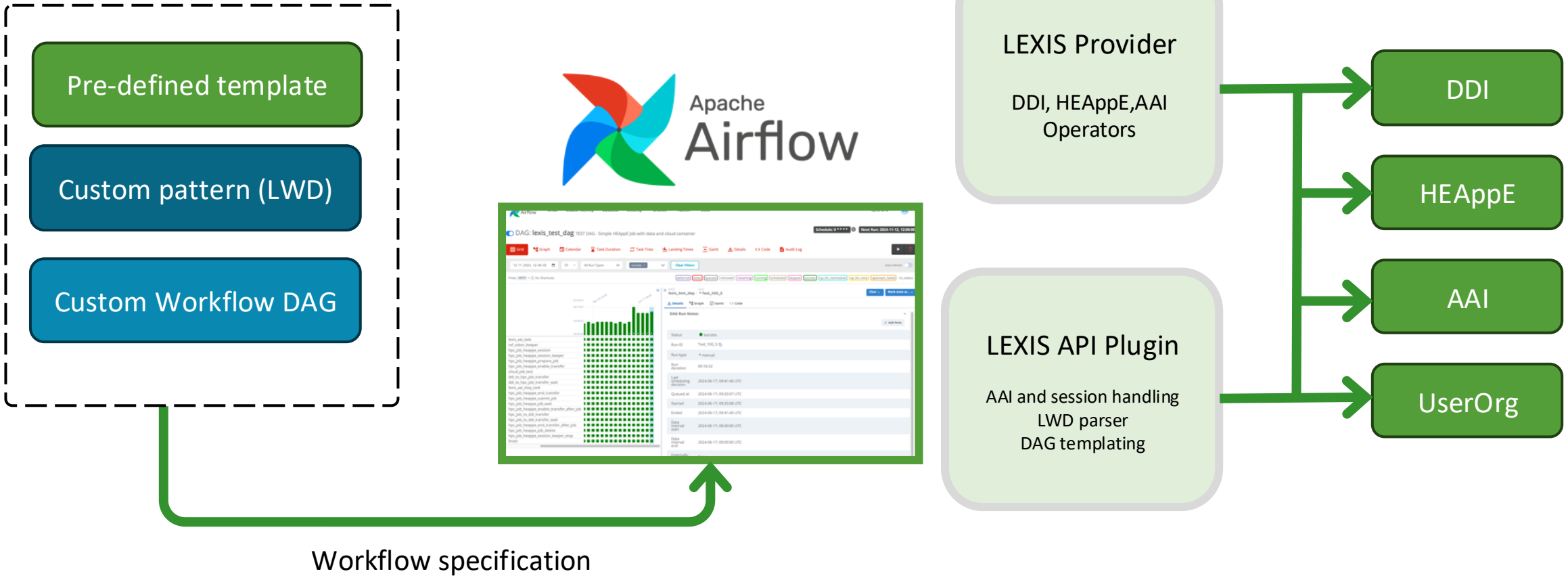


Part of the HEAppE API



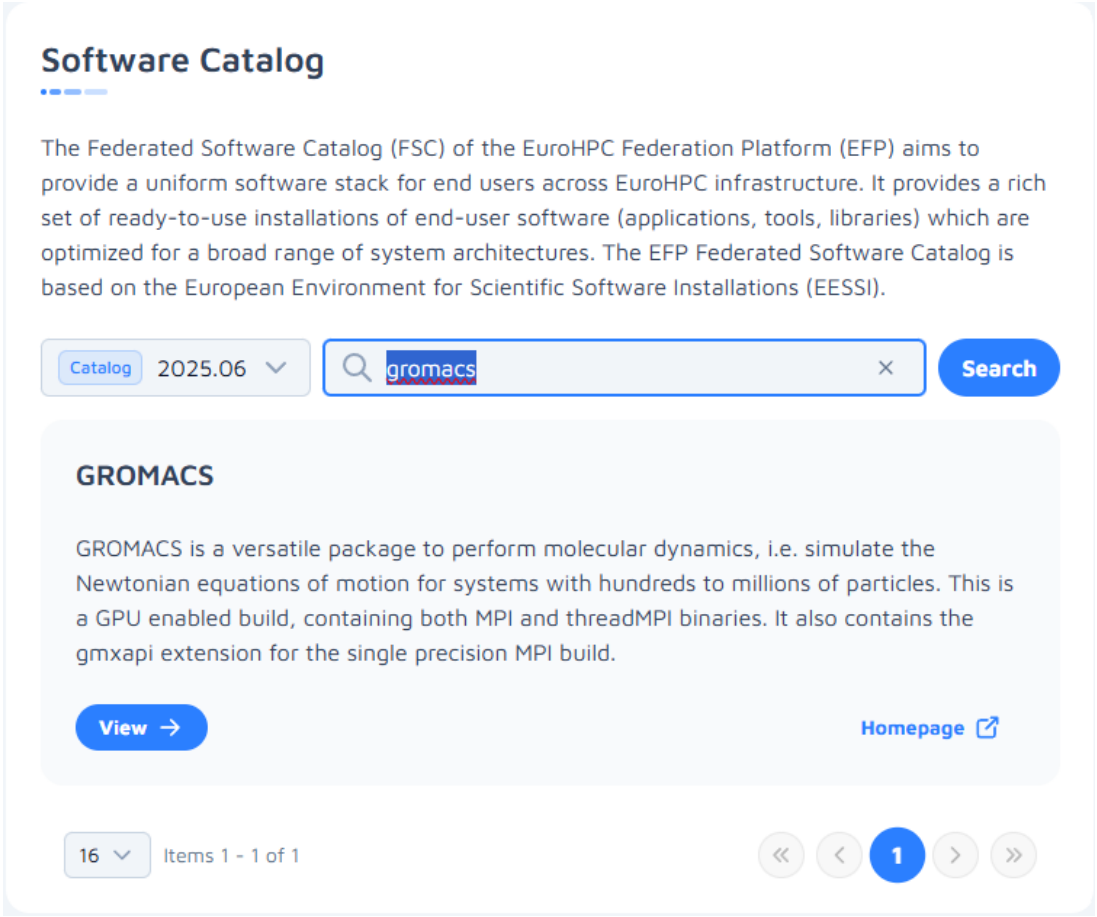
Visit HEAppE web
https://heappe.eu

Apache Airflow in LEXIS Platform



Software Catalog

- Curated software catalog powered by EESSI **available on all EuroHPC systems**
- Aim is to never compromise performance for portability
- Powers apps of EFP Interactive component
- Access mechanism can vary by site, see documentation
- https://my-eurohpc.eu/software-catalog



Let’s simulate some proteins in GROMACS

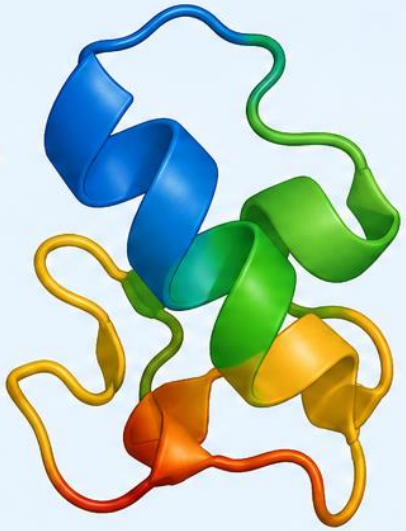
Crambin

A very small protein from the seeds of Crambe abyssinica (Abyssinian cabbage), a plant related to mustard and rapeseed.

- 46 amino acids
- ~20,000 atoms (with solvent)
- Small, stable and well known structure
- Convenient test system for molecular simulations



Crambe abyssinica (Abyssinian cabbage)



3D structure of Crambin (46 amino acids)

Molecular dynamics

Atoms move, vibrate and interact over time according to physical forces.



Time (1,000 steps)

What the benchmark does

Simulates the movement and interactions of all atoms in the crambin protein using molecular dynamics (GROMACS).

Calculates 1,000 time steps, following the laws of physics.

Distributed across multiple compute nodes, with MPI parallelization, to demonstrate that GROMACS runs correctly in a multi-node HPC environment.

Parallel execution on HPC



Verifies correct multi-node execution

Demonstrates parallel computing

Useful test case before larger simulations

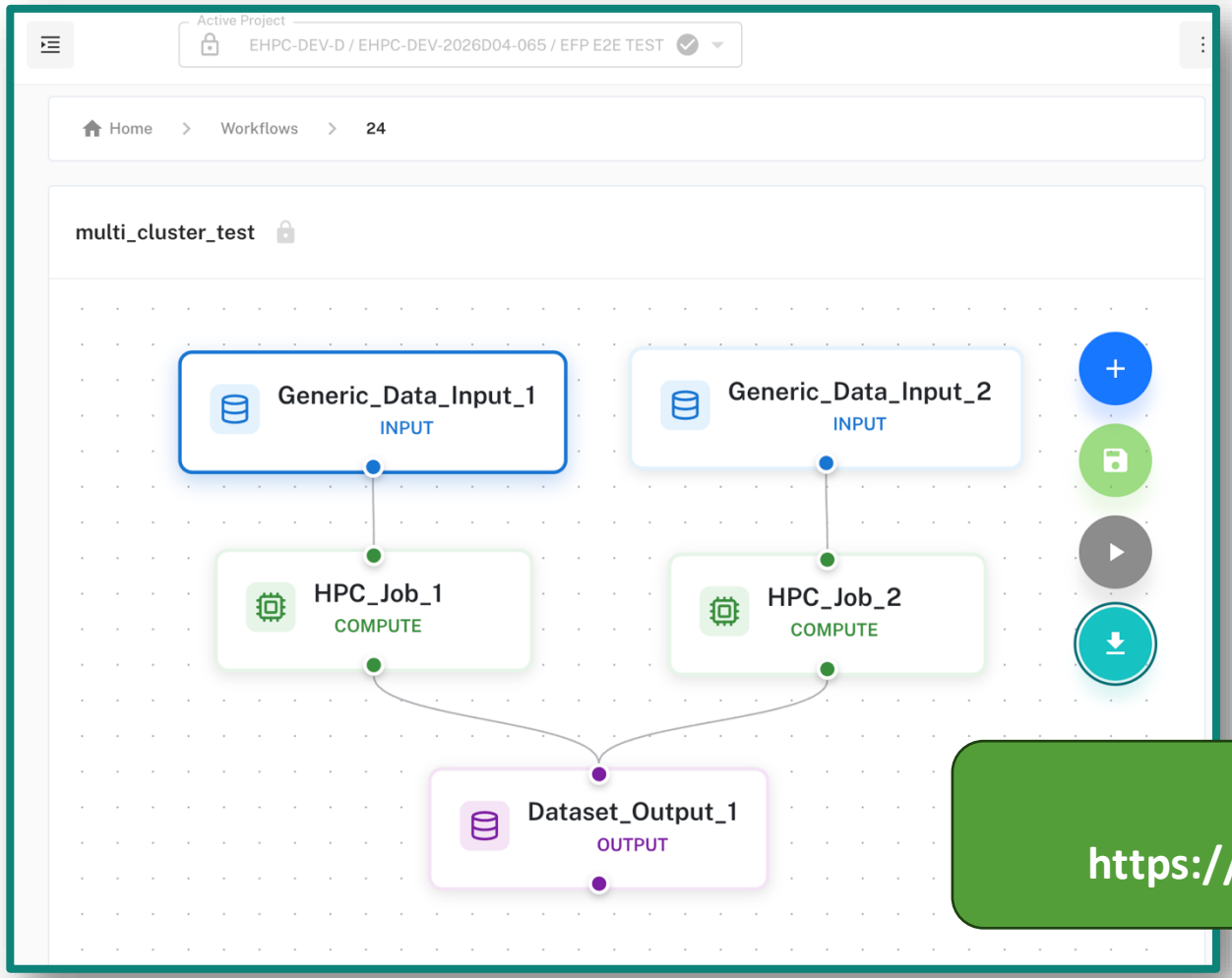
FAST. FLEXIBLE. FREE. GROMACS

LEXIS2 Platform

EESSI EUROPEAN ENVIRONMENT FOR SCIENTIFIC SOFTWARE INSTALLATIONS

Custom workflows

Graphical builder



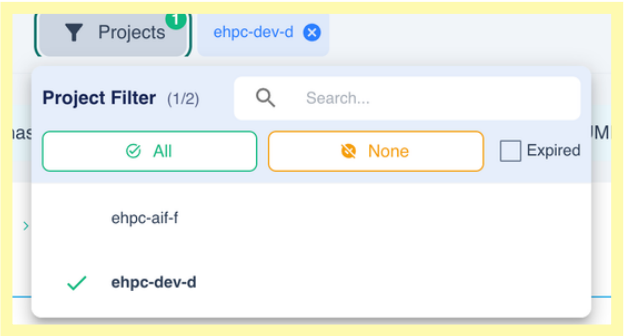
LEXIS Workflow Description (LWD)

```
id: ehpc-dev-d_multi_cluster_test
desc: Workflow generated from Builder  application
project_shortname: ehpc-dev-d
jobs:
  HPC_Job_1: ⋯
  HPC_Job_2:
    requirements:
      command_template_name: TestTemplate
      node_type_name: debug
      locations:
        - location_name: LUMI
          location_resource: project_465002827
      walltime_limit: 400
      max_cores: 10
      template_parameters:
        inputParam: Hello from LUMI
      environment_variables: {}
    data_inputs:
      - source: ddi://1af11ada-64cf-11f1-8efb-e2bb3f2b926a/
        target: /
    data_outputs:
      - source: /output
        metadata:
          $name: Dataset_Output_1
          title: TEST_Output_from_all
          ccess: project
          : ddi://~/
          e:
          urce: project_465002827
          tion: LUMI iRODS
  start_date: "2026-10-25T17:54:15.389Z"
  catchup: false
```

See https://docs.lexis.tech

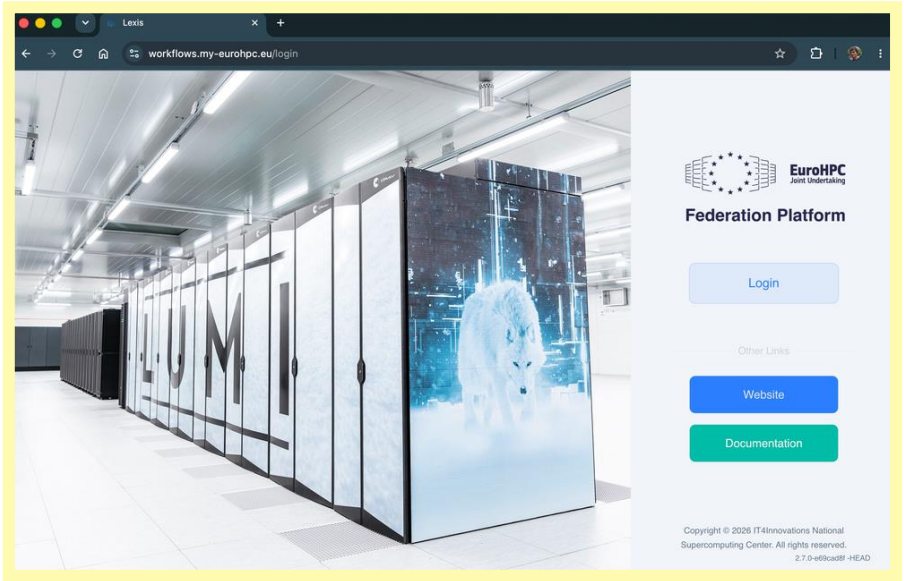
Accessing the EFP Workflows

Your EuroHPC allocation will automatically appear in EFP Workflows as a project



Visit main web interface at:

https://workflows.my-eurohpc.eu



Check the documentation at

https://docs.my-eurohpc.eu/workflows/overview

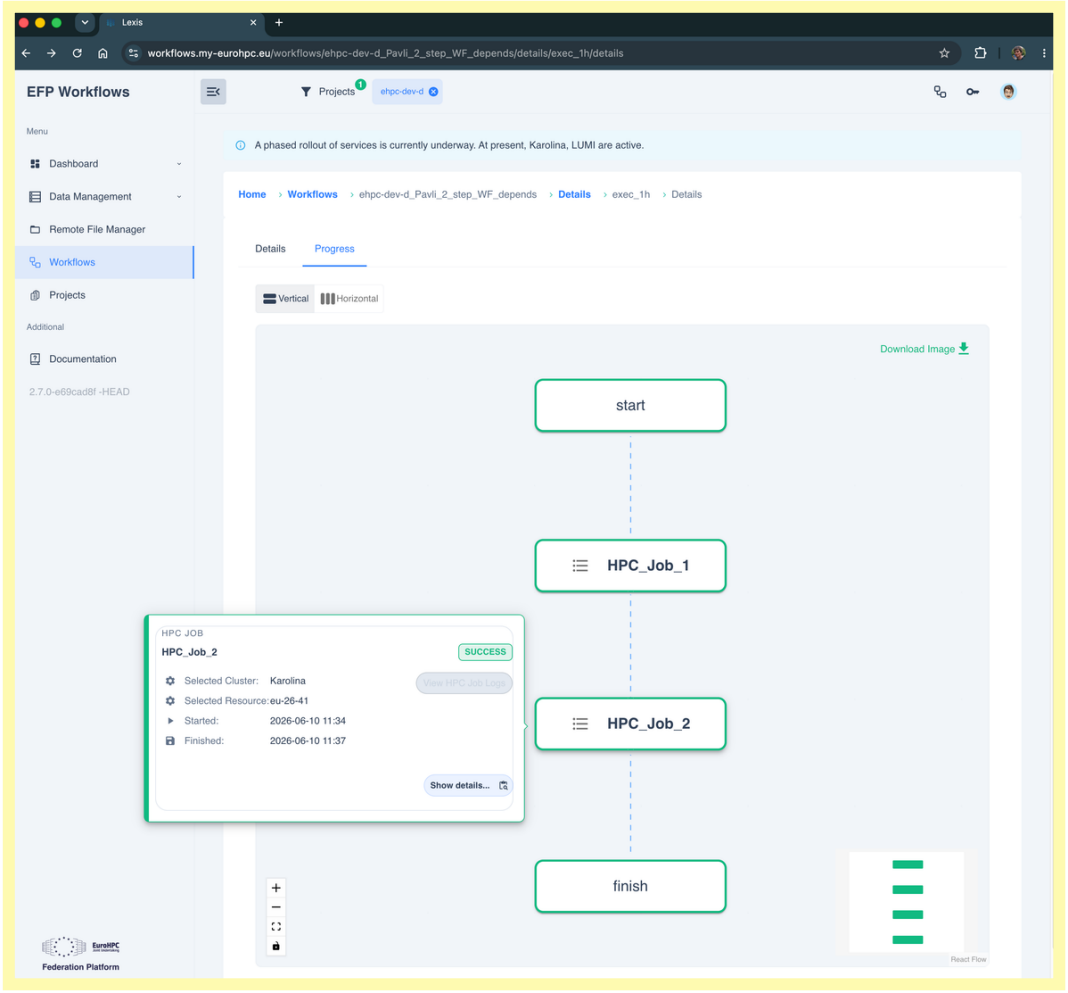
https://docs.lexis.tech

Getting help for EFP Workflows

Contact EFP Helpdesk at: helpdesk@my-eurohpc.eu

We can help you with

- **Managing your data in EFP Workflows**
- **Onboarding your applications**
- **Defining custom workflow patterns**
- **… and many more**



EFP webinars

Initial series of 5 webinars introduction the EuroHPC Federation Platform (Feb-June 2026) - **Recordings are available: https://docs.my-eurohpc.eu/training**

New series of webinars scheduled for October 2026:

Mon 5 Oct 2026, 14:00 CEST — **Introduction to the EuroHPC Federation Platform (EFP)**
*speaker: Alberto Lanzanova (CSC - IT Center for Science) – **RECORDING AVAILABLE***

Mon 12 Oct 2026, 14:00 CEST — **Getting Started with EFP: Registration and On-Boarding**
*speakers: Josh Howlett (GÉANT), Ahti Saar (University of Tartu) – **RECORDING AVAILABLE***

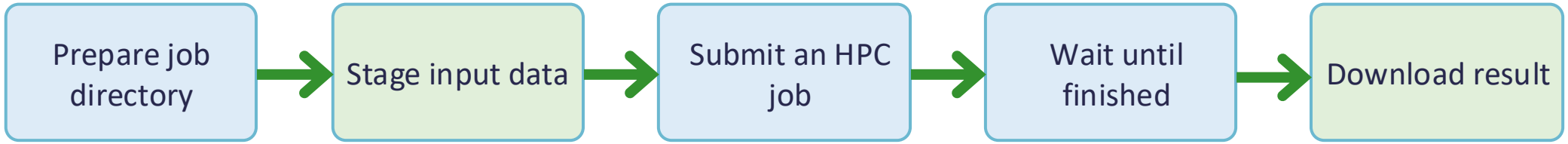
Mon 19 Oct 2026, 14:00 CEST — **EFP Features Showcase: Managing projects, direct SSH, federated software catalog, interactive web interface**
speaker: Alan O'Cais (Ghent University)

Mon 25 October 2026, 14:00 CET — **EFP Workflows: use cases**
speaker: Martin Golasowski (IT4Innovations)

Scan for more information on the EFP webinars!

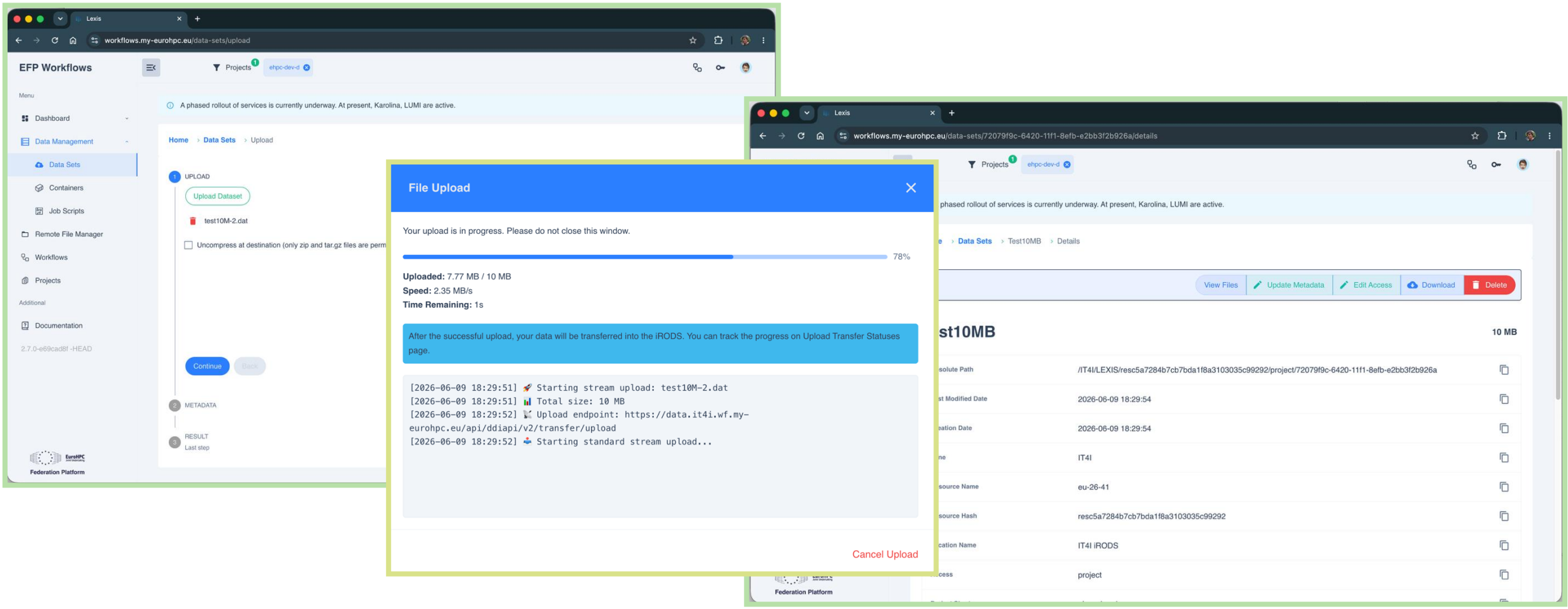
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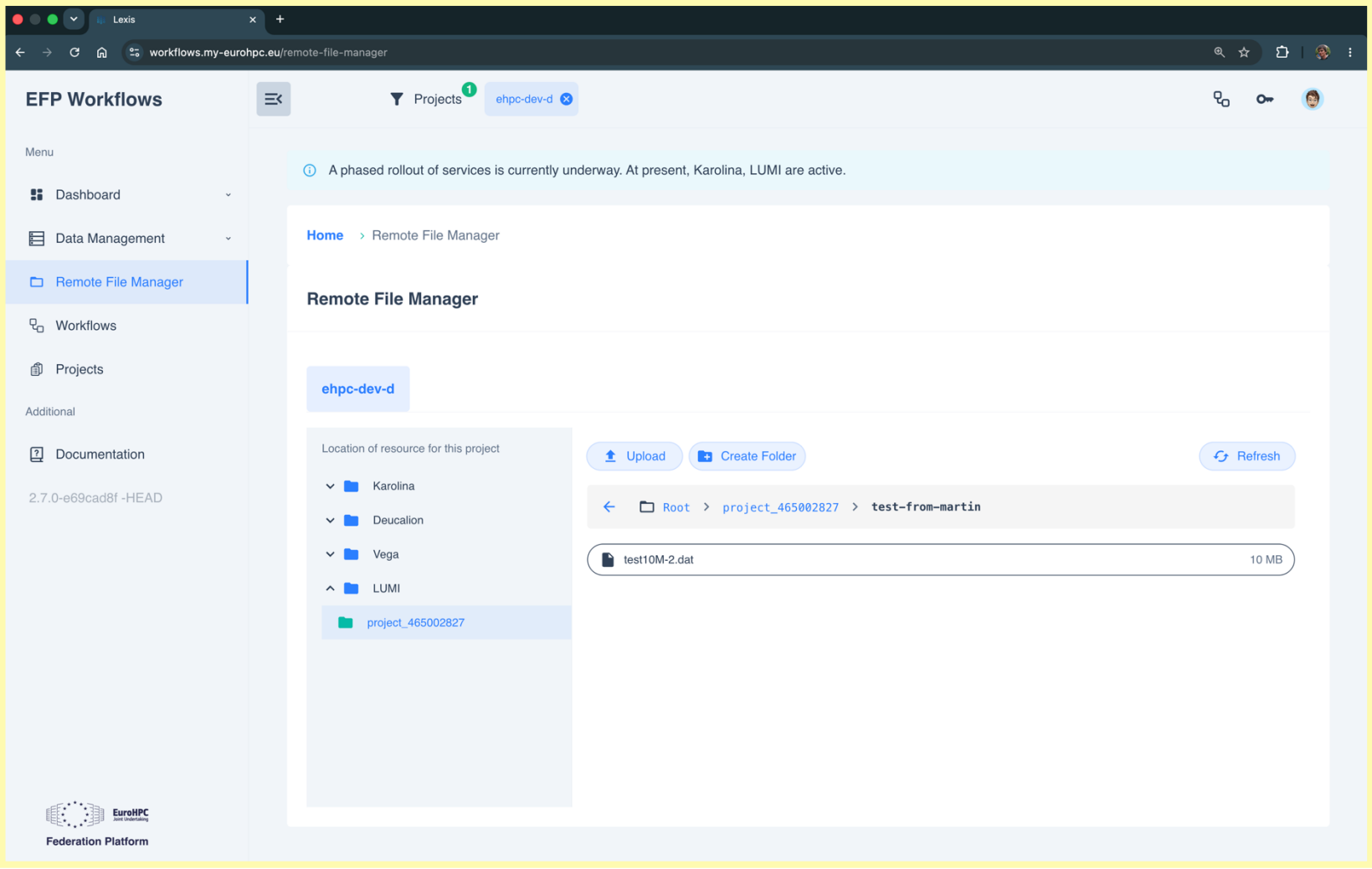


Simple HPC workflow steps

Step 1a. Upload input dataset with metadata

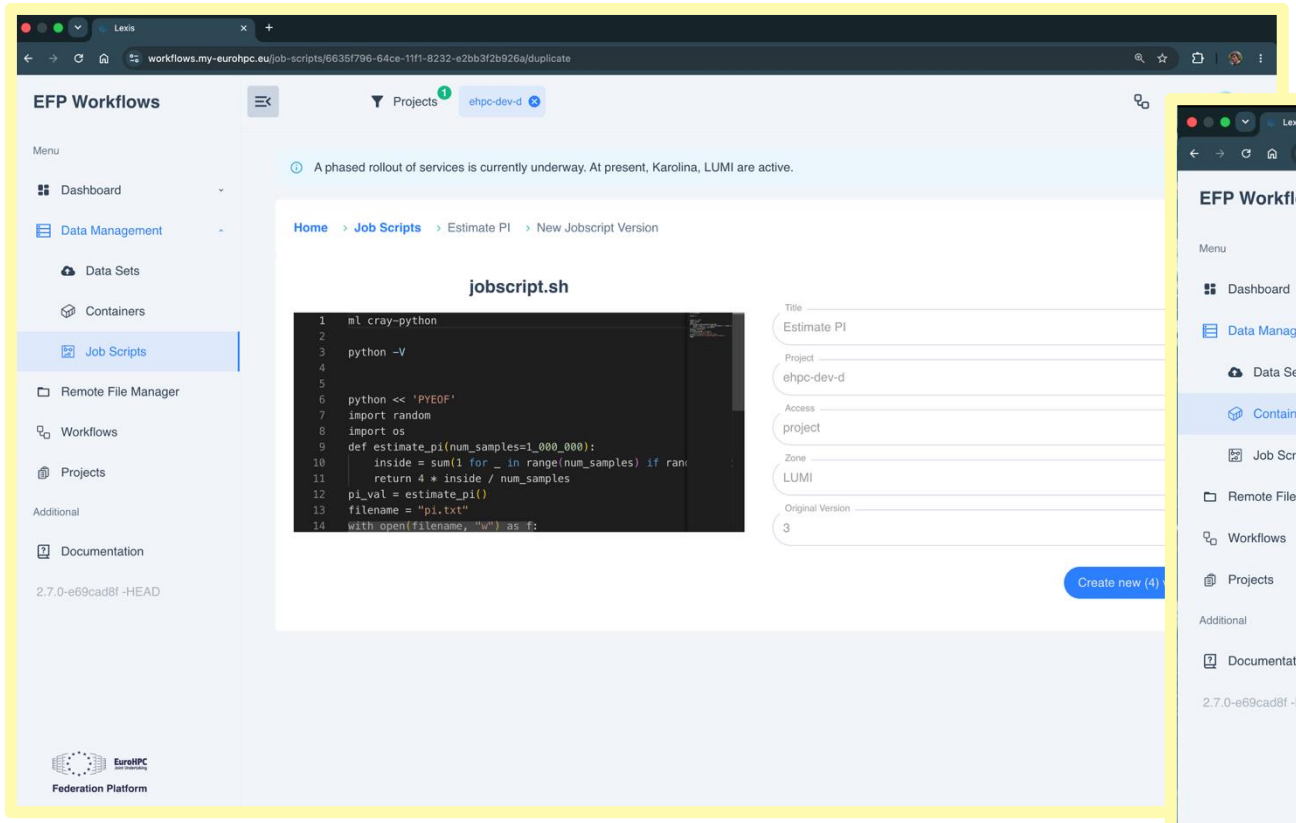


Step 1b. Upload data directly to HPC cluster

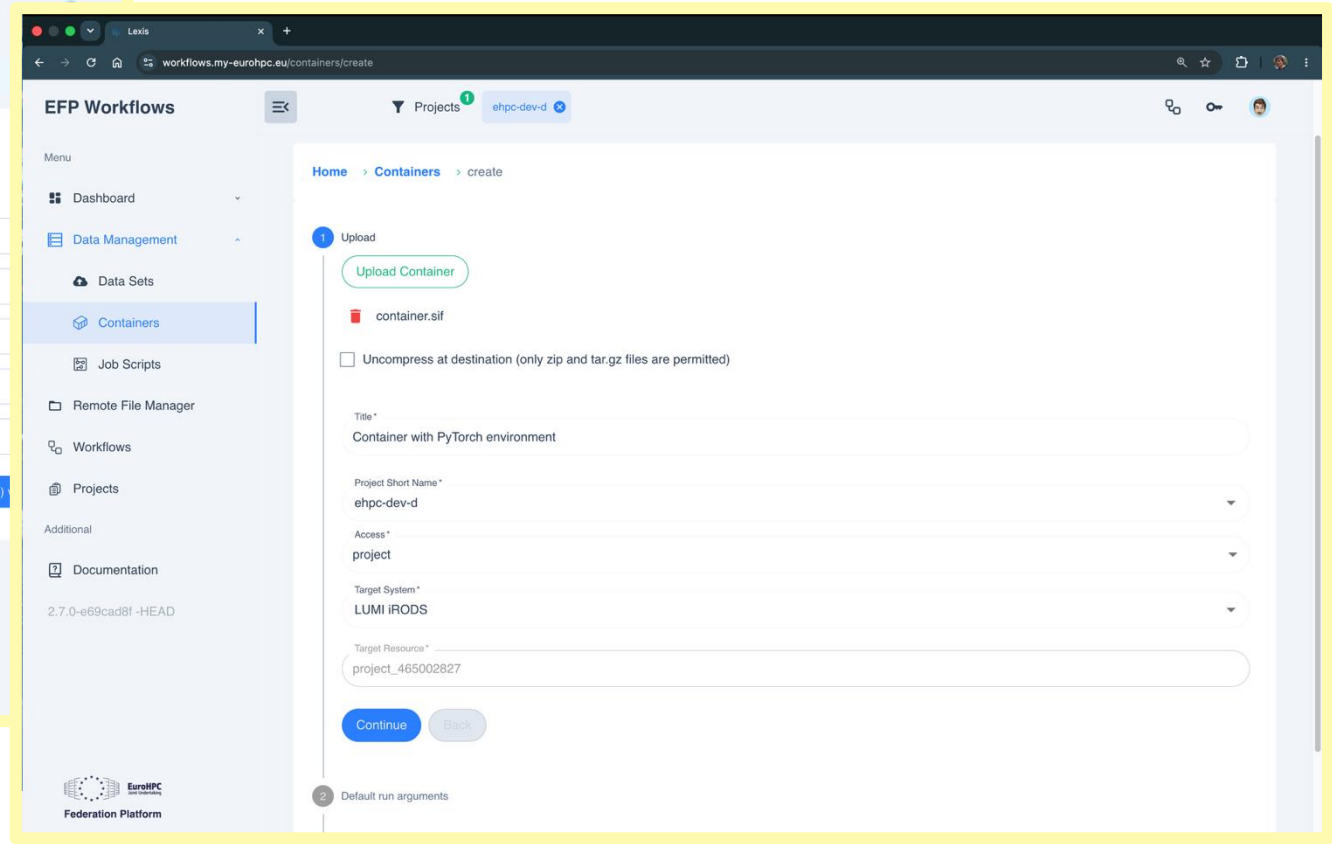


- Use direct upload and download to the HPC cluster
- Access to a directory assigned to the allocation (scratch) via web UI
- Based on HTTP/2 streaming API
- Bulk data copy between clusters included

Step 2. Create a job script or upload a container

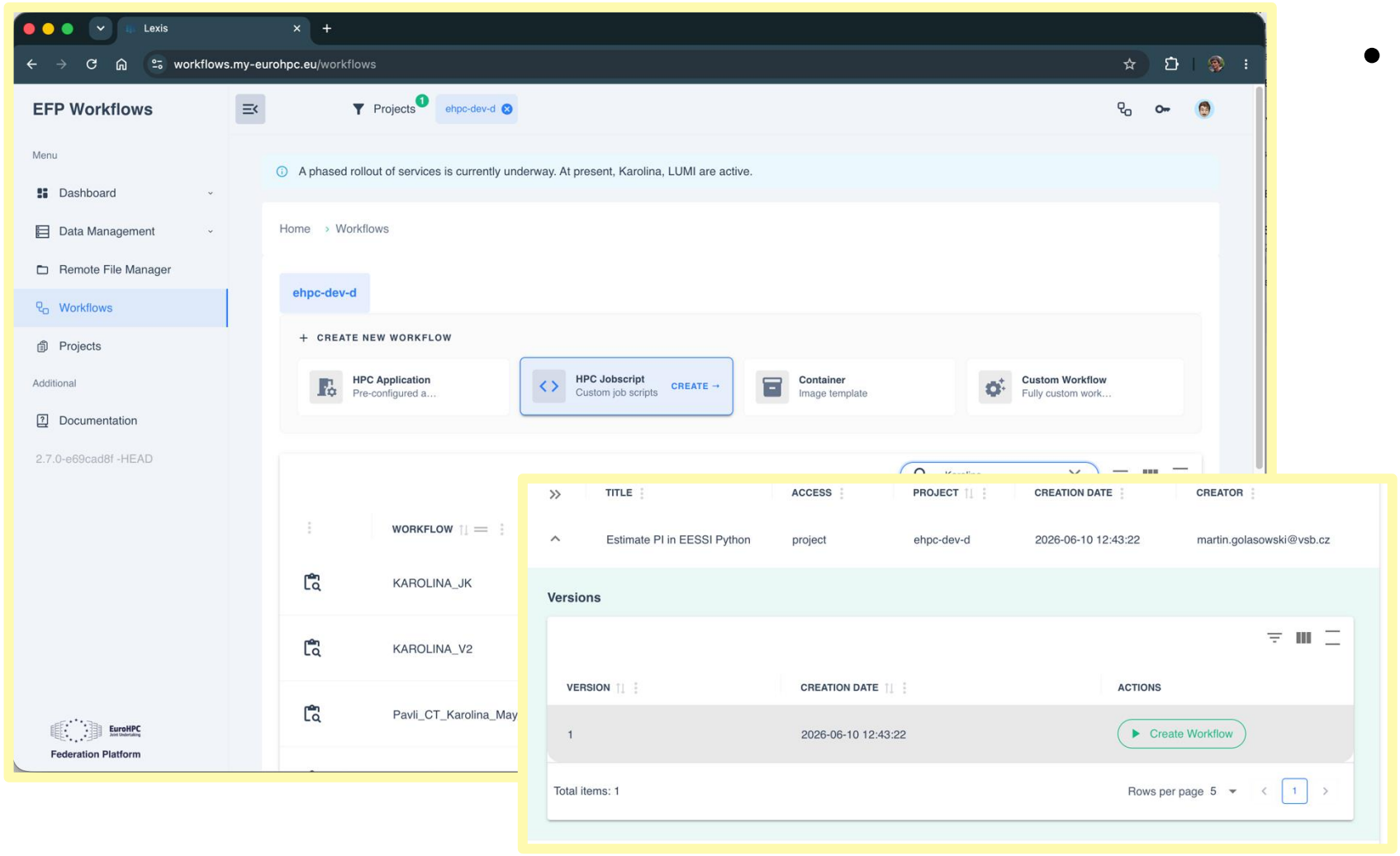


Custom job script



Apptainer container (SIF file)

Step 3. Create a workflow – select a pattern

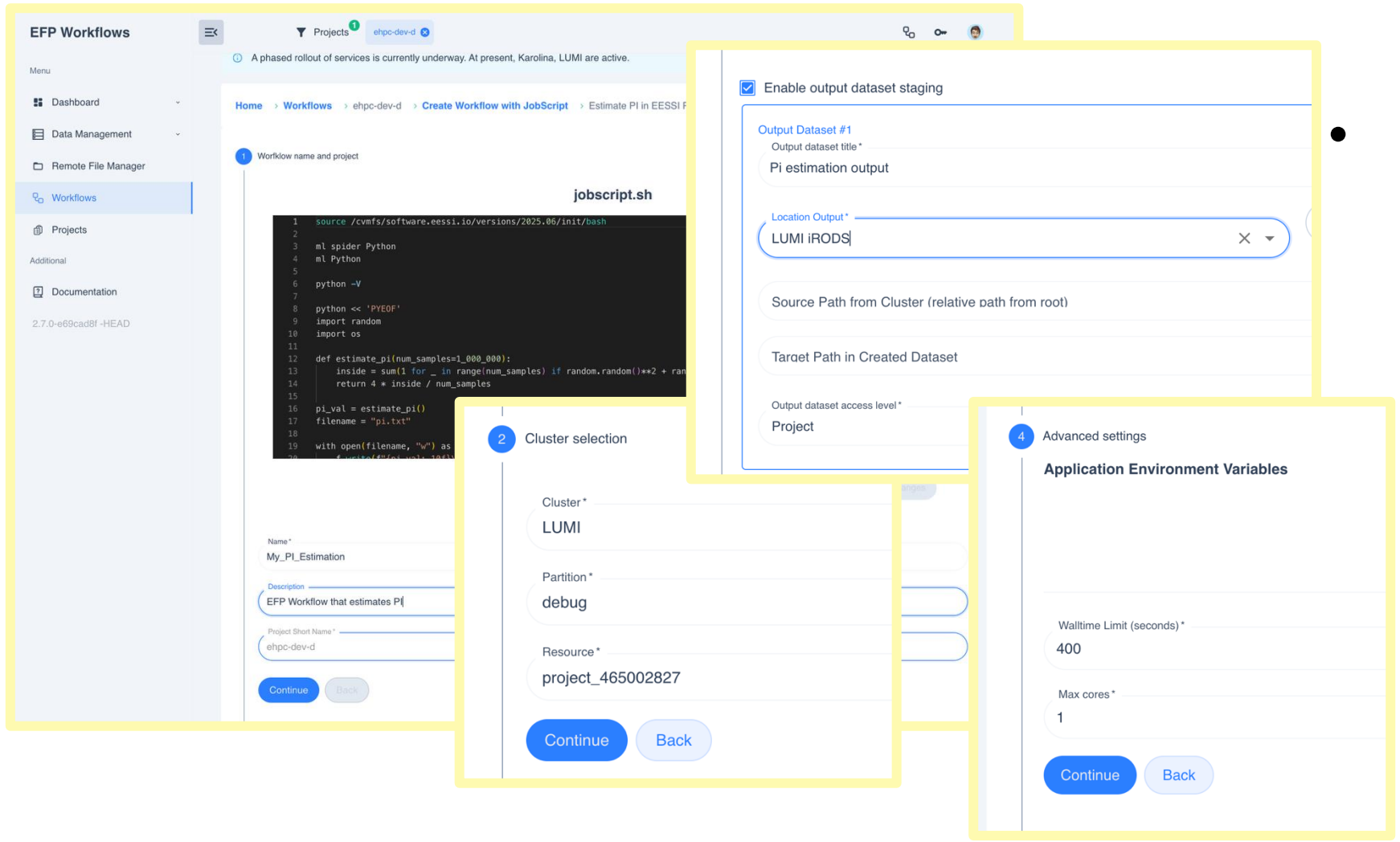


- Use a pre-defined HPC workflow template with
  - Pre-defined job script (e.g. CWL runtime)
  - Custom job script
  - Container

Or create a custom workflow using

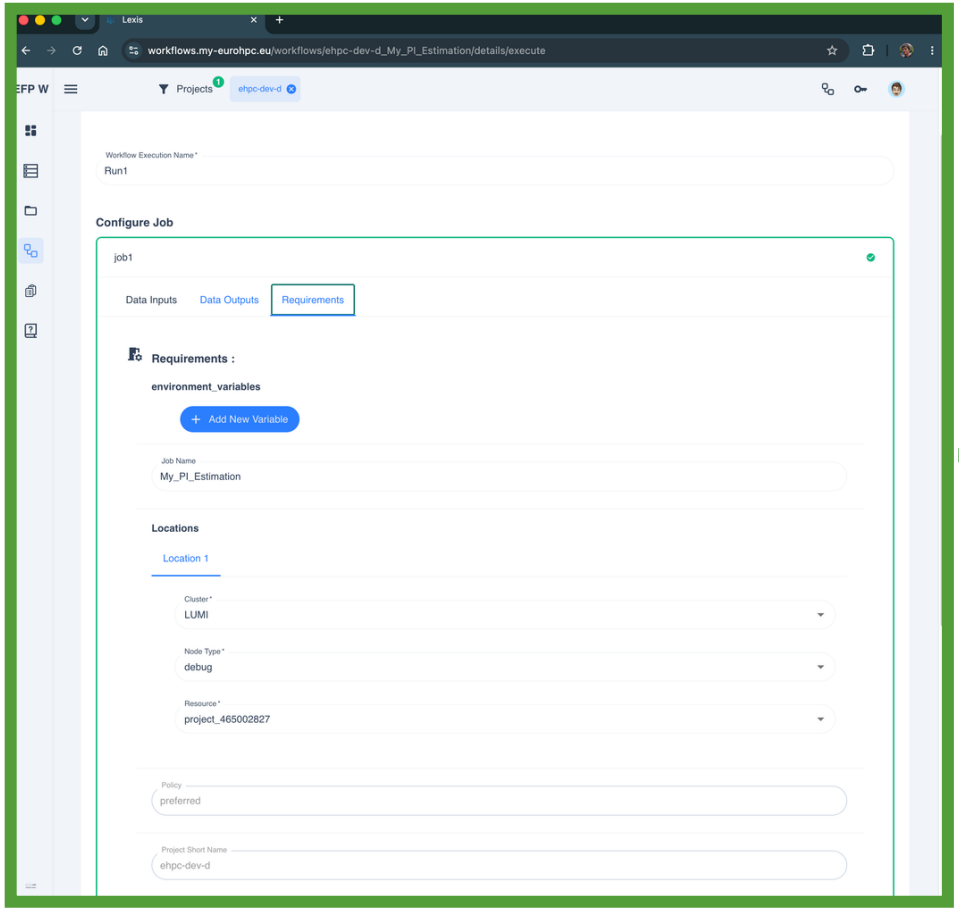
- YAML syntax
- Visual workflow builder

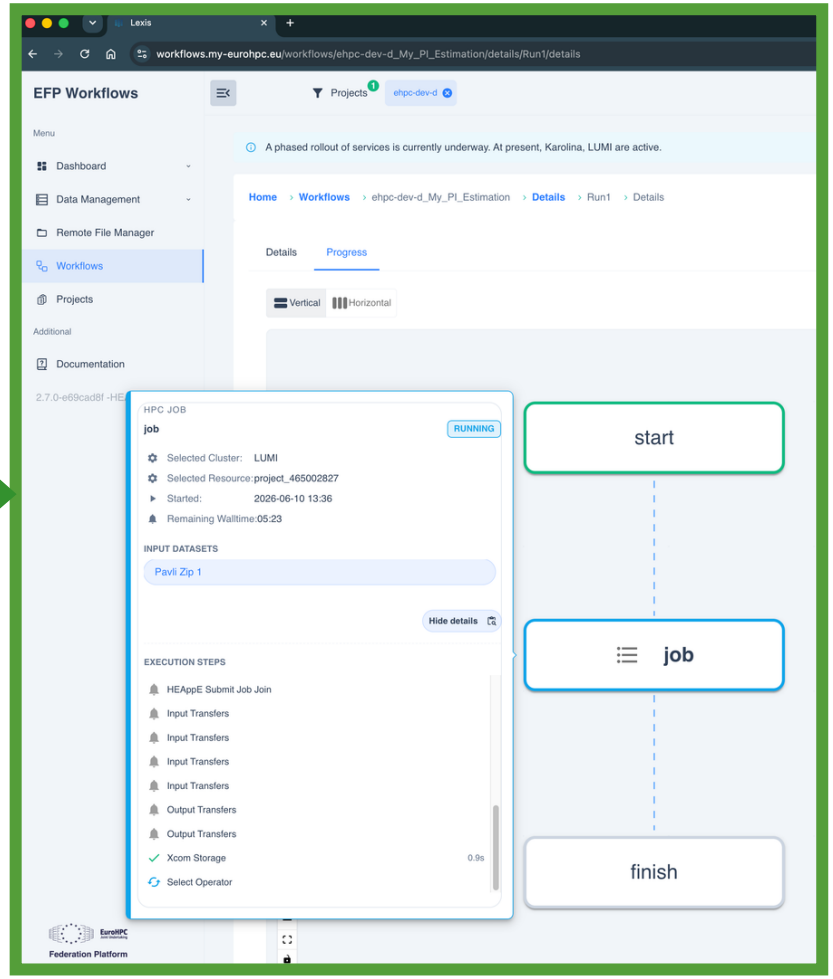
Step 3. Create a workflow – default parameters



- Set default parameters for your HPC workflow via Graphical wizard
  - Title & description
  - Optional data input & output staging
  - Default location
  - Walltime, Cores/GPUs
  - Environment vars

Step 4. Execute the worklow

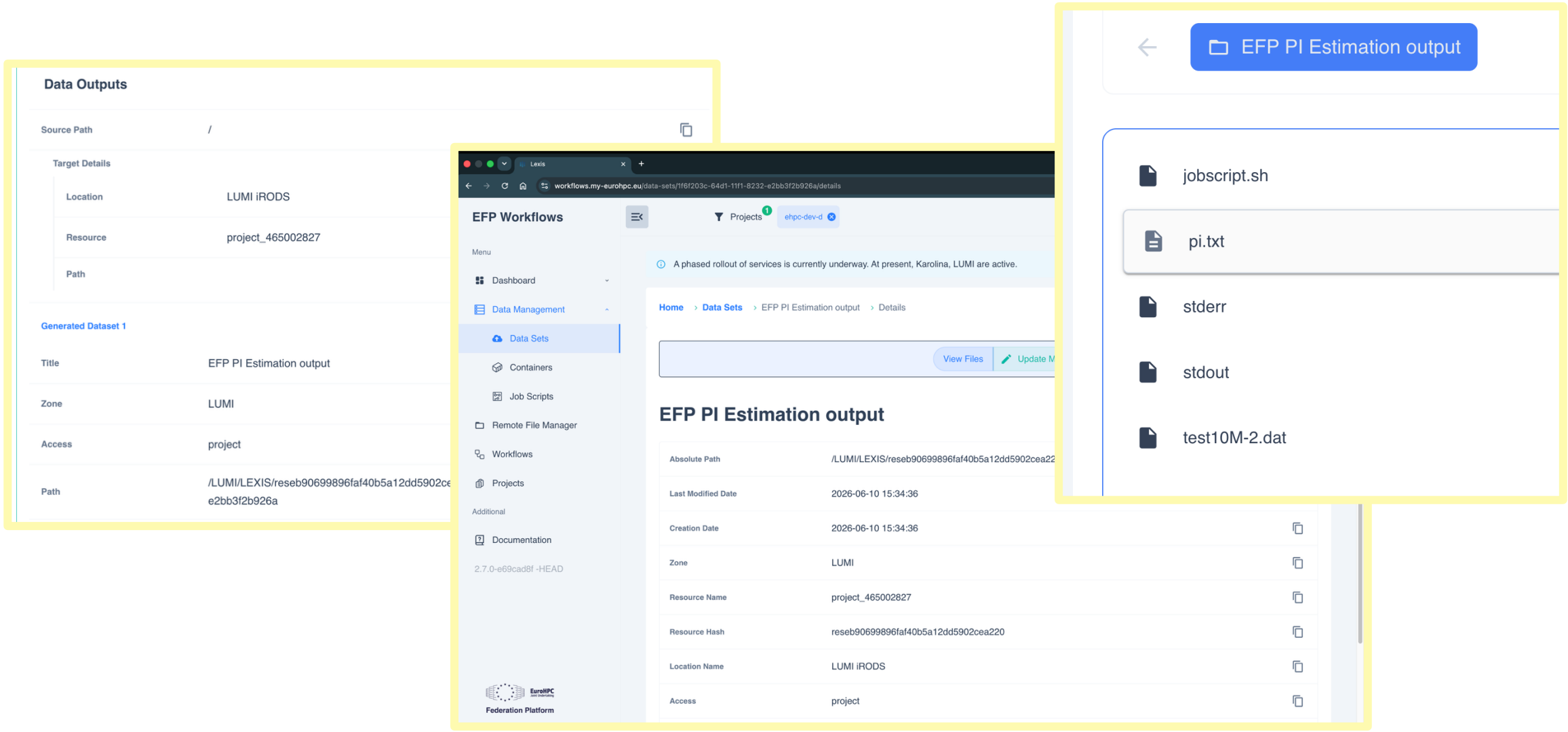




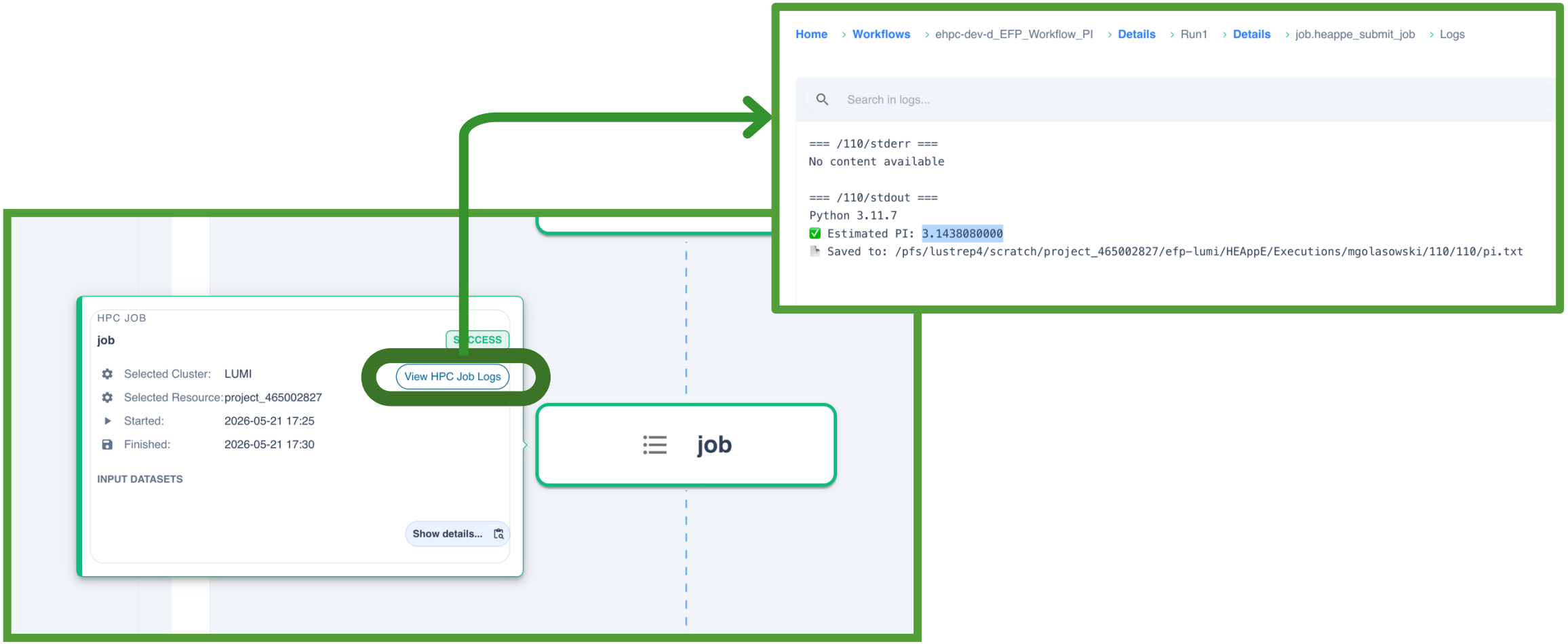
Modify run-time parameters and execute

Watch the progress

Step 5. Access output data



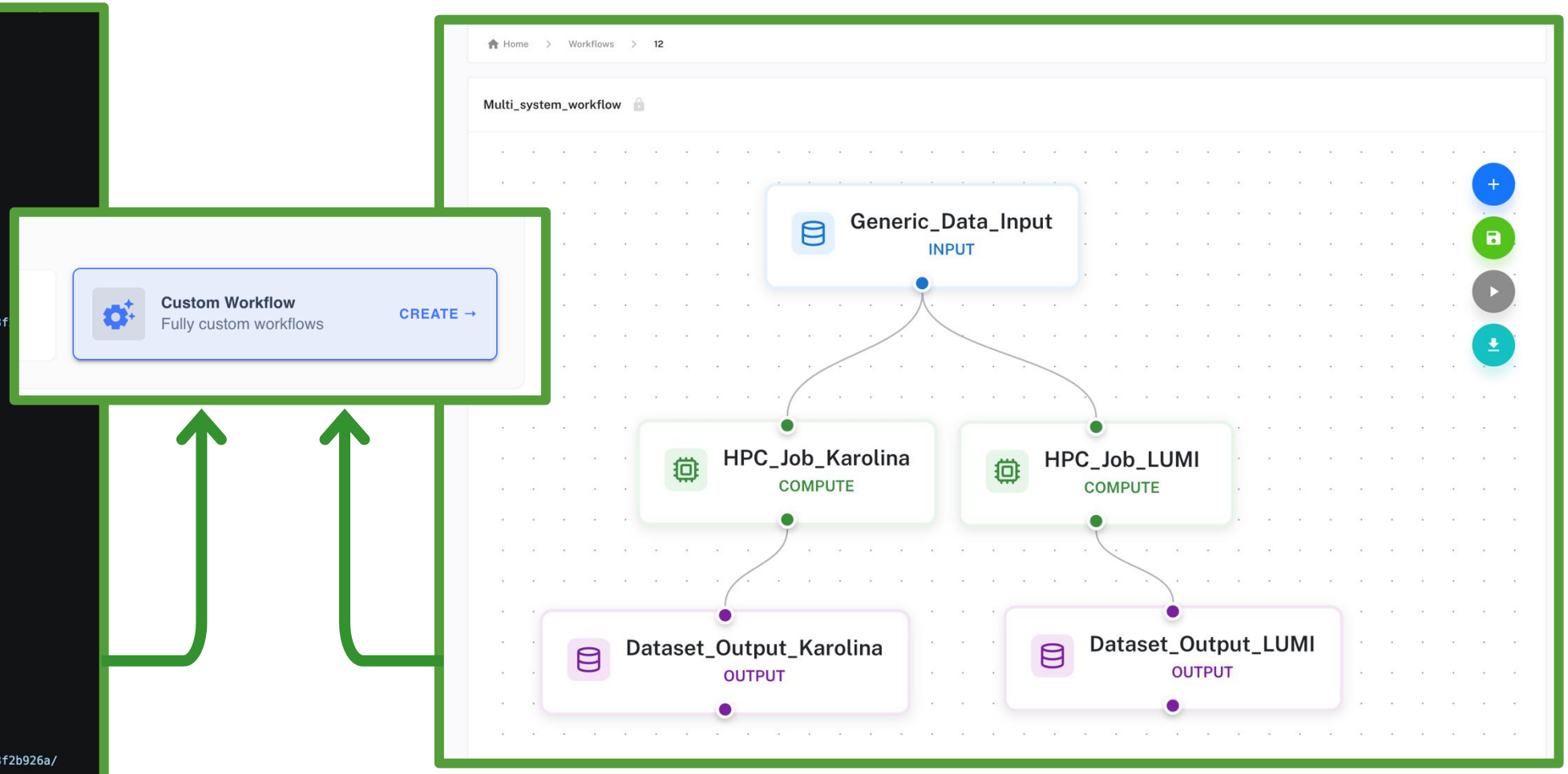
Step 5. Access HPC job logs



Extra: Define custom workflow patterns

```yaml
id: ehpc-dev-d_Multi_system_workflow
desc: Workflow generated from Builder  application
project_shortname: ehpc-dev-d
jobs:
  HPC_Job_Karolina:
    requirements:
      command_template_name: TestTemplate
      node_type_name: qcpu
      locations:
        - location_name: Karolina
          location_resource: eu-26-41
      walltime_limit: 600
      max_cores: 0
      template_parameters:
        inputParam: Hello from Karolina
      environment_variables: {}
    data_inputs:
      - source: ddi://0feff268-64cb-11f1-8efb-e2bb3f
        target: /
    data_outputs:
      - source: /
        metadata:
          $name: Dataset_Output_Karolina
          title: Output
          access: project
        target: ddi://~/
        storage:
          resource: eu-26-41
          location: IT4I iRODS
  HPC_Job_LUMI:
    requirements:
      command_template_name: TestTemplate
      node_type_name: qcpu
      locations:
        - location_name: Karolina
          location_resource: eu-26-41
      walltime_limit: 400
      max_cores: 11
      template_parameters:
        inputParam: Hello from LUMI
      environment_variables: {}
    data_inputs:
      - source: ddi://0feff268-64cb-11f1-8efb-e2bb3f2b926a/
        target: /
    data_outputs:
```

YAML Specification



Visual workflow builder with templates

Extra: Access the EFP Worfklows via Py4Lexis

