Using Supercomputers from the Collaboratory (v2)

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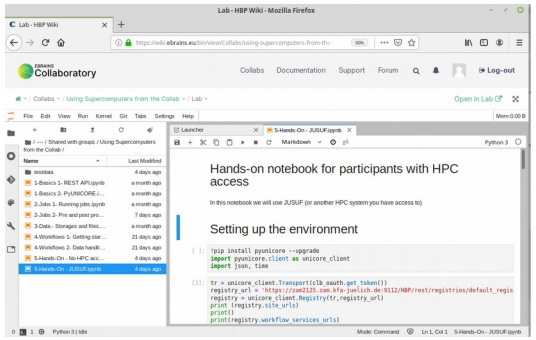
Outline

- The Collaboratoy and HPC
- UNICORE
- Demo / Hands-on

The Collaboratory and HPC



HBP identity management (OIDC)

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HPC Resource | HPC Resource | HPC Resource

Site local accounts
Projects
Compute quotas

- Run simulations
- Access and move data
- ...

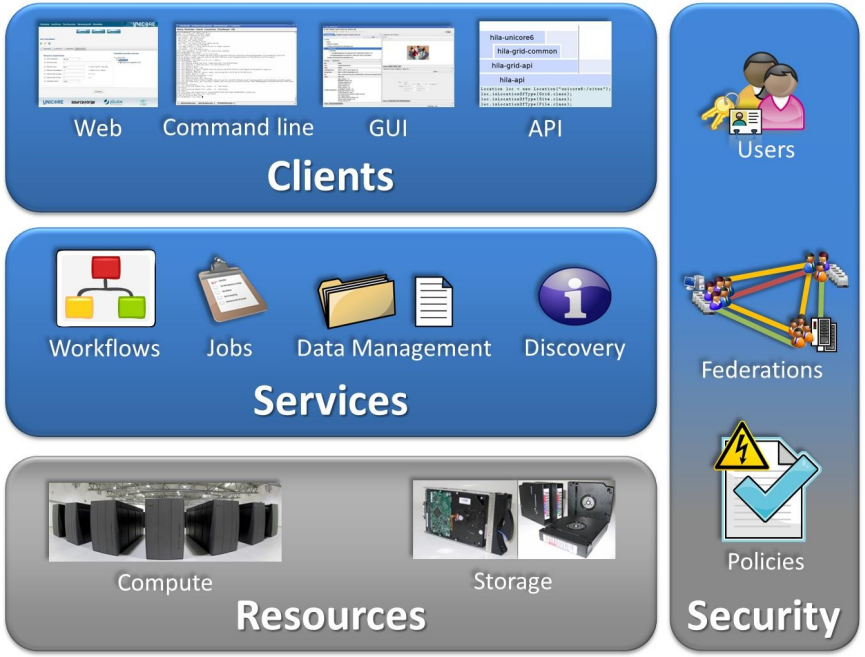
Wish list

- Authentication via OIDC token – single sign-on
- Provide delegation – service can use other services on user's behalf
- Map users to their local account(s) transparently
- Common APIs
- Workflow capabilities

- Computing time projects
- Principal investigators / project members

FENIX RESEARCH INFRASTRUCTURE

- UNiform Interface to COmputing and data REsources (https://www.unicore.eu/about-unicore/history)
- Middleware components for integration of HPC into federated environments
- REST APIs for jobs, data and workflows
- Transparent and flexible security & user mapping
- Maintained as Open Source (BSD license) https://github.com/UNICORE-EU



Building blocks

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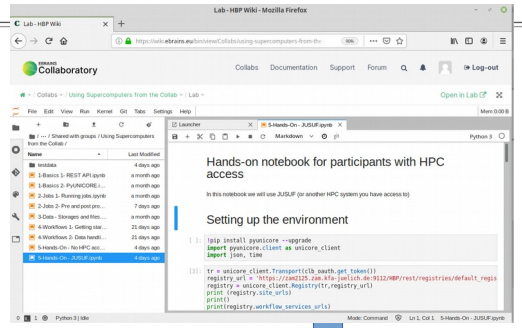

Login

HBP Login

REST / JSON over https

Registry

Workflow

HPC Site(s)

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Service discovery

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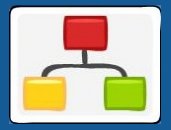
Workflow processing



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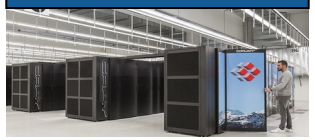
Jobs and data



HPC Site

REST APIs

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Job submission

Data access

Local user mapping (authorization)

Target System Interface

UFTPD

User authentication

Unity
(operated at JSC)

Authentication & user mapping

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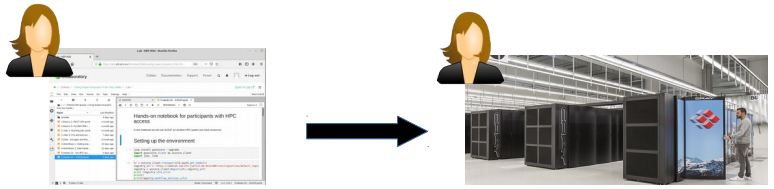
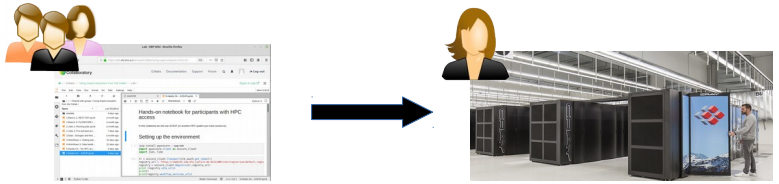
- Default: per-user mapping
  - The current user is mapped to their personal HPC account(s)
  - OIDC token from collaboratory



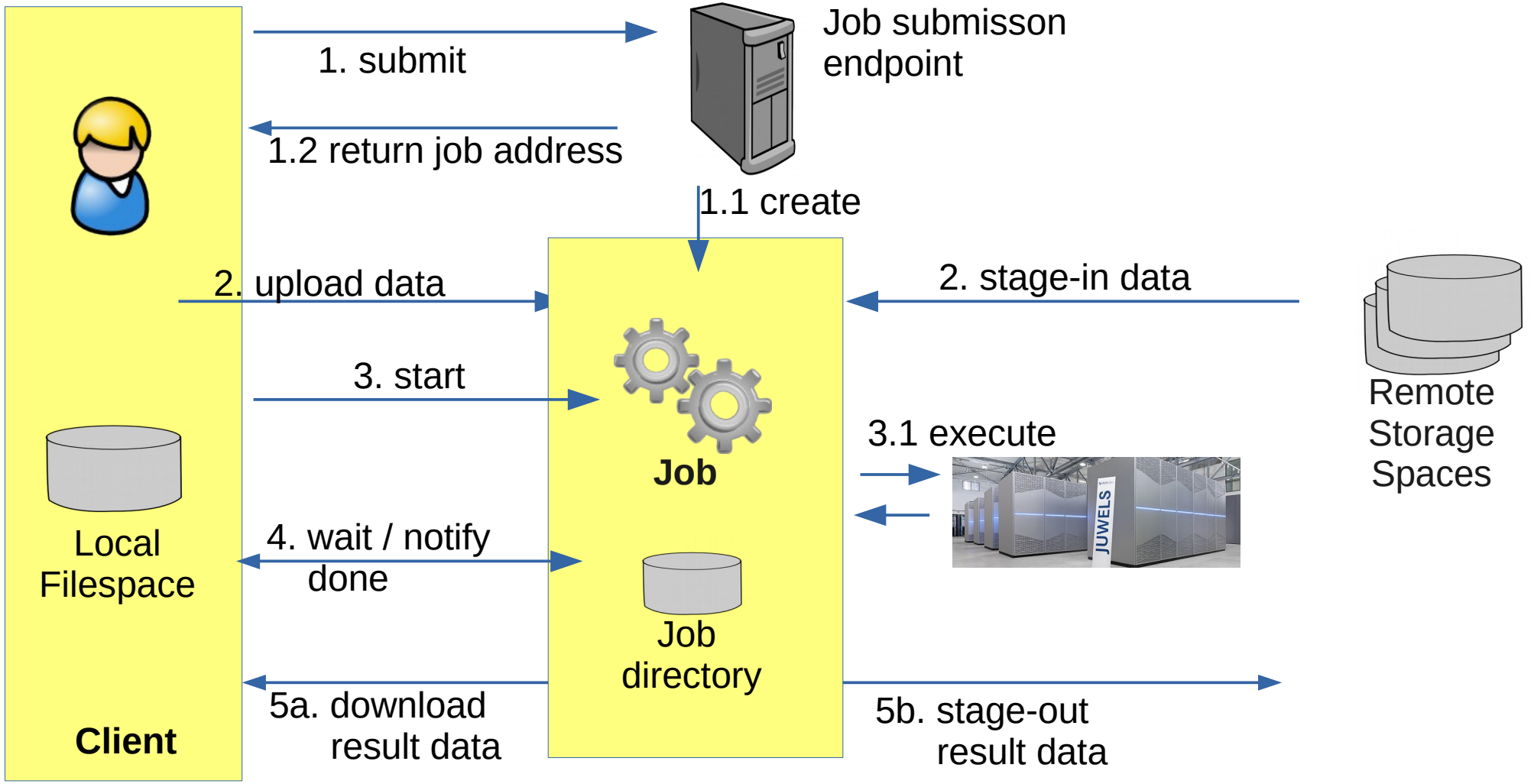
- Special use case: platform-level services
  - One or more „service accounts“ used for multiple users
  - → proxy services for job submission



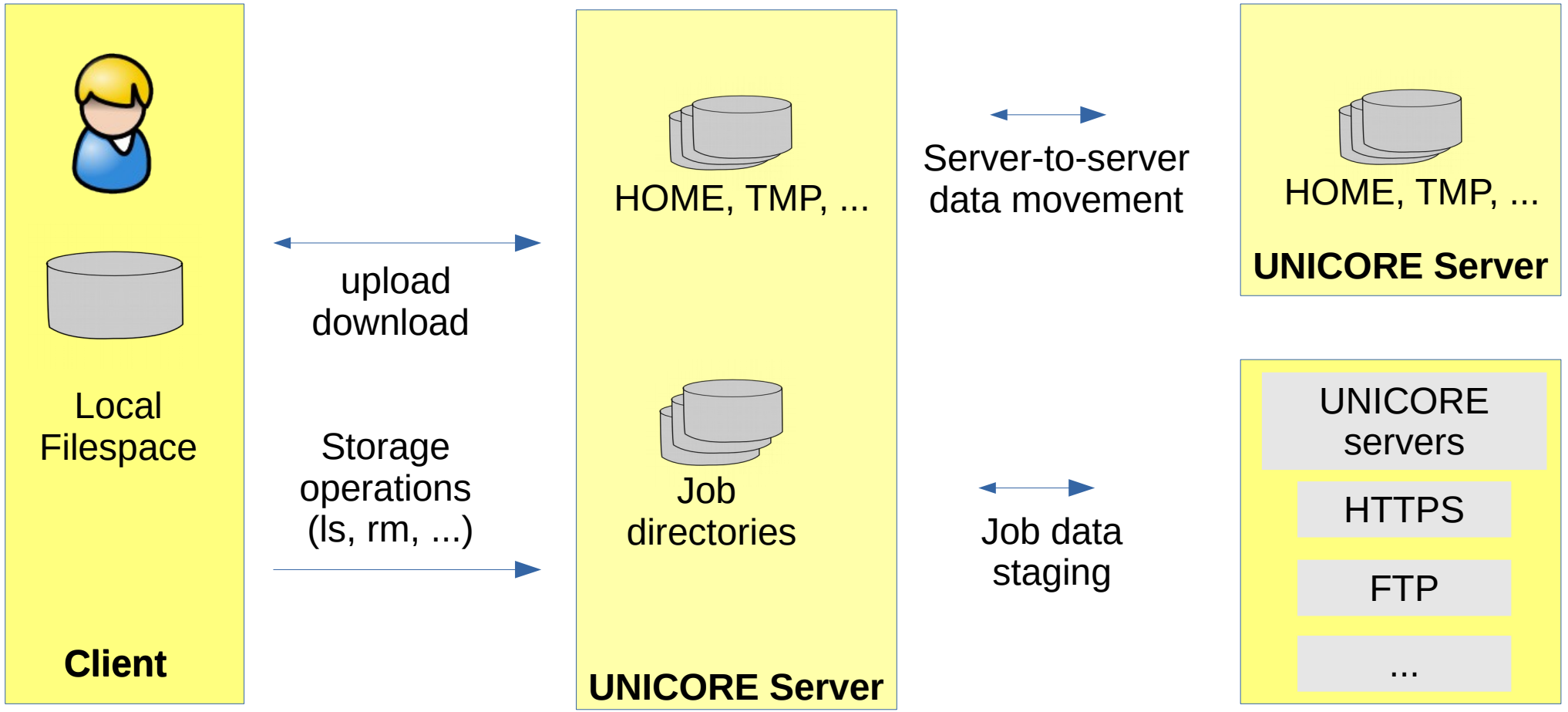
Jobs

- Unique working directory – accessible at any time in the job‘s lifetime
- Data stage-in from remote servers
- Pre-command(s)
- Main execution
  - On compute node(s) via batch scheduler (default) or login node
- Post command(s)
- Data stage-out to remote servers

Job execution model



Storages


Local Filespace
Client
upload
download
Storage operations (ls, rm, ...)
HOME, TMP, ...
Job directories
UNICORE Server
Server-to-server data movement
Job data staging
HOME, TMP, ...
UNICORE Server
UNICORE servers
HTTPS
FTP
...

Endpoints

UNICORE

- UNICORE is resource / object oriented
  - E.g. a job or a storage
  - Per-user, access-controlled

https://sourceforge.net/p/unicore/wiki/REST_API

- RESTful APIs and semantics
  - Properties (GET) and operations (PUT, POST, DELETE)
  - Error codes

- Linked system of inter-related endpoints
  - Site-level
    - Job submission, storages, server-server data transfers
  - Federation
    - Workflows, Registry

Clients and APIs

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- ***RESTful APIs***
  - curl, Python Requests, …
  - PyUNICORE client library
- ***Command line tools***
  - UNICORE Commandline Client (UCC)
  - UFTP client for high-performance data access

Summary

- UNICORE
  - Access to HPC compute and data via REST APIs
  - Handles authentication and authorization transparently and flexibly
  - Job submission/management
  - Data access, data movement
  - Workflows
- „Glue technology“ for many integration use cases

Hands-on

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- ***Public collab with example notebooks***

  https://wiki.ebrains.eu/bin/view/Collabs/using-supercomputers-from-the-collab/

- API Documentation

  https://sourceforge.net/p/unicore/wiki/REST_API

- PyUNICORE on GitHub

  https://github.com/HumanBrainProject/pyunicore/

Thank you!

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