



Co-funded by
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Human Brain Project

Using the HPAC supercomputers from the collaboratory

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OUTLINE



- The HPAC supercomputers
- UNICORE middleware – motivation & brief overview
- Demos
- Hands-on
 - Jupyter notebooks in the Collab (v1)
 - <accessing some HPC machine>

HPAC



- High-performance compute and data resources
- Services for job submission, data access, data movement, ...
- Allow integration with the Collaboratory and other Platforms
- Enable and support complex user workflows

Visualisation Systems



Platform services, APIs, policies, support, ...

HPC, Storage, Cloud VMs



HPC, Storage



HPC, Storage



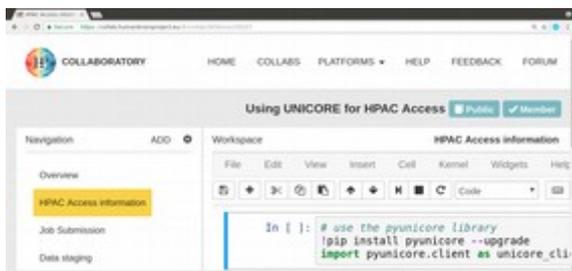
HPC, Storage, Cloud VMs



ENABLE MULTISITE WORKFLOWS



Jupyter notebook or app



HBP accounts



3. Use

Visualization Service

CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

1. Launch simulation

HPC simulation

JÜLICH
FORSCHUNGSZENTRUM

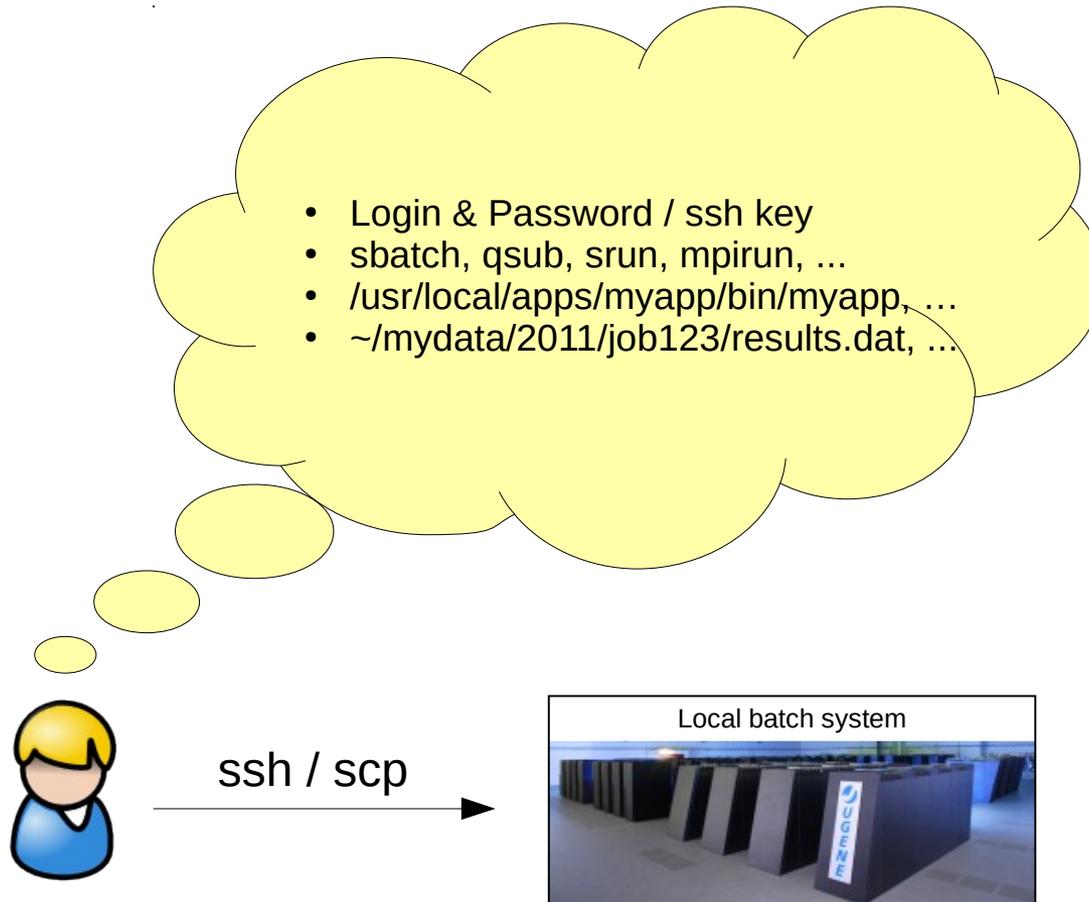
Data access

Storage

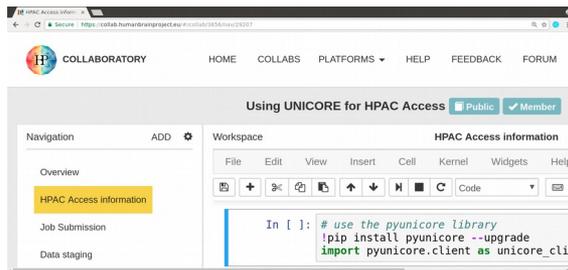
CINECA

2. Results

TRADITIONAL HPC USE



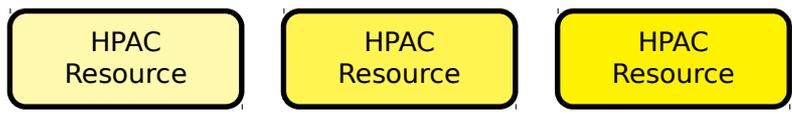
COLLABORATORY AND HPAC



HBP accounts
(OIDC)



- Login with HBP account
- HBP account automatically mapped to local account(s)
- Delegation – service can use other services on user's behalf



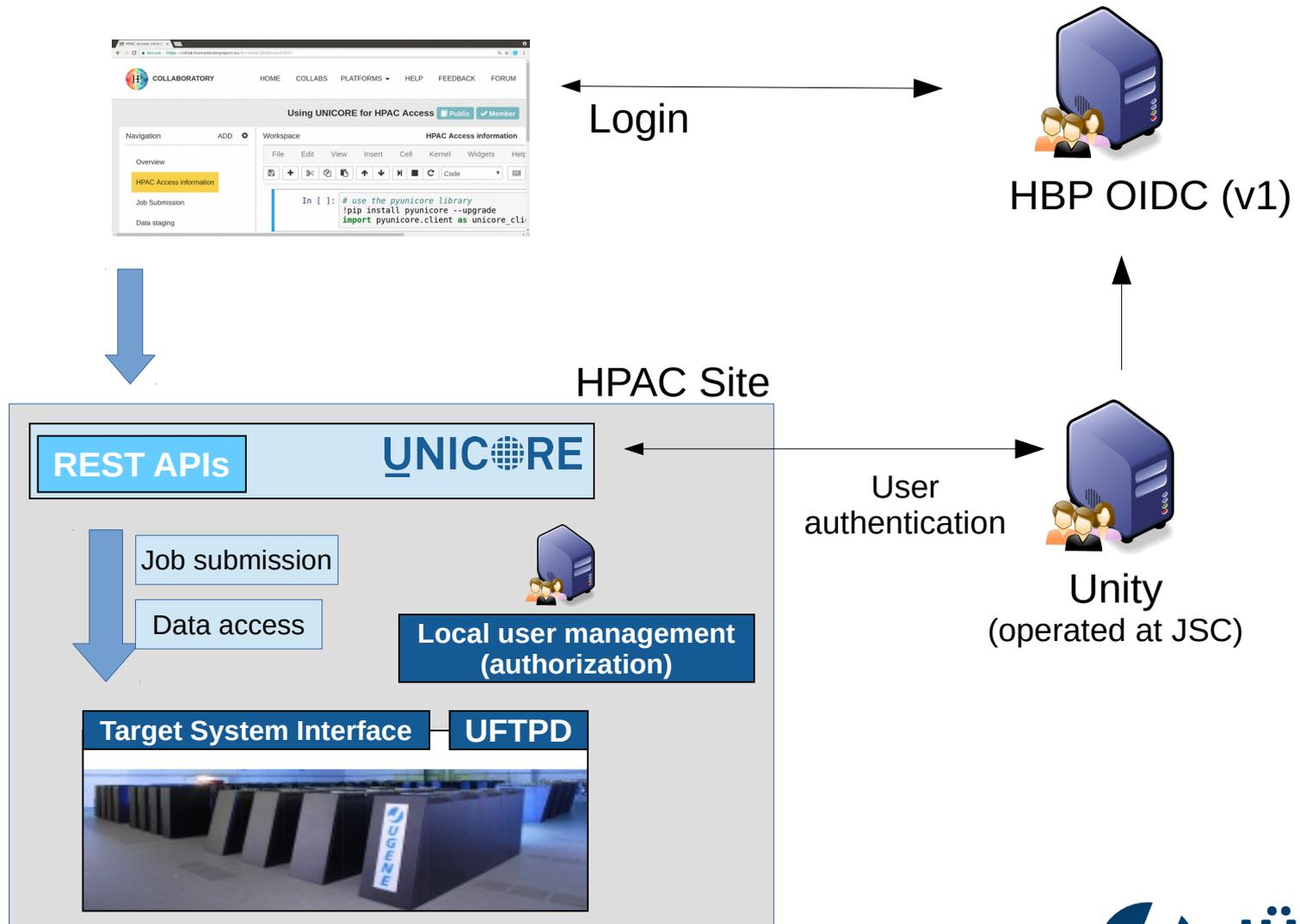
- Run simulations
- Access and move data
- ...



Site local accounts
Projects
Groups
Compute quotas



ACCESSING A HPAC SITE



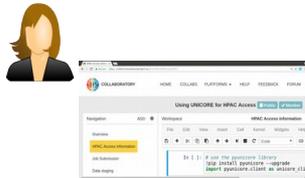
KEY FEATURES

UNICORE



- UNiform Interface to COmputing and data REsources (established 1997, <https://www.unicore.eu/about-unicore/history>)
- Middleware components for integration of HPC into federated environments
 - Federated authentication, site-local authorization, account mapping (UNIX login & groups)
 - Batch system abstraction
 - File system access
 - High-performance data transfer (UFTP)
- REST APIs for jobs, data, workflows

BUILDING FEDERATED SYSTEMS



HBP OIDC (v1)

Service Registry

UNITY
Federated identity

Workflow enactment
service

Client tier

Shared
services
(defining the
federation)



UNICORE
HPC site(s)

UNICORE

Web Command line GUI API

Clients

Workflows Jobs Data Management Discovery

Services

Compute Storage

Resources

Users

Federations

Policies

Security

- Open source (BSD license)
<https://www.unicore.eu>

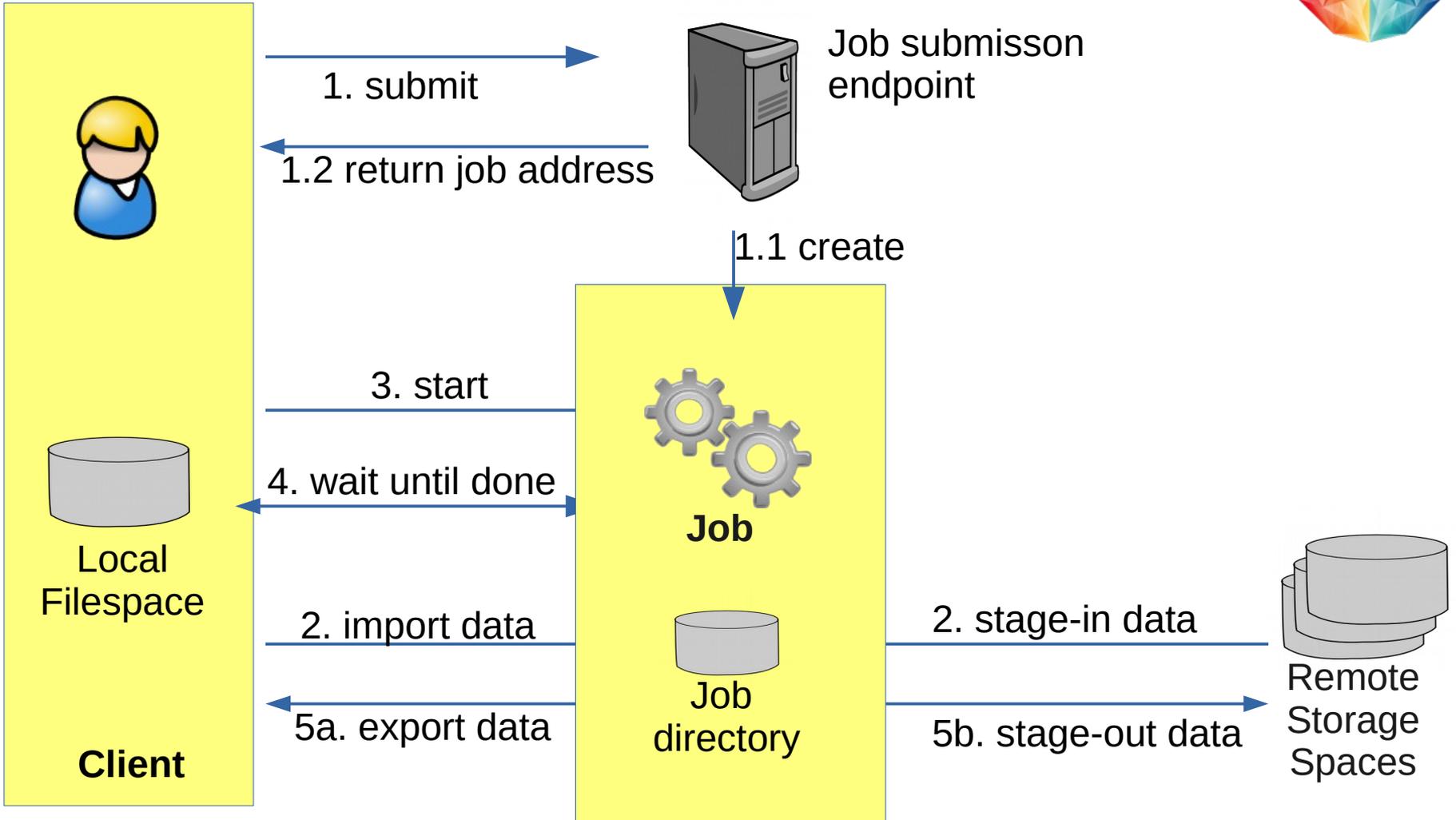
RESOURCE MODEL



- UNICORE is resource / object oriented
 - E.g. a batch job or a storage
 - HTTPS endpoints / URLs with operations to manipulate them
 - Per-user, access-controlled

- APIs
 - REST / JSON
 - SOAP / XML

JOB EXECUTION



JOB EXECUTION



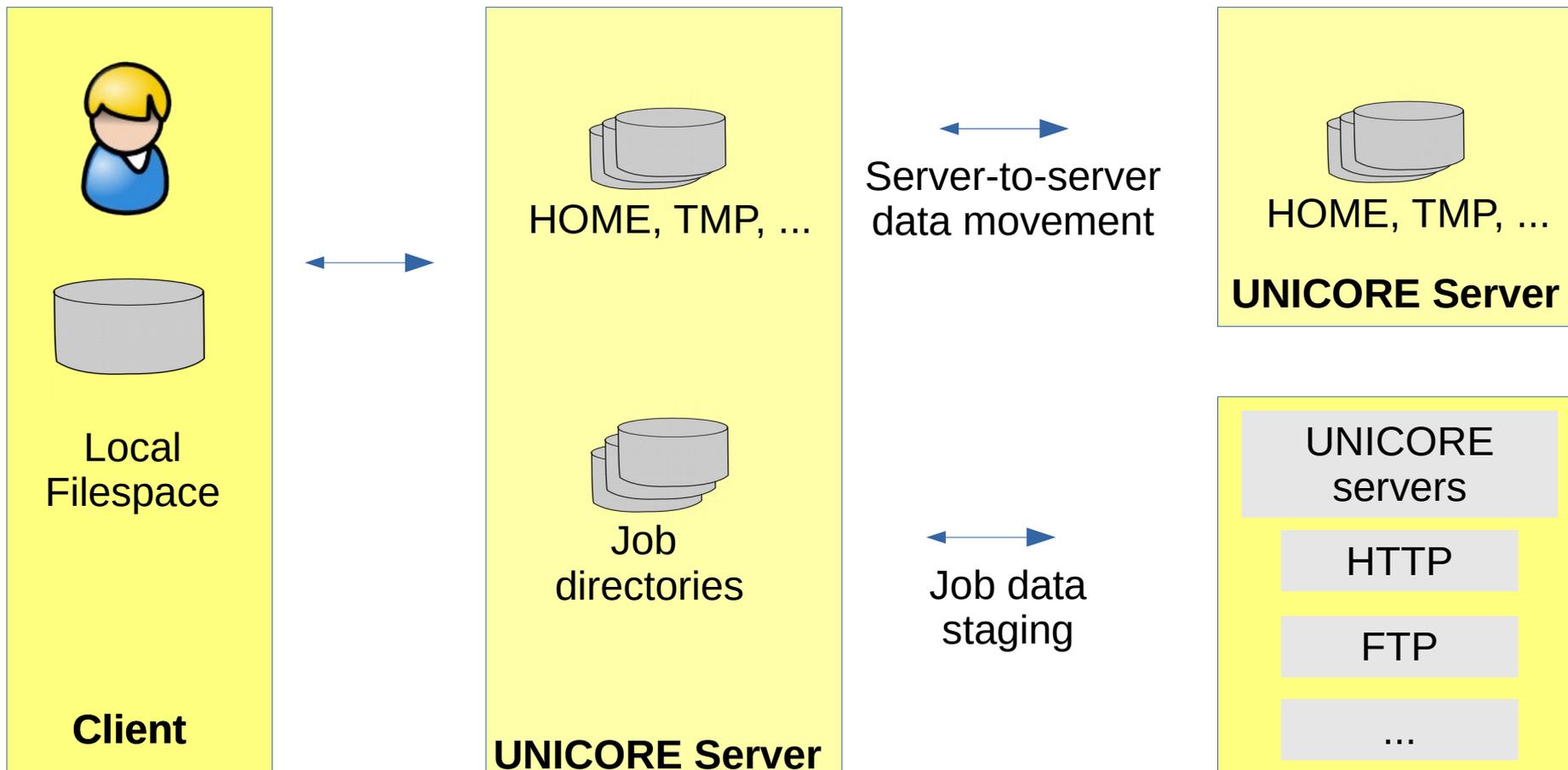
- A UNICORE job includes:
 - Data stage-in from remote servers
 - Pre-command(s)
 - Main execution / submission to batch system
 - Post command(s)
 - Data stage-out to remote servers

JOB MANAGEMENT



- A UNICORE job has:
 - Properties (status, log, ...)
 - Working directory (sandbox) that can be accessed at any time
 - Control operations (abort, restart, delete)

DATA AND STORAGE SERVICES



STORAGE MANAGEMENT



- “Abstract” storage instances like HOME, SCRATCH, ...
- List, create directories, remove files, ...
- Upload/download files
- Send/receive files from other UNICORE servers
- Data movement via https (default) or UFTP
- Properties
 - Free space, ...

CLIENTS



- REST APIs
 - curl, Python Requests, PyUNICORE client library, ...
- Command line (supporting OIDC via oidc-agent)
 - UNICORE Commandline Client (UCC)
 - UFTP client for high-performance data access

SUMMARY



- HPAC platform
 - Federated infrastructure for HPC, data and VM-based services
 - Consists of heterogeneous, distributed resources
 - Co-design approach: scientists and infrastructure need to work together to realise complex use cases

SUMMARY



- UNICORE
 - Access to HPC compute and data via REST APIs
 - Handles authentication and authorization
 - Job submission/management, data access, data movement

- Enables HPC for
 - Web-based environments like the Collaboratory
 - Commandline environments
 - Applications requiring access to HPC

HANDS ON



- Requires Collab (v1) account
<https://collab.humanbrainproject.eu>
- Training collab: “HPAC Training: Using UNICORE”
<https://collab.humanbrainproject.eu/#/collab/34731/nav/240789>
- Low level API documentation
https://sourceforge.net/p/unicore/wiki/REST_API