



Co-funded by
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Human Brain Project

Using the HPAC supercomputers from the collaboratory

Bernd Schuller

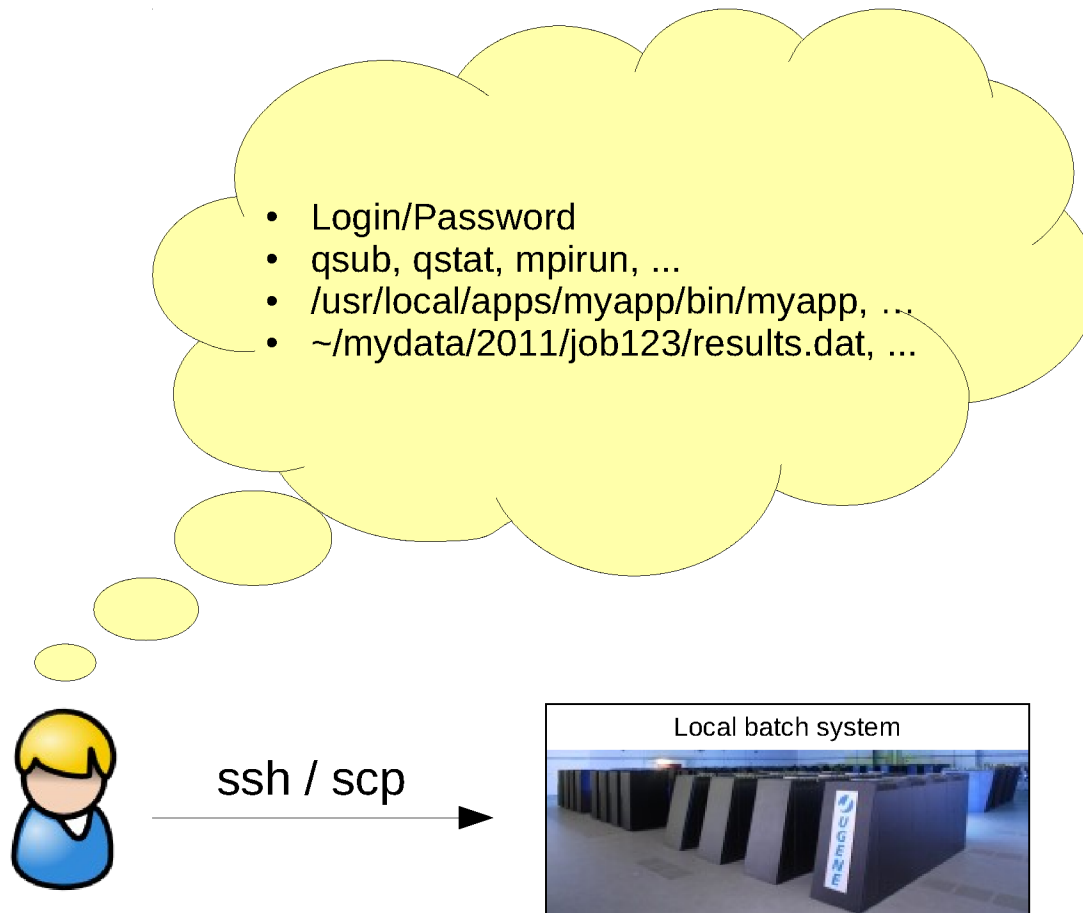
Forschungszentrum Jülich GmbH

OUTLINE



- The HPAC supercomputers
- UNICORE middleware – brief overview
- Hands-on
 - Jupyter notebooks
 - CSCS Piz Daint

TRADITIONAL HPC USE



- Common authentication – single sign on
- APIs for job submission, data access, data movement, ...
- Allow integration with the Collaboratory
- Enable user workflows

Visualisation Systems



UNICORE

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

HPC, Storage, Cloud VMs



HPC, Storage



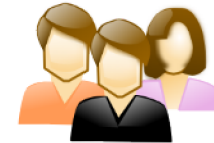
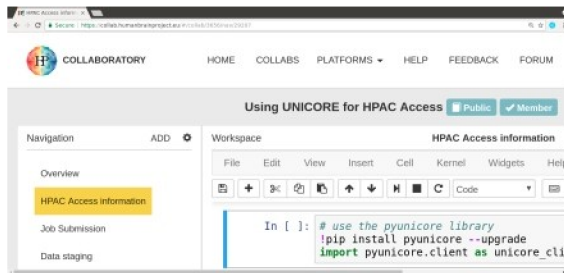
HPC, Storage



HPC, Storage, Cloud VMs

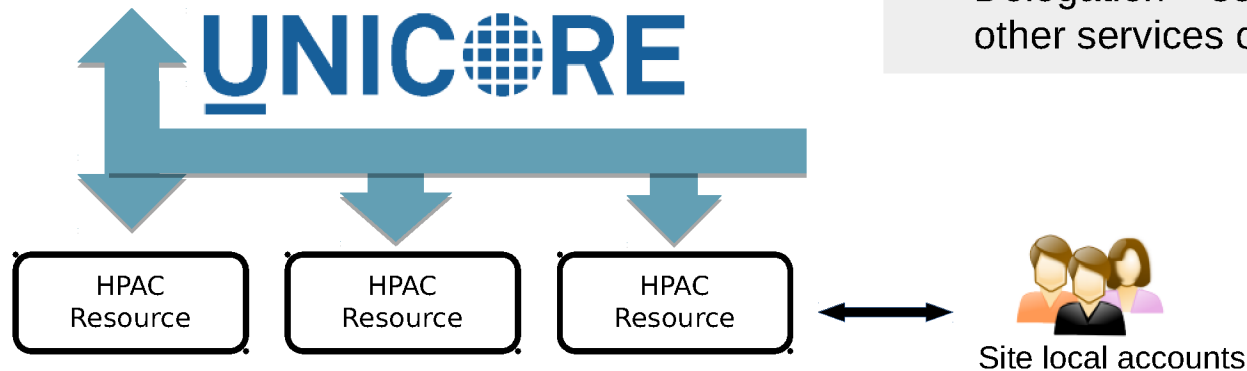


SINGLE SIGN ON / COLLABORATORY

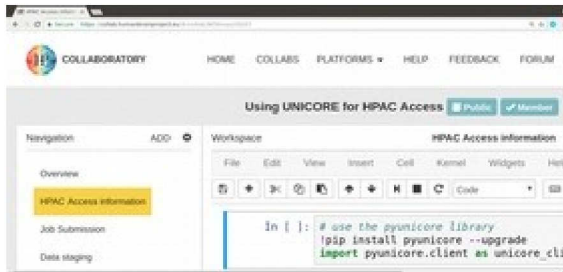


HBP accounts

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



ENABLE USER WORKFLOWS



HBP accounts

3. Use

Visualization Service



1. Launch simulation

HPC simulation



2. Results

Storage

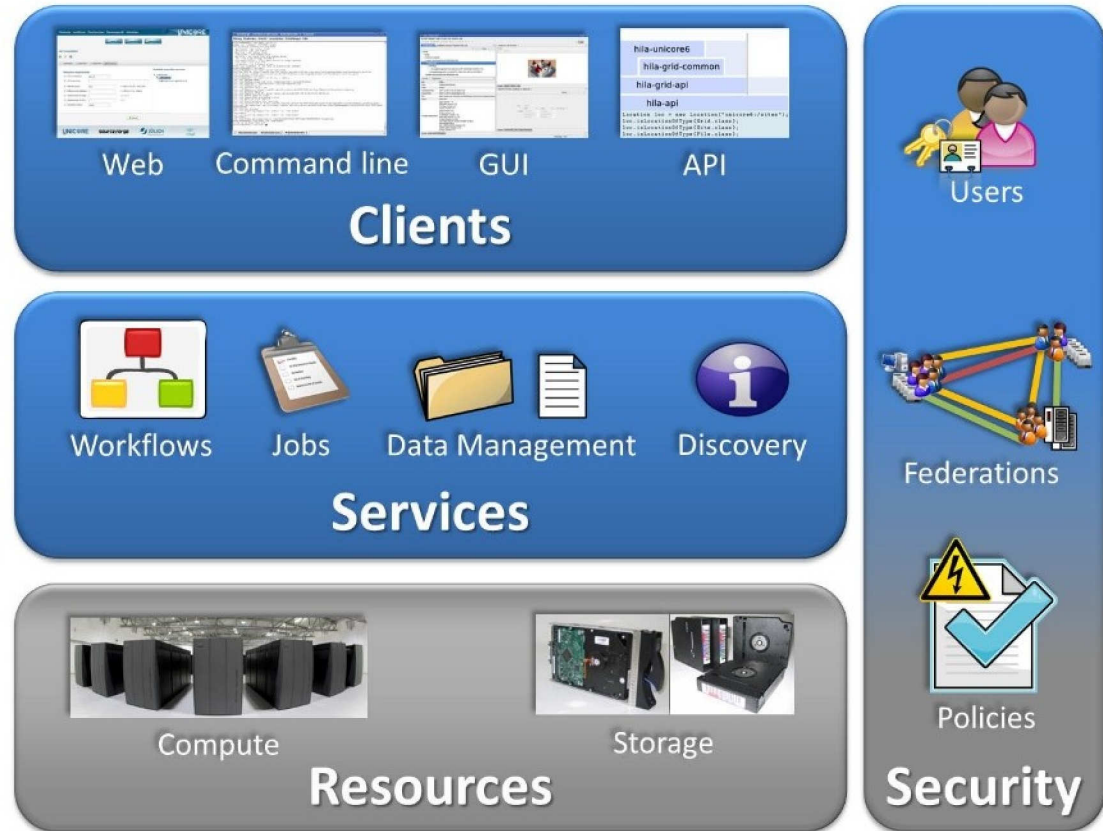


Data access



- Middleware components for integration of HPC into federated environments
 - Federated authentication, site-local authorization, account mapping
 - Batch system abstraction
 - File system access
- REST APIs for jobs, data, workflows
- Simplifies HPC use for non-experts (Application concept, abstract resource model, predefined applications, workflow templates, ...)

UNICORE



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



- Workflow enactment
- Task execution
- Job submission
- Job management
- Reservations
- Storages
- File transfer
- Metadata
- Service Registry
- Resource Broker



Compute

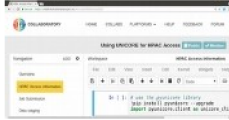


Storage

Resources

- Batch systems
(Slurm, LSF, ...)
 - SSH tunnel to remote servers
 - Direct execution
(e.g. on Windows)
 - ... (extensible)
- File systems
 - S3, CDMI
 - ... (extensible)

UNICORE COMPONENTS



Service Registry

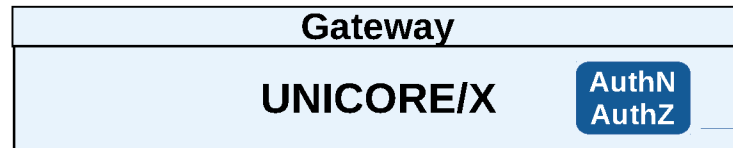
Federated identity
UNITY

Workflow enactment
service

Client tier

Shared
services
(defining the
federation)

Components
at each HPC
site



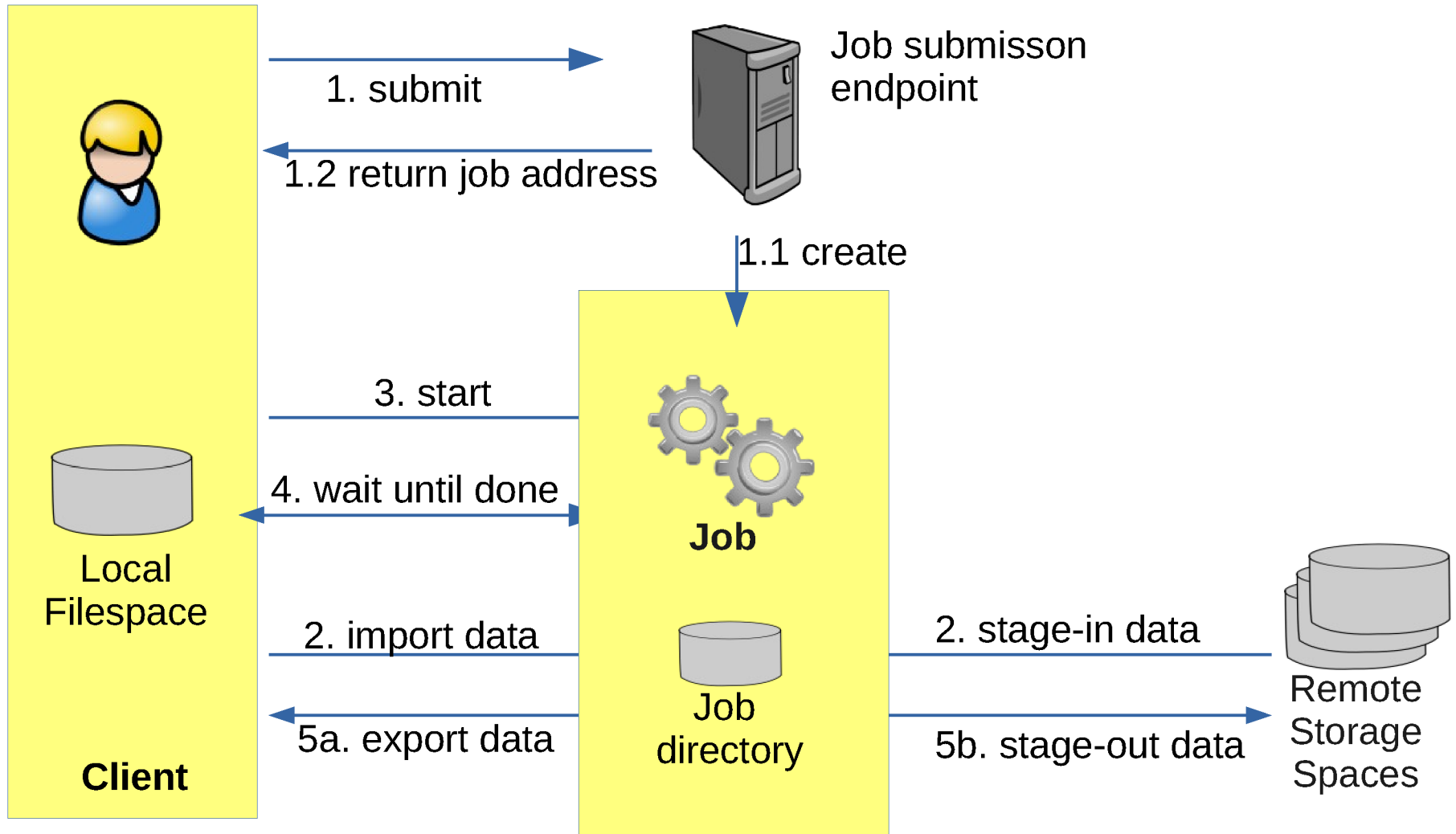
mapping of users
to local logins



RESOURCE MODEL

- UNICORE is resource / object oriented
 - E.g. a batch job or a storage
 - Endpoints / URLs with operations to manipulate them
 - Per-user, access-controlled
- APIs
 - SOAP / XML
 - REST / JSON

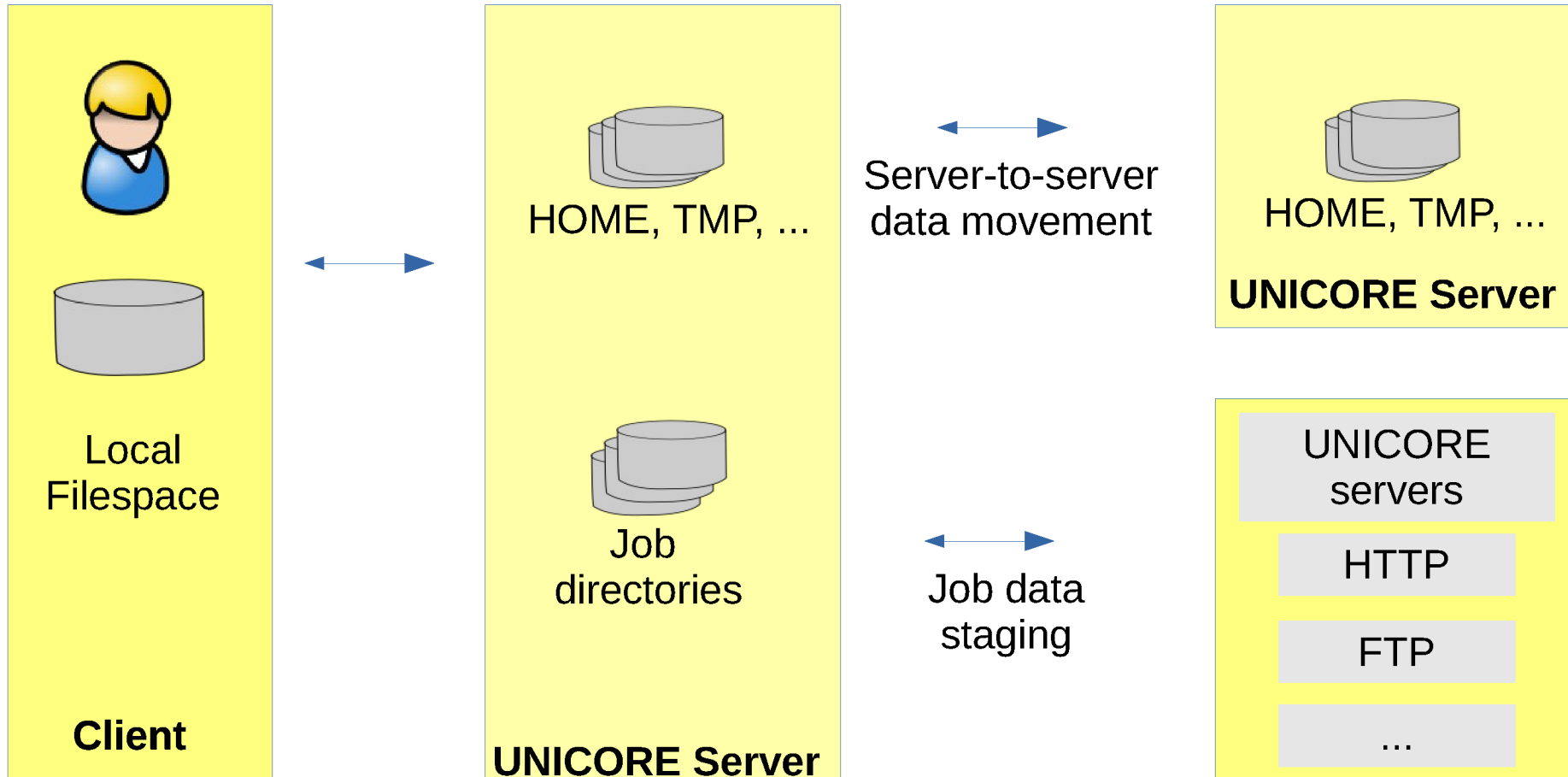
JOB EXECUTION



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
- Jobs can be re-started (includes pre, main, post, stage-out)

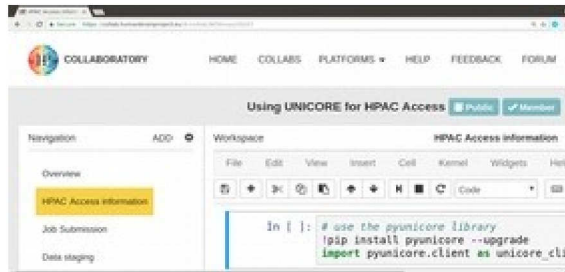
DATA AND STORAGE SERVICES



EXAMPLE USER WORKFLOWS



Jupyter notebook or app



HBP accounts

3. Use

Visualization Service



1. Launch simulation

HPC simulation



Data access

Storage

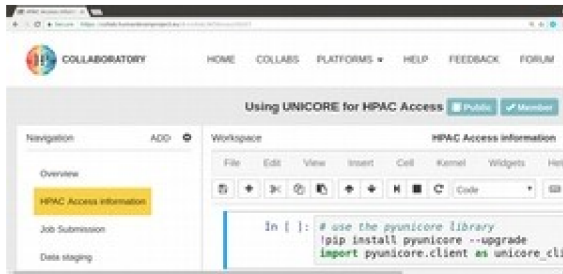


2. Results

EXAMPLE USER WORKFLOWS



Jupyter notebook or app



HBP accounts

1. Launch simulation A

2. Launch task B



Access
results from
simulation A

SUMMARY

- HPAC platform
 - Federated infrastructure for HPC, data and VM-based services
 - Access from HBP Collaboratory via UNICORE REST APIs
 - Co design approach: scientists and infrastructure need to work together to realise complex use cases

HANDS ON

- Requires Collab account
- 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