# Using the HPAC supercomputers from the collaboratory

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Human Brain Project
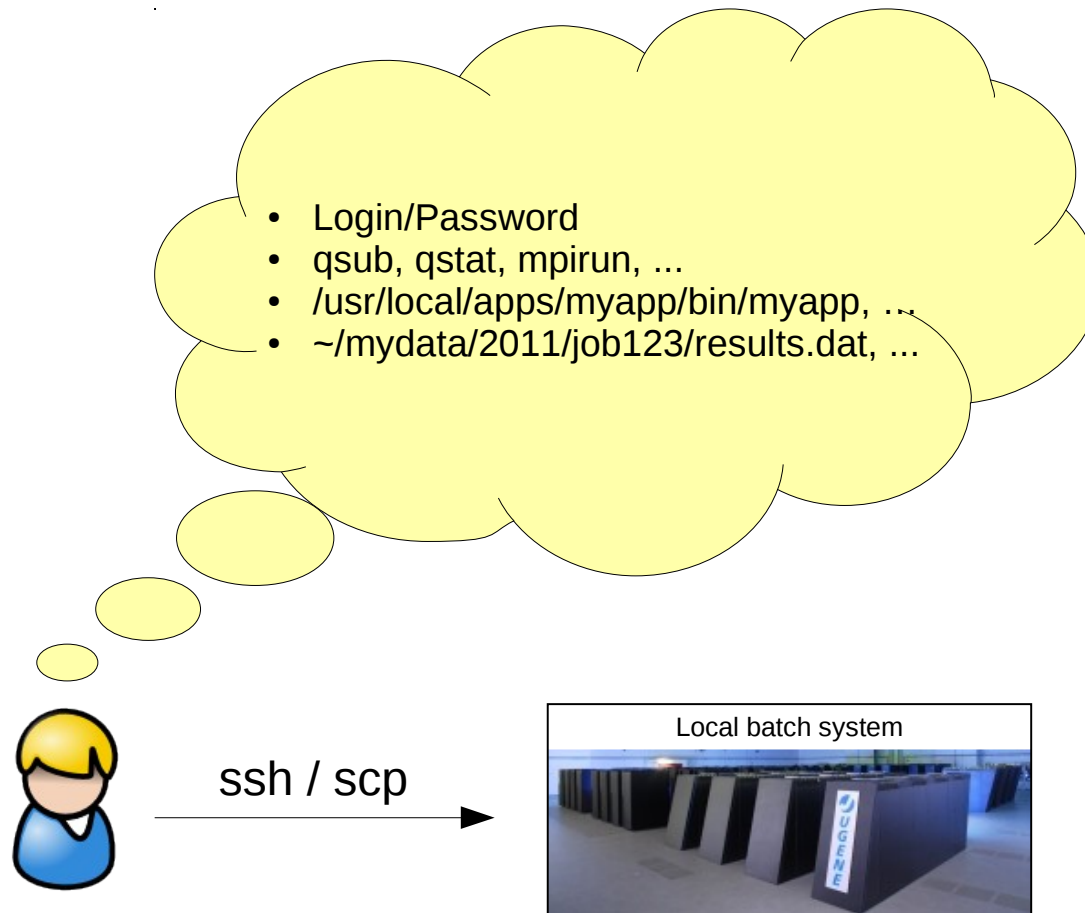
# OUTLINE

- The HPAC supercomputers

- UNICORE middleware – brief overview

- Hands-on

  - Jupyter notebooks

  - CSCS Piz Daint

# TRADITIONAL HPC USE

- Login/Password
- qsub, qstat, mpirun, ...
- /usr/local/apps/myapp/bin/myapp, ...
- ~/mydata/2011/job123/results.dat, ...

ssh / scp

Local batch system

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# HPAC

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

Visualisation Systems

Storage

UNIC☉RE

**Platform services, APIs, policies, support, ...**
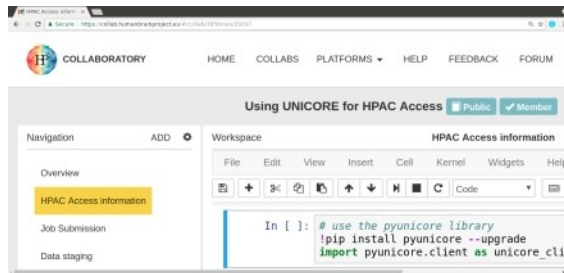
HPC, Storage, Cloud VMs

HPC, Storage

HPC, Storage
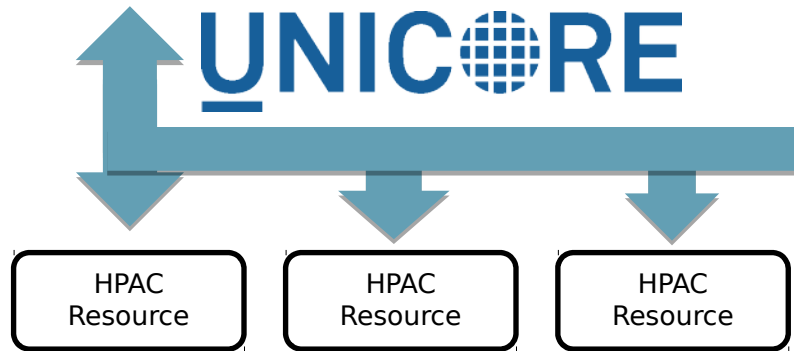
HPC, Storage, Cloud VMs

# SINGLE SIGN ON / COLLABORATORY



HBP accounts

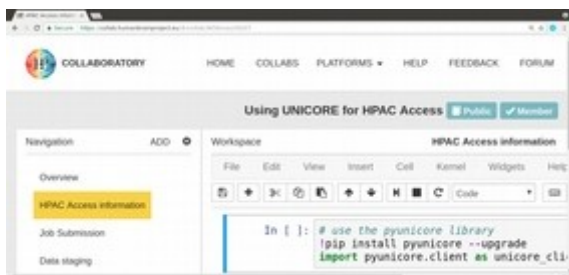- Single login with HBP account
- HBP account automatically mapped to local account
- Delegation – service can use other services on user's behalf

UNIC●RE

| HPAC Resource | HPAC Resource | HPAC Resource |
|---|---|---|

Site local accounts

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# ENABLE USER WORKFLOWS



HBP accounts

3. Use

**Visualization Service**

**CSCS**
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

1. Launch simulation

Data access

**HPC simulation**

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2. Results

**Storage**

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# KEY FEATURES

**UNIC⬦RE**

- 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, …)

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

Workflows    Jobs    Data Management    Discovery

**Services**

- Workflow enactment
- Task execution

- Job submission
- Job management
- Reservations

- Storages
- File transfer
- Metadata

- Service Registry
- Resource Broker

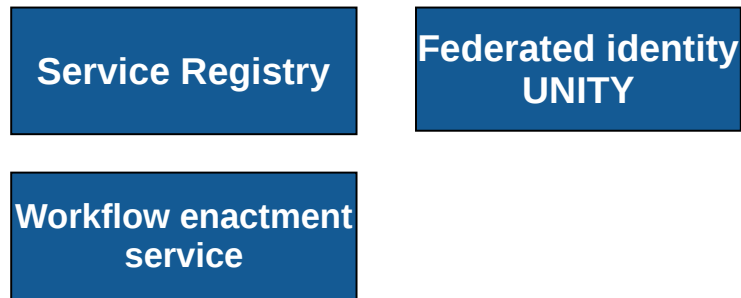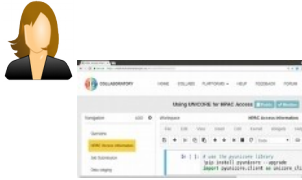JÜLICH
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Compute  Storage

## Resources

- Batch systems
  (Slurm, LSF, ...)

- SSH tunnel to remote servers

- Direct execution
  (e.g. on Windows)

- ... (extensible)

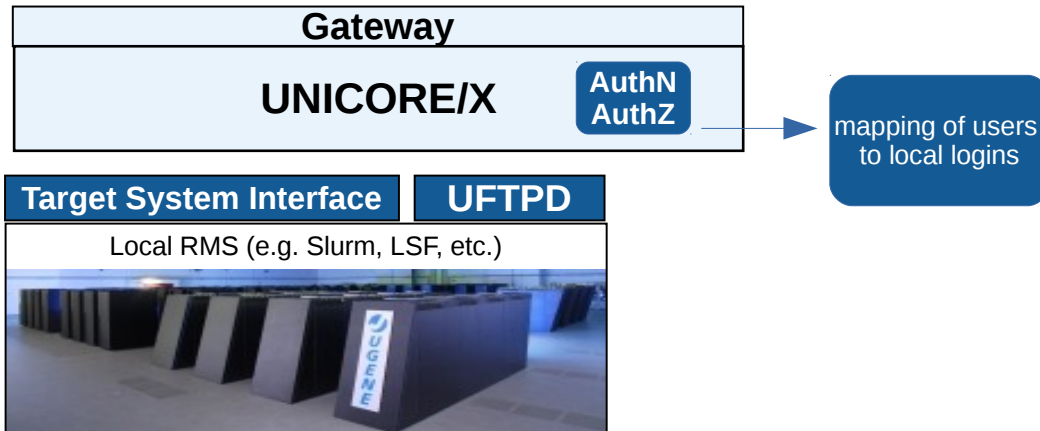- File systems

- S3, CDMI

- ... (extensible)

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# UNICORE COMPONENTS

Client tier

**Service Registry**

**Federated identity UNITY**

**Workflow enactment service**

Shared services (defining the federation)

**Gateway**

**UNICORE/X** | **AuthN AuthZ** → mapping of users to local logins

**Target System Interface** | **UFTPD**

Local RMS (e.g. Slurm, LSF, etc.)

Components at each HPC site

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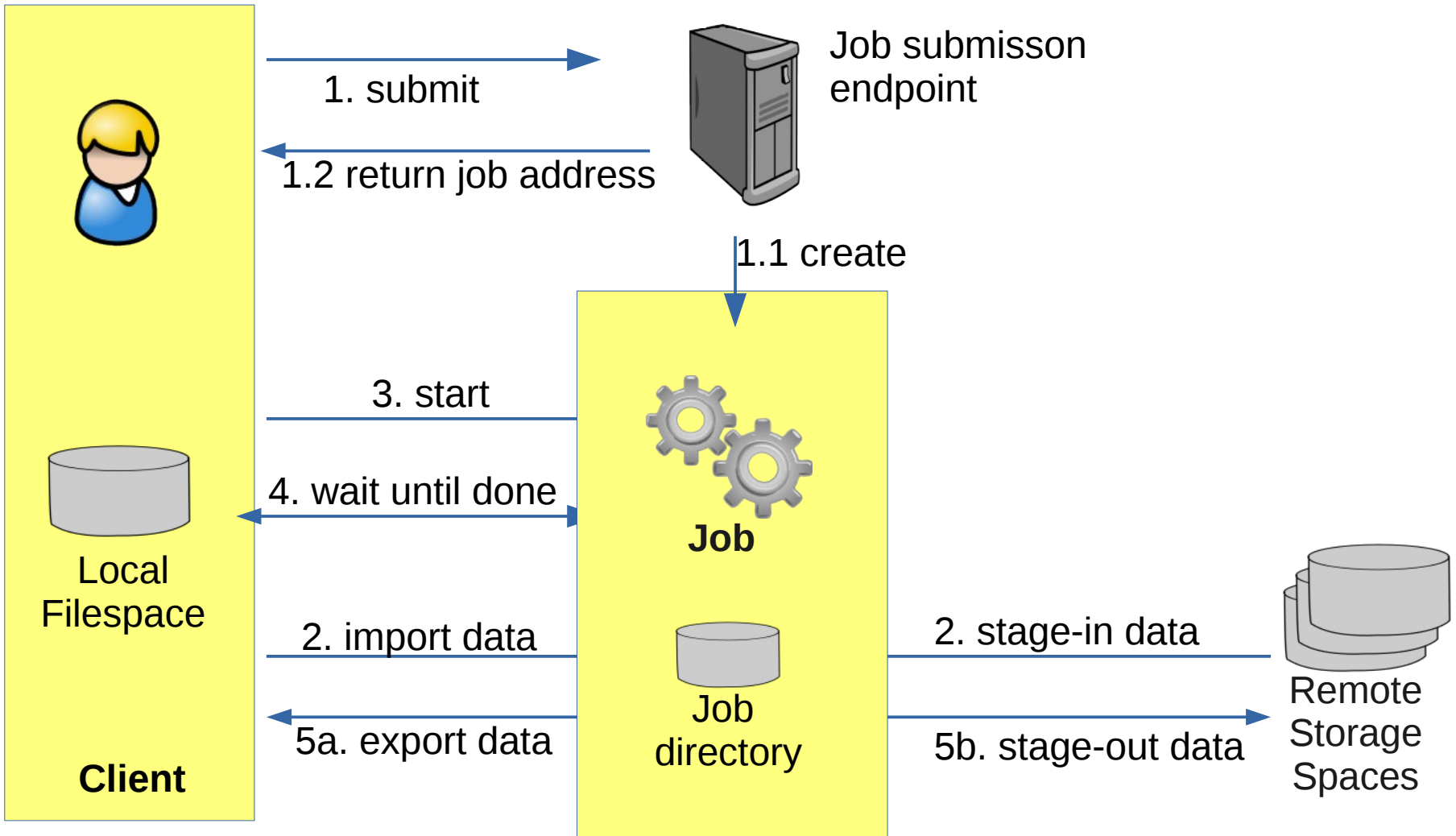
# RESOURCE MODEL

- UNICORE is resource / object oriented

  - E.g. a batch job or a storage

  - Endpoints / URLs with operations to manipulate them

  - Per-user, access-controlled
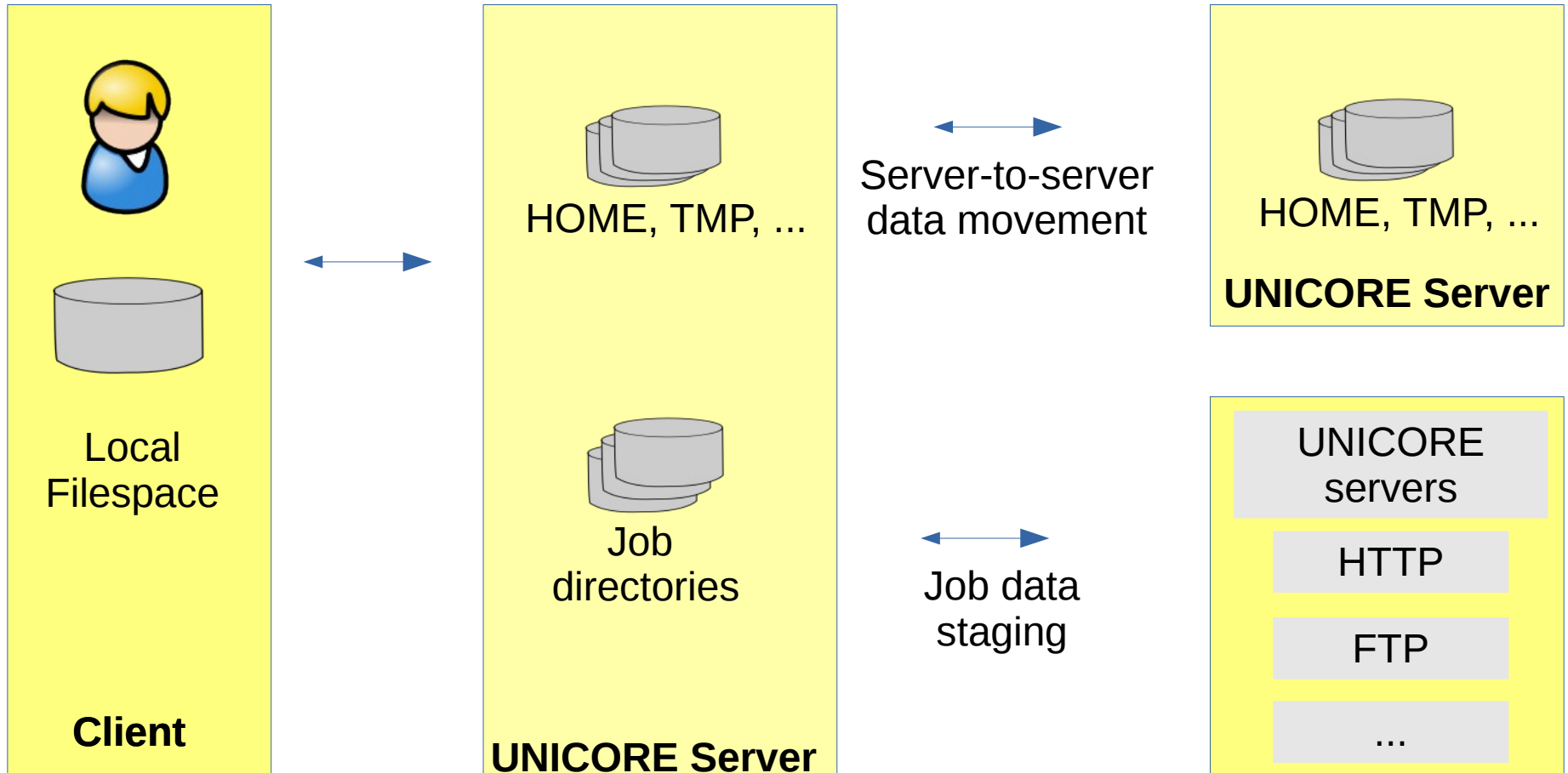
- APIs

  - SOAP / XML

  - REST / JSON

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# JOB EXECUTION

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- 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

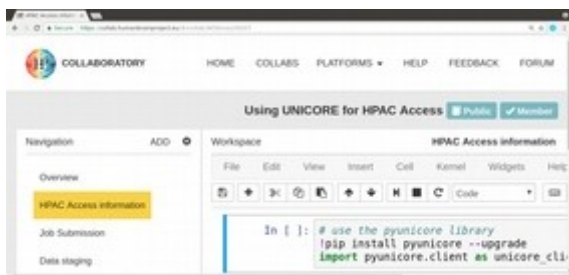- Jobs can be re-started (includes pre, main, post, stage-out)

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# DATA AND STORAGE SERVICES

# EXAMPLE USER WORKFLOWS

Jupyter notebook or app

HBP accounts

Visualization Service

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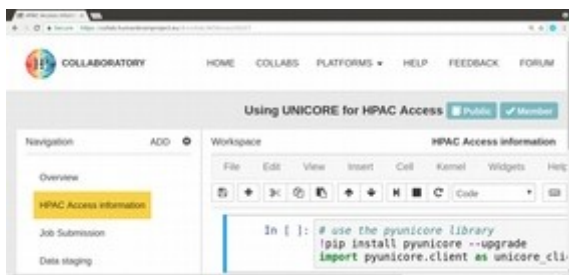
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# EXAMPLE USER WORKFLOWS



Jupyter notebook or app

HBP accounts

1. Launch simulation A

2. Launch task B

**HPC simulation**

**HPC simulation**

Access results from simulation A

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# 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 infrastucture need to work together to realise complex use cases

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# 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

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