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
ENABLE MULTISITE WORKFLOWS

1. Launch simulation
   - Jupyter notebook or app

2. Results
   - HPC simulation

3. Use
   - Visualization Service
     - CSCS
     - CINECA

Data access

HBP accounts
TRADITIONAL HPC USE

- Login & Password / ssh key
- sbatch, qsub, srun, mpirun, ...
- /usr/local/apps/myapp/bin/myapp, ...
- ~/mydata/2011/job123/results.dat, ...

Local batch system
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
...
ACCESSING A HPAC SITE

Login

HBP OIDC (v1)

HPAC Site

User authentication

Unity
(operated at JSC)

REST APIs

UNICORE

Job submission
Data access

Local user management
(authorization)

Target System Interface

UFTPD
KEY FEATURES

• 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

Client tier

Shared services (defining the federation)

Service Registry

UNITY Federated identity

Workflow enactment service

UNICORE Site

UNICORE Site

UNICORE Site

HBP OIDC (v1)

UNICORE Site

UNICORE HPC site(s)
• Open source (BSD license)
  https://www.unicore.eu
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**

1. submit
   - 1.1 create
     - Job directory
     - Job submission endpoint

2. import data
   - 2. stage-in data
     - Remote Storage Spaces

3. start

4. wait until done
   - 4. wait until done

5a. export data
   - 5a. export data

5b. stage-out data
   - 5b. stage-out data

**Client**

**Local Filespace**
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
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
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