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

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

Local batch system
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

UNICORE

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

HPC, Storage, Cloud VMs

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HPC, Storage, Cloud VMs

Mitglied der Helmholtz-Gemeinschaft
SINGLE SIGN ON / COLLABORATORY

- 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

1. Launch simulation

2. Results

3. Use

Data access

Visualization Service

HBP accounts

HPC simulation

Storage

CINECA

CSCS

Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre
KEY FEATURES

• 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, …)
• 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
- 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

Gateway

UNICORE/X

AuthN AuthZ

Target System Interface

UFTPD

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

mapping of users to local logins

Client tier

Shared services (defining the federation)

Components at each HPC site
RESOURCES 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

1. submit
1.2 return job address
3. start
4. wait until done
2. stage-in data
5a. export data
5b. stage-out data

Client
Local Filespace

Job submission endpoint

Job directory

Remote Storage Spaces
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

Local Filespace

Client

HOME, TMP, ...

Job directories

UNICORE Server

Server-to-server data movement

Job data staging

UNICORE Server

UNICORE servers

HTTP

FTP

...
EXAMPLE USER WORKFLOWS

1. Launch simulation

HPC simulation

2. Results

Visualization Service

Data access

3. Use

Jupyter notebook or app

HBP accounts
EXAMPLE USER WORKFLOWS

1. Launch simulation A

HPC simulation

Access results from simulation A

2. Launch task B

HPC simulation

HBP accounts

Jupyter notebook or app
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