UNICORE in the Human Brain Project

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Outline

- Motivation
- UNICORE overview
- REST API
- Deployment in the Human Brain Project
- Outlook
HBP Hardware infrastructure for High-performance computing

- HBP High Fidelity Visualisation Systems
- HBP Supercomputer
- HBP Molecular Dynamics Supercomputer
- HBP Massive Data Analytics Supercomputer
- HBP Cloud Storage
- HBP Development System

PRACE network
User access?

- Login/password or ssh key
- qsub, qstat, runjob, mpirun, ...
- Cores, nodes, GPUs, memory, ...
- /usr/local/apps/myapp/bin/myapp, ...
- ~/mydata/2016/job123/ergebnisse.txt, ...
User access?

How can I ...
- ... use multiple, heterogeneous systems seamlessly and securely
- ... manage my job input data and results?
- ... across systems? Workflows?
- ... integrate HPC/data resources into applications/portals?
A federation software suite

- Secure and seamless access to compute and data resources
- Java/Python based
- Complies with typical HPC centre policies
- Open source, BSD licensed
Services

- Workflow enactment
- Task execution
- TargetSystemFactory
- TargetSystem
- JobManagement
- Reservations
- StorageFactory
- StorageManagement
- FileTransfer
- Metadata
- Registry
- Resource Broker
- Batch systems
  (Torque, Slurm, LoadLeveler, GridEngine, ...)
- Apache Hadoop (YARN)
- Direct execution
  (e.g. on Windows)
- ... (extensible)

- File systems
- S3
- Apache HDFS
- CDMI
- ... (extensible)
Deploying UNICORE in HBP

- HBP Molecular Dynamics Supercomputer
- HBP Data Analytics Supercomputer
- HBP Development System
- HBP Supercomputer
- HBP Cloud Storage
Clients

- Portal
- Third-party science gateways
- UCC
- Eclipse-base Rich Client
- REST API
- Java API
Demo: using the REST API

- Using small UNICORE deployment on 'localhost'
1. Authentication

Token

OIDC Server

2. Use REST API for job submission, data movement etc.

3. Authentication, validate token

Unity

REST API

UNICORE

HBP Collaboratory and other clients / applications

HBP Molecular Dynamics Supercomputer

HBP Data Analytics Supercomputer

HBP Development System

HBP Supercomputer

HBP Cloud Storage

LDAP

BSC

CINECA

CSCS

JÜLICH

KIT
HBP single sign-on

- **Starting point: HBP account**
- **Authentication via Unity**
  - Required to access the services
  - Bridges UNICORE to HBP OIDC infrastructure
  - Supports REST, Web and SOAP/WS clients
- **Authorization**
  - Required to actually be able to consume resource
  - Users apply for and are granted resources (→ review process)
  - User IDs and groups are mirrored to HPC sites (LDAP), access via UNICORE is configured automatically
Running NEST on a HPC machine

- Login via ssh to JUQUEEN
- Manage working directory, code, input params
- Create/submit LoadLeveler script

```bash
#@job_name         = slns_demo
#...
#@bg_size             = 32
#@wall_clock_limit = 00:10:00

module load python3/3.4.2
export TMPDIR=$WORK/tmp
export PYTHONPATH=/homeb/slns/slns007/local/opt/...

runjob --ranks-per-node 1 --exp-env ... : /bgsys/.../python3 microcircuit.py
```
Admin defines UNICORE Application “NEST” for JUQUEEN

```xml
<idb:IDBApplication>
  <idb:ApplicationName>NEST</idb:ApplicationName>

  <jsdl:POSIXApplication>
    <jsdl:Executable>runjob --ranks-per-node 1 --exp-env ... : .../python3</jsdl:Executable>
    <jsdl:Argument Type="filename">$NESTCODE?</jsdl:Argument>
    <jsdl:Argument Type="filename"># $PARAMETERS?</jsdl:Argument>
  </jsdl:POSIXApplication>

  <idb:PreCommand>#@environment = COPY_ALL</idb:PreCommand>
  <idb:PreCommand>module load python3/3.4.2</idb:PreCommand>
  <idb:PreCommand>export TMPDIR=$WORK/tmp</idb:PreCommand>
  <idb:PreCommand>export PYTHONPATH=/usr/local/...:$PYTHONPATH</idb:PreCommand>

  <idb:PostCommand>find -name *gdf | xargs zip output.zip</idb:PostCommand>
</idb:IDBApplication>
```
Running NEST via UNICORE

- Complexity is now on hidden by UNICORE
- **Users** can use a UNICORE Application “NEST” and need only provide relevant data

```json
{
  ApplicationName: NEST,

  Parameters: [
    NESTCODE: microcircuit.py, PARAMETERS: parameters.py,
  ],

  Imports: [ ... ],

  Resources: { Nodes: 32, Runtime: 1200 },
}
```
Outlook: The UNICORE deployment in HBP

- Deploy the Workflow system
  - Useful for automation tasks
  - Required e.g. by the Polarized Light Imaging (PLI) use case
  - REST API available for workflow submission and management
- Analyse and realise data management use cases
- Integrate neuromorphic systems
Outlook: Collaboratory integration

- Task framework
  - THE way to integrate scientific computations into the Collaboratory
  - Autogenerated Web UI, provenance support etc
  - But: currently only uses local resources

- HPC support in the Collaboratory
  - Via UNICORE
  - OIDC support, REST API
  - Job submission and management
  - Data management
Summary

- **UNICORE**: **Secure** and **easy** access to HBPs compute and storage resources
- Compute and storage abstractions. Acts as **integration layer** for a unified view on the underlying resources
- **Single sign-on** via HBP OIDC infrastructure

... more on UNICORE: http://www.unicore.eu