2015 HBP SUMMIT

COLLABORATE
BUILD
SHARE

ICOMEM, MADRID SPAIN 27-30 SEPTEMBER
UNICORE in the Human Brain Project

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Jülich Supercomputing Centre
Hardware infrastructure

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

Internet

PRACE network
Systems access?

- Login/password or ssh key
- `qsub`, `qstat`, `runjob`, `mpirun`, ...
- Setting cores, nodes, memory, ...
- `/usr/local/apps/myapp/bin/myapp`, ...
- `~/mydata/2011/job123/ergebnisse.txt`, ...
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?
1. authenticate
   returns OIDC token

OIDC server

3. pass OIDC token
   returns signed SAML

Unity

3.1 validate OIDC

Collaboratory, other portals and applications

2. access REST APIs
   pass OIDC token

REST API

SOAP/WS API

UNICORE

BSC
HPC site

CINECA
HPC site

CSCS
HPC site

JSC
HPC site

KIT
S3 storage
Single sign-on

- Unity
  - Bridges UNICORE to HBP OIDC infrastructure
  - Supports REST and Web clients
  - Support for SOAP/WS clients (legacy)

- User management
  - Users are granted resources (-> review process)
  - User IDs and groups are mirrored to HPC sites (LDAP)
  - Access via UNICORE is configured automatically

- Go get an HBP account and compute time!
Running NEST - without UNICORE

- 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
```
Running NEST - using UNICORE

- Complexity is now hidden by UNICORE
- User can use a UNICORE Application “NEST”
- User need only invoke the application and provide relevant data

ApplicationName: NEST,

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

Imports: [ ... ],

Resources: { Nodes: 32, Runtime: 1200 }
Running NEST - using UNICORE

- 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>
```
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 and REST API are available
  - Job submission and management is very easy
  - Data management needs to be better defined
Summary

- Secure and easy access to HPC compute and storage resources
- UNICORE provides compute and storage abstractions. Acts as integration layer for a unified view on the underlying resources
- Allows integration of HCP/Storage into custom applications using the REST API
- HBP single sign-on via OIDC supported

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