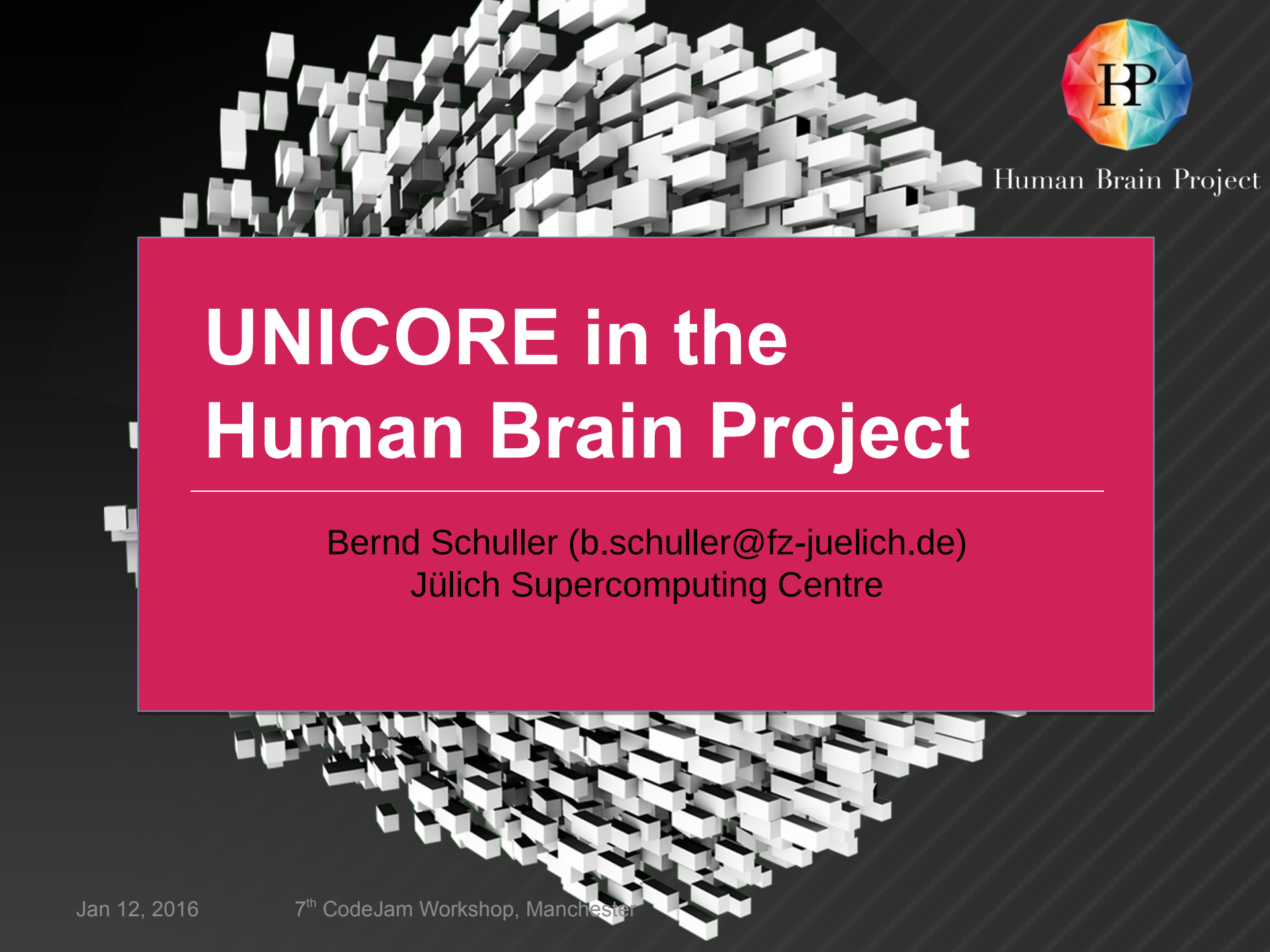

UNICORE in the Human Brain Project

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Outline

- Motivation
- UNICORE overview
- REST API
- Deployment in the Human Brain Project
- Outlook

HBP Hardware infrastructure for High-performance computing

Human Brain Project

HBP High Fidelity Visualisation Systems

RWTH AACHEN UNIVERSITY

HBP Cloud Storage

KIT Karlsruhe Institute of Technology

HBP High Fidelity Visualisation Systems

EPFL ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

dedicated

Internet

dedicated

HBP Supercomputer

JÜLICH FORSCHUNGSZENTRUM

HBP Molecular Dynamics Supercomputer

BSC Barcelona Supercomputing Center Centro Nacional de Supercomputación

HBP Massive Data Analytics Supercomputer

HBP Development System

CSCS Centro Svizzero di Calcolo Scientifico Swiss National Supercomputing Centre

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, ...

ssh / scp

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?

UNICORE

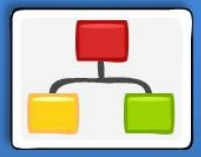

Web


Command line


GUI

API

Clients


Workflows


Jobs


Data Management


Discovery

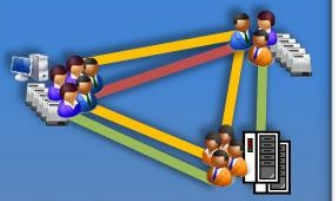
Services


Compute


Storage

Resources


Users


Federations


Policies

Security

UNICORE

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

- 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

Human Brain Project

UNICORE

HBP Molecular Dynamics Supercomputer

HBP Data Analytics Supercomputer

HBP Development System

HBP Supercomputer

HBP Cloud Storage

- 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'

HBP Collaboratory and other clients / applications

1. Authentication

Token

OIDC Server

LDAP

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

3. Authentication, validate token

Unity

REST API

UNICORE

HBP Molecular Dynamics Supercomputer

HBP Data Analytics Supercomputer

HBP Development System

HBP Supercomputer

HBP Cloud Storage

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

```
#@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
```

Configuring NEST in UNICORE

- **Admin** defines UNICORE Application “NEST” for JUQUEEN

```
<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

```
{
   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