FEDERATED COMPUTING

with UNICORE

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OUTLINE

- Federating HPC with UNICORE and Unity
- Administrative concerns
- Use cases at JSC and their implementation
- Outlook on UNICORE 8

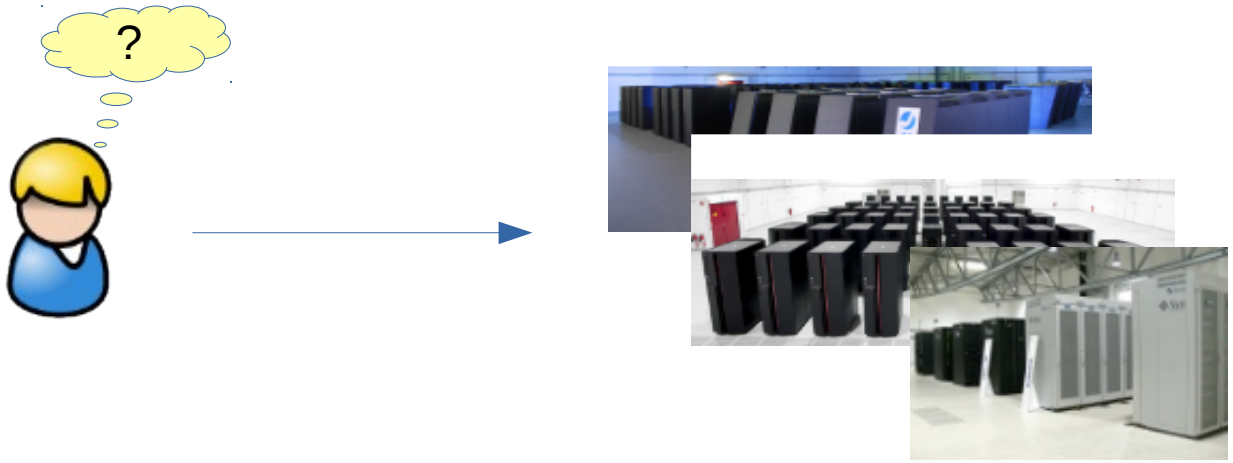
MOTIVATION

- Login/Password
- qsub, qstat, mpirun, ...
- /usr/local/apps/myapp/bin/myapp, …
- ~/mydata/2011/job123/ergebnisse.txt, ...

ssh / scp

Local batch system LoadLeveller

MOTIVATION



How can I…

- … use multiple, heterogeneous systems seamlessly?
- … manage my job input data and results?
- … across systems? Workflows?
- ... integrate HPC into custom applications and portals?

UNICORE


Web


Command line


GUI

API

Clients


Workflows


Jobs


Data Management


Discovery

Services


Compute


Storage

Resources


Users


Federations


Policies

Security

UNICORE KEY FEATURES

- A set of software components for integration of HPC into federated environments
- Federated authentication, local authorization, site keeps full control
- REST APIs for jobs, data, workflows
- Simplifies HPC use for non-experts (Application concept, abstract resource model, workflow templates, …)
- Flexible and non-intrusive
- Independence of the OS and batch system

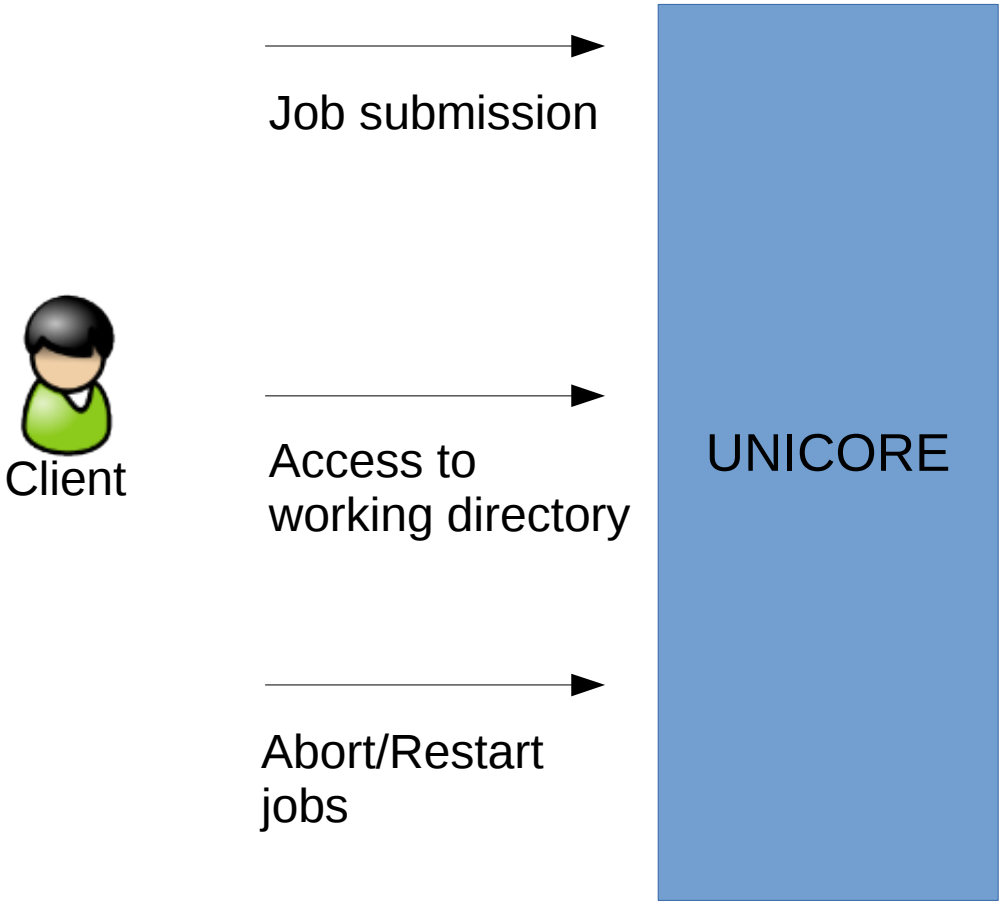
- Workflow enactment
- Task execution

- Job submission
- Job management
- Reservations

- File systems
- Storage access
- Metadata
- File transfers

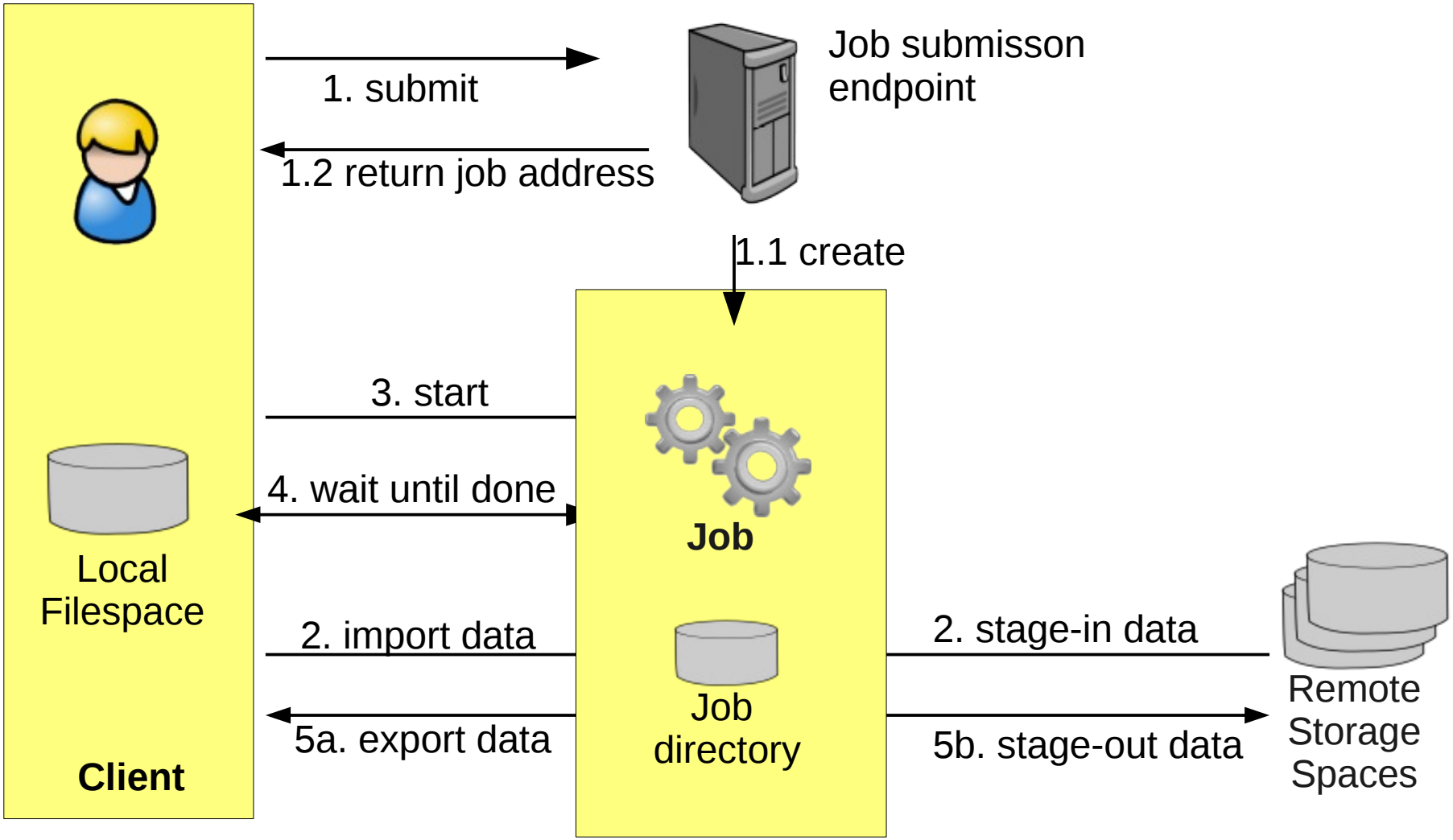
- Service registry
- Resource brokering

JOB SUBMISSION AND MANAGEMENT



- Cluster managers (Slurm, LSF, …)
- YARN
- SSH tunnels

JOB EXECUTION



UNICORE'S "APPLICATION" CONCEPT

To setup a simulation run you need to ...

- … manage working directory, code, input params
- … create and submit batch scheduler 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
```

UNICORE'S "APPLICATION" CONCEPT

- Admin (or power user) defines UNICORE application

```
<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>
```

UNICORE'S "APPLICATION" CONCEPT

Complexity is now hidden!

- Users need only provide *relevant* parameters
- … jobs can even be 100% the same on different compute clusters

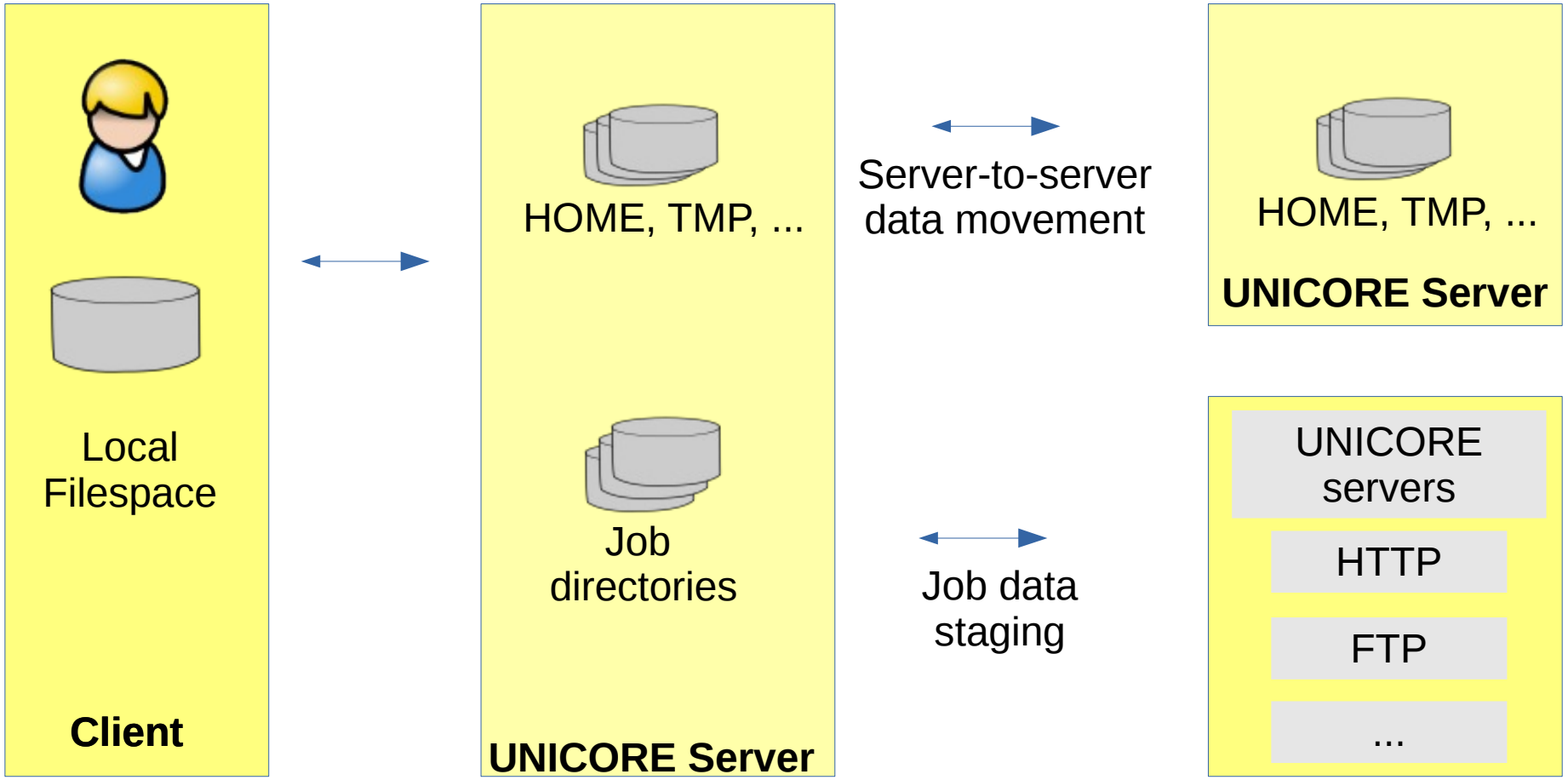
```
{
   ApplicationName: NEST,

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

   Imports: [ ... ],

   Resources: { Nodes: 32, Runtime: 1200 },
}
```

DATA AND STORAGE SERVICES



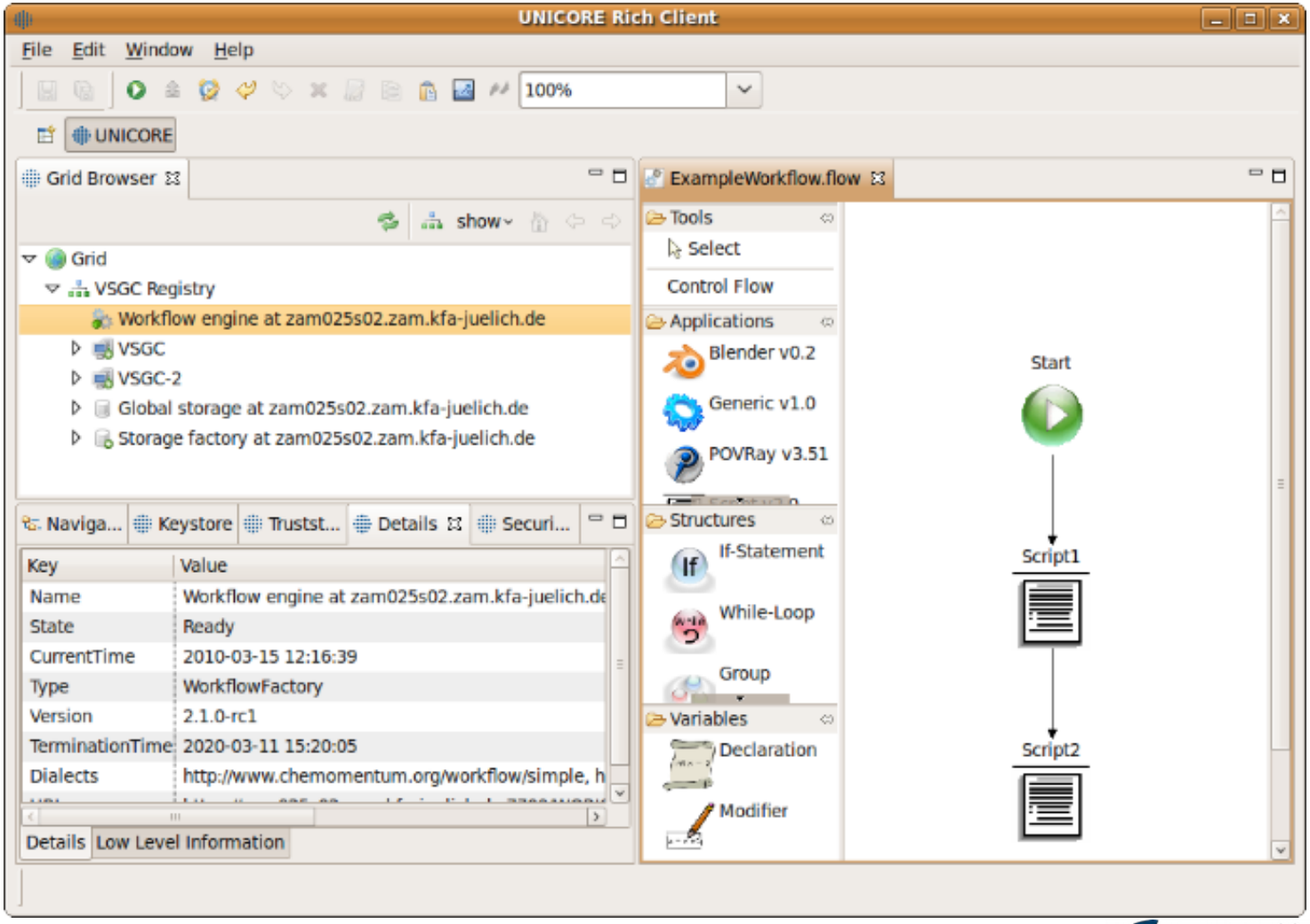
DATA MANAGEMENT FEATURES

- Posix-like operations (ls, stat, mkdir, cp, rm, …)
- File transfers (client-server, server-server)
- Metadata management
  - Schema-free, key-value
  - Indexed via Lucene, searchable
- Rule-based data processing
  - New files automatically trigger actions
  - Possible use cases: file registration, metadata extraction, compression, etc

WORKFLOWS

- Built on single jobs
- Powerful constructs
  - Graphs
  - Loops
  - Conditions, variables
  - Hold/continue (with variable changes)
- Data management
  - Input / output / intermediate files

WORKFLOW EDITOR

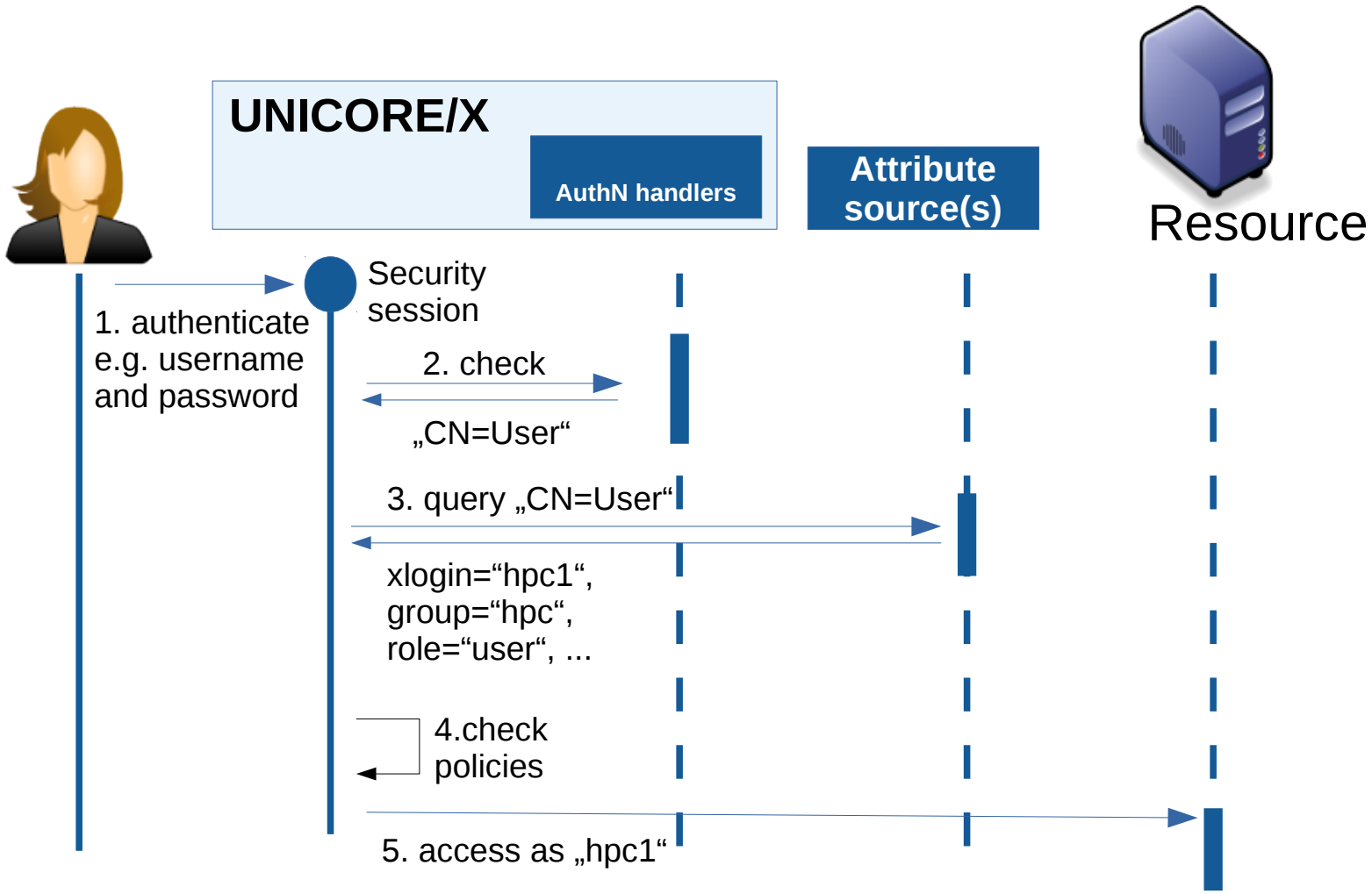


SECURITY, AUTHENTICATION, ETC.

USER AUTHENTICATION

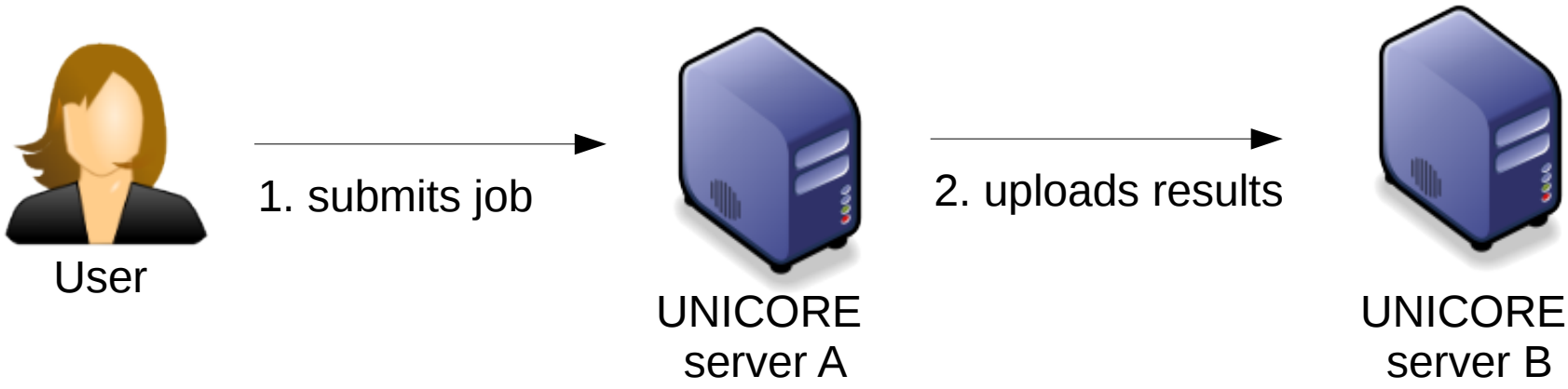
- Via Unity
  - Username/password (PAM, LDAP, Unity internal)
  - OAuth
  - SAML IdPs
- X509 certificates (better not)

AUTHN / AUTHZ FLOW



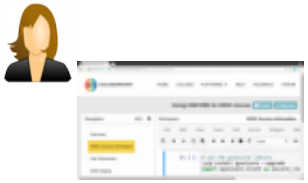
DELEGATION

- Allows services to work on behalf of the user
- Without storing and passing actual user credentials
- SAML-based (SOAP/WS)



DEPLOYMENT

UNICORE COMPONENTS



Client tier

Workflow service

Service orchestrator

Service Registry

Federated identity UNITY

Shared services (federation)

UNICORE/X

Target System Interface

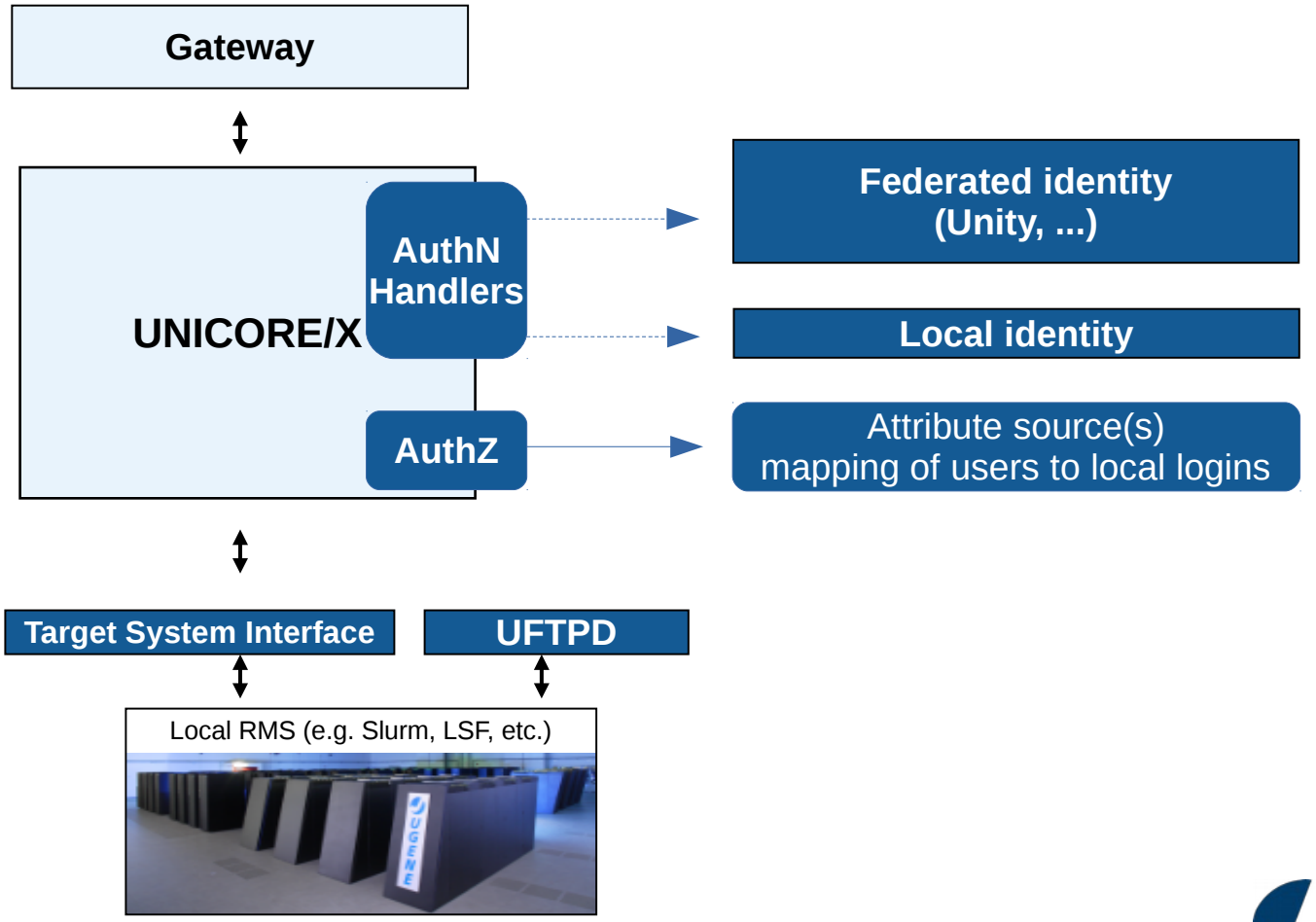
UFTPD

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

Components at the HPC site

UNICORE COMPONENTS

- Access to a single cluster



COMPONENT OVERVIEW / DEPLOYMENT

- **Gateway (optional)**
  - „Firewall entry point“ for all client requests
  - Gateway address must be accessible for clients and for UNICORE/X server – all other components can run in the intranet
  - Used to access multiple servers „behind“ it (multiple UNICORE/X, Registry, Workflow, …)

- **UNICORE/X**
  - Main server, connects to all other components
  - One UNICORE/X per resource (i.e. cluster + associated file systems) is required
  - Requires memory and processing power

COMPONENT OVERVIEW / DEPLOYMENT

- **TSI (target system interface)**
  - Needs to be installed on the resource (e.g. cluster login node)
  - Needs access to file systems, resource management system (submit jobs, check queues etc)
  - Needs to run as root for multi-user operation

- **UFTPD (UNICORE file transfer protocol daemon) (OPTIONAL)**
  - High-performance file transfer daemon
  - Similar requirements as TSI: runs as root on a cluster access node
  - UFTPD „listen“ port must be accessible from the internet, firewall must be configured for FTP)

COMPONENT OVERVIEW / DEPLOYMENT

- **XUUDB („Extended UNICORE user database“) (OPTIONAL)**
  - Default attribute source
  - Maps Grid users to local Unix accounts and roles (user, admin, ...)
  - Can be used by multiple services at a site (multiple UNICORE/X, Registry, Workflow etc)

- **Registry (OPTIONAL)**
  - Useful when more than one resource are to be accessed via UNICORE
    - At a single site
    - In a larger, multi-site installation
  - Very much like UNICORE/X in terms of configuration (except it does not connect to a TSI or UFTPD)

COMPONENT OVERVIEW / DEPLOYMENT

- **Workflow server (OPTIONAL)**
  - Workflow submission and management interfaces
  - Workflow enactment
  - Very similar to a UNICORE/X server

- **Service Orchestrator (OPTIONAL)**
  - Resource broker
  - Executes single workflow tasks (jobs)
  - Very similar to a UNICORE/X server

COMPONENT OVERVIEW / DEPLOYMENT

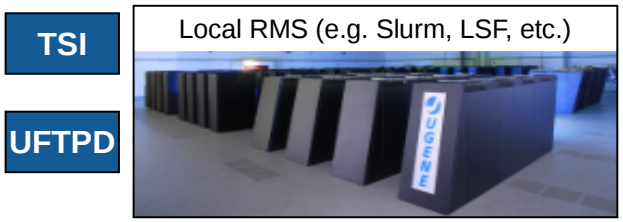
- **Unity (federated identity) (OPTIONAL)**
  - Maps authentication options to Grid users
    - SAML, username/password, OAuth, …
    - Integration with third-party AAI systems (e.g. EduGAIN)
  - Can be used by all UNICORE/X-like services in the Grid
- Must: configure Unity public key as „trusted SAML issuer certificate“ in all UNICORE/X servers
- Optional: REST API authentication in UNICORE/X

PERFORMANCE NOTES

- More than one UNICORE service can be installed on a single machine
- Choose machines that can stand the expected load
- Especially UNICORE/X, Workflow, Service Orchestrator require memory and CPU (512 MB per component, 2 cores per component)
- UNICORE/X, Workflow, Service Orchestrator require storage for their state
  - File system (simple, but creates load)
  - MySQL server (reduces load)

MINIMAL

- Single cluster accessed via UNICORE
- One Linux machine for Grid components
  - Gateway (optional), UNICORE/X
- Cluster frontend node
  - TSI, UFTPD (optional)



STORAGES CONFIGURATION

- Configure directories that can be used as UNICORE storages
  - WORK, SCRATCH, HOME, …
- „Storage factory“ service
  - Allows users to create storage instances dynamically
  - Think remote „mkdir“ on a shared space
  - Good for temporary data
  - Recommended if a workflow system is to be used
  - Should be installed only on systems with large and fast storage capacity

FILE TRANSFER: UFTP

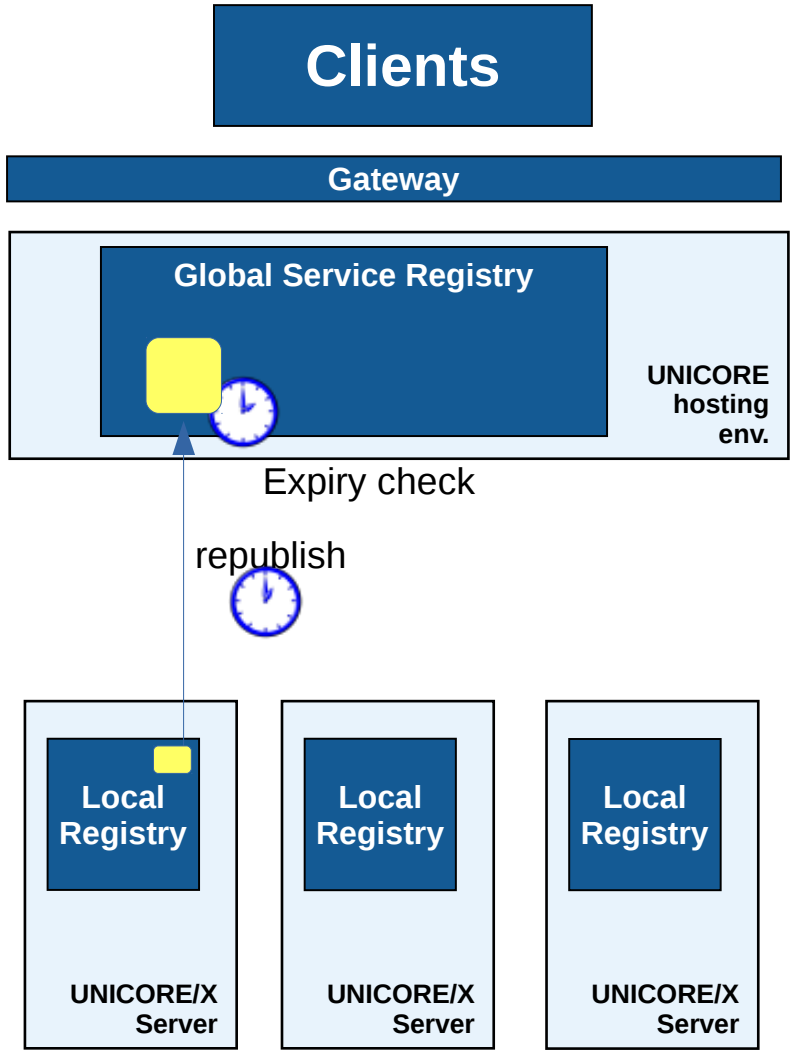
- Default file transfer through HTTPS: simple (zero config) and reasonably fast (some MB/sec.)
- High performance option: UFTP („UNICORE FTP“)
- Warmly recommended for environments / users who want to move lots of data
- Requires additional server (UFTPD) on a system with access to the filesystems (e.g. login node)
- Fast (typically many 10s of MB/sec) on single files
- UFTPD is a separate download (tgz, rpm, deb) and comes with detailed installation instructions

ATTRIBUTE SOURCES

- Mapping of Grid identity (DN) to local attributes (role, local Unix login, local Unix groups)
- Currently three options exist
  - File: simple, easy to use, local to a UNICORE/X
  - XUUDB: web service interface, can be used by multiple UNICORE/X servers at a UNICORE site, admin commandline tool
  - Unity: SAML web service interface, can be used by all sites in a UNICORE Grid, very powerful, but complex
- Attribute sources can be chained for maximum flexibility and administrator control
- Full details are given in the UNICORE/X manual

REGISTRY

- Aggregates service information from multiple UNICORE sites
- An Entry contains at minimum:
  - Service address
  - Service type
  - Server DN
- Content is held up-to-date
  - Services register with local registry
  - Local registries push info to global registry
  - Entries in global registries expire if not re-published in time



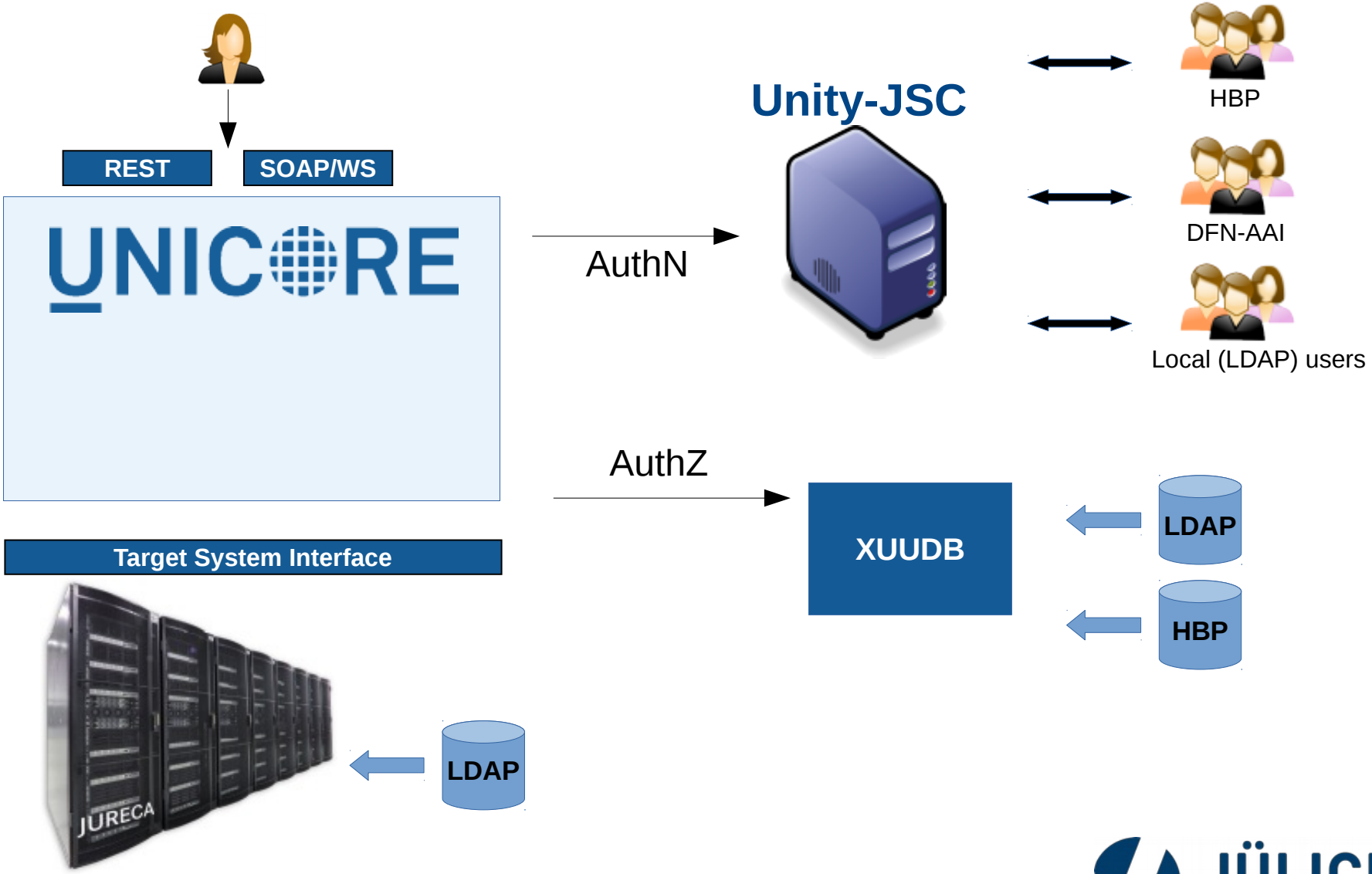
UNICORE @ JSC

UNICORE @ JSC

End-user clients
(ucc, Rich Client, ...)

Human Brain Project

UNICORE @ JSC


REST
SOAP/WS
UNICORE
AuthN
Unity-JSC
HBP
DFN-AAI
Local (LDAP) users
AuthZ
XUUDB
LDAP
HBP
Target System Interface
JURECA
LDAP

UNICORE @ JSC

- Authentication via Unity
  - Multiple user communities served via different endpoints
  - E.g. HBP users vs Jupyter users
- Authorization: automated management of entries in UNICORE’s user database
- JSC HPC LDAP / user DBs as primary information source

UNICORE @ JSC

- One UNICORE/X per system (JURECA, JUWELS, …)
  - Shared XUUDB
  - Shared MySQL for persistence
- Multiple Registry instances (HBP, FZJ …)
- Multiple workflow service instances (HBP, FZJ, ...)
- Single UFTPD instance accessing the (shared) GPFS

EXAMPLE USE CASE: JUPYTERHUB

- Goal: secure and easy-to-use setup for accessing JSC's machines via Jupyterhub

- Authentication
  - Users log in with JSC LDAP username/password

- Authorization
  - XUUDB User DB entries taken from JSC LDAP (automated)

SUMMARY: UNICORE FOR FEDERATING HPC

- Main challenges
  - Open up HPC to non-traditional use cases
  - Access from community portals like HBP Collaboratory
  - Data sharing
- Solutions
  - UNICORE – compute, storage, workflows
  - Unity – federated identity management
  - UFTP – high-performance data transfer with sharing capabilities

OUTLOOK: UNICORE 8

- Reduce complexity
- Strengthen core use cases
- REST API as the primary API

REDUCE COMPLEXITY

- Remove some unused features

- Simplify config files
  - Remove internal details, simple property format

- Back-end resource definition and description
  - Introduce simpler format (JSON)
  - Auto-generate e.g. from Slurm information

REDUCE COMPLEXITY

- Simplify workflow system
  - Drop “tracer” component
  - Join Workflow/Servorch components by default

- Out-of-the-box RESTful authentication without Unity
  - PAM module (username/password)
  - SSH keys support

STRENGTHEN CORE USECASES

- Model current clusters
  - Heterogeneous, modular, many partitions and node types
- Improve abstract batch submission
  - extend “Application” concept
- Support low-level batch system interaction
  - Sometimes UNICORE is the only way for a user to access the system. We do not want to limit what the user can do.

REST API AS PRIMARY API

- Full support for delegation
  - Using JWT (“JSON web tokens”) specification
- Dual SOAP/REST clients
- SOAP APIs will be dropped in UNICORE 9

UNICORE 8 ROADMAP

- 7.x maintenance mode – further releases only as necessary
- First release of UNICORE 8 planned for Spring/Summer 2019