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UNICORE

JÜLICH
FORSCHUNGSZENTRUM

Data management and data processing using UNICORE

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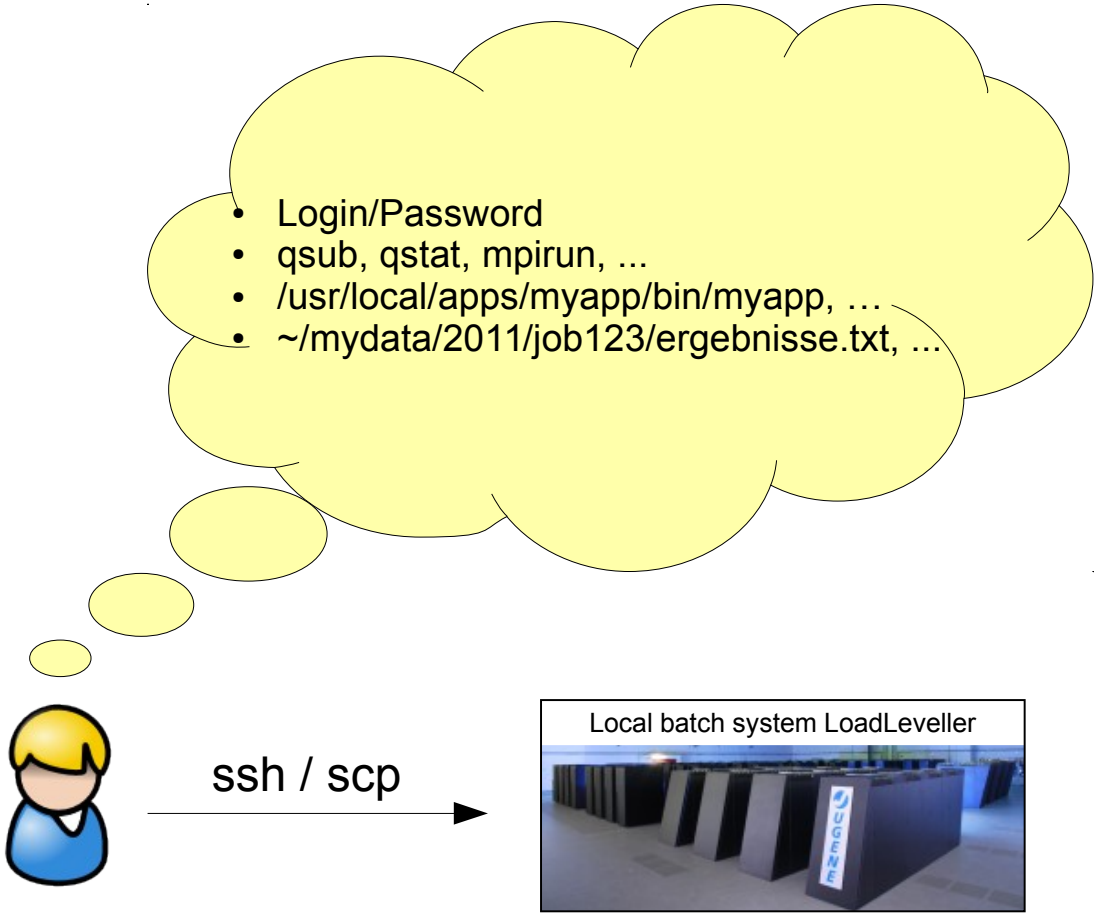
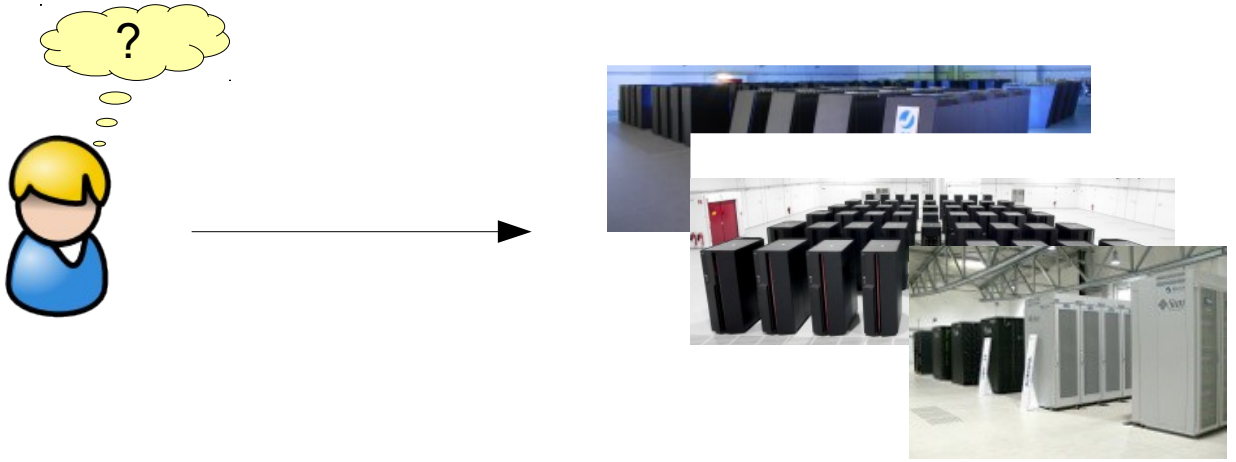
ScaDS Herbstschule, Dresden

Outline

- UNICORE
  - Overview, services, security, clients, ...
- Data management
  - Services, storage backends, …
    - *Demo*
- Processing
  - Jobs, workflows and all that
    - *Demo*
  - Data-driven processing
    - *Demo*


Login/Password
qsub, qstat, mpirun, ...
/usr/local/apps/myapp/bin/myapp, …
~/mydata/2011/job123/ergebnisse.txt, ...
ssh / scp
Local batch system LoadLeveller
JUGENE



How can I ...

- … use multiple, heterogeneous systems seamlessly,
- … manage my jobs
- … manage input data and results? Metadata?
- … across systems? Workflows?

UNICORE

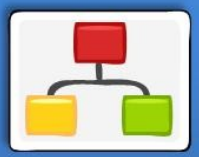

Web


Command line


GUI

API

Clients


Workflows


Jobs


Data Management


Discovery

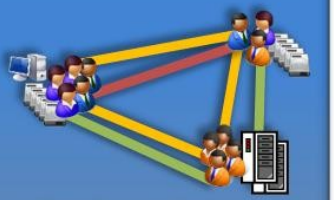
Services


Compute


Storage

Resources


Users


Federations

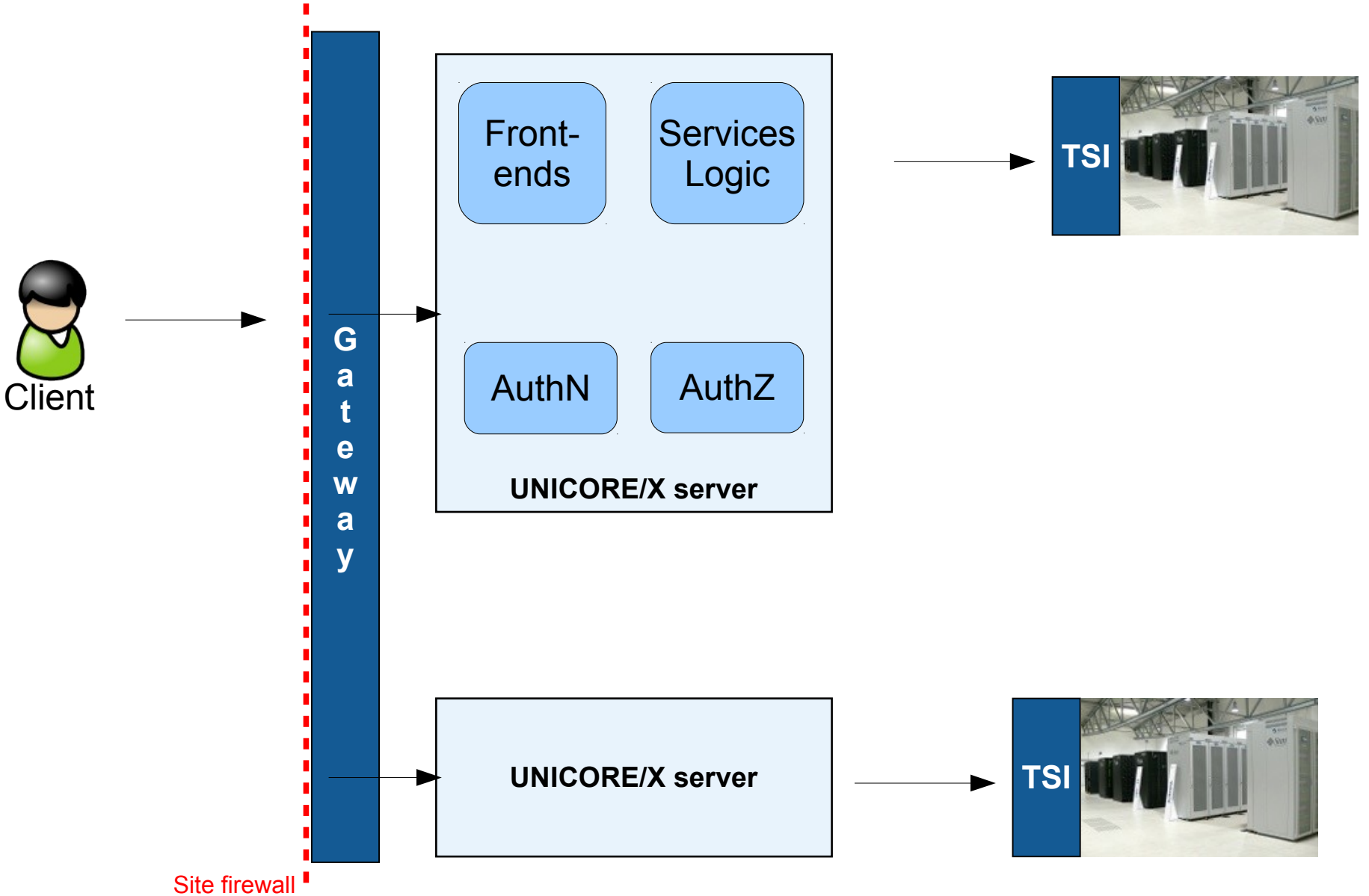

Policies

Security

A (subjective) UNICORE timeline

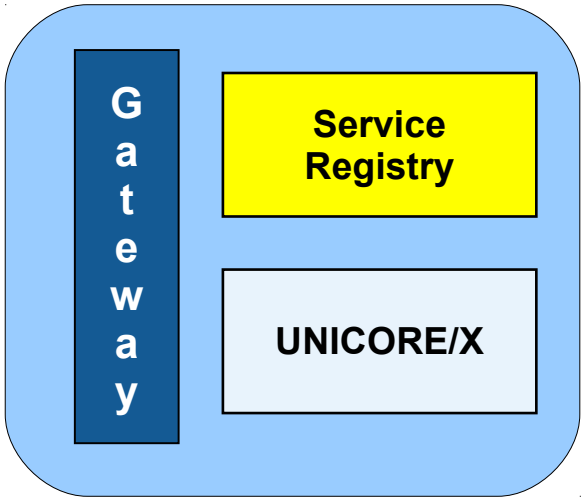
- **1996**: first UNICORE project (Germany only)
- **2002: UNICORE 5** → Eurogrid project, UNICORE goes Open Source (I started to work at Jülich on the OpenMolGRID project)
- 2005: UniGRIDS project : SOAP/WS(RF) interfaces defined, **2007: UNICORE 6.0** release
- **2014: UNICORE 7.0** release
  - … we're still going (thanks to projects and institutional funding)
- 2016 UNICORE 8 release?

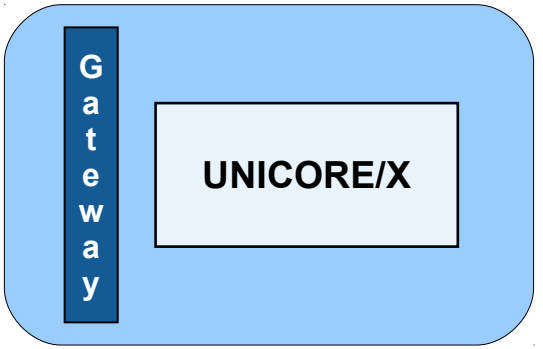
Components at a typical site

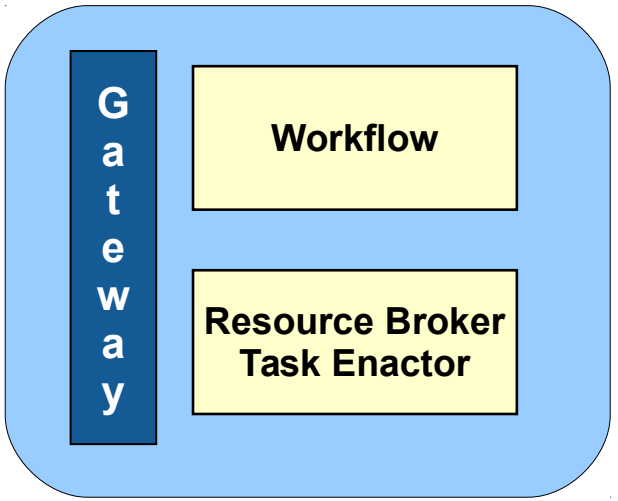


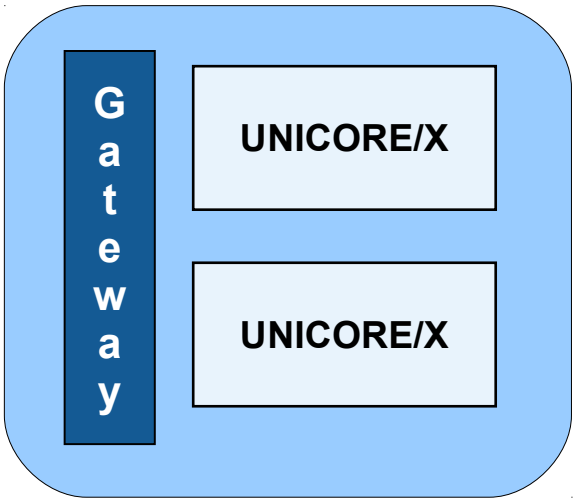
A UNICORE Grid ...

Clients

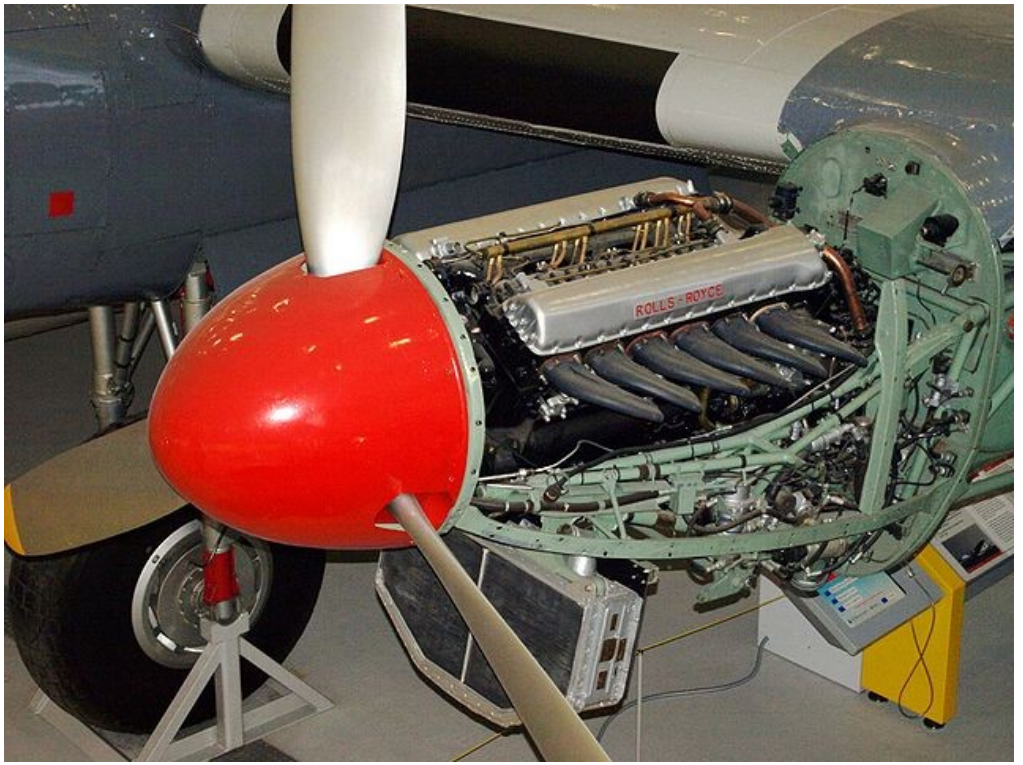








UNICORE : under the hood



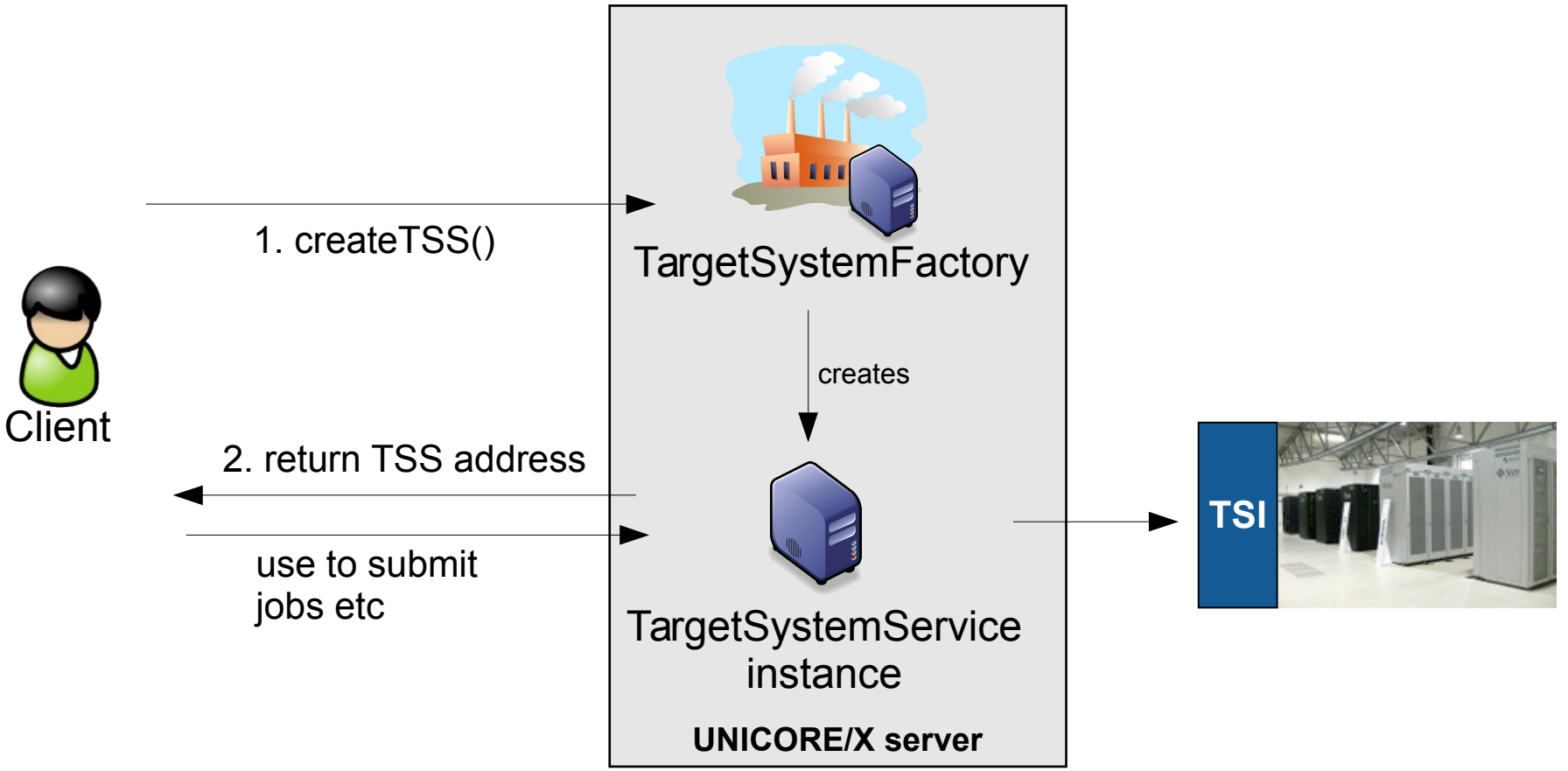
- Workflow enactment
- Task execution

- TargetSystemFactory
- TargetSystem
- JobManagement
- Reservations

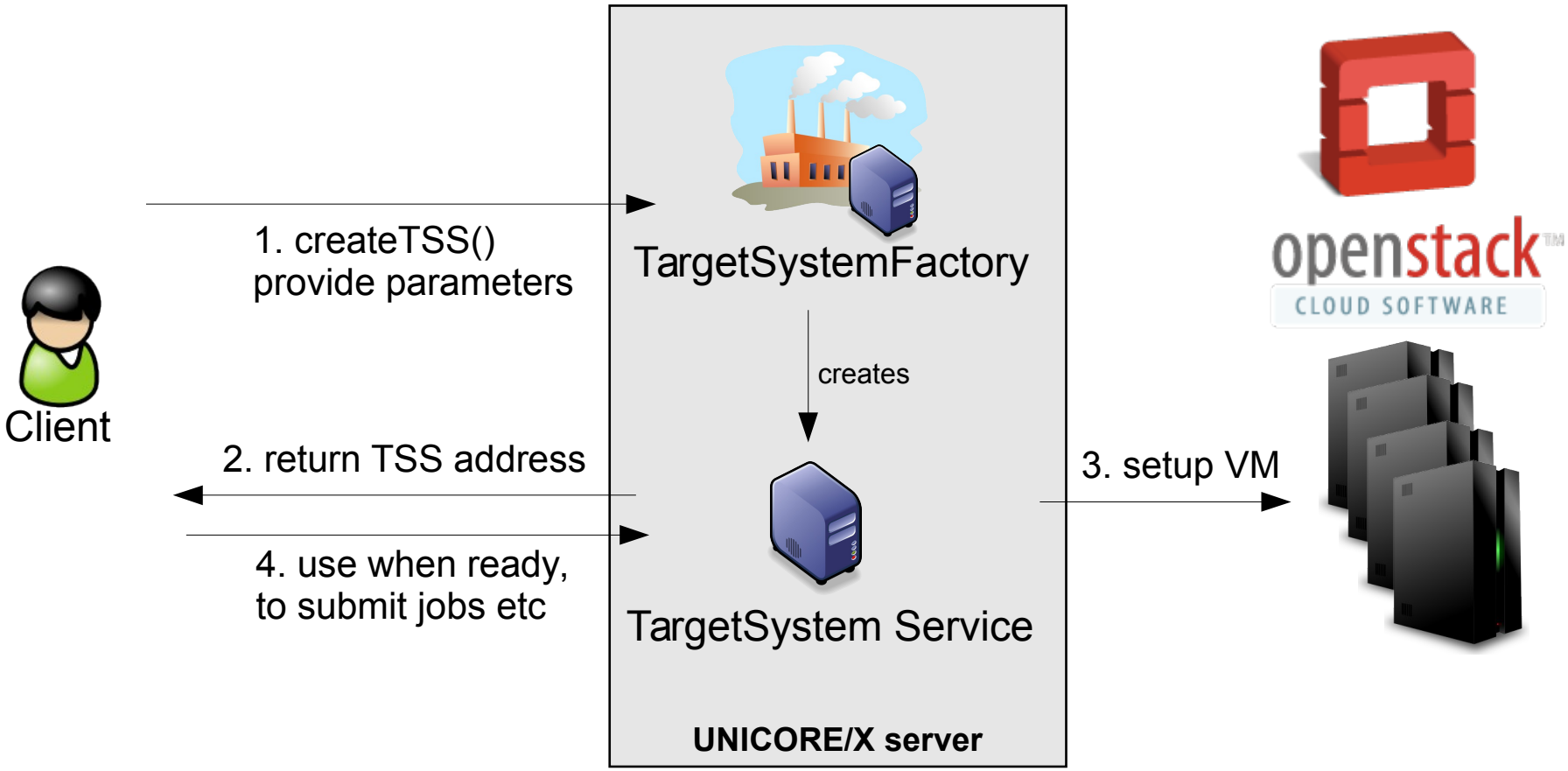
- StorageFactory
- StorageManagement
- FileTransfer
- Metadata

- Registry
- Resource Broker

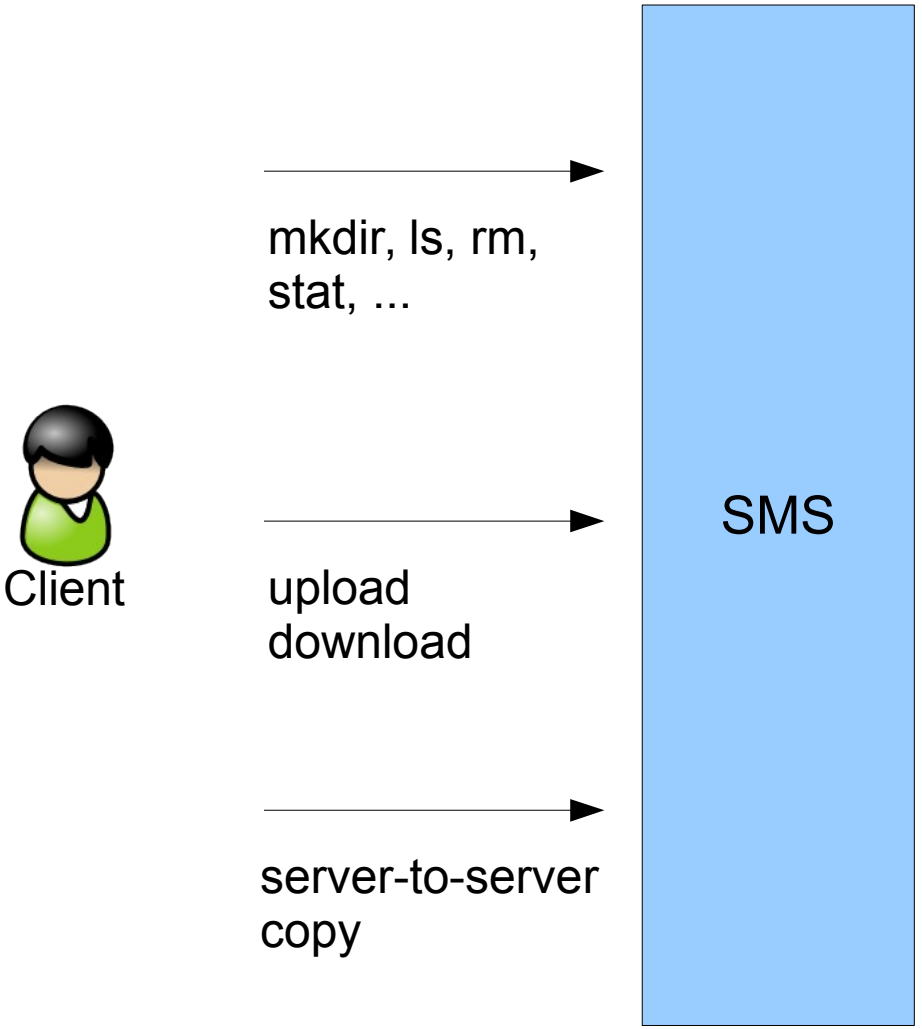
„Factory“ services



„Factory“ services: virtualisation support



UNICORE Storage Management Service



- File systems
- Apache HDFS
- **S3**
- iRODS (prototype)
- ...

Storage Management Service

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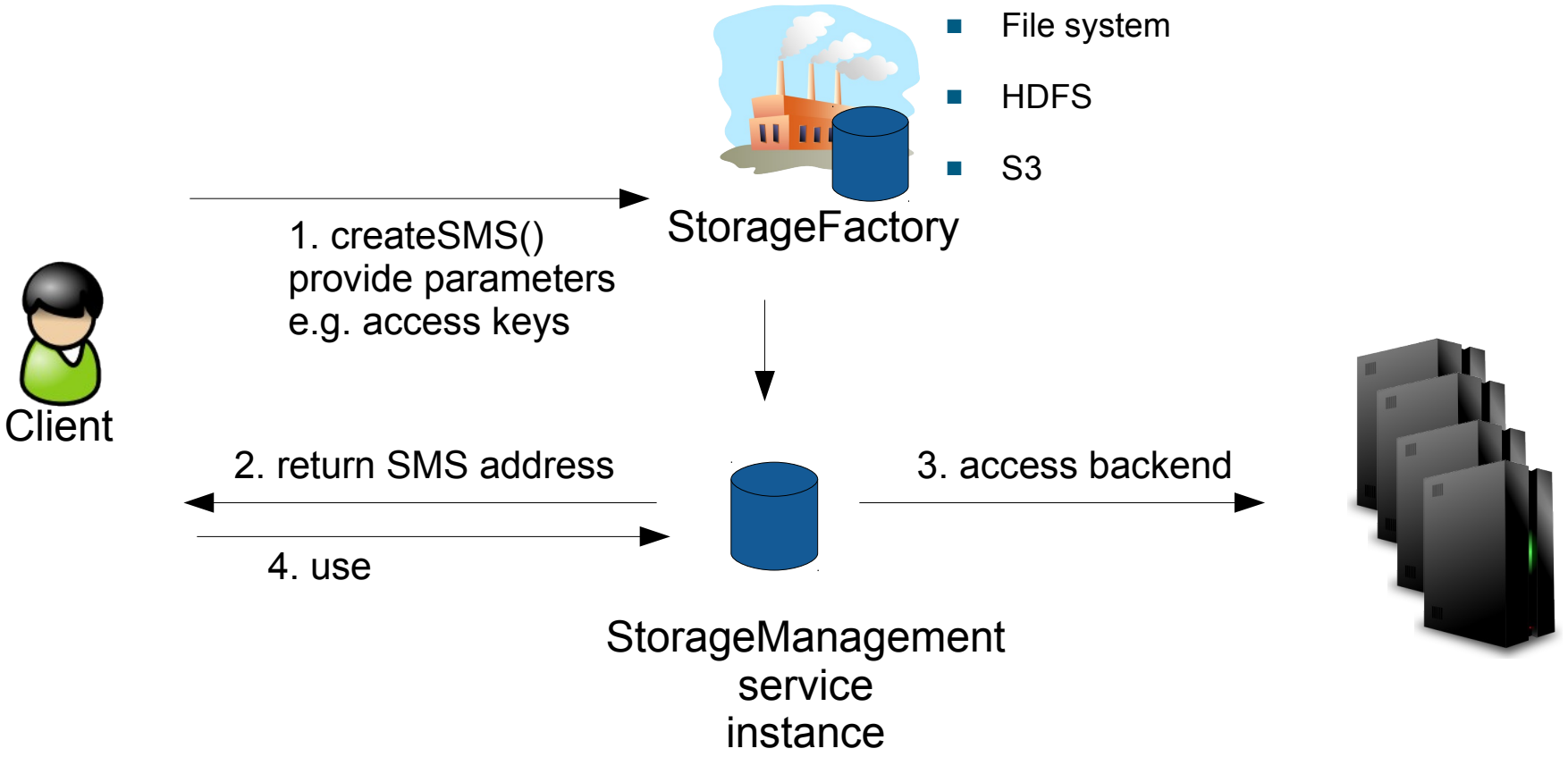
- Initiate file transfers
  - Multi-protocol support
- Metadata management
  - Schema-free, key-value
  - Indexed via Lucene, searchable
- Rule-based data processing
  - New files automatically trigger actions
  - e.g. metadata extraction, compression, etc

StorageFactory service: user-owned storages



- Different types of storage backends can be supported
- User can select and provide required parameters

UNICORE Services Environment

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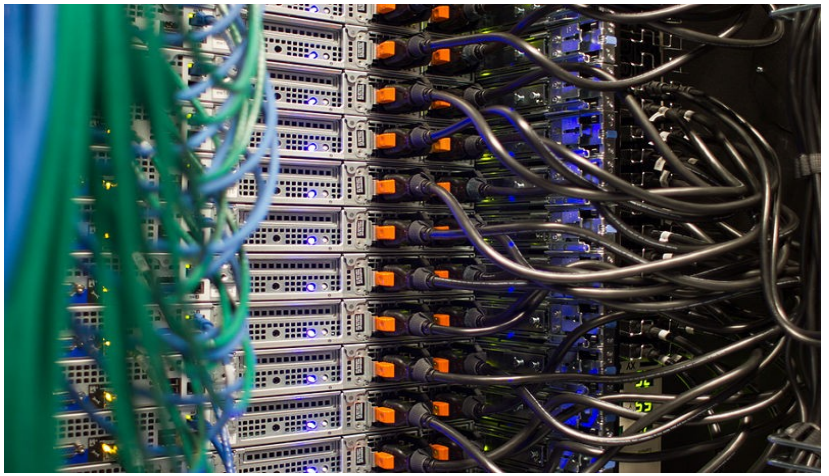
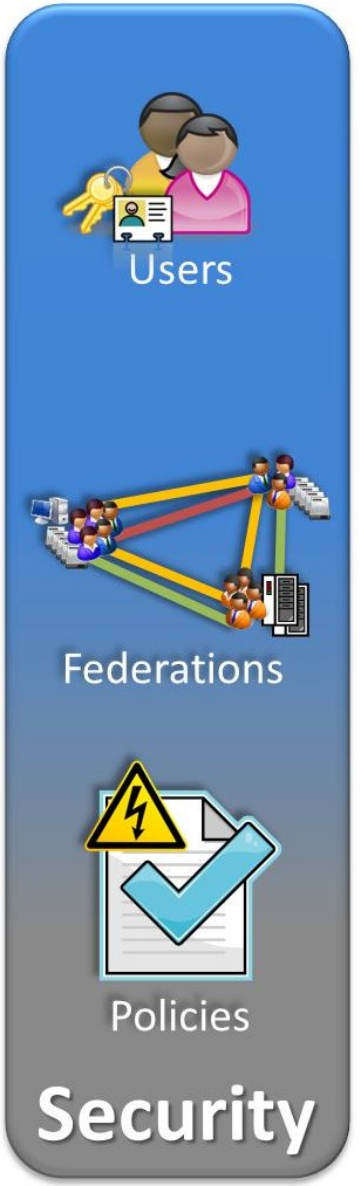
- Implemented in Java
- Based on Apache CXF (http://cxf.apache.org/)
  - Very mature and up-to-date services stack
  - SOAP web services
  - REST via JAX-RS

- Numerous other open source libraries

Federated access: security is key



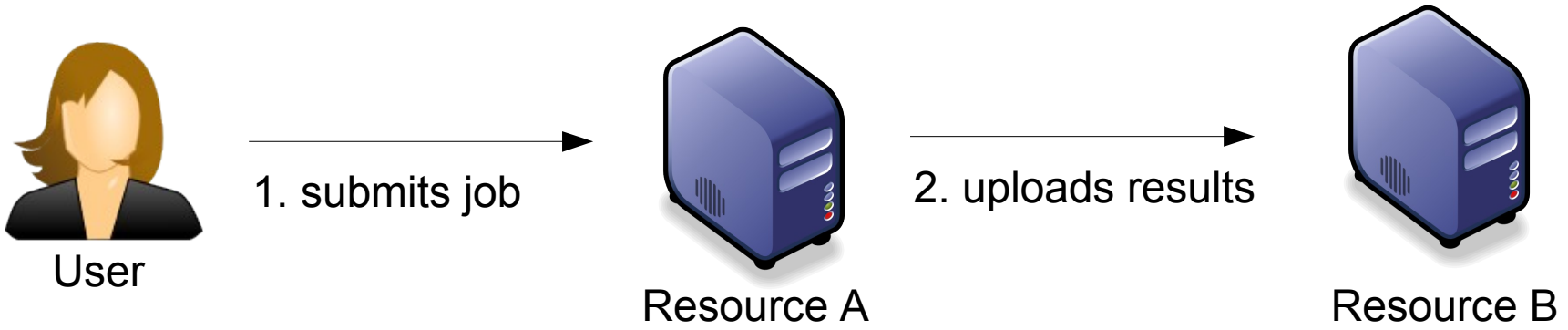


Basic security flow

- **User invokes a UNICORE service**
  - **Authentication**: who is the user?
    - *Results in the user's X.500 DN („CN=..., O=..., C=...“)*
  - **Assign attributes** to the DN
    - *Standard attributes: role, Unix ID, groups, etc.*
    - *Custom attributes: (e.g. S3 access and secret keys)*
  - **Authorisation**
    - *Add context: e.g. who owns the service?*
    - *Check local policies (XACML)*
- **Allow or deny** the request

Delegation

- Allow Service to work on behalf of the user
- UNICORE solution based on SAML
  - Use chain of signed assertions
  - Trust always delegated to particular server
  - Can be validated and audited



End-user authentication in UNICORE

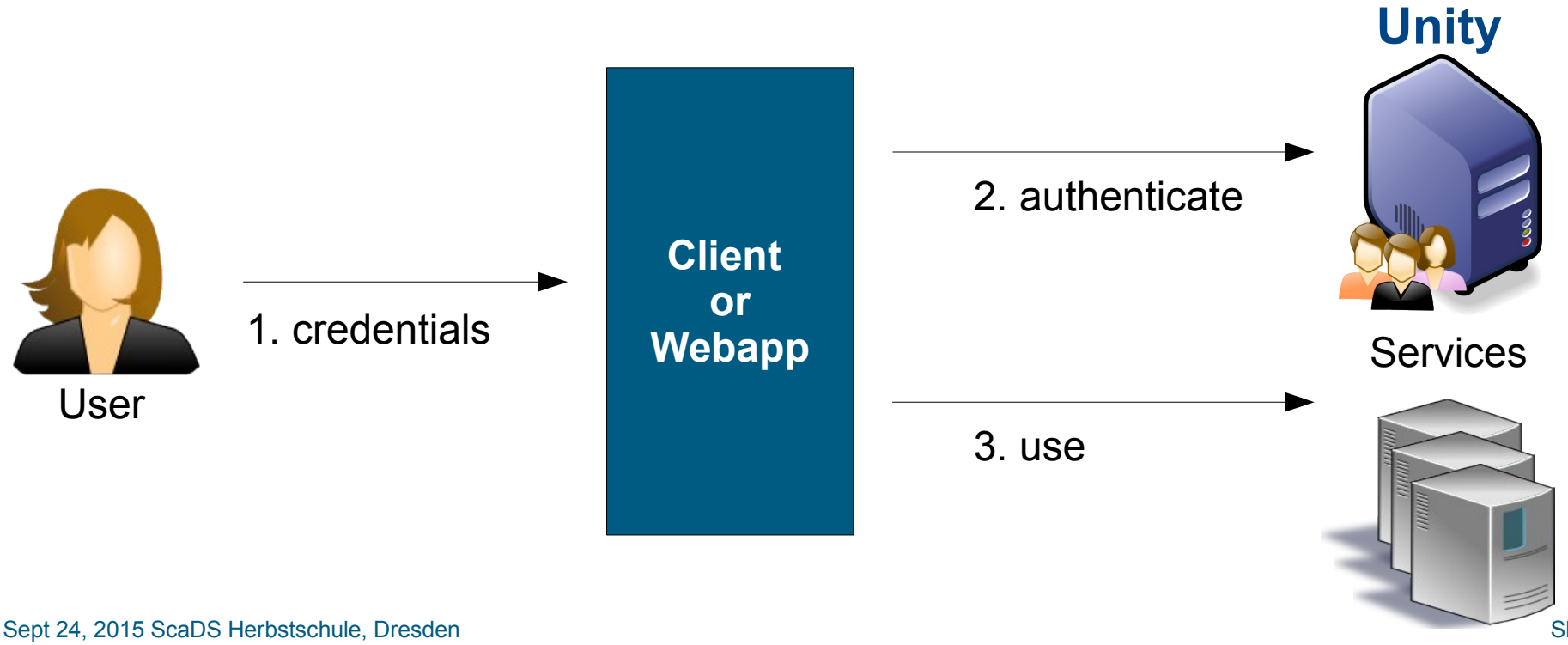
- Pre-UNICORE 7: X.509 client certificates REQUIRED for end-users
- Users tend to hate them
  - All sorts of usage issues
- Lack of understanding leads to lack of security (copying keys to other machines, no/weak encryption, etc)
- Users understand passwords
  - and it is relatively easy to teach basic security measures

Certificate-less end-user authentication

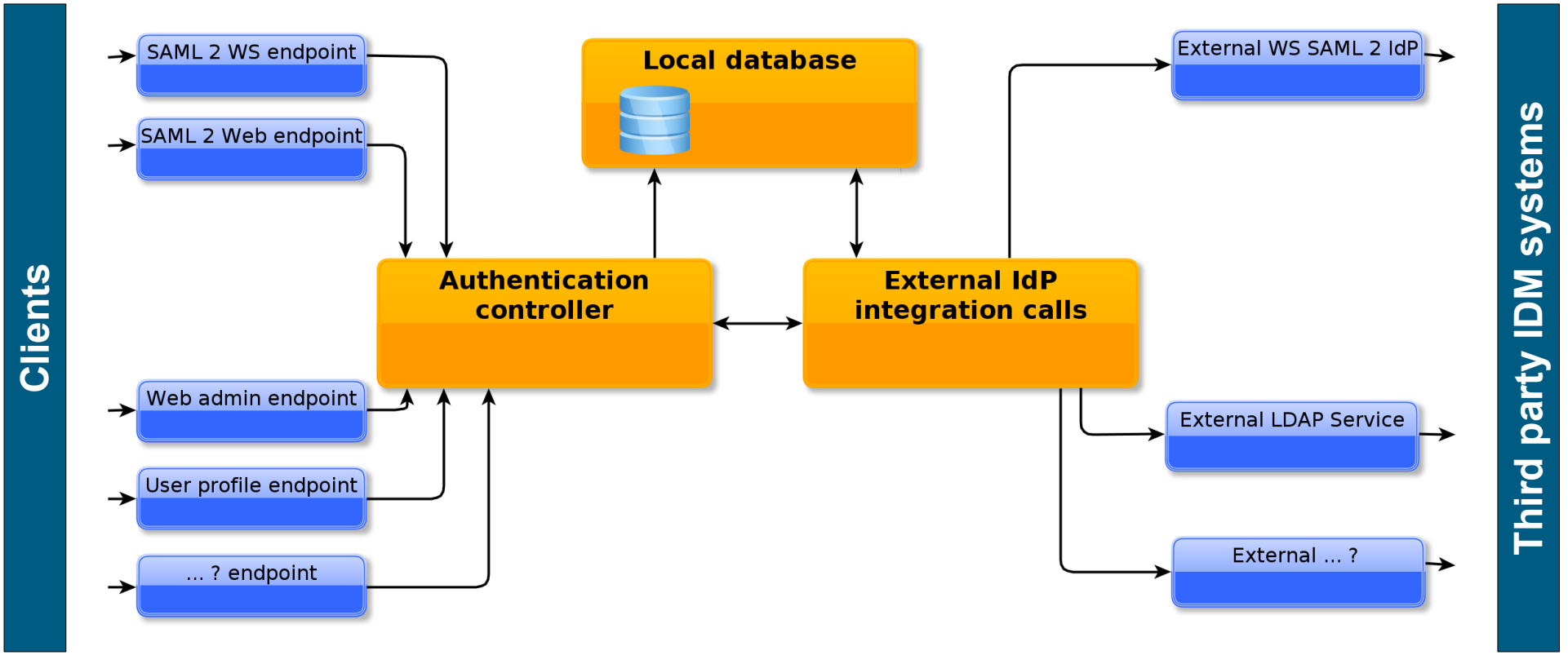
- **No end-user certificates** (not even short-lived)
- Approach
  - Use *signed SAML assertions*
  - Issued and signed by the trusted server
  - MANY options, e.g. support for existing SAML IdPs , federations like DFN AAI, OAuth2, OpenID Connect, etc
  - Flexible solution is required
- Implications
  - Client – server TLS is not client-authenticated any more
  - End-user cannot sign anything (no more „non-repudiation“)

Introducing Unity

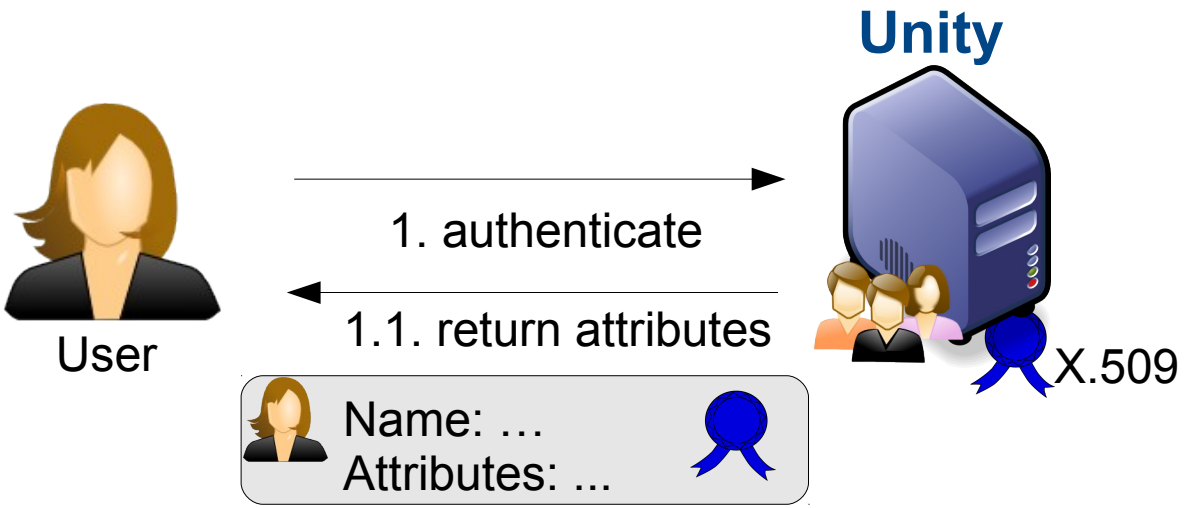
- Complete **Authentication and Identity Management** solution
- Manage users and user attributes, group membership
- Developed by **ICM / Univ. of Warsaw** (PL)
- Separate product: www.unity-idm.eu
- Already widely deployed: Human Brain Project, EUDAT, ...



Unity architecture



Example: authentication assertion



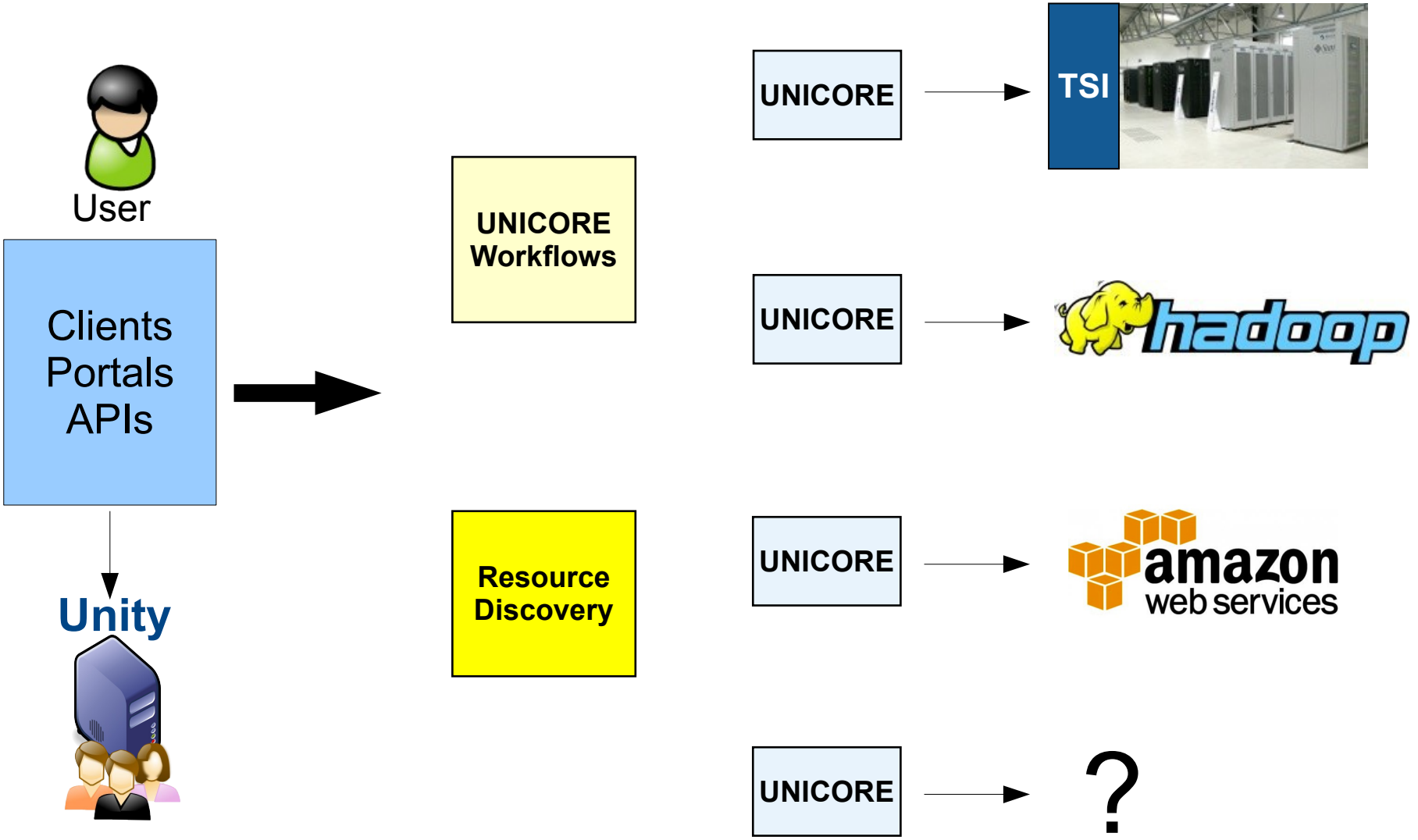

```
<urn:Assertion>...
  <dsig:Signature... </dsig:Signature>
  <urn:Subject>
    <urn:NameID
      Format="urn:oasis:names:tc:SAML:1.1:nameid-format:X509SubjectName">CN=Demo User,O=UNICORE,C=EU</urn:NameID>
    <urn:SubjectConfirmation Method="urn:oasis:names:tc:SAML:2.0:cm:sender-vouches">
      <urn:SubjectConfirmationData NotOnOrAfter="2014-11-16T10:30:23.334Z"/>
    </urn:SubjectConfirmation>
  </urn:Subject>
  <urn:AttributeStatement>
    <urn:Attribute Name="cn">
      <urn:AttributeValue>Demo User</urn:AttributeValue>
    </urn:Attribute>
    <urn:Attribute Name="email">
      <urn:AttributeValue>test@example.com</urn:AttributeValue>
    </urn:Attribute>
    <urn:Attribute Name="memberOf">
      <urn:AttributeValue>/portal</urn:AttributeValue>
      <urn:AttributeValue>/</urn:AttributeValue>
    </urn:Attribute>
  </urn:AttributeStatement>
</urn:Assertion>
```

Resource sharing

Example: user wants to securely share S3 storage

- UNICORE 7.3 introduces per-service ACLs
- Managed by owner of the resource
- Allow read/modify access based on DN, local UID/GID, UNICORE role, VO membership

Single sign-on and resource federation



- Batch systems (Torque, Slurm, LoadLeveler, GridEngine, ...)
- Apache Hadoop (YARN)
- Direct execution (e.g. on Windows)

- File systems
- Apache HDFS
- Amazon S3
- ...

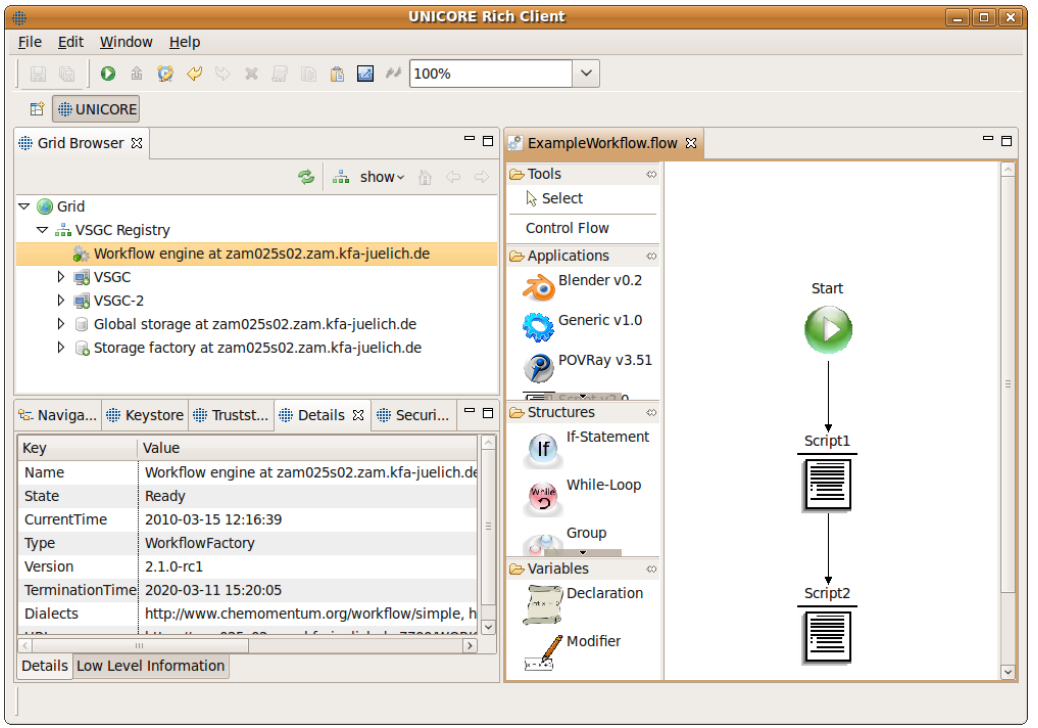
- Portals
- Science Gateways

- UCC

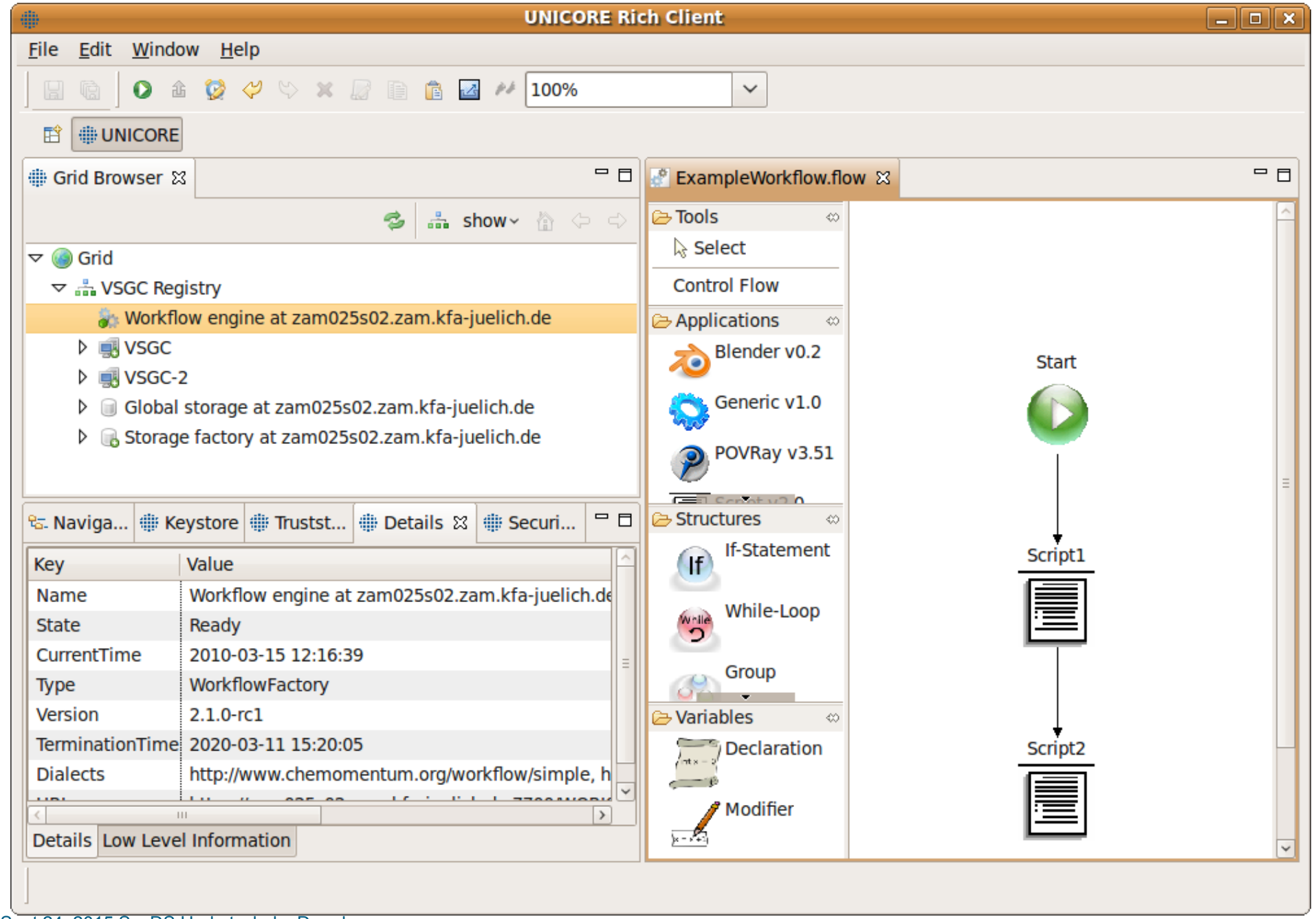
- Eclipse-based Rich Client

- RESTful API
- Java APIs

Rich client



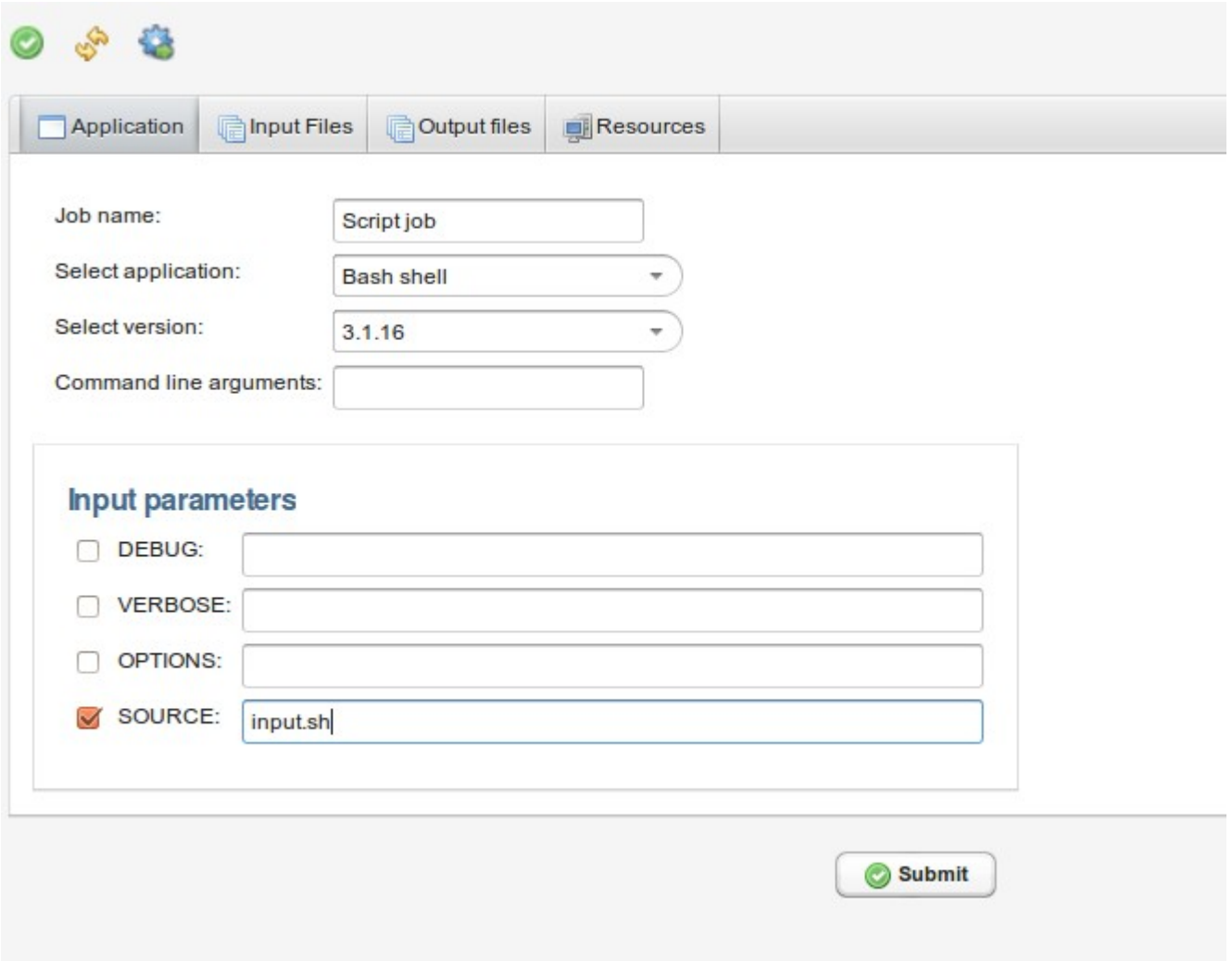
- Building, submitting and monitoring jobs and workflows
- Integrated data and storage management
- X.509 and Unity for AuthN
- “Simple view” for novice users
- Based on the Eclipse framework
- Extensibility through plug-ins
- Installation/update mechanism for plug-ins and Application GUIs


UNICORE Rich Client
File
Edit
Window
Help
100%
UNICORE
Grid Browser
show
Grid
VSGC Registry
Workflow engine at zam025s02.zam.kfa-juelich.de
VSGC
VSGC-2
Global storage at zam025s02.zam.kfa-juelich.de
Storage factory at zam025s02.zam.kfa-juelich.de
Naviga...
Keystore
Truststr...
Details
Securi...
Key
Value
Name
Workflow engine at zam025s02.zam.kfa-juelich.de
State
Ready
CurrentTime
2010-03-15 12:16:39
Type
WorkflowFactory
Version
2.1.0-rc1
TerminationTime
2020-03-11 15:20:05
Dialects
http://www.chemomentum.org/workflow/simple, h
Details
Low Level Information
ExampleWorkflow.flow
Tools
Select
Control Flow
Applications
Blender v0.2
Generic v1.0
POVRay v3.51
Structures
If-Statement
While-Loop
Group
Variables
Declaration
Modifier
Start
Script1
Script2

UNICORE Portal

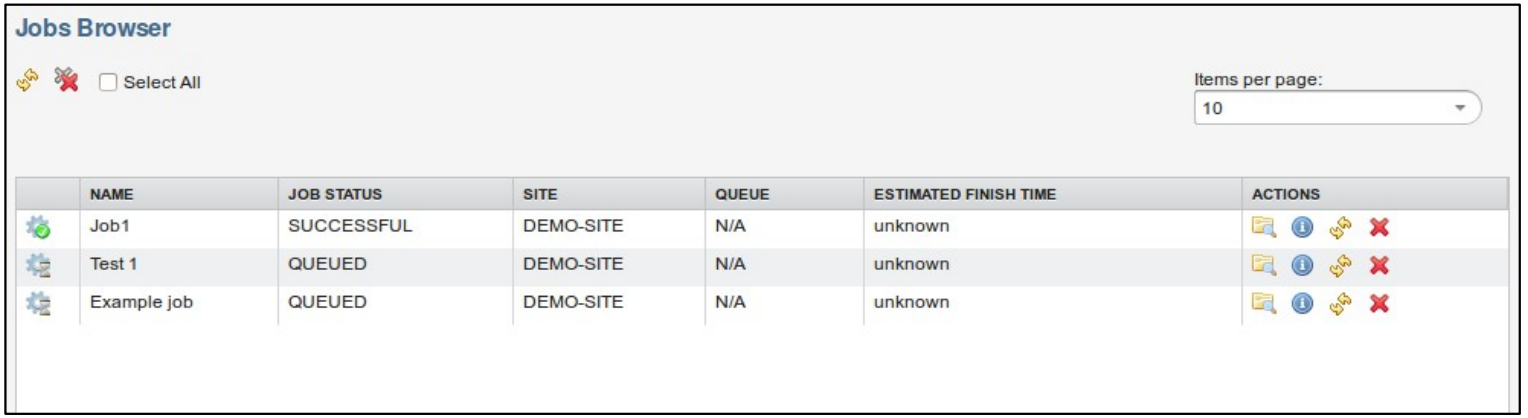
- Aim for a simple, easy-to-use web application
- Flexible authentication and user registration
  - support Unity
- Implementation choices
  - Java-based, VAADIN web framework
  - Use UNICORE Java APIs

UNICORE Portal – Job creation view

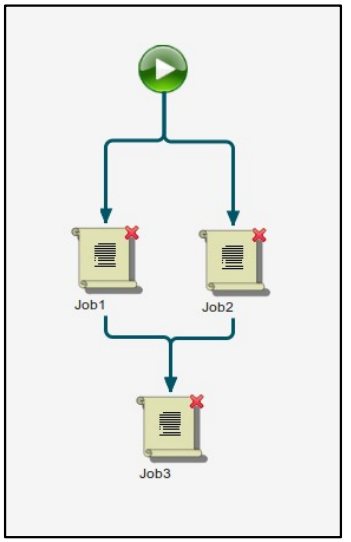


UNICORE Portal – various

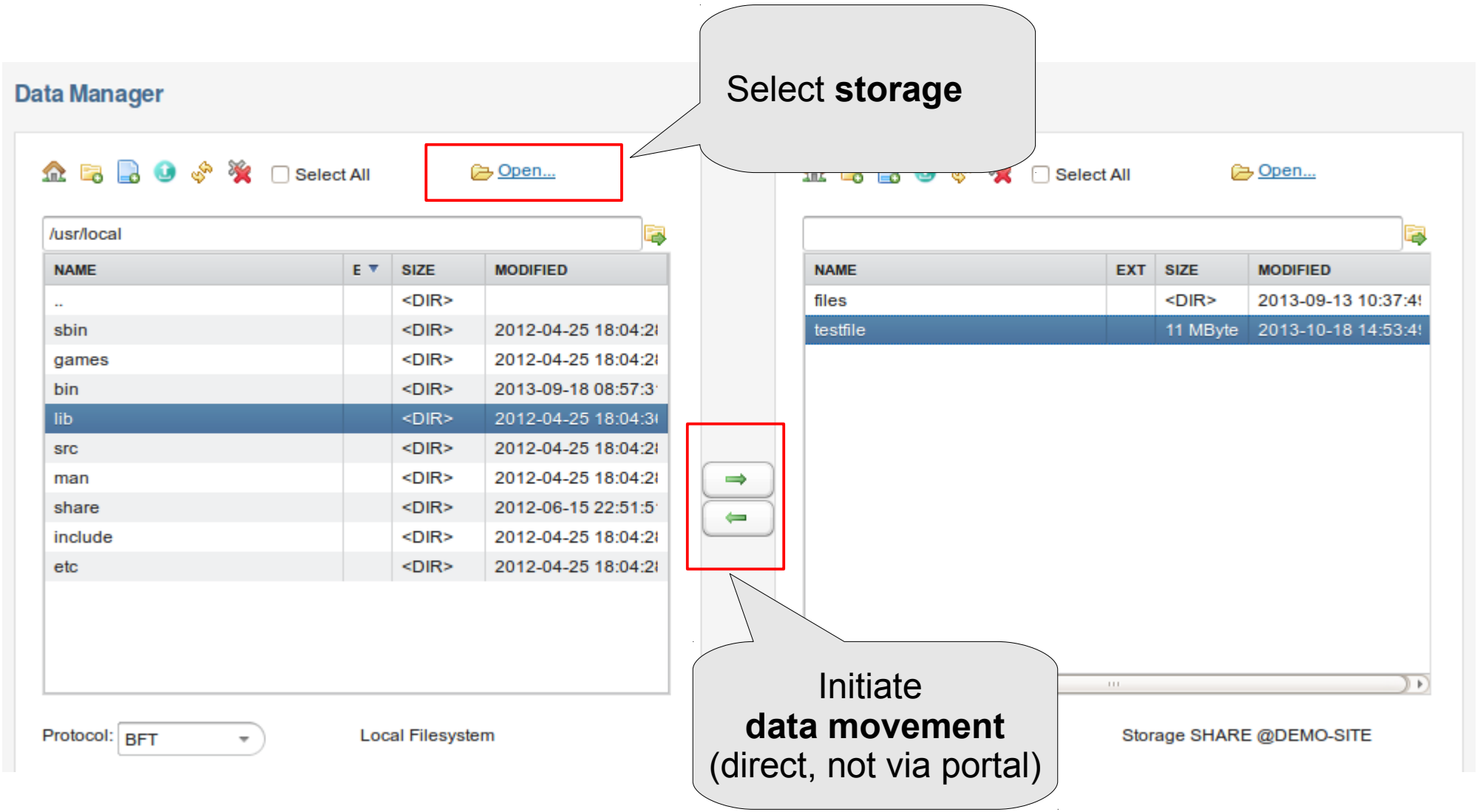
- Several „list“ views, e.g. jobs, sites



- Workflow creation
- JavaScript
- Initially only simple graphs



UNICORE Portal: Data manager



RESTful interfaces

- REST
  - Document / Resource oriented approach
  - HTTP semantics (GET, POST, PUT, DELETE)
  - Simple JSON (and HTML) data exchange formats and resource representations
  - Clients exist in all languages (even *curl* or *wget*)
  - Excellent support in Java (JAX-RS)

REST vs SOAP/WS

- REST: **simpler integration** with community solutions / portals
  - e.g. Human Brain Project portal: JavaScript and Python would not play well with SOAP/XML and WS-Security
- **Performance** gains (side effect)
  - SOAP/ XML and WS-Security is rather heavy!
- Stay consistent and backwards compatible
  - Keep SOAP/WS(RF) services
  - Access to same jobs, data, etc
  - Consistent security layer (user DNs, attributes mapping, access control)

Example: job submission

```
job.u:
{
  Executable: "/bin/echo" ,
  Arguments: ["Hello World"],
}
```

```
$> curl -X POST -H “Content-Type: application/json“
   --data-binary @job.u
   https://server:8080/DEMO-SITE/rest/core/jobs
```

```
HTTP/1.1 201 Created
Content-Type: application/json;charset=ISO-8859-1
Date: Mon, 17 Nov 2014 22:08:17 GMT
Location: https://server:8080/DEMO-SITE/rest/core/jobs/ \
       74198236-e970-429d-b55c-a7d59c831f14
```

Example: JSON representation of a job

```
$> curl -X GET -H “Accept: application/json“
   https://localhost:8080/DEMO-SITE/rest/core/jobs/...
```


```
{
   "owner": "CN=Demo User,O=UNICORE,C=EU",
   "currentTime": "2014-11-17T21:51:49+0000",
   "terminationTime": "2014-12-17T20:09:15+0000",
   "resourceStatus": "READY",

   "status": "SUCCESSFUL",
   "queue": "N/A",
   "submissionTime": "2014-11-17T20:09:15+0000",
   "statusMessage": "",
   "exitCode": "0"

   "_links": {
      "action:abort": {
         "href": "https://localhost:8080/DEMO-SITE/rest/core/jobs/.../actions/abort",
         "description": "Abort"
      },
      "action:restart": {
         "href": "https://localhost:8080/DEMO-SITE/rest/core/jobs/.../actions/restart",
         "description": "Restart"
      },


   }
}
```


Generic part

Job specific

Links

REST APIs: speedup some (indicative) performance data

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Get resource properties

Client threads	Requests/sec WSRF	Requests/sec REST
1	27	79
2	57	193
4	80	286
8	76	332

Job submission

Client threads	Requests/sec WSRF	Requests/sec REST
1	5	34
2	11	54
4	12	75

A major use case: the Human Brain Project's HPC platform

HBP portals,
other applications

1. authenticate

returns token

OIDC server
user login

3.1 validate

2. access UNICORE
job submission, data movement, ...

3. validate token

OK

Unity

REST API

UNICORE

HBP Molecular Dynamics Supercomputer

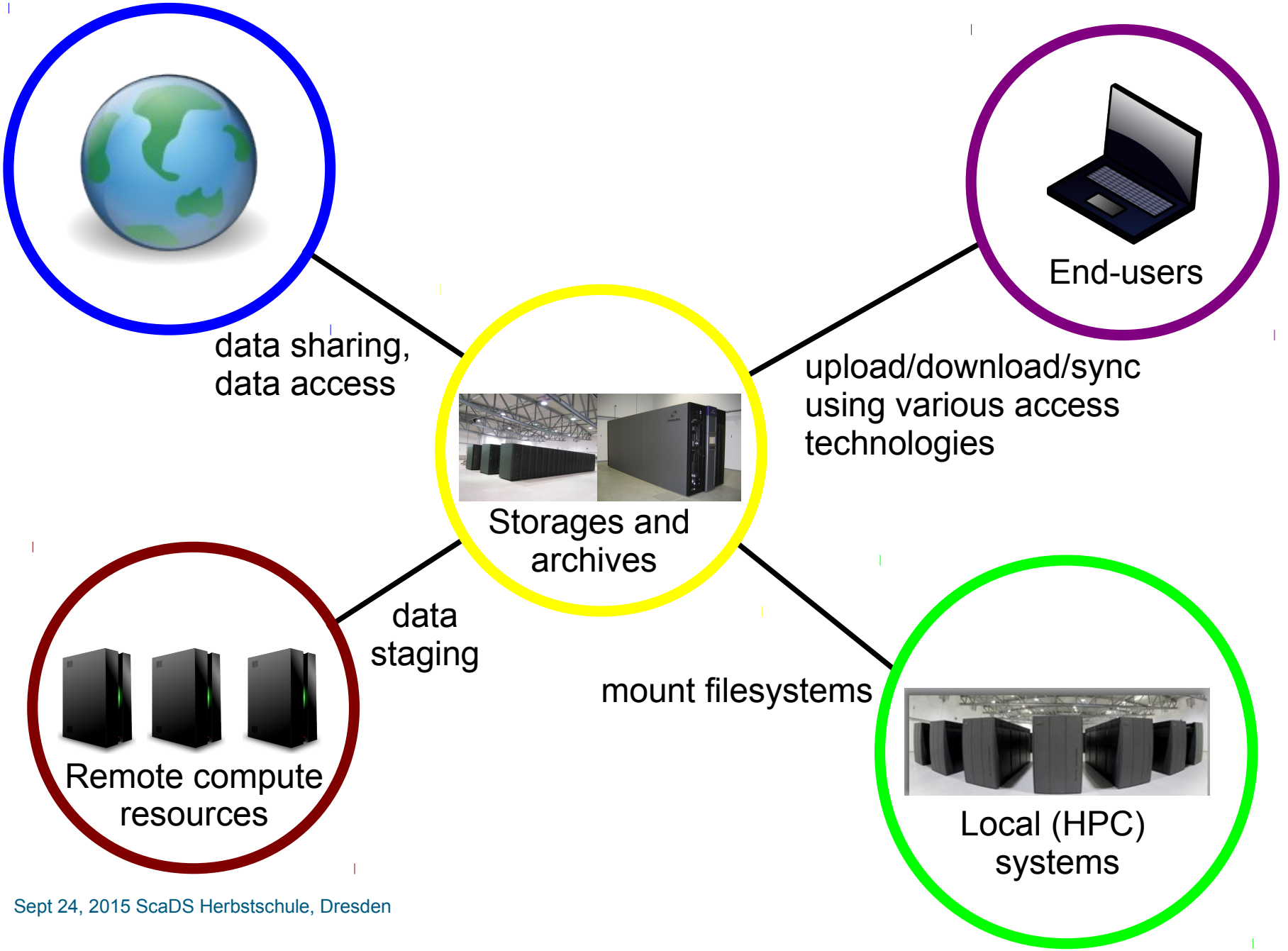
HBP Data Analytics Supercomputer

HBP Development System

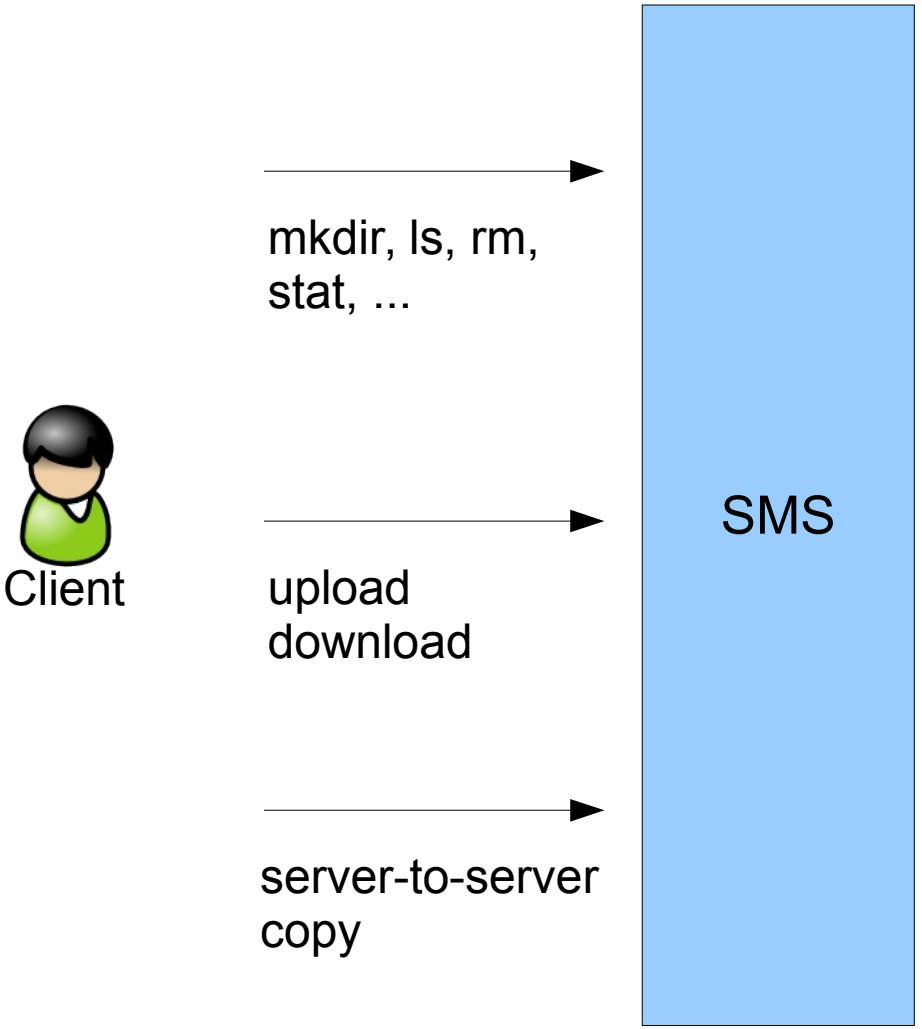
HBP Supercomputer

HBP Cloud Storage

Data management



UNICORE Storage Management Service



- File systems
- Apache HDFS
- **S3**
- iRODS (prototype)

Storage Management Service

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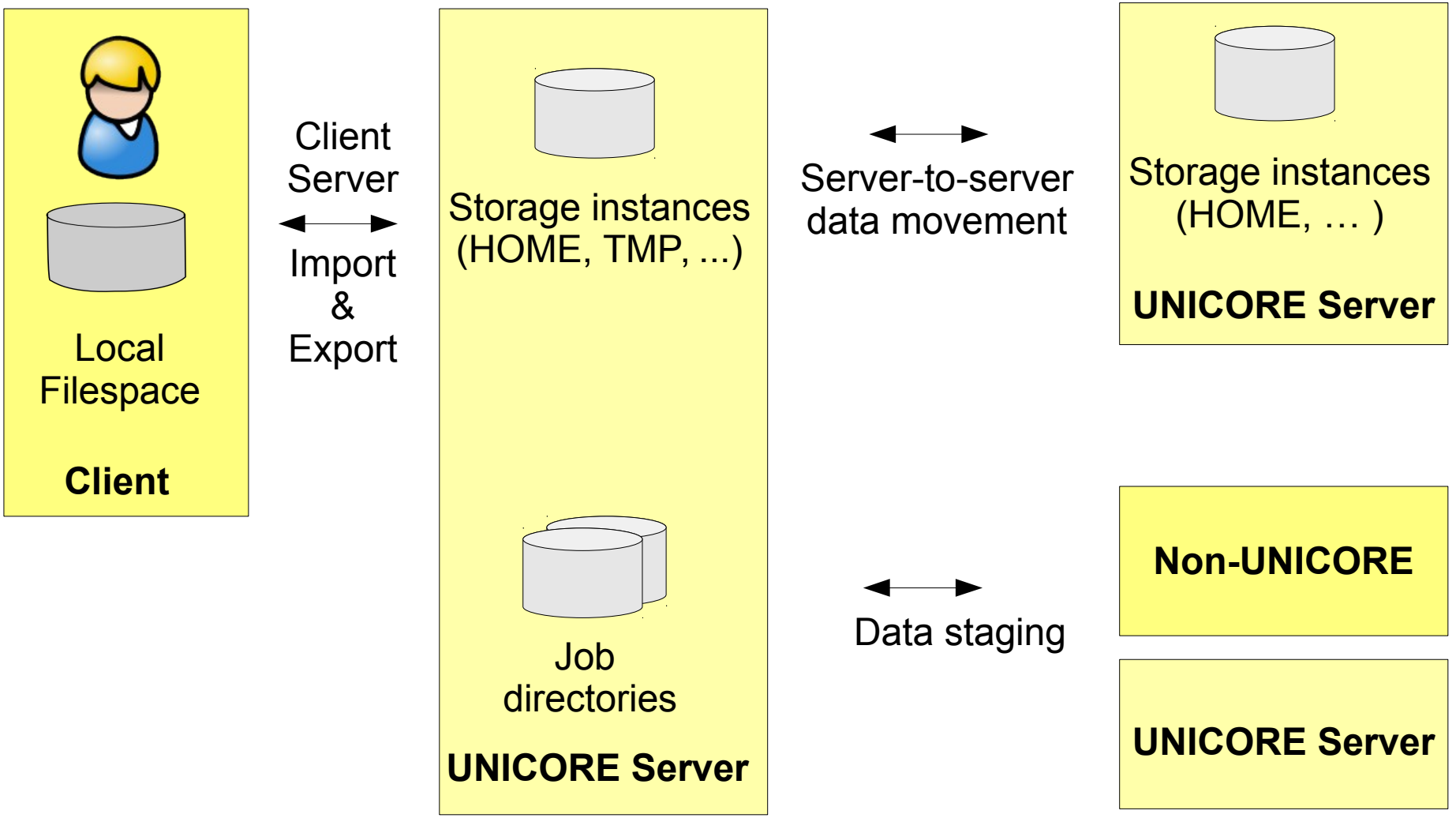
- File system operations
- Initiate file transfers
  - Upload/download, server-to-server
  - Multi-protocol support
- Metadata management
  - Schema-free, key-value, indexed via Lucene, searchable
- Rule-based data-driven processing
  - … more details later

Storages and data movement



File transfer

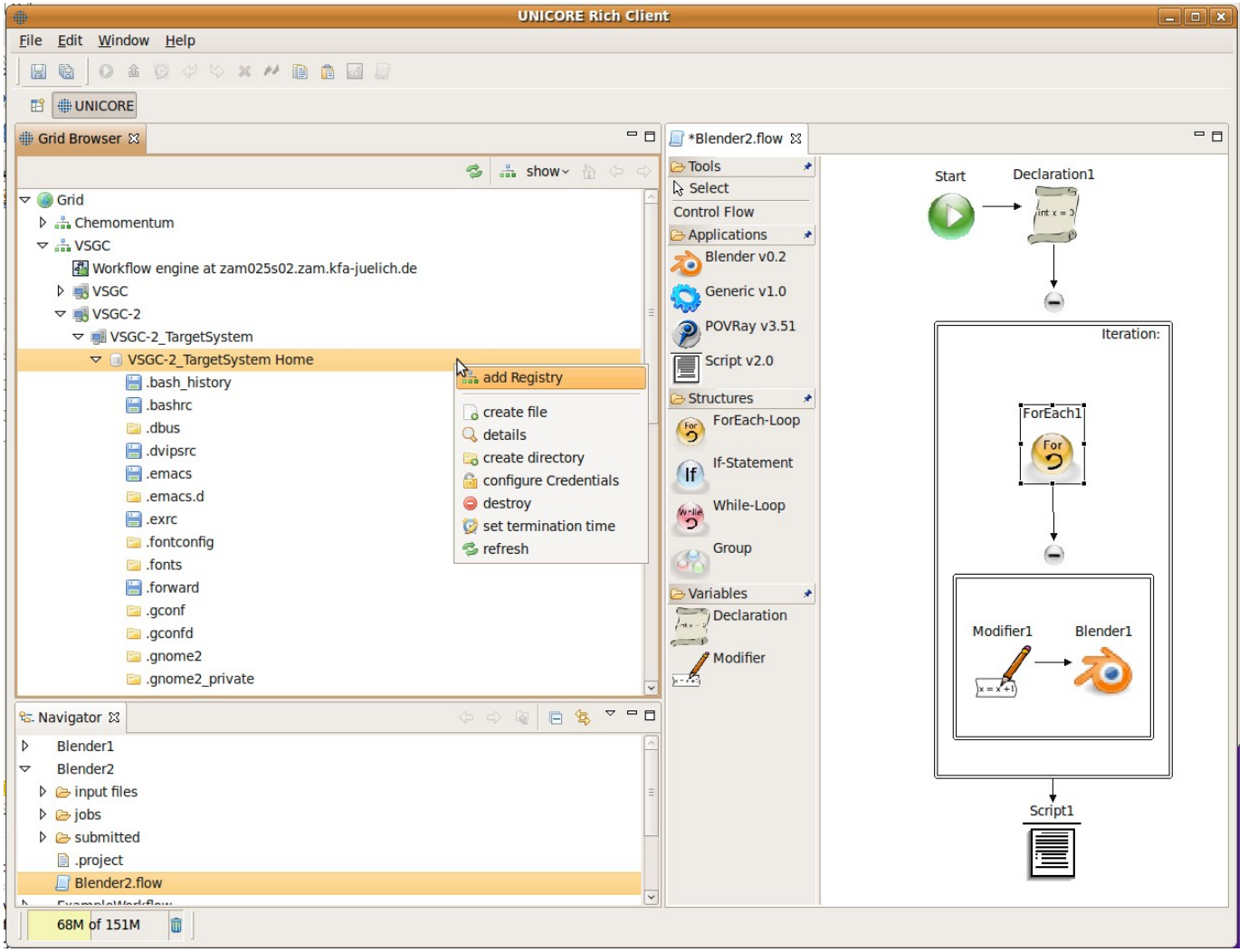
- Both client-to-server and server-to-server FT available
- Builtin: HTTPS based transfer („BFT“)
  - Single open port needed, (almost) full UNICORE security
  - Simple interface (bulk write, read supports byte ranges), **decent performance** (several MB/sec.)
- Builtin: OGSA ByteIO (uses SOAP messages)
  - Single port, full UNICORE security
  - Rich interface (POSIX-like, block read/write, etc), slow (~400kB/sec)
- **High-performance** UFTPD file server available as an extension

Additional options for data staging

- GridFTP
  - Uses existing globus-url-copy
  - Proxy generated on the client and sent with the job
- Plain HTTP and HTTPS
- FTP and SCP (including client credentials)
- „mailto“ for stage-out :-)

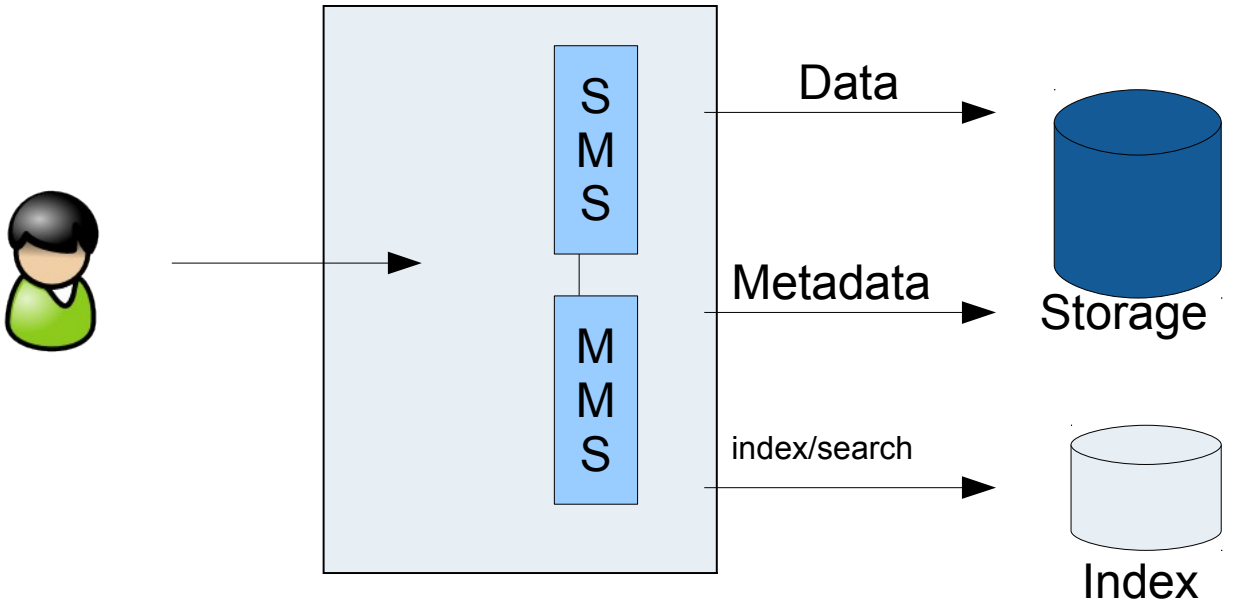
Integrated storage management in the UNICORE Rich Client

- Create files
- Drag and drop from/to desktop environment
- Copy and paste
- Remote file editing



Metadata management

- De-centralized approach: „metadata management service“ (MMS) associated with each storage service („SMS“)
- Schema-free: metadata is key-value pairs
- User can create, edit, delete metadata, trigger automated extraction
- Metadata indexing



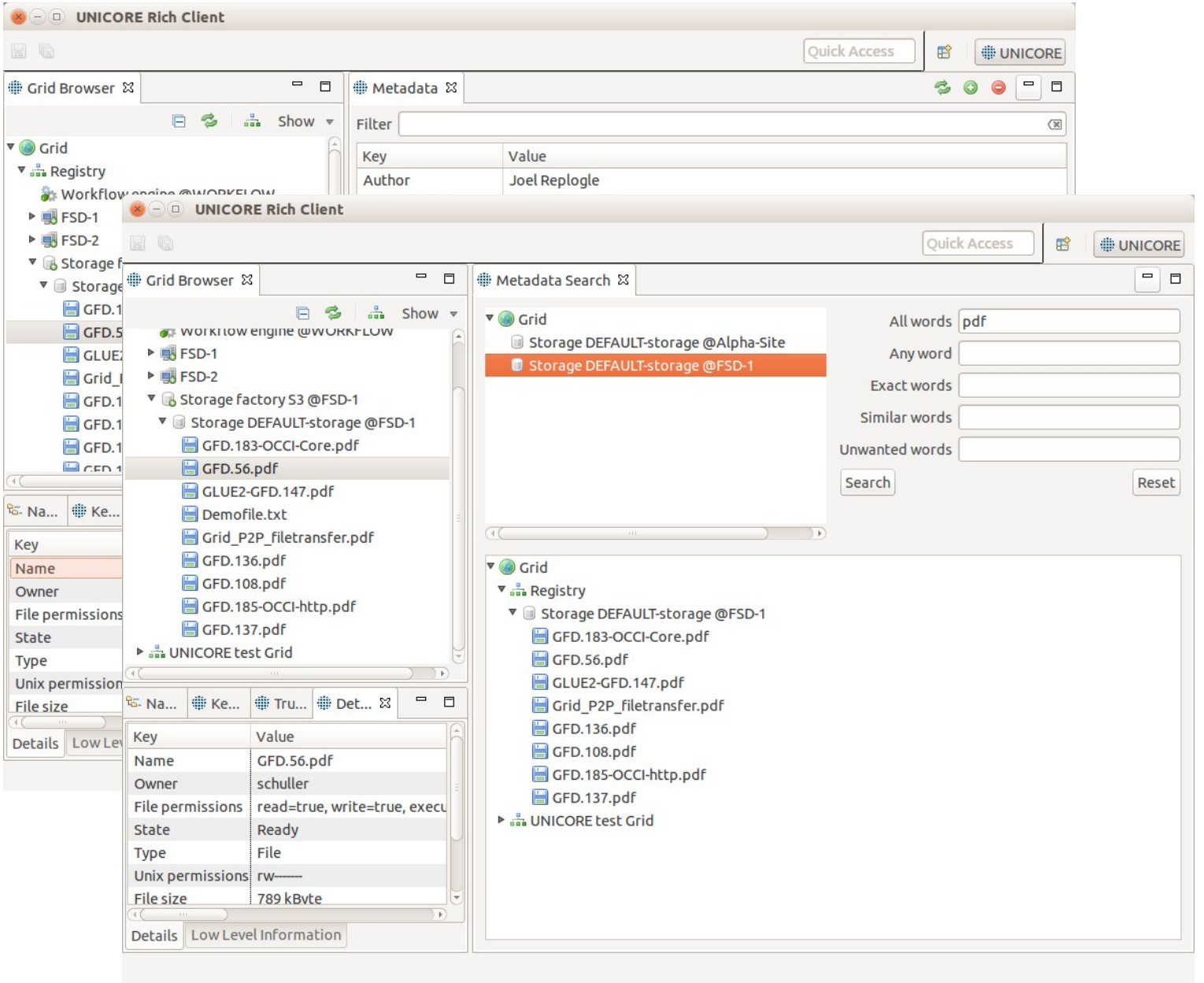
Metadata management: implementation

- Metadata storage directly as files on the storage
- Uses well-known open source libraries
- Indexer and search engine: Apache Lucene
- Metadata extraction framework: Apache Tika
- Supported via UCC, URC, REST APIs
  - Example: list file properties including metadata

```
schuller@zam994-t400:/$ ucc-vsgc ls -l u6://VSGC-2/Home/Documents/refcard-hadoop.pdf -m
-rw-        1670701 2011-02-24 09:26 /Documents/refcard-hadoop.pdf
{
  "Content-Type": "application/pdf",
  "Creation-Date": "2010-09-23T16:25:05Z",
  "Last-Modified": "2010-09-23T16:25:11Z",
  "created": "Thu Sep 23 18:25:05 CEST 2010",
  "creator": "Adobe InDesign CS5 (7.0)",
  "producer": "Adobe PDF Library 9.9",
  "resourceName": "/Documents/refcard-hadoop.pdf",
  "trapped": "False",
  "xmpTPg:NPages": "6"
}
```

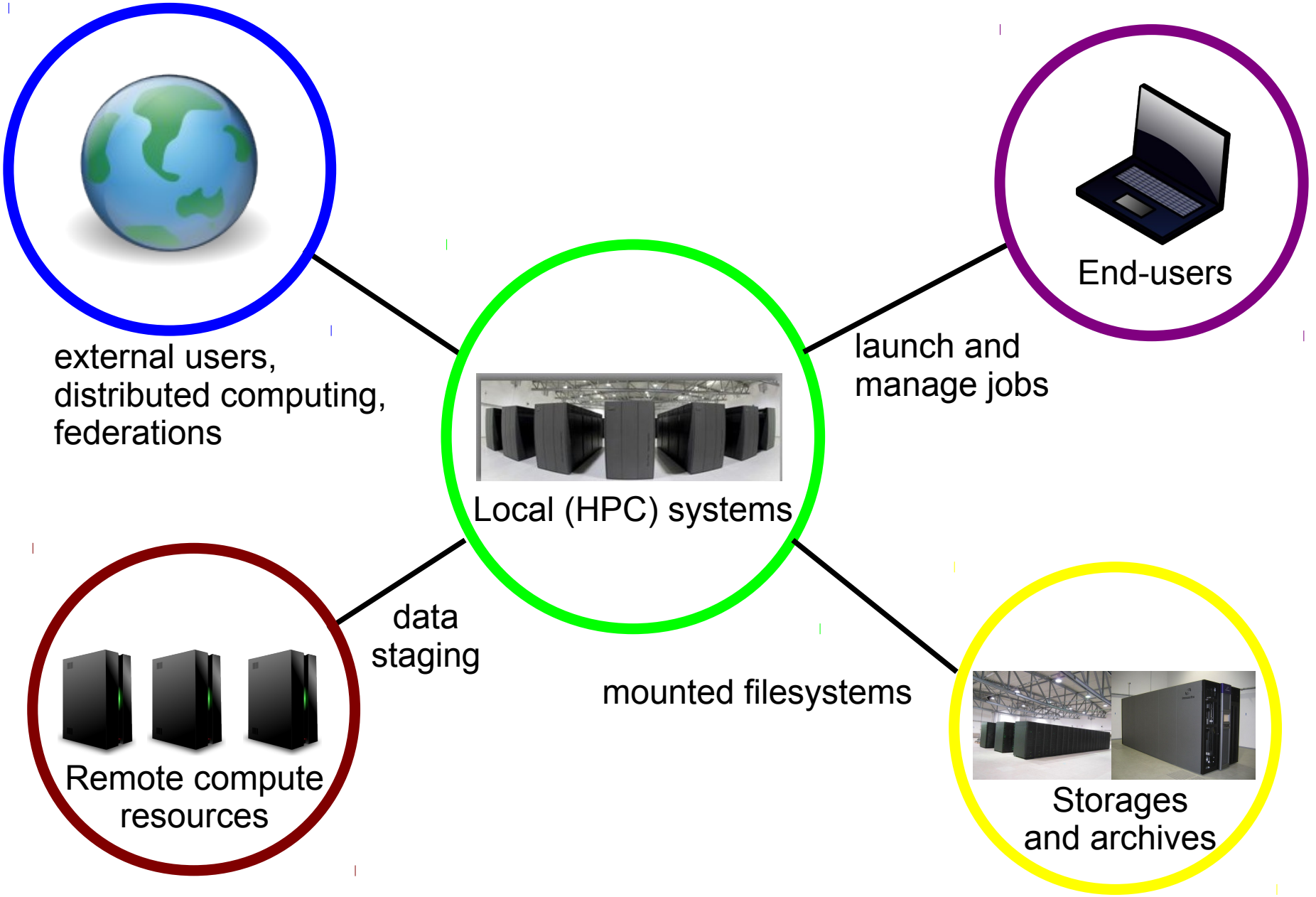
Integrated metadata management in the UNICORE Rich Client

- Edit
- Trigger auto-extraction
- Search



Demo: storages and metadata using URC

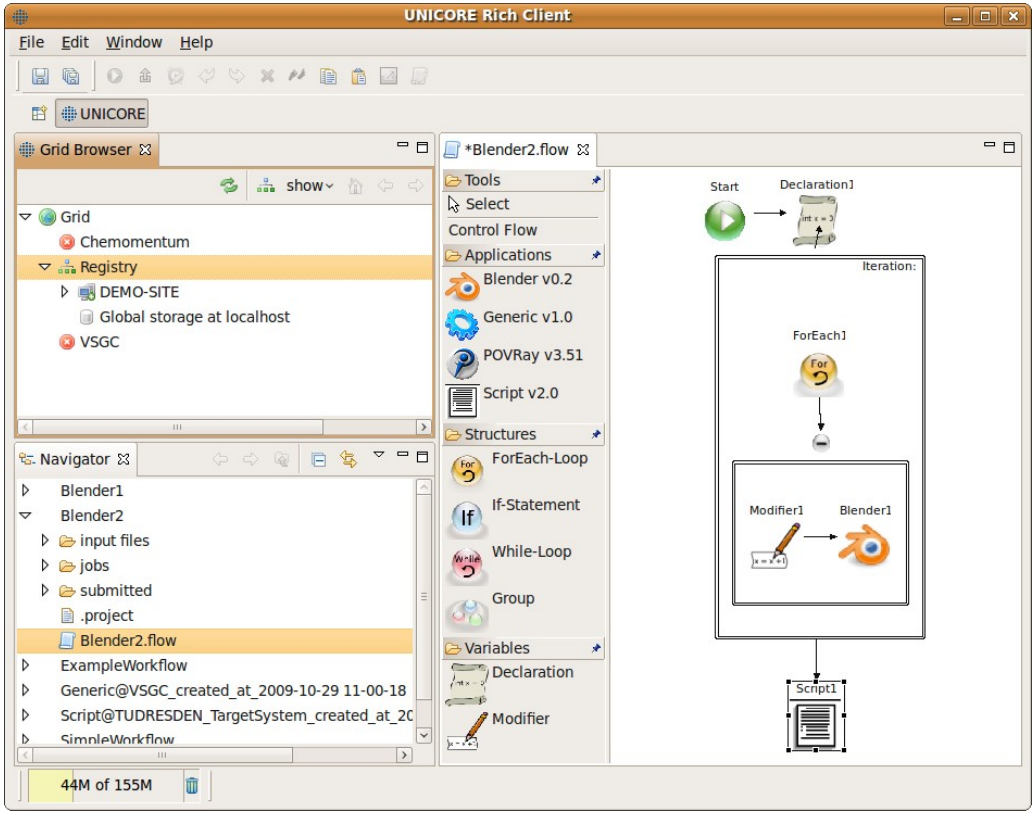
Data processing



Data processing using UNICORE

- Single jobs
- Workflow system
- Data-driven

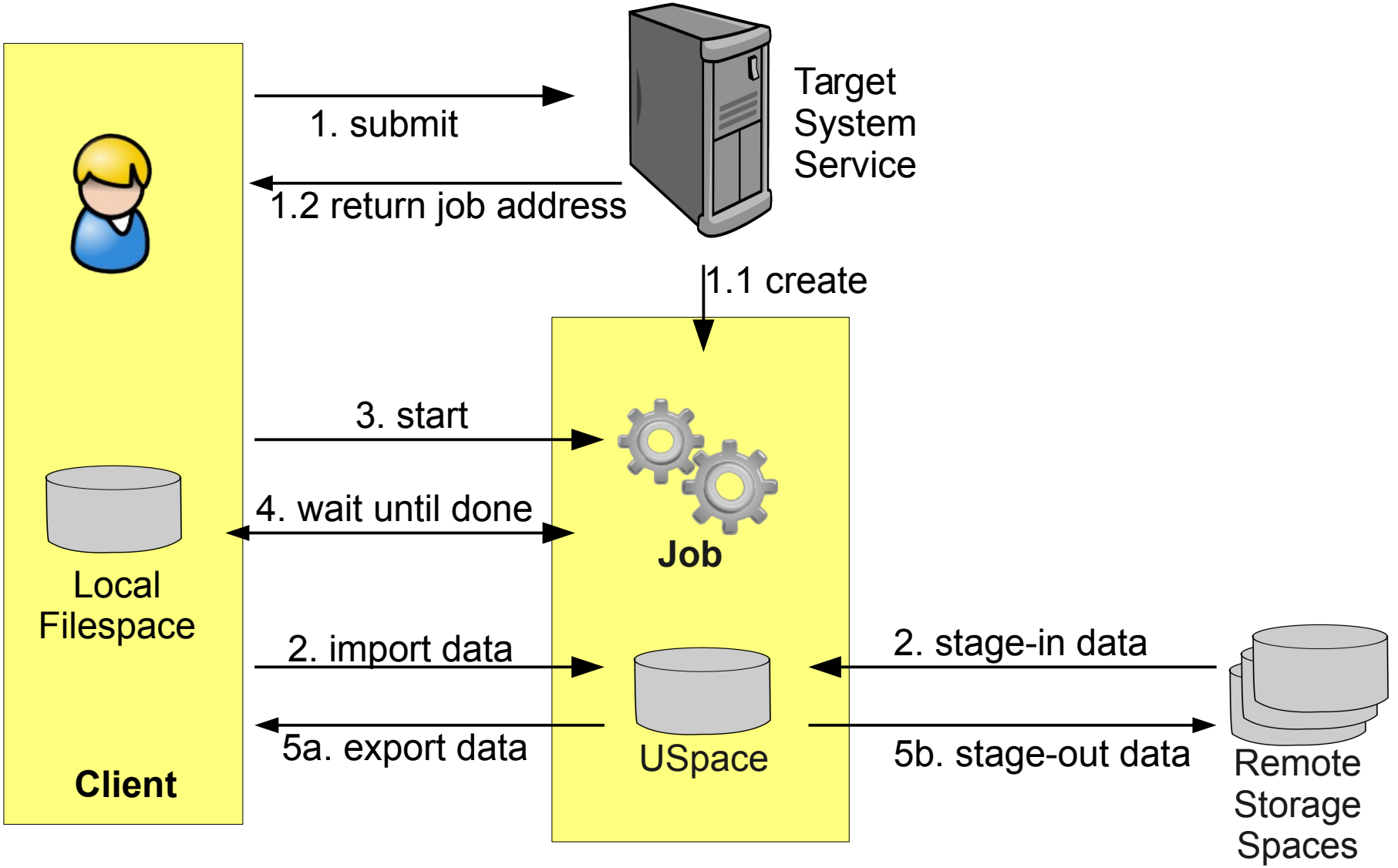
- End-user clients
  URC / UCC / Portal
  REST APIs
  Java APIs



Single jobs

- Batch job oriented
  - Data stage-in
  - Execution
  - Data stage-out
- End-user must ...
  - Setup job definition
  - Select site (broker is available)
  - Upload input data from local machine
  - Submit

Single job execution



Workflow system

- Sequences / Graphs / Control
- Based on single jobs
- End-user client tasks
  - Setup workflow definition
  - Upload input data
  - Submit
- Pros
  - Easy automation of complex processes
  - Control constructs available
  - Low load on client side
  - Powerful GUI client
- Cons
  - High overhead on servers
  - Data staging can be a limiting factor

Demo: jobs and workflows using URC

„Data-driven“ processing

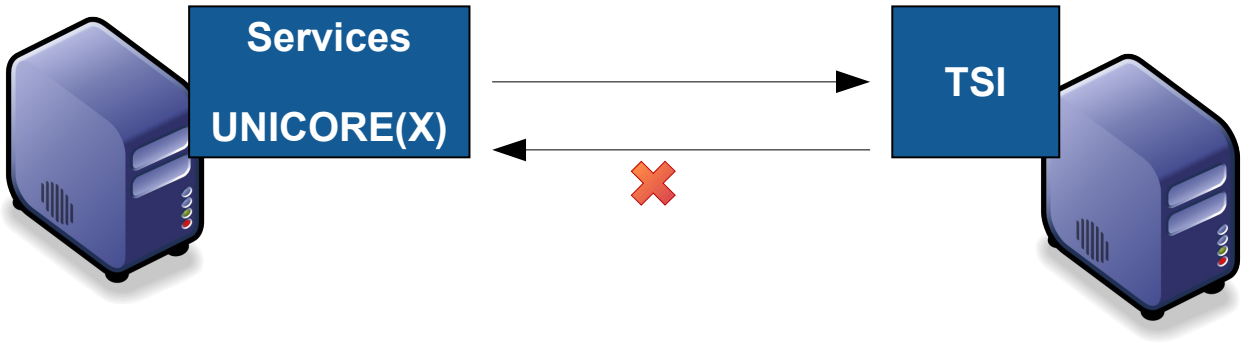
- As opposed to „job-oriented“
- Driven purely by data
- No end-user involvement required (apart from setup)
- Kind of like a „cron job“

Basic UNICORE architecture - I

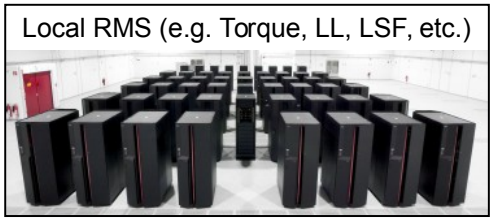
- User centric
- Everything is „owned“ by a user (submission services, jobs, storages, file transfers ...)
- Fully compatible with Unix file permissions
- UNICORE never operates as a „superuser“

Basic UNICORE architecture - II

- Services / logic lives on the UNICORE/X server
- File system and batch system accessed via TSI agent
- TSI accessed via request/response
- No file system notifications possible with current TSI



Cluster access node



UNICORE Storage Management Service

Client

mkdir, ls, rm, stat, ...

upload
download

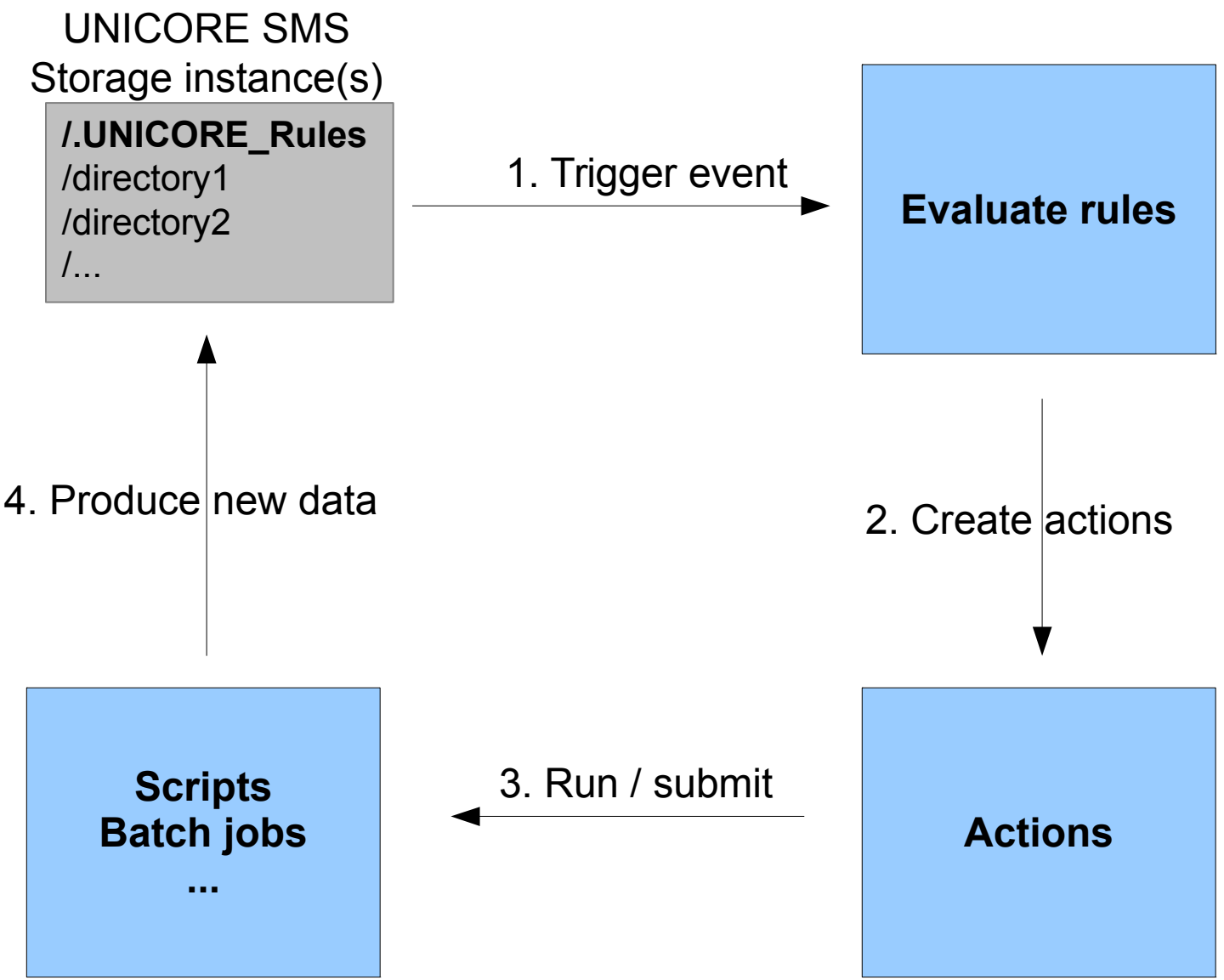
server-to-server copy

SMS

- File systems
- Apache HDFS

- S3

- iRODS (prototype)


UNICORE SMS
Storage instance(s)
/.UNICORE_Rules
/directory1
/directory2
/...
1. Trigger event
Evaluate rules
2. Create actions
Actions
3. Run / submit
Scripts
Batch jobs
...
4. Produce new data

Periodic directory scan

- Files can be written independently of UNICORE
- Scan interval configurable
- Directory include/exclude patterns

Types of actions

- Local script
  - Executed via TSI
  - TSI node (cluster login node)
- Local batch job
  - Executed via XNJS/TSI
  - Compute node(s)
  - UCC-like job description
- Metadata extraction

Required setup

- Create a storage (service instance) where data-driven processing is enabled
  - by the user
  - pre-configured by the admin
- Configure (edit .UNICORE_Rules file)

Example

- Goal: calculate checksums (md5) of PDF files in a certain directory using batch jobs
- Rule (job is defined in the usual JSON job syntax)

```
Name: computeMD5Sum, Match: ".*\\.pdf",
Action: {
    Type: BATCH,
    Job:  {
      Executable: "/usr/bin/md5sum",
      Arguments: ["${UC_FILE_PATH}"],
      Exports: [
        {From: "stdout",
        To: "file://${UC_BASE_DIR}/checksums/${UC_FILE_NAME}.md5"},
      ],
    }
```

Summary

A federation software suite

- Secure and seamless access to compute and data resources
- Excellent application and workflow support
- Wide variety of clients: GUI, commandline, APIs, ...
- Portable code, supports UNIX, MacOS, Windows and many resource management systems (Torque, Slurm, SGE, …)
- Easy to install, configure, administrate and monitor
- Active developer team, responsive to user wishes ;-), quick and efficient support
- **Open source, BSD licensed, visit http://www.unicore.eu**

Team / Thank you

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- Richard Grunzke and others at Technical University Dresden
- Students: Burak Bengi, Maciej Golik, Konstantine Muradov
- … many others who reported bugs, suggested features, contributed code and provided patches