



UNICORE

Uniform Access to the JSC Resources

23. NOVEMBER 2018 | BJÖRN HAGEMEIER, FEDERATED SYSTEMS AND DATA

MOTIVATION

Differences of machines



Slurm → srun, ...



LoadLeveler → llsbmit, ...



MOTIVATION

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Slurm → srun, ...



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MOTIVATION

Various RMS on machines

- JUQUEEN: IBM LoadLeveler
- JURECA: Slurm
- Different job description languages for specifying
of nodes, memory requirements, wall time, ...

- Admittedly, not important anymore at JSC

UNICORE

- unify and simplify supercomputer access

```
#@job_name      = hybrid_code
#@comment      = "16x4 configuration"
#@output       = test_$(jobid).out
#@error        = test_$(jobid).err
#@environment  = COPY_ALL
#@job_type     = bluegene
#@notification  = never
#@bg_size      = 512
#@bg_connectivity = torus
#@wall_clock_limit = 14:00:00
#@queue

runjob --np 8192 --ranks-per-node 16\
      --env OMP_NUM_THREADS=4 : app.x -i input
```

LoadLeveler Job Script

```
#!/bin/bash

#SBATCH --ntasks=6
#SBATCH --ntasks-per-node=2
#SBATCH --cpus-per-task=24
#SBATCH --output=mpi-out.%j
#SBATCH --error=mpi-err.%j
#SBATCH --time=00:20:00
#SBATCH --partition=batch

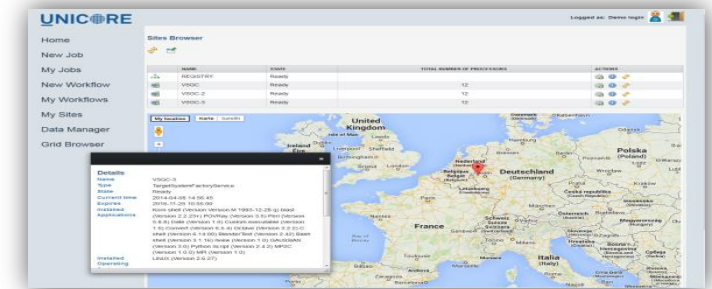
export OMP_NUM_THREADS=${SLURM_CPUS_PER_TASK}
srun ./hybrid-prog
```

Slurm Job Script

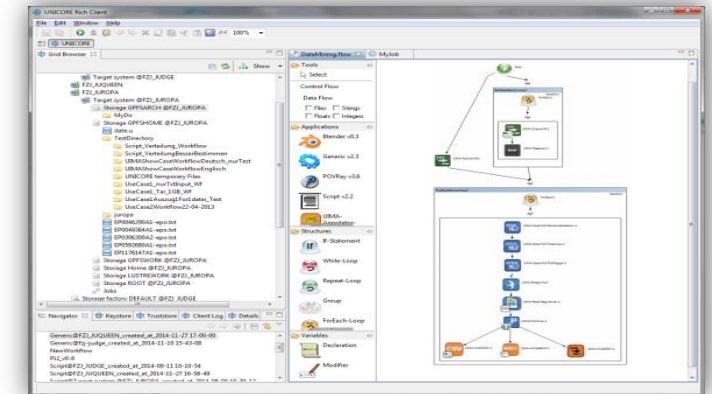
WHY UNICORE?

ADVANTAGES

- Hides system specific commands
- Create, submit and monitor jobs
 - Seamless, secure, and intuitive access to distributed computing and data resources
- Multiple clients, including web portal
- Easy to install and to configure clients
 - Linux, Windows, MacOS versions of stand-alone clients
- Integrated **data management**
- **Federated** identities
- Open Source



Web portal



UNICORE Rich Client (URC)

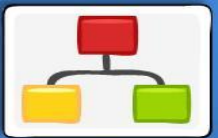
- Commandline Client
- REST API






Web
Command line
GUI
API

Clients





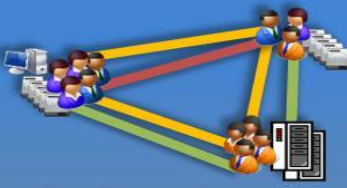

Workflows
Jobs
Data Management
Discovery

Services




Compute
Storage

Resources


Users
Federations
Policies

Security

APPLICATION INTEGRATION

Abstractions of applications on the HPC systems

- Selection by name and version
- Support for user-defined applications, no need to ask an administrator
- Application metadata for generating application-specific GUI
- Hide or rather pre-configure module load ...

*Generic

Job name: Generic

Select application: CP2K

Select version: 4.1-plumed-elpa

Command line arguments:

Application Parameters

☒ INPUT: /tmp/cp2k_geo_opt.inp Browse ...

☐ OUTPUT:

☒ CHECK: true

☐ ECHO: true

☐ MPI_MAPPING:

☐ XML: true

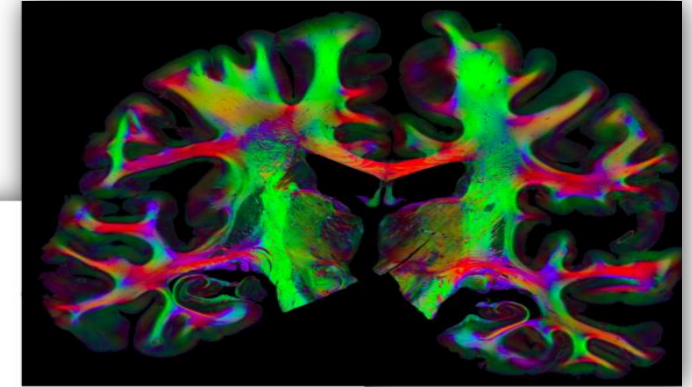
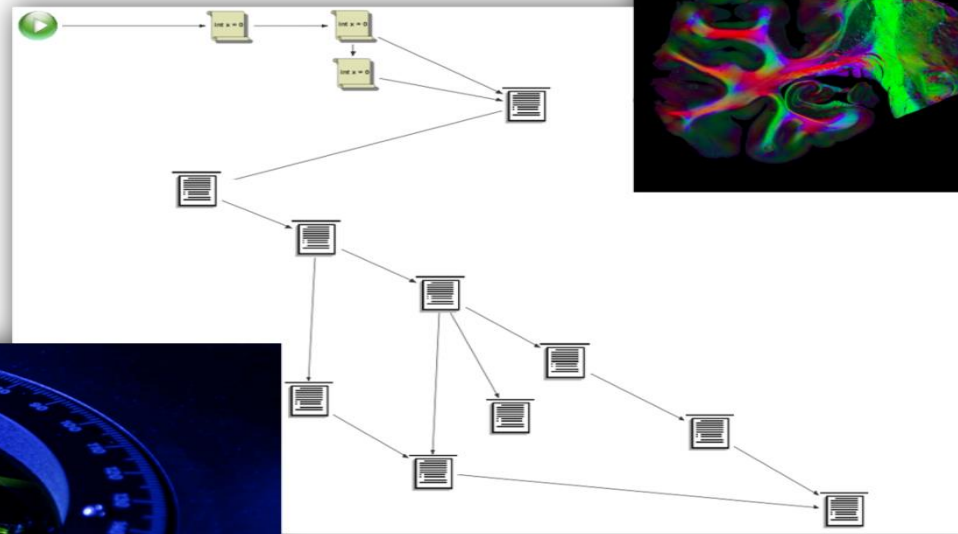
☐ OPTIONS:

Generic Files Variables Resources

```
<jsdl:Argument Description="Check input file"
  Type="boolean"
  Default="..."
  ValidValues="true false"
  DependsOn="..."
  Excludes="..."
  IsEnabled="false"
  IsMandatory="false">-c$CHECK?</jsdl:Argument>
```

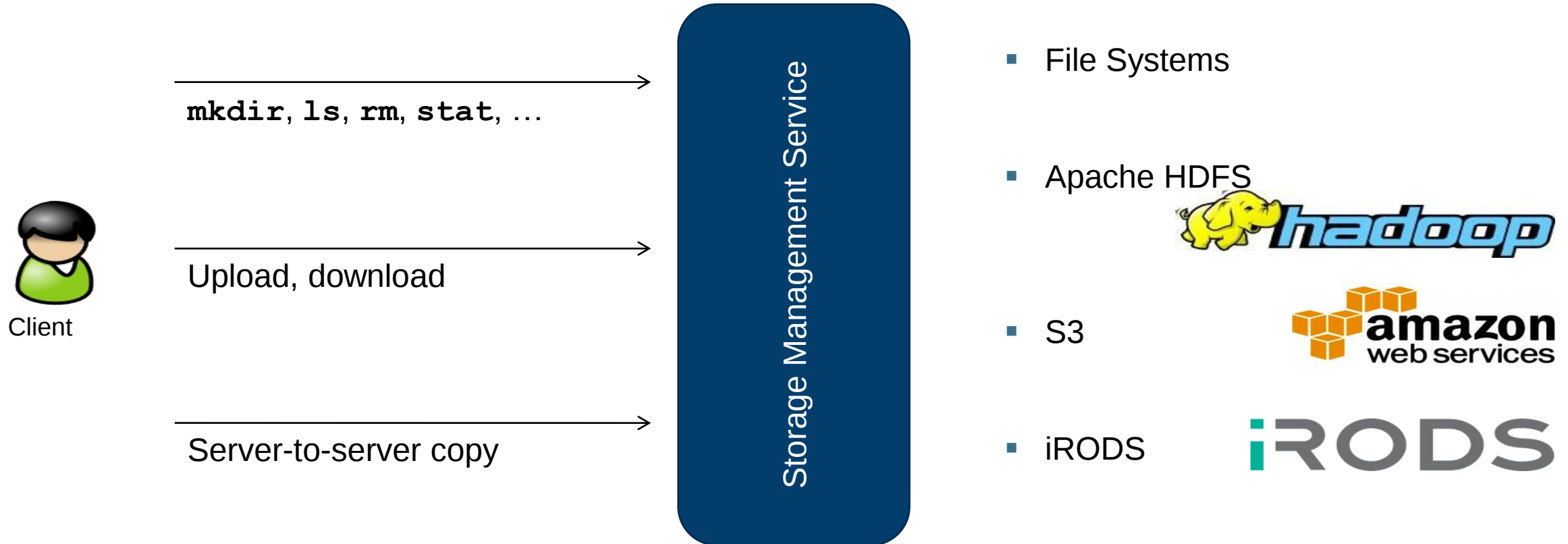
SCIENTIFIC WORKFLOWS

- Create reproducible, complex execution chains
- Automate pre and post processing
- Reduce makespan as compared to manual orchestration



UNICORE

DATA MANAGEMENT AND FILE TRANSFER

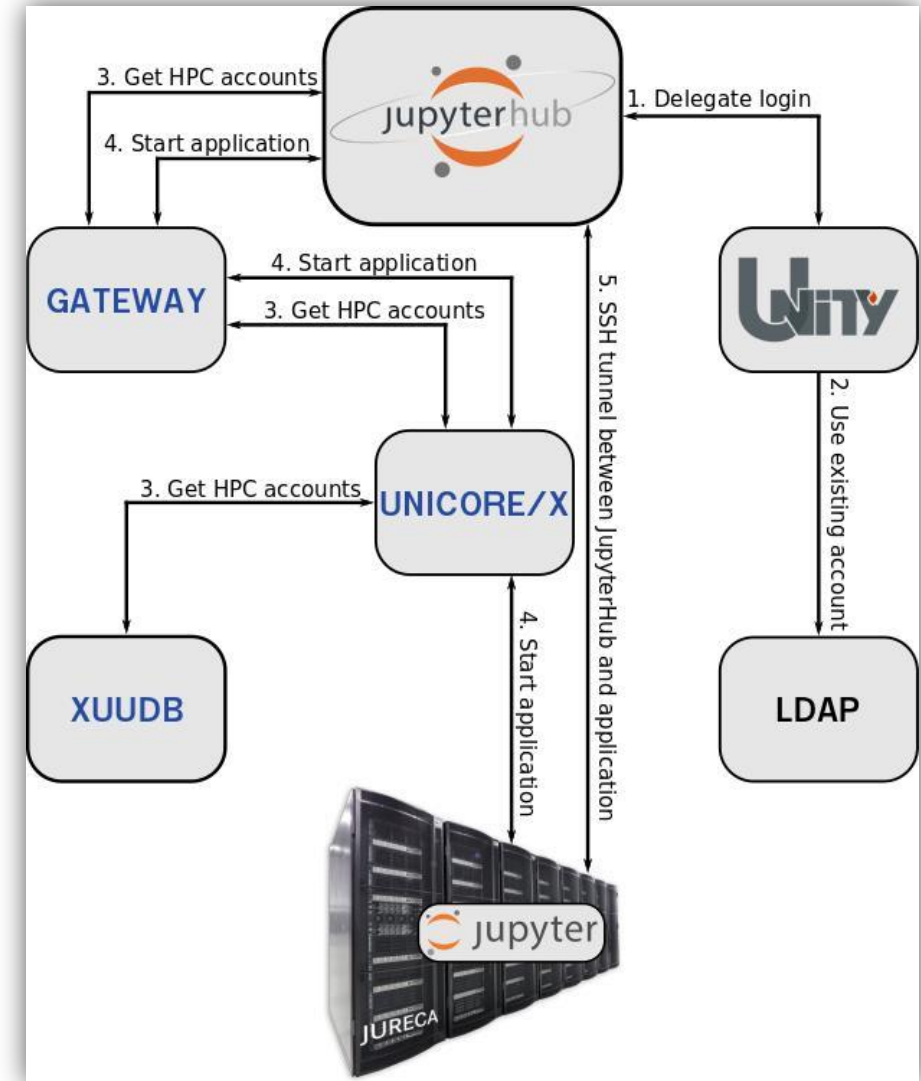


EFFICIENT FILE TRANSFER WITH UNICORE FTP (UFTP)

- Data **streaming** library and **file transfer** tool
- Fully integrated into UNICORE
- Standalone (non-UNICORE) client available
- Client-server and 3rd-party data transfer
- Data staging among UFTP-enabled sites
- Efficient **synchronization** of individual local and remote files using the **rsync** algorithm
- Optional **compression** and **encryption** of data streams

JUPYTER HUB @JSC

- UNICORE is an integral part of the Jupyter offering at JSC
- Access JUWELS, JURECA, or JURON
- <https://jupyter-jsc.fz-juelich.de/>



ADDITIONAL INFORMATION AND SUPPORT

UNICORE

- Project web site: <https://www.unicore.eu/> for downloads and documentation
- Product Support: unicore-support@lists.sourceforge.net

UNICORE at FZJ

- User support email: ds-support@fz-juelich.de
- Portal: <https://unicore-portal.fz-juelich.de/>
- Registry:
https://fzj-unic.fz-juelich.de:9112/FZJ/services/Registry?res=default_registry