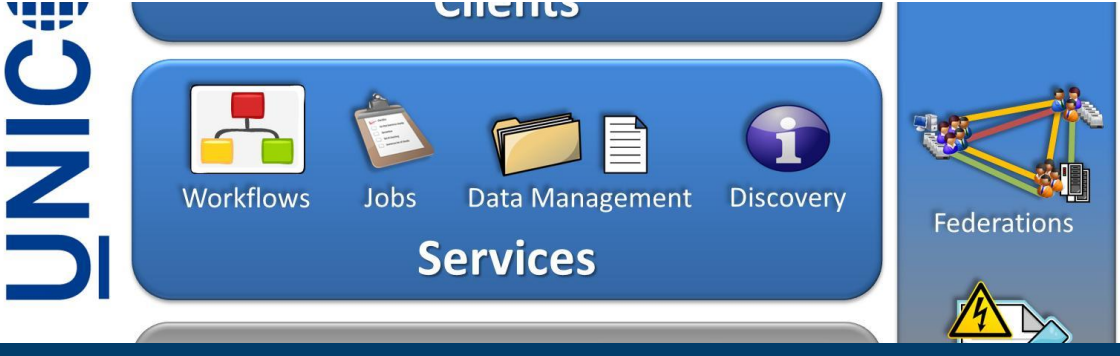
Uniform Resource Access
Compute and Cloud Resources at JSC

2024-11-12 | Björn Hagemeier | Juelich Supercomputing Centre



Part I: UNICORE

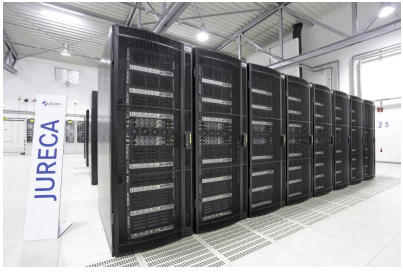
Motivation

Differences of systems

Uniform **I**nterface to **Co**mputing **Re**sources

Various RMS on systems

- JUQUEEN: IBM LoadLeveler
- JURECA: Slurm
- Different job description languages for specifying # of nodes, memory requirements, wall time, ...
- Different parameters on the command line
- Unify and simplify supercomputer access



Slurm

Load Leveler

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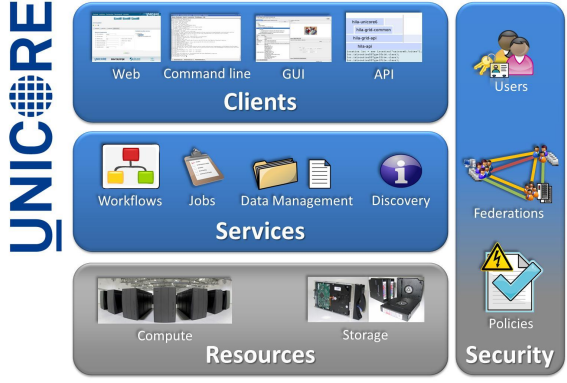
Slurm

Slurm

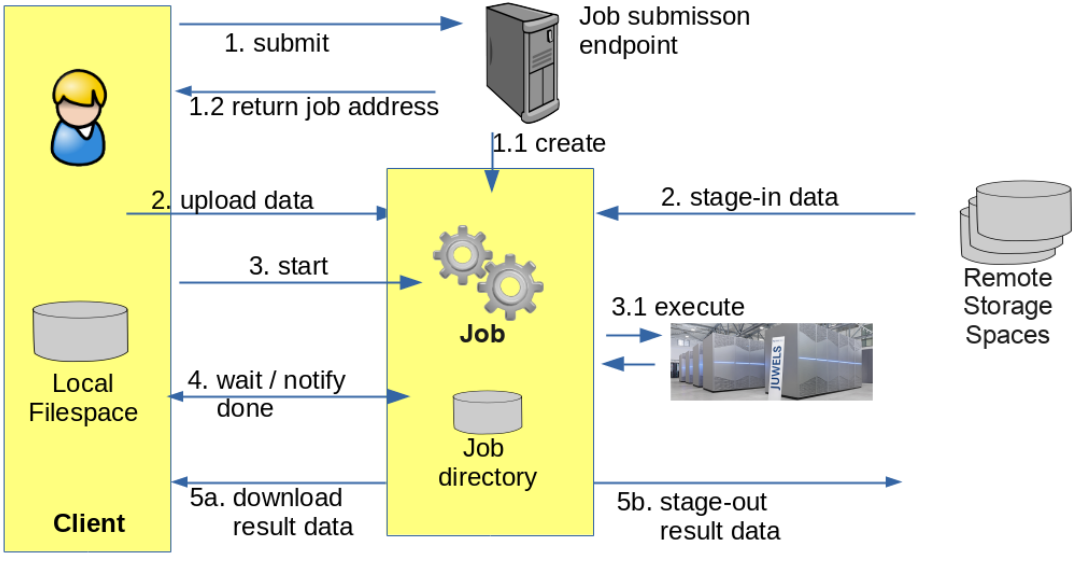
Why UNICORE

Advantages

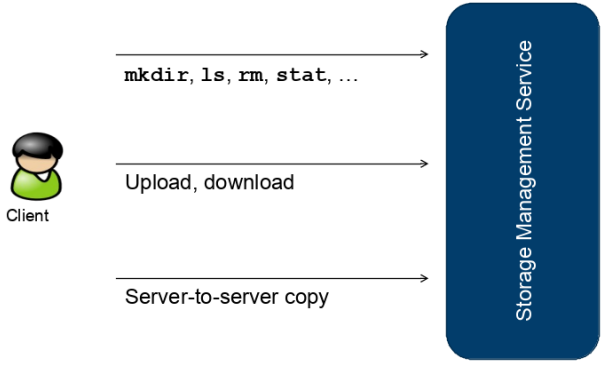
- Hide system specific commands
- Create, submit and monitor jobs
  - Seamless, secure, and intuitive access to distributed compute and data resources
- Multiple clients
- Integrated **data management**
- **Federated identities**
- Open Source: `https://github.com/UNICORE-EU`



Job execution model



Data management and file transfer



- File Systems
- Apache HDFS
- S3
- iRODS

Efficient file transfer

UFTP

- Data **streaming** library and **file transfer** tool
- Fully integrated into UNICORE
- Standalone (non-UNICORE) client available
- Client to server and server to server data transfers
- 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

Efficient file transfer

UFTP

Source: SC Asia web site

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- Awarded “best systemic approach” in SC Asia Data Mover Challenge 2020

PyUNICORE API

Features

- Job submission and monitoring
- File transfer handling
- Mounting filesystems remotely via UFTP
- Workflow management

```
$ pip install pyunicore[crypto,fs,fuse]
```

```
import pyunicore.client as uc_client
import pyunicore.credentials as uc_credentials
import json

base_url = "https://localhost:8080/DEMO-SITE/rest/core"

# authenticate with username/password
credential = uc_credentials.UsernamePassword("demouser", "test123")
transport  = uc_client.Transport(credential)

client = uc_client.Client(transport, base_url)
print(json.dumps(client.properties, indent = 2))
```

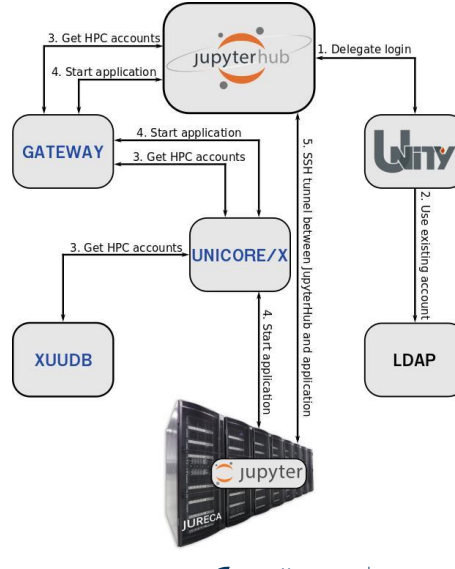
Clients and APIs

- Commandline tools
  - UNICORE Commandline Client (UCC): `https://sourceforge.net/projects/ \ unicore/files/Clients/Commandline%20Client/`
  - UFTP client for high-performance data access: `https: //sourceforge.net/projects/unicore/files/Clients/UFTP-Client/`
- RESTful APIs
  - curl, Python Requests
  - `https://sourceforge.net/p/unicore/wiki/REST_API/`
  - PyUNCIORE client library: `https://github.com/HumanBrainProject/pyunicore`

Jupyter Hub @JSC

HPC in your web browser

- UNICORE is an integral part of the Jupyter offering at JSC
- Start Jupyter Labs on JUWELS, JURECA-DC, JUSUF, DEEP, HDFML, or a cloud based VM
- `https://jupyter-jsc.fz-juelich.de/`
- Foundation for NFDI base service Jupyter4NFDI



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`
- Registry: `https://fzj-unic.fz-juelich.de:9112/FZJ/rest/registries/default_registry`
- Documentation: `https://www.fz-juelich.de/en/ias/jsc/services/user-support/jsc-software-tools/unicore`

Part II: JSC Cloud

Overview

- OpenStack Infrastructure-as-a-Service (IaaS) environment
  - Compute, storage, network, orchestration, load balancing
  - Run VMs to provide services **linked to LARGEDATA**
  - Orchestration using OpenStack Heat
  - Load Balancer as a Service (LBaaS) using OpenStack Octavia
- Intended and existing workloads
  - Scientific services connected to HPC
  - Jupyter JSC
- Further information and reference: `https://go.fzj.de/jsc-cloud`

	JSC Cloud
vCPU	9312
Memory	30.5 TB
GPU	12x NVIDA A100 80GB 16x NVIDIA V100 16GB 4x AMD MI210
NVMe	32x 1TB 6x 3.84 TB

OpenStack

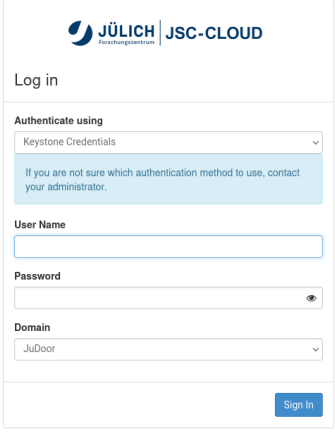
Software and services

- OpenStack Zed release
  - released 2022-10-05
  - we try to balance stable operation and tracing current versions
- Services
  - Keystone – authentication and service registry
  - Horizon dashboard – convenient Web UI appropriate for many simple tasks
  - Nova compute – virtual machine (VM) service
  - Neutron networking – software defined networks
  - Cinder volume – virtual block devices
  - Glance images – template images for VMs
  - Heat orchestration – infrastructure management
  - Octavia load balancing – load balancing as a service
  - Neutron VPNaaS – cross-site (or project) VPNs
  - Sahara – data processing through virtual clusters

Authentication

There are two ways to authenticate

- JSC account
  - username and password
  - usable from both commandline interface and Web UI
- Helmholtz login
  - directly usable only from Web UI
  - commandline access through application credentials
- However: you need a project and allocated resources before using JSC Cloud



Nova

Virtual machine service

Nova manages the lifecycle of virtual machines (VMs) that have

- a number of CPUs
- an amount of main memory
- storage: **system**, ephemeral, swap
- data storage: volumes
- network ports
- a template image containing an operating system

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← Cinder

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← Cinder

← Neutron

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} Nova

- data storage: volumes ← Cinder
- network ports ← Neutron
- a template image containing an operating system ← Glance

Nova

Flavors

We are using as subset of the Sovereign Cloud Stack (SCS) flavors of the form

Example

SCS-16L:32:20n or SCS-nL:m:l-features

with

- n $\rightarrow$ number of CPUs (L for low performance or high oversubscription)
- m $\rightarrow$ amount of main memory (RAM) in GB
- l $\rightarrow$ size of root disk in GB (n for network shared storage)

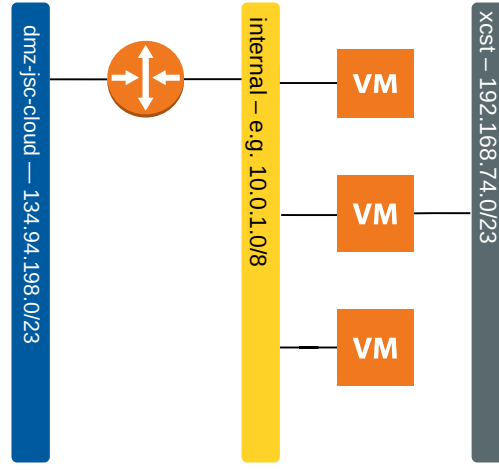
Use `openstack flavor list` or the Web UI to see available flavors. Some examples:

- SCS-2L:4:20n
- SCS-16L:64:20n-z2-nvme
- SCS-1L:1:20n

Networking

Specific networks at JSC

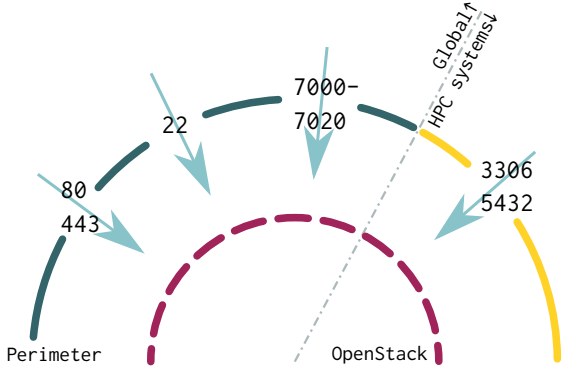
- **floating IPs** realized in router as DNAT/SNAT
- VMs without floating IPs not accessible from the outside and SNATed in outbound connections
- all new projects will be equipped with a **router** and **internal network**, such that you can immediately start working. JSC's **DNS servers** will be configured in the internal network
- **xcst** is a special purpose network for accessing DATA HPC file system



Network setup

Security groups and perimater firewall

- OpenStack firewall freely configurable
- Restrictions apply for inbound connections in perimeter firewall
  - Globally available services and ports: HTTP (80), HTTPS (443), SSH (22), 7000–7020
  - Available from HPC systems: MySql (3306), PostgreSQL (5432)
- Outbound connections: anything but MTA (25) aka. SMTP



Commandline interface

Prerequisites

- Python virtual environment
- Download credential files from the web interface (cf. authentication)

Run the following in your shell:

```
$ python3 -m venv openstack
$ source openstack/bin/activate
$ pip install python-openstackclient
```

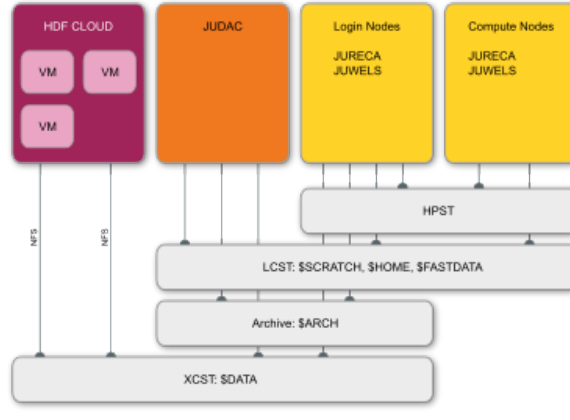
Authentication:

- Option 1: Download and `source openrc.sh`
- Option 2: Download clouds.yaml, put it in one of
  - current working directory as `clouds.yaml` or
  - ∼ `/.config/openstack/clouds.yaml`

JSC Storage Landscape

Availability of file systems

- XCST
  - $DATA on JUDAC and login nodes
  - dedicated NFS export to VMs
- Archive
  - $ARCH on JUDAC and login nodes
- LCST
  - $SCRATCH, $HOME, $FASTDATA, $PROJECT on JUDAC, login and compute nodes
- HPST
  - Login and compute nodes



Data access

VMs and the DATA file system

- JSC Cloud / OpenStack cluster
  - Hosts virtual machines (VMs) for communities
  - Potentially administered by externals, bound by acceptable use policy
- Enable access to data beyond perimeter of SC facility
  - Web interfaces, databases, post processing, …
  - Users of service likely unknown to SC directory information service
- Access Method
  - POSIX file systems ($DATA) accessible in VMs via NFS mount from CES servers
  - Server side UID squashing
    - ensures consistency
    - requires services to manage data accordingly
    - read-write or read-only

OpenStack and cloud training

- February 18, 2025 **online**
- Details to be announced
- Topics
  - OpenStack core services: Nova, Neutron, Cinder, Glance
  - Advanced services: Kubernetes, Heat, Loadbalancers

Summary

JSC Cloud

OpenStack

- Project web site: `https://www.openstack.org/`
- Documentation: `https://docs.openstack.org/`

JSC Cloud:

- User support: `sc@fz-juelich.de`
- Web dashboard: `https://cloud.jsc.fz-juelich.de/`
- Documentation: `https://go.fzj.de/jsc-cloud`