



# RDM FOR DATA FROM HPC

07.04.2025 | Sander Apweiler, Benedikt von St. Vieth, Rajveer Saini | JSC

1. HPC Systems

2. Stagesystems

3. Transfertools

4. B2SHARE

5. DataPub

6. Jülich DATA

7. Comparison of Data services

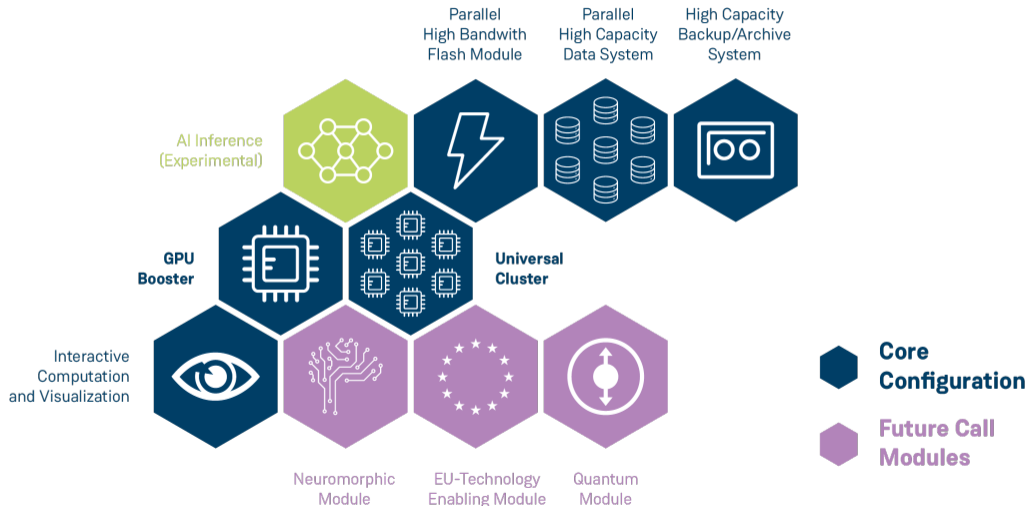
# HPC Systems

# HPC Systems - ... to the present

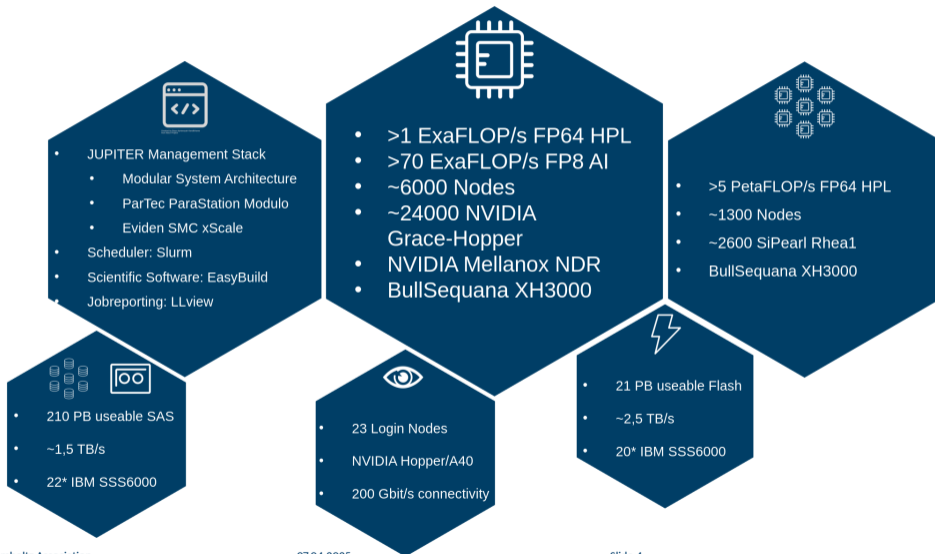
	JUWELS		JURECA	
	Cluster	Booster	Data Centric	HWAI
Peak Petaflops/s	12,3	75	18,5	8,5
Nodes	2567	936	768	32
Accelerators	224 GPUs	3744 GPUs	768 GPUs	128 GPUs

- Beside of the large HPC clusters
  - Prototype as a blueprint for modular super computers: DEEP
  - Small cluster for user from campus or specific communities: HDF-ML, JUZE A1
  - Data access cluster: JUDAC
  - Others: JSC Cloud (combination of JUSUF and HDF Cloud)

# HPC Systems - Jupiter High Level Architecture



# HPC Systems - Jupiter High Level Architecture



# Beyond HPC Systems - JSC cloud

	JSC cloud
Installation	2023/2024
Software Foundations	OpenStack IaaS
vCPUs	12384 (on 72 nodes, mostly AMD)
Memory	36,5 TB
Accelerators	16x NVIDIA V100 16GB 12x NVIDIA A100 80GB 32x NVIDIA RTX A6000 4x AMD MI210
PCI Passthrough Devices	32x 1TB NVMe 30x 3,84 TB NVMe
Storage	4 PB (NFS on top of GPFS, Migration to Ceph ongoing)
Resources via	Different projects participating in funding
End of life	-

# Storagesystems

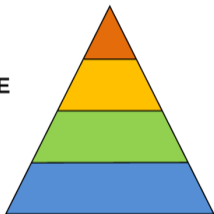
# Storagesystems

SCRATCH

PROJECT/HOME

DATA

ARCHIVE



## JUWELS, ...

IBM SSS6000

IBM SSS6000

XCST/IBM SSS6000

4 Shared Libraries, HSM (IBM DSS), Spectrum Protect

## JUPITER

ExaFLASH (SSS6000)

ExaSTORE (SSS6000)

ExaSTORE (SSS6000)

# Storagesystems

## ExaFLASH

- 29 PB raw
- 2,1 TB read /  
3,1 TB write
- 30 TB NVME
- IBM SSS6000
- IBM Storage  
Scale
- InfiniBand  
only

## ExaSTORE

- 308 PB raw
- 1,4 TB read /  
1,1 TB write
- 22 TB disk
- IBM SSS6000
- IBM Storage  
Scale
- InfiniBand and  
100GE

## JUST6

- 154 PB raw
- 700 GB read /  
500 GB write
- 22 TB disk
- IBM SSS6000
- IBM Storage  
Scale
- 100 GE fabric  
(like JUST5)

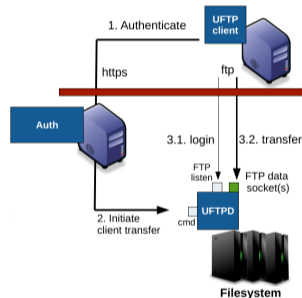
## Tape

- 664 PB raw
- 4 libraries
- 117 Drives
- 53205 Media
- IBM Storage  
Protect
- Backup/Archive

# Transfertools

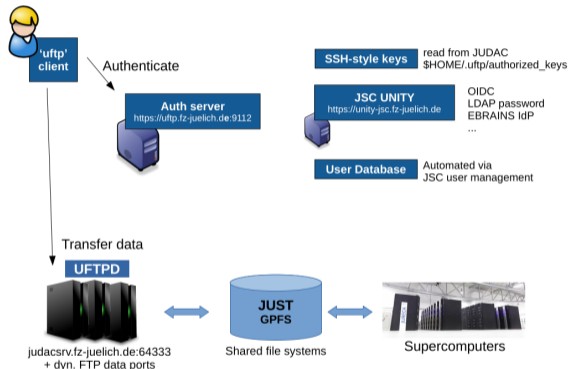
# Transfertools - UFTP

- „UNICORE FTP“ ⇒ it grew out of the need for a high-performance data transfer for the UNICORE federated middleware
- Client/server file transfer system, based on FTP, with flexible, federated authentication
- Extended with
  - Compression and/or encryption of data stream(s)
  - Multiple TCP streams per data connection
  - Bandwidth management (both server and client)
- UFTPD Server supports partial file reads/writes
- UFTPD creates multiple sessions in parallel for scalability
- Multiple UFTPD backends are possible (round-robin)



# Transfertools - UFTP

- Share data with other users via UFTP
- Command line tool with well known commands like:  
cp, ls, ...
- Authentication via
  - ssh-style keys (recommended, at JSC it must differ from ssh key)
  - OAuth tokens
  - username/password
- Available at JSC, HLRS and LRZ



Full presentation about UFTP at DOI:10.23728/b2share.83b63c4bf4674e638711ef9bddb93bfb or PID: 11304/7d62b0f3-02a3-4d82-aa47-436fa9778cda

# B2SHARE

# B2SHARE

- Developed by EUDAT CDI
- Provided by JSC as community instance
- URL: <https://b2share.fz-juelich.de>
- Audience: researchers from Forschungszentrum Jülich and related communities
- Quota: 50GB per file; 200GB per deposit
- Listed as repository on re3data
- Accepted repository for Springer publication
- Harvested by B2FIND



# B2SHARE

- Attaches DOI to each deposit and PID to each deposit and all files
- Supports multiple versions of a deposit
- Supports individual (community) metadata schemas
- Usage with web UI or REST API
- Command line tool for basic usage available
- Link to other data storage is possible, if the data is stored somewhere else
- More information: <https://go.fzj.de/B2SHARE>




[HELP](#) [COMMUNITIES](#) [UPLOAD](#) [CONTACT](#)
[sa.apweiler@fz-juelich.de](mailto:sa.apweiler@fz-juelich.de)
[RECORDS](#) - 3F5C3F8E853148D2806867A93EECD4E0

Latest Version - Apr 29, 2021

## TOAR-II Database Infrastructure presentation for WMO virtual conference on Earth system data exchange in the 21st century, 16 - 19 Nov 2020

by Schröder, Sabine; Epp, Eleonora; Leufen, Lukas; Mozaffari, Amirpasha; Romberg, Mathilde; Schultz, Martin; Sun, Jianing;

Apr 29, 2021

**Abstract:** Innovative Air Quality Services: The TOAR Database Infrastructure

The Tropospheric Ozone Assessment Report database of global air quality observations includes multi-faceted metadata and was built according to Open Data and FAIR principles.

We now collect OpenAQ data and exploit high-resolution geospatial data.

This presentation was shown at the poster session of the WMO virtual conference on Earth system data exchange in the 21st century, 16 - 19 Nov 2020 (<https://meetings.wmo.int/WMO-Data-Conference/SitePages/Conference%20Scheme.aspx>).

**Disciplines:** 3.2.4 → Chemistry → Atmospheric chemistry;

**Keywords:** tropospheric ozone, global air quality, air quality monitoring;;

**DOI:** [10.34730/3f5c3f8e853148d2806867a93eecd4e0](https://doi.org/10.34730/3f5c3f8e853148d2806867a93eecd4e0)

**PID:** [21.11125/dac26910-1581-46c0-9c33-a4131865e827](https://nbn-resolving.org/urn:nbn:de:hbz:5:1-63862-p0011-7)



### Files

Member of the Helmholtz Association

 07.04.2025  
Size

### Basic metadata

Open Access Slide 16 True ✓

License

Creative Commons Attribution (CC-BY)

# DataPub

# DataPub

- URL: <https://datapub.fz-juelich.de/>
- Solution for files which do not fit in B2SHARE
- Audience: researchers from Forschungszentrum Jülich
- Listed as repository on re3data
- Stores only data but no metadata and does not assign identifiers
- Accessible via https
- Datarepository can be managed by single users or groups
- Usage must be requested

# Jülich DATA

# Jülich DATA

- URL: <https://data.fz-juelich.de/>
- Based on Dataverse
- Service provided by ZB (central library) as central solution
- Connected via OpenID Connect to Helmholtz AAI
- Provides DOIs
- Storage for metadata and small files (up to 2GB)
- Link to other storages with URIs
- Storage tiering if institutes provide their own S3 storage
- Individual metadata schemas are possible

# Comparison of Data services

	B2SHARE	DataPub	Jülich Data
Filesize	50GB	unlimited	2GB
Recordsize	200GB	unlimited	-
Metadata	Yes	No	Yes
PID/DOI	Yes	No	Yes
Access	FZJ Internal	External	FZJ Internal
Retention	10Y	10Y	10Y
Registry	re3data, Fairsharing, DataCite	re3data	re3data
External repository	No	Yes	Yes