

Easier Access to ESM Data: Implementation at Jülich Supercomputing Centre (JSC)



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Scientific Motivation

The Challenge

- km-scale ESM produce $\mathcal{O}(GB)$ per variable & level Driven by advances in computing performance of HPC systems
- Challenge on storing and processing data
- petabyte-scale capacity file storage @ HPC centers
- Prohibitive bottleneck especially for local user systems
- Demand for FAIR data, in particular findable data ESM=Earth System Models

HPC=high performance computing FAIR=Findable, Accessible, Interoperable, and Re-usable

Easier Module within WarmWorld project

- Provide harmonized access to ICON modelling system alongside IFS-based solutions and observational Simplification of data access
 - Preparation to manage km-scale/exascale data streams
- Prototype exascale analysis workflows Combining simulations and observations
- Performance in WarmWorld Better & Faster

ICON=Icosahedral Nonhydrostatic[1]: a numeric ESM model by DWD, MPI-M, DKRZ, KIT, C2SM

Joined Approach at DKRZ & JSC

- Federated catalog for data centers
- Common interfaces to access data & analysis
- direct/local access, download, zarr over HTTP
- Easier use-case drives developments:
 - hosting of IFS data @ JSC and ICON data @ DKRZ for analysis by University of Cologne

IFS=Integrated Forecast System of ECMWF[2] DKRZ=German Climate Computing Center ECMWF=European Centre for Medium-Range Weather Forecasts

Ingredients for developments at JSC

Data Backend: Fields DataBase (FDB)

Object store for geospatial data[3, 4]

- Operational storage for recent results at ECMWF
- Access to data via metadata (MARS language)
- Storage of data in POSIX structure
 - Directory \rightarrow file \rightarrow grib file (multiple fields)
 - Structure defined by metadata (configurable)

SpatioTemporal Asset Catalog (STAC)

Metadata catalog for geospatial data[5]

- Based on JSON: Machine and human readable
- JSC: Hosting API specification with Postgres backend[6]
- Federated catalog hosted at DKRZ
- More details: Kameswar Rao Modali et al. (EGU25-10288 at Hall X4 | X4.107)

Test Dataset

- IFS dataset (306 600 fields) 365 days with two runs/day and 12 forecast steps
- 5 model levels
- 7 atmospheric and 1 surface variable
- $0.25^{\circ} \times 0.25^{\circ}$ resolution $(0.25^{\circ} \approx 27 \text{ km})$
- \approx 2 MB per field

UNICORE - UNiform Interface to COmputing REsources

Access to HPC resources via RESTful API through different interfaces[7]

- Start and control of jobs on HPC systems (e.g. SLURM)
- Port forwarding from external systems to compute nodes
- Access to storage cluster, e.g. FUSE mounts
- Allows data driven execution of scripts

UNIC#RE

OpenID Connect (OIDC) provider for Helmholtz centers and other scientific institutions[8]

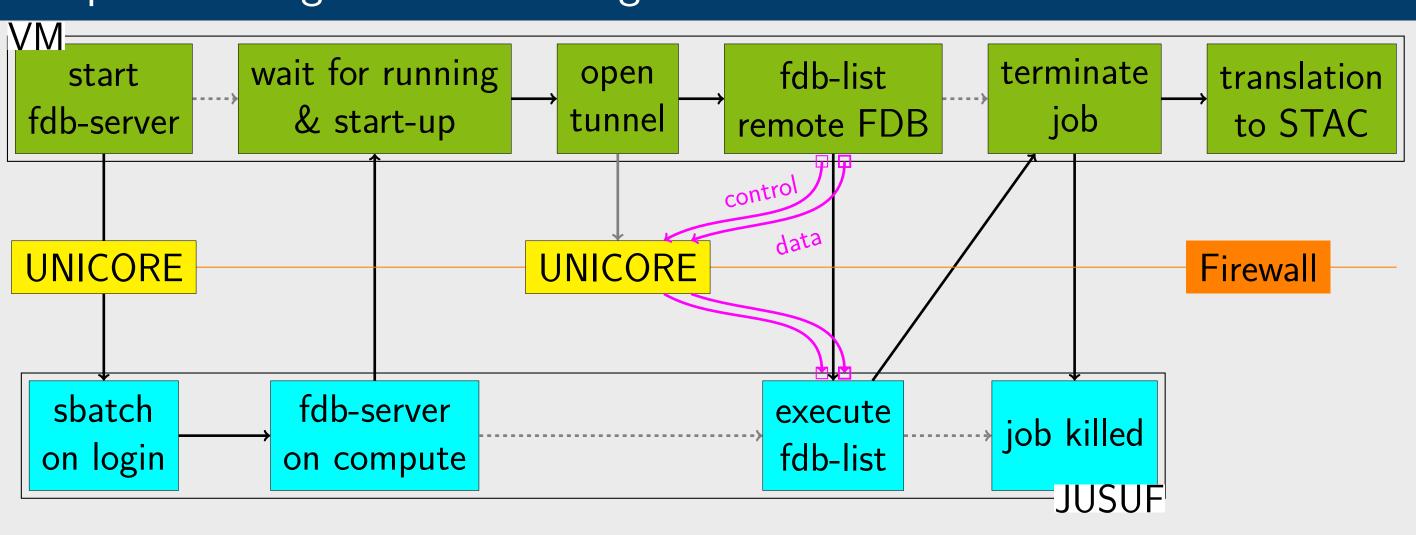
Federated AAI also including social Identity Providers (ORCiD, github, google)

Helmholtz ID as Authorization and Authentication Infrastructure

- Login through infrastructure of identity provider/home institution
- Authorization via different scopes possible, e.g. handling of "virtual organisations"



Recipe for Filling a STAC Catalog with Metadata from an FDB

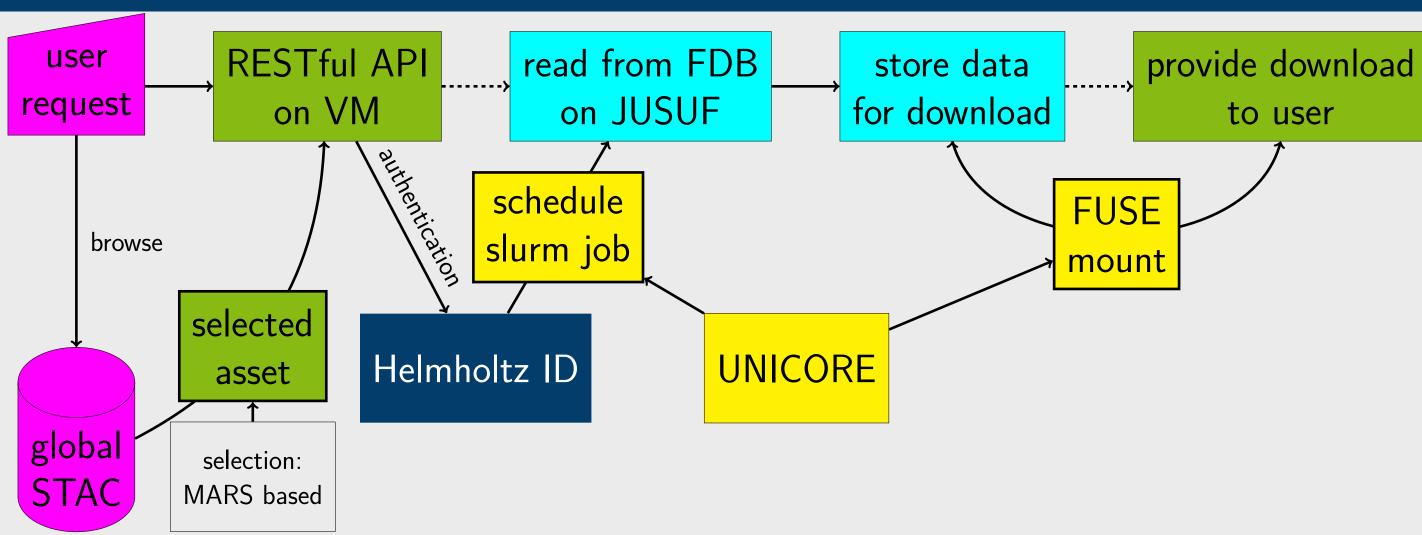


<u></u>

400

JUSUF: Jülich Support for Fenix, see https://go.fzj.de/jusuf

Recipe for Download Service



Outcome: Benchmarks for Accessing Data in FDB

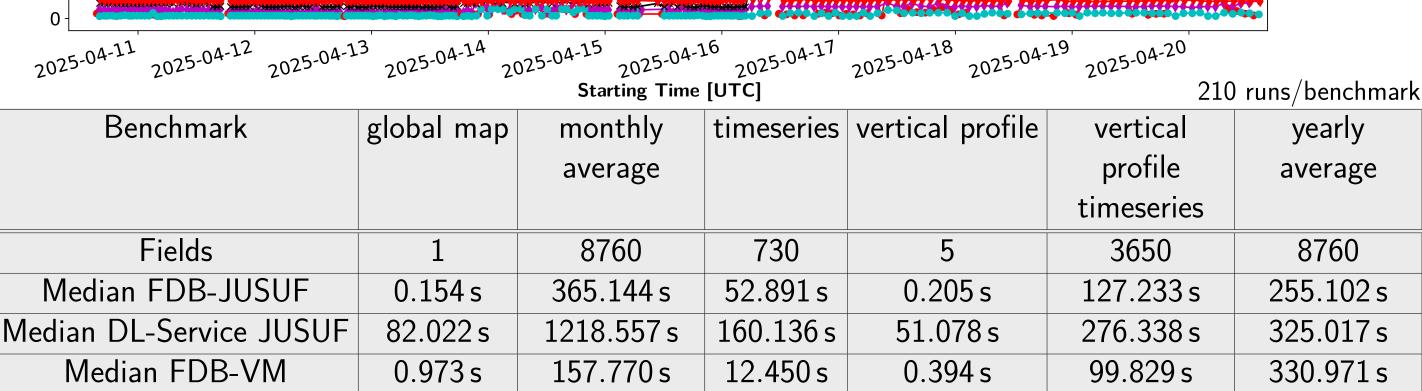
- Case 1: Local operation on JUSUF, direct access to FDB
 - JUSUF as HPC system has access to shared storage cluster JUST hosting the FDB - FDB @ \$SCRATCH
- Recent simulations will be written \$SCRATCH Case 2: Remote user with access to FDB
 - through JSC-Cloud - No direct access to FDB
 - Cloud has no access to \$SCRATCH - Cloud hosts services to download data
- Case 3: Local operation on VM
 - FDB on dedicated volume
- Cloud as host for data management services (e.g. fill catalog)

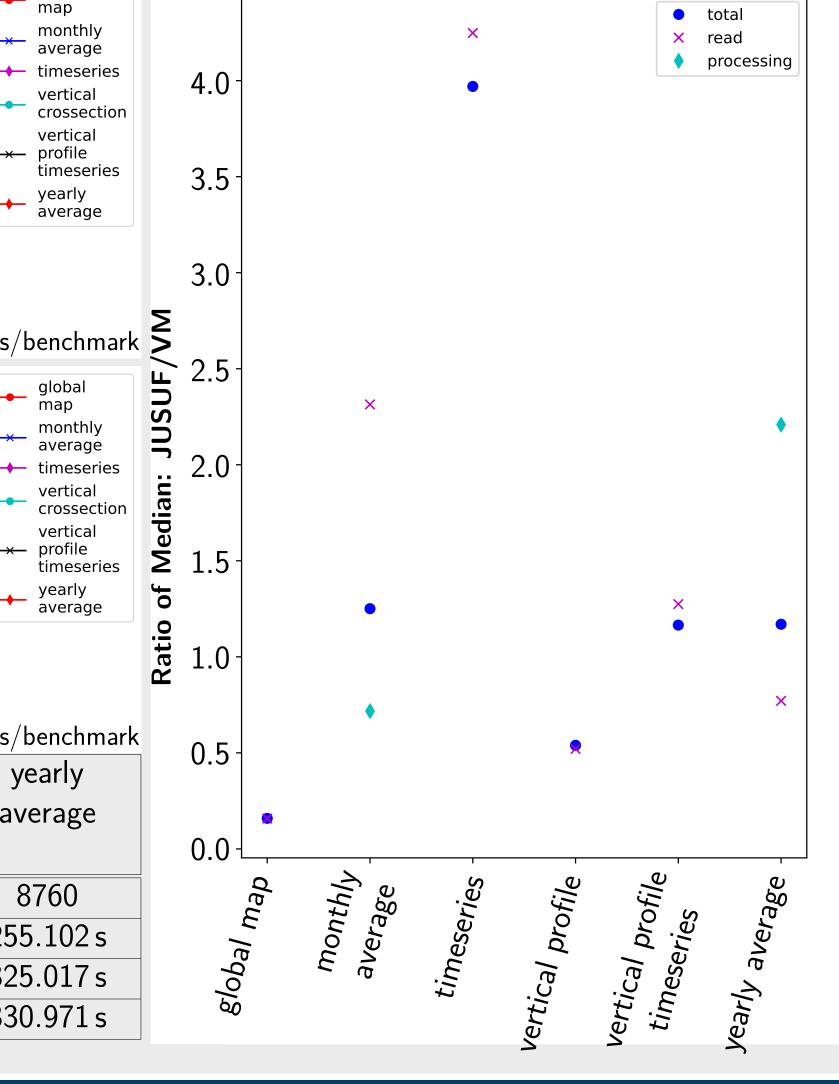
Hardware			
	VM @ JSC-CLoud	JUSUF	
CPU	4 cores@2.25 GHz	2× AMD EPYC 7742 64	
		cores @2.25 GHz	
RAM	7.75 GB	16 × 16 GB DDR4 @	
		3200 MHz	
Volume	15 TB	access to JUST	
		$\mathcal{O}(TB)$ to $\mathcal{O}(PB)$	
		C19760	

JUST: Jülich Storage Cluster JUST specification for details:

300 ق 2025-04-09 2025-04-06 Starting Time [UTC] 330 runs/benchmark Case 2: Access through Download Service 4000 of JSC-Cloud download through ्र ह्य 3000 download through UNICORE storage resource UNICORF-FUSE mount 2000 2000 1000 -2025-04-16 2025-04-13 2025-04-12 2025-04-14 2025-04-15 Starting Time [UTC] Benchmark global map monthly timeseries vertical profile vertical profile average timeseries

Case 1: JUSUF (Single Node, Direct FDB Access)





Case 3: JUSUF & JSC-Cloud

Conclusions

- Storage cluster and HPC provide a compatible performance to VM Data size requires storage cluster like JUST for km-scale simulations
- Access through service is slower (job allocation, copying on HPC system & download)
- Access for project partners through Helmholtz ID

Outlook

- Improved data access services
- Hosting of a service to access FDB data as zarr via HTTP (development by ECMWF)
- Hosting of a *polytope*[9] service
- Optimization of data extraction for download & job allocation
- Extended authorization using a "Virtual organisation" concept of the Helmholtz ID
- Portal for ESM data services provided by JSC within WarmWorld

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