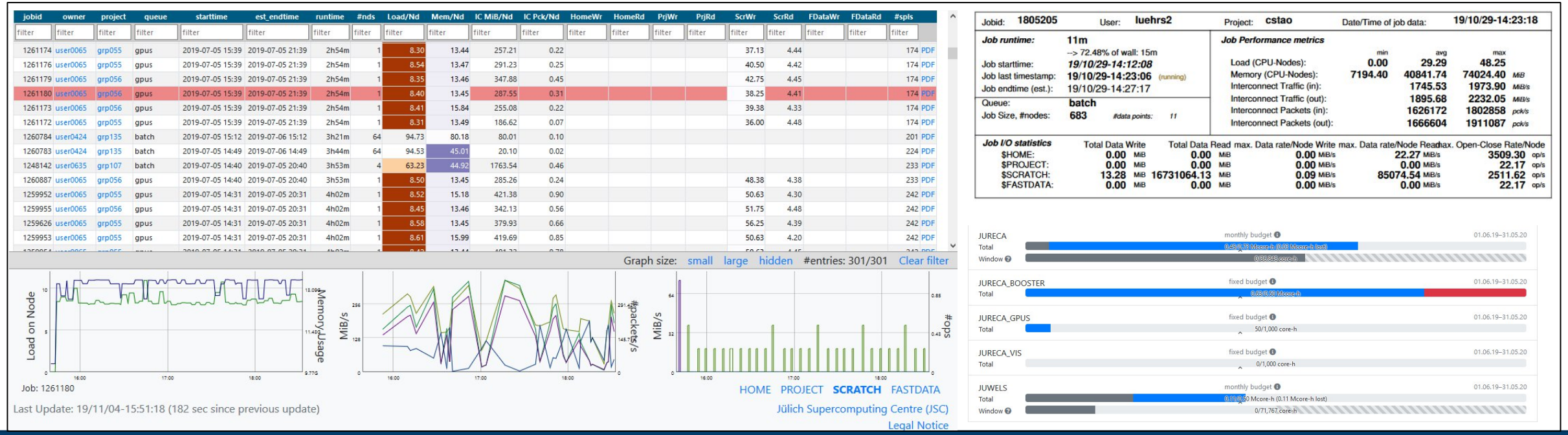
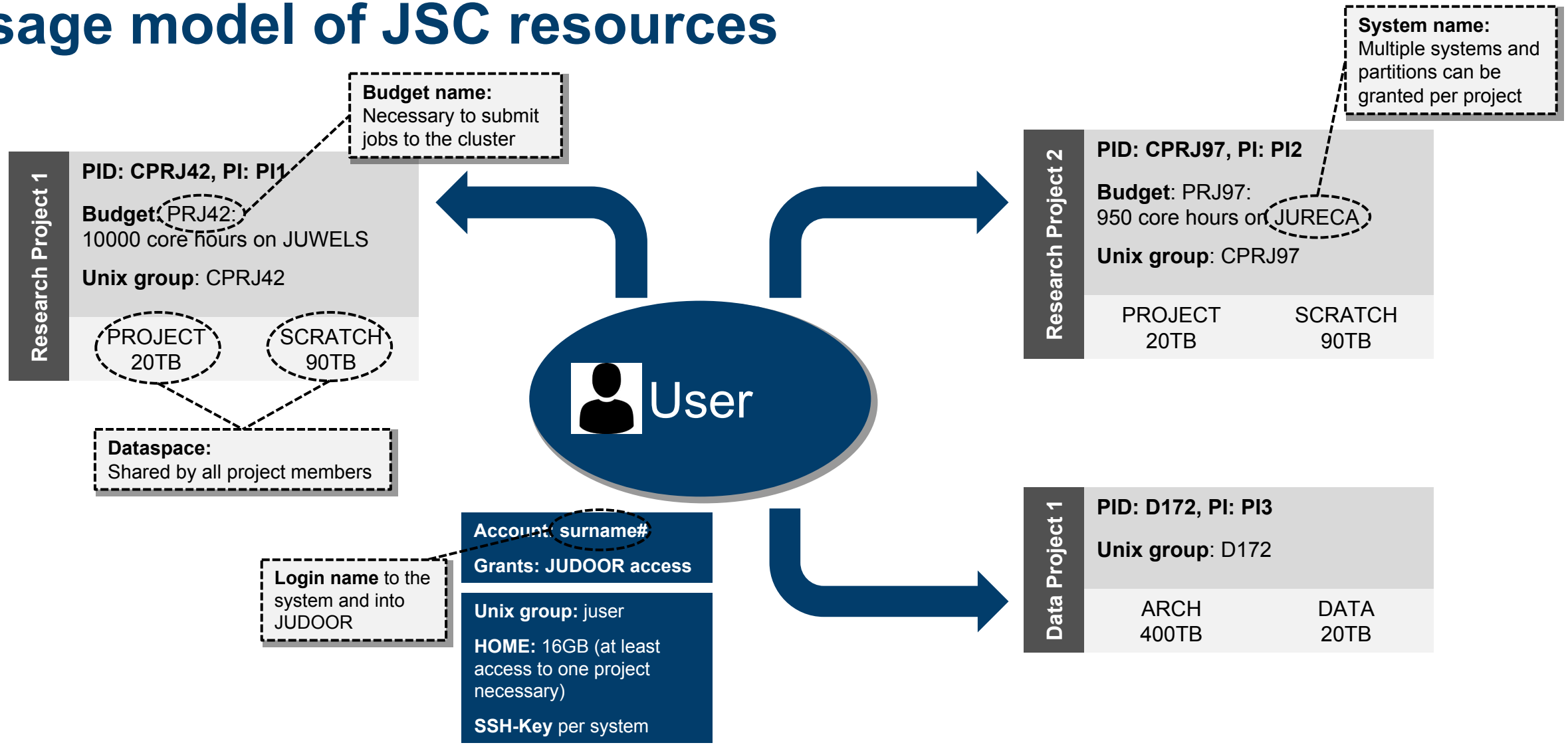


First Steps: User Portal and Job Monitoring

Webportals and Support-Tools @ JSC

30.05.2023 I Dr. Jolanta Zjupa

Usage model of JSC resources



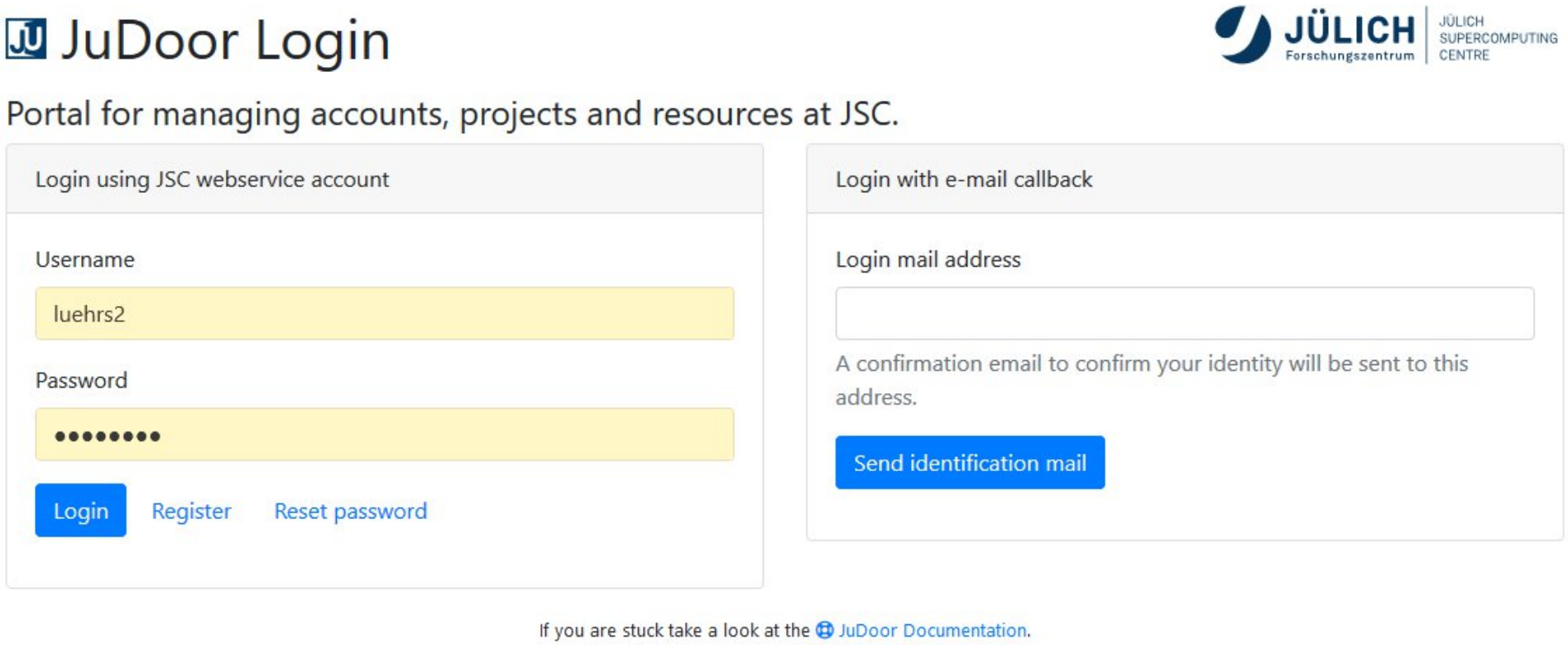
Compute project vs. data project

	Compute project	Data project
Call	Twice per year	Continuously open
Computing time		
Grants system access	• JUWELS • JURECA • JUDAC …	• JUDAC
Filesystem access on all systems	• PROJECT • SCRATCH	• ARCHIVE • FASTDATA • DATA • SOFTWARE

Note: $SCRATCH has **no backup** and files that have not been touched 90 days are **automatically deleted**

3 Steps to access the HPC systems

Step 1: JUDOOR account registration



https://judoor.fz-juelich.de

Step 2: Join a project

Two alternatives

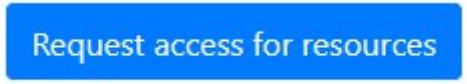
in JUDOOR if you know the project ID

Follow invitation link send by PI or PA

https://judoor.fz-juelich.de/projects/join/...

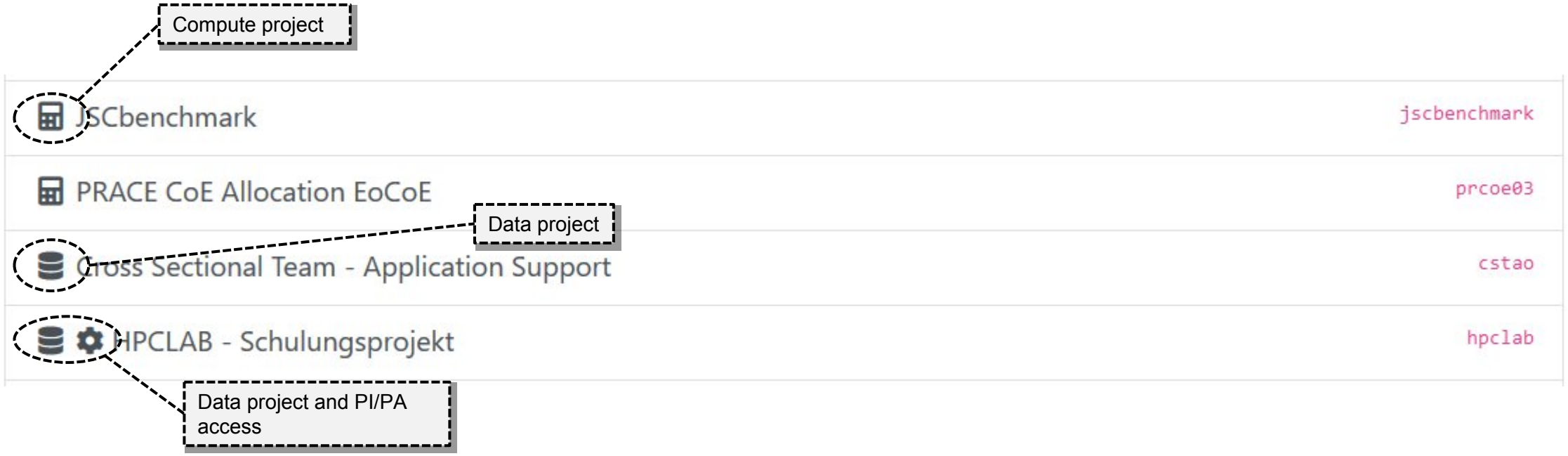
PI/PA receives notification and grants project resource specific access

If you are already a project member but don't see all available project systems, you can use



JUDOOR Overview

An user can be part of multiple compute and data projects



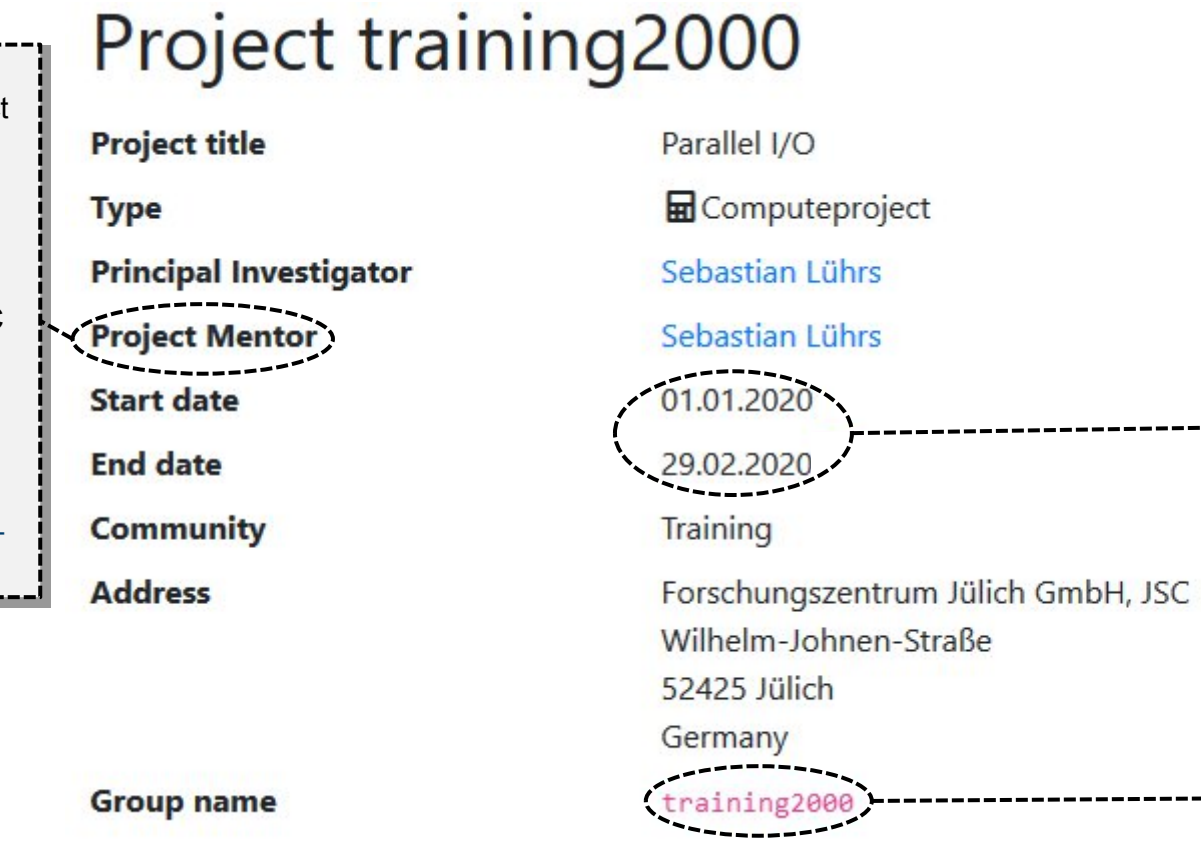
JUDOOR Overview

Project details

Project Mentor:
Project specific permanent contact point at JSC, in addition to sc@fz-juelich.de.

The mentor is available for requests concerning further support and training offers by JSC or helps to arrange in-depth code analyses.

More details:
https://www.fz-juelich.de/en/ias/jsc/services/user-support/project-mentoring



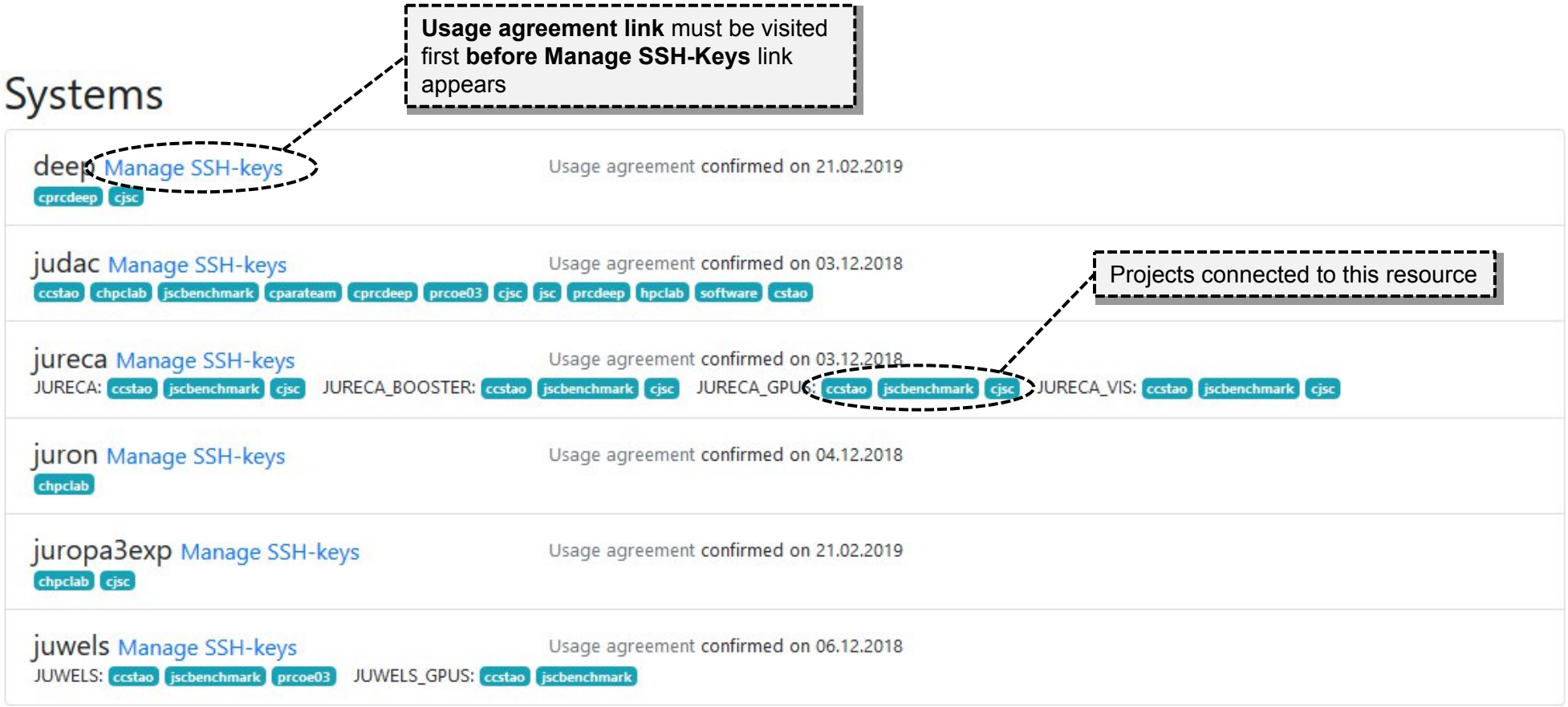
Data access is possible up to 3 month after the end of the project via JUDAC.

Project duration:
Job execution is only possible during the runtime of the project if there is an available budget.

Project unix group:
Unix group for project related top level folders

JUDOOR Overview

Each projects grants access to various systems and partitions.



JÜLICH Forschungszentrum

Step 3: Upload your SSH-key

How to Login

Terminal

```
ssh [-X] userX@jureca.fz-juelich.de
```

- This will bring you to $HOME on JURECA, analogously other systems

  Note: $HOME has only 16GB and is *not* meant for production - go to: $PROJECT or $SCRATCH

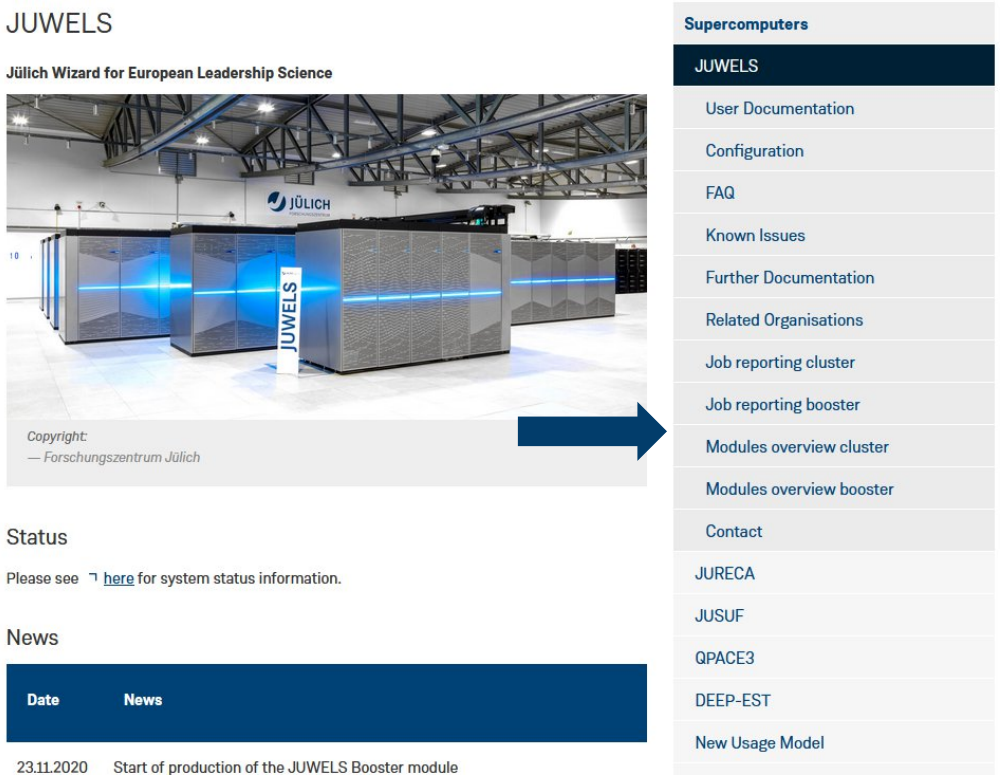
- On your local machine you can edit `.ssh/config` to set shortcuts

- **JupyterLab** (through the browser) **Talk today by J.-H. Göbbert (JSC)**

- Setup SSH connection through your favourite editor (VSC, Sublime, Atom, Kate, … many others)

- Mount the Filesystem to your local machine through a mount point **Hands on**

Overview preinstalled software



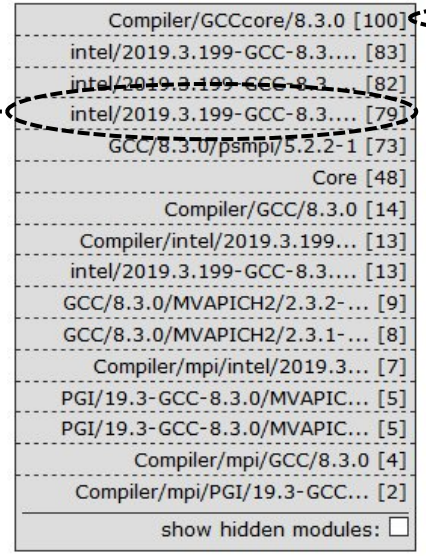
JURECA: https://apps.fz-juelich.de/jsc/llview/jureca_modules/

JUWELS Cluster: https://apps.fz-juelich.de/jsc/llview/juwels_modules/

JUWELS Booster: https://apps.fz-juelich.de/jsc/llview/juwels_modules_booster/

Overview preinstalled software

Software toolchains



One software toolchain: Intel compiler & ParaStationMPI

MPI/intel/2019.3.199-GCC-8.3.0/psmpi/5.2.2-1

ABINIT/8.10.2	LAMMPS/12Dec2018	Silo/4.10.2
ARPACK-NG/3.7.0	MUMPS/5.1.2	SuiteSparse/5.4.0-
ASE/3.17.0-Python-3.6.8	MUST/1.6-rc3-Python-3.6.8	METIS-5.1.0
Boost/1.69.0-Python-2.7.16	Meep/1.7.0	Valgrind/3.14.0
Boost/1.69.0-Python-3.6.8	NAMD/2.13	VampirServer/9.6.1
CDO/1.9.5	NCL/6.6.2	YAXT/0.6.0
CGAL/4.13.1-Python-2.7.16	NCO/4.7.9	buildenv/intel-para
CGAL/4.13.1-Python-3.6.8	OSPRay/1.8.4	darshan-runtime/3.1.7
CP2K/6.1-plumed-elpa	PETSc/3.11.1	darshan-util/3.1.7
CPMD/4.3	PETSc/3.11.1_complex	ecCodes/2.12.0
ELPA/2016.05.004	PETSc/3.11.1_int8	h5py/2.9.0-Python-2.7.16
ELPA/2018.11.001	PLUMED/2.5.1	h5py/2.9.0-Python-3.6.8
ELPA/2018.11.001-gpu	ParMETIS/4.0.3	imkl/2019.3.199
ELPA/2018.11.001-single	ParMETIS/4.0.3-double	mpi4py/3.0.1-Python-2.7.16
ESMF/7.1.0r	PyFerret/7.5.0-Python-2.7.16	mpi4py/3.0.1-Python-3.6.8
Elemental/0.87.7	QuantumESPRESSO/6.4.1	mpiP/3.4.1
Extrae/3.7.0	R/3.5.3	netCDF-C++4/4.3.0
FFTW/3.3.8	R/3.5.3.bak_20190521110136	netCDF-Fortran/4.4.5
GPAW/1.5.2-Python-3.6.8	RELION/3.0.4	netCDF/4.6.3
GROMACS/2019.1	SCOTCH/6.0.6	netcdf4-python/1.5.0.1-
GROMACS/2019.1.bak_20190712181534	SIONlib/1.7.2	Python-2.7.16
GROMACS/2019.3	SLEPc/3.11.1	netcdf4-python/1.5.0.1-
HDF5/1.10.5	Scalasca/2.5	Python-3.6.8
Harminv/1.4.1	Score-P/5.0	parallel-netcdf/1.11.0
Hypre/2.15.1	Score-P/6.0	petsc4py/3.11.0-
Hypre/2.15.1-bigint	Score-P/default	Python-3.6.8
	Siesta/4.0.2	sprng/1
		sprng/5-14042019
		sundials/3.2.1
		sundials/4.1.0

Can be loaded on the system by using:

```
module load Intel
module load ParaStationMPI
module load netCDF
```

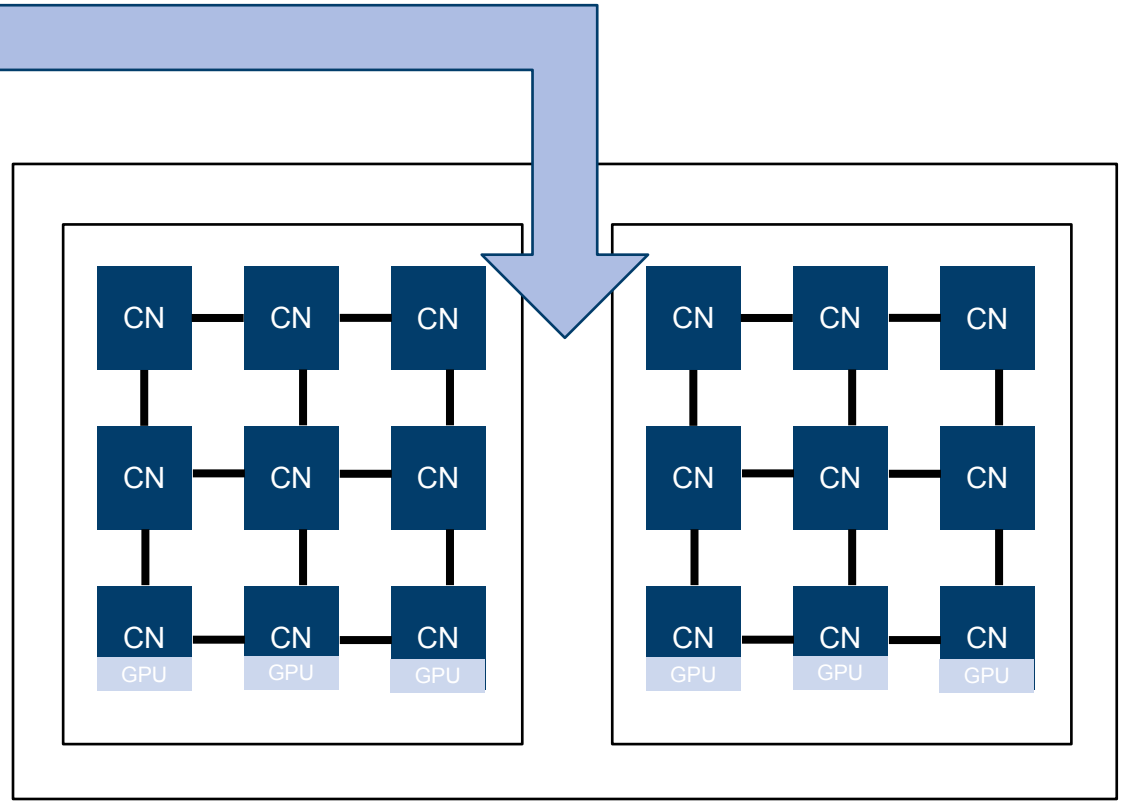
Talk tomorrow by R. Schöbel (JSC)

Slurm job submission

```
#!/bin/bash -x
#SBATCH --mail-type=BEGIN,END,FAIL
#SBATCH --mail-user=

#SBATCH --account=
#SBATCH --job-name
#SBATCH --output=
#SBATCH --error=
#SBATCH --time=24:00:00
#SBATCH --nodes=
#SBATCH --ntasks-per-node=
#SBATCH --partition=

srun ./mycode
```

Login node

Terminal: `sbatch job_jureca.sh`



Compute nodes

Talk tomorrow by C. Paschoulas (JSC)

Quota calculation

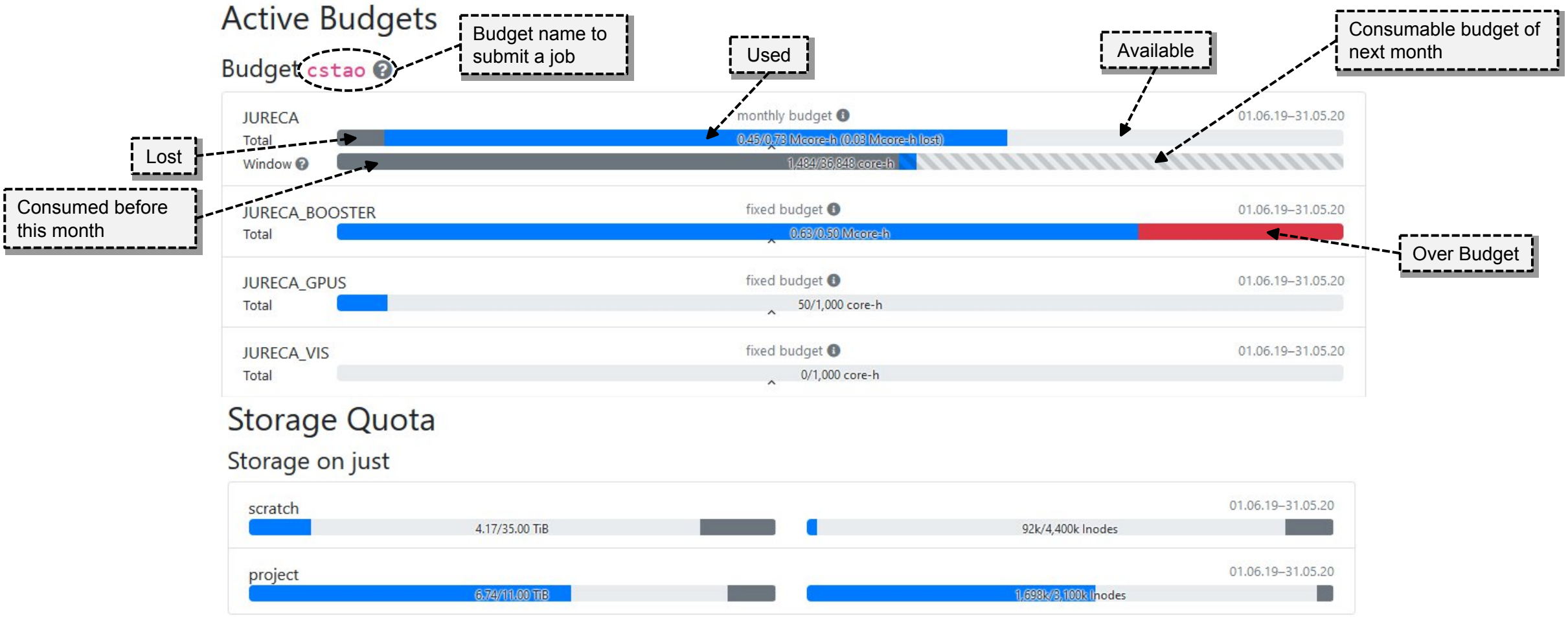
`#nodes x #physical_cores_per_node x runtime`

- **`#physical_cores_per_node`**:
  - JUWELS or JUWELS_BOOSTER: 48
  - JURECA-DC or JUSUF: 128

- **`runtime`**: actual job runtime, not the provided walltime of the job

- There is no node-sharing on compute nodes
- The quota is fully placed on the day when the job ended
- The quota of a job is not taken into account in advance
- The base priority of a job based on the overall project quota and is updated on a daily basis

JUDOOR Quota status



`Jutil` tool & budget monitoring

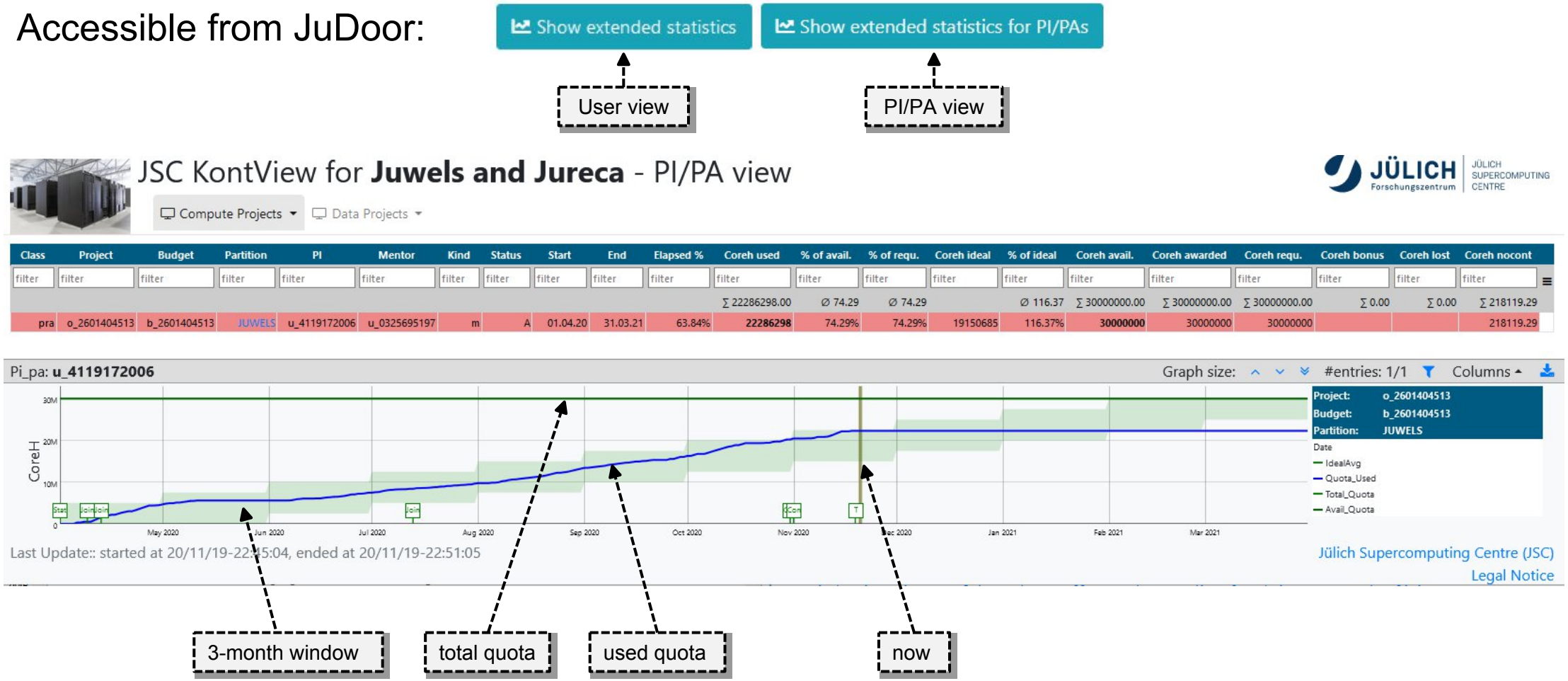
The budget can be provided on a per job basis (using the `--account` or `-A` option in SLURM), or the command line tool `jutil` can be used to monitor the budget or to activate a specific budget by default for a running Shell:

```
# See your projects
jutil user projects

# See your compute allocation
jutil user cpuquota

# See your disk quota
jutil user dataquota

# Activate environment (and optionally default budget) for a given project
# Sets $PROJECT and $SCRATCH
jutil env activate -p <project> [-A <budget>]
```

https://apps.fz-juelich.de/jsc/hps/just/jutil.html

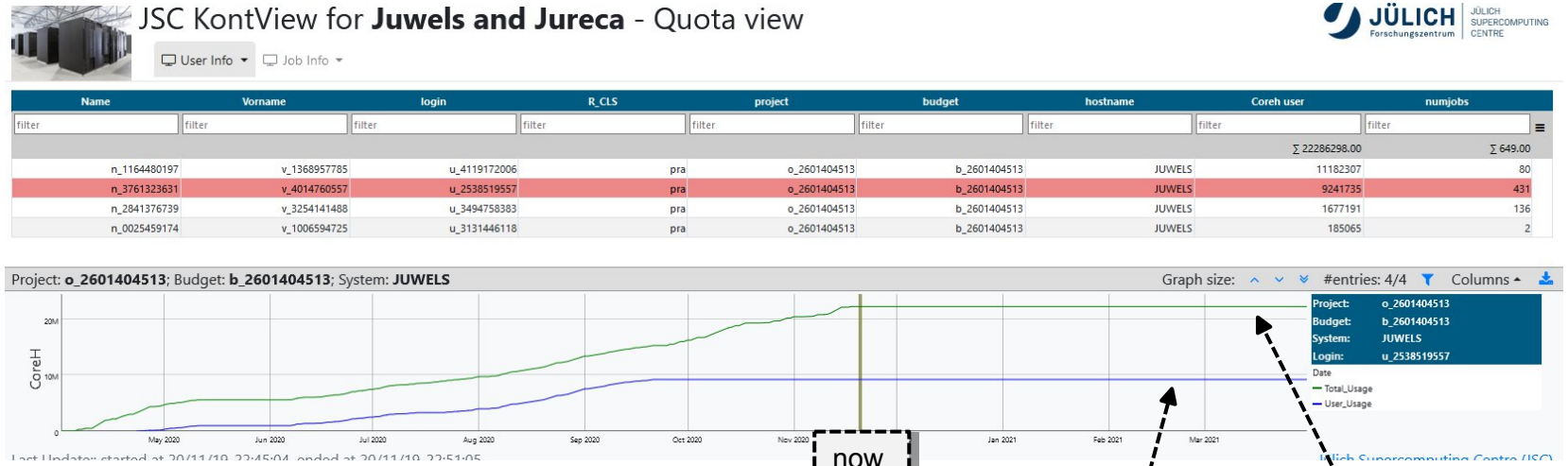
Project quota overview: KontView

Accessible from JuDoor:

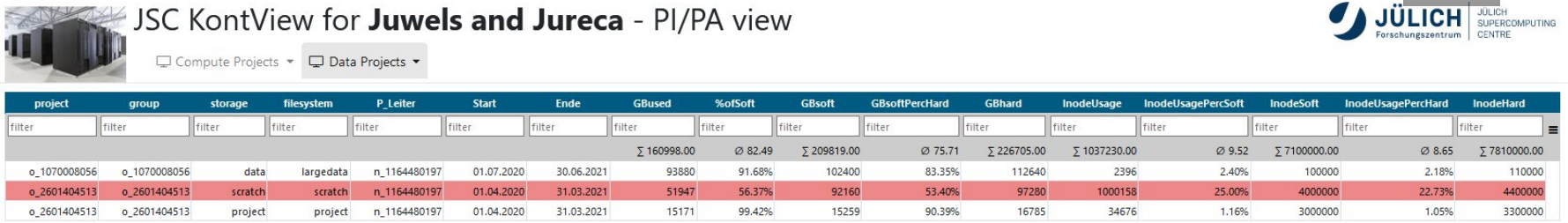


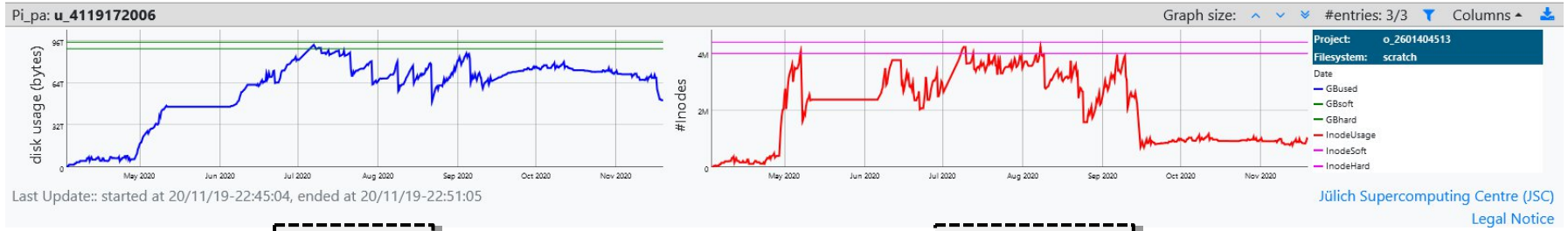
Project quota overview: KontView

PI/PA view:
display quota per user:



Storage utilization:





disc usage

inodes usage

Documentation

JUWELS

Jülich Wizard for European Leadership Science

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Supercomputers

- JUWELS
  - User Documentation
  - Configuration
  - FAQ
  - Known Issues
  - Job Reporting
  - Modules overview
  - Related Organisations
- JURECA
- JUSUF
- Apply for test access
- Apply for computing time

Supercomputers: https://www.fz-juelich.de/en/ias/jsc/systems/supercomputers(/<system>)

Storage systems: https://www.fz-juelich.de/en/ias/jsc/systems/storage-systems(/<system>)

Service status

– Cluster Systems

JUWELS Booster	Next Maintenance at 3. Mai 2022, 08:00:00	JUWELS Cluster	Next Maintenance at 3. Mai 2022, 08:00:00
JURECA Booster	Next Maintenance at 3. Mai 2022, 08:00:00	JURECA DC	Next Maintenance at 3. Mai 2022, 08:00:00
JUSUF HPC	Next Maintenance at 3. Mai 2022, 08:00:00	JUDAC	Next Maintenance at 3. Mai 2022, 08:00:00
HDF-ML	Next Maintenance at 3. Mai 2022, 08:00:00	JUZEA1	Next Maintenance at 3. Mai 2022, 08:00:00
QLM	Next Maintenance at 3. Mai 2022, 08:00:00		

– File Systems

$HOME	Next Maintenance at 3. Mai 2022, 08:00:00	$PROJECT	Next Maintenance at 3. Mai 2022, 08:00:00
$SCRATCH	Next Maintenance at 3. Mai 2022, 08:00:00	$ARCHIVE	Next Maintenance at 3. Mai 2022, 08:00:00
$CSCRATCH	Next Maintenance at 3. Mai 2022, 08:00:00	$DATA	Next Maintenance at 3. Mai 2022, 08:00:00
$FASTDATA	Next Maintenance at 3. Mai 2022, 08:00:00		

– Services

JuDoor		Jupyter-JSC	Next Maintenance at 3. Mai 2022, 08:00:00
Backup	Next Maintenance at 3. Mai 2022, 08:00:00	UNICORE	Next Maintenance at 3. Mai 2022, 08:00:00
HDF Cloud	Next Maintenance at 3. Mai 2022, 08:00:00	JUSUF CLOUD	Next Maintenance at 3. Mai 2022, 08:00:00
Cloud Object Storage	Next Maintenance at 3. Mai 2022, 08:00:00	JUSTCOM	Next Maintenance at 3. Mai 2022, 08:00:00

– Support

SC Support

JUWELS

Jülich Wizard for European Leadership Science

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Supercomputers

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- Known Issues
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- Modules overview
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- JURECA
- JUSUF
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- Apply for computing time

Status

e the JSC Service Status Page for system status information:

System messages JUWELS Cluster

System messages JUWELS Booster

https://status.jsc.fz-juelich.de/

Read the MOTD

Service status

JUWELS Cluster

The Cluster partition of the JUWELS Supercomputer

JUWELS Cluster is currently degraded

Unavailable login nodes
- juwelsvis01.fz-juelich.de

Degraded base services

$CSCRATCH

Current state

Issues in cell 03

28. Feb. 2022, 14:20:00 - unknown

Today, on Monday 2022-02-28, at 14:20, a series of hardware failures resulted in a malfunction in the power and cooling systems of cell 03 in JUWELS Cluster. As a result the InfiniBand network suffered instabilities that affected other cells, and some jobs failed. The cell is now disconnected from the fabric and the system is stable.

We apologize for the inconvenience.

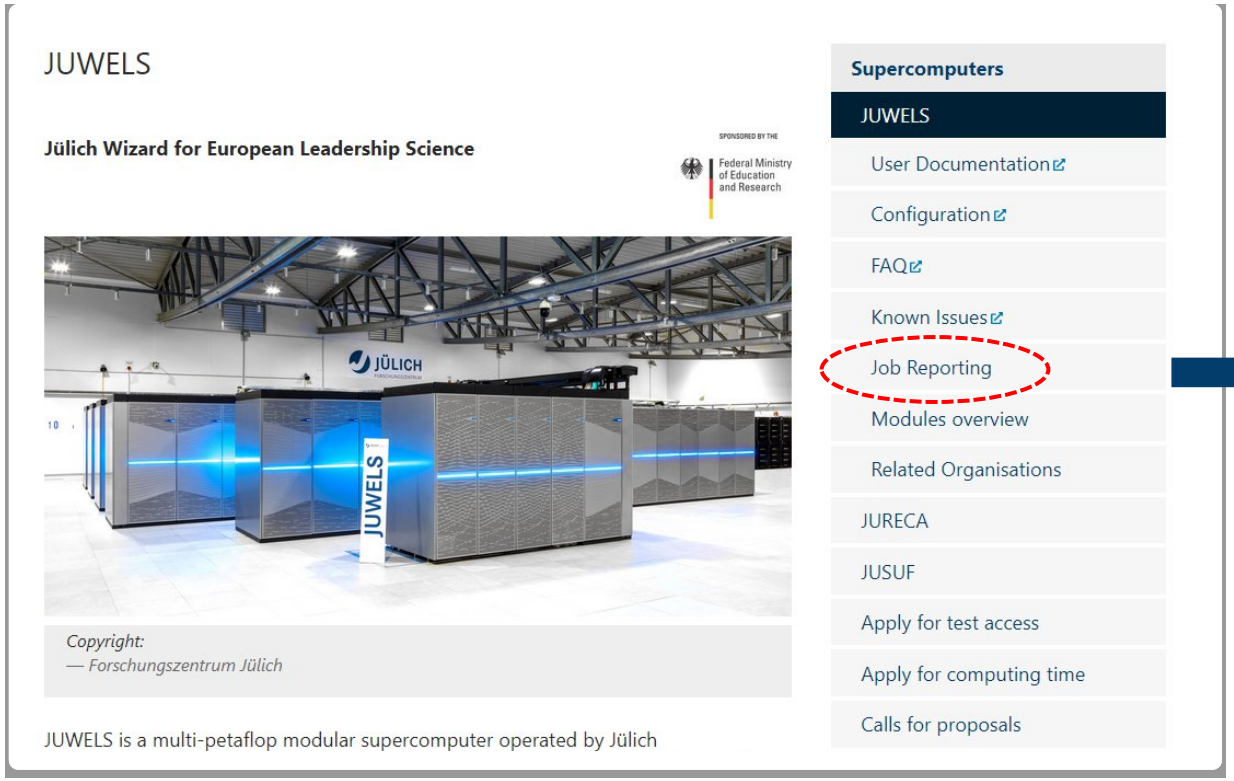
History

New software stage

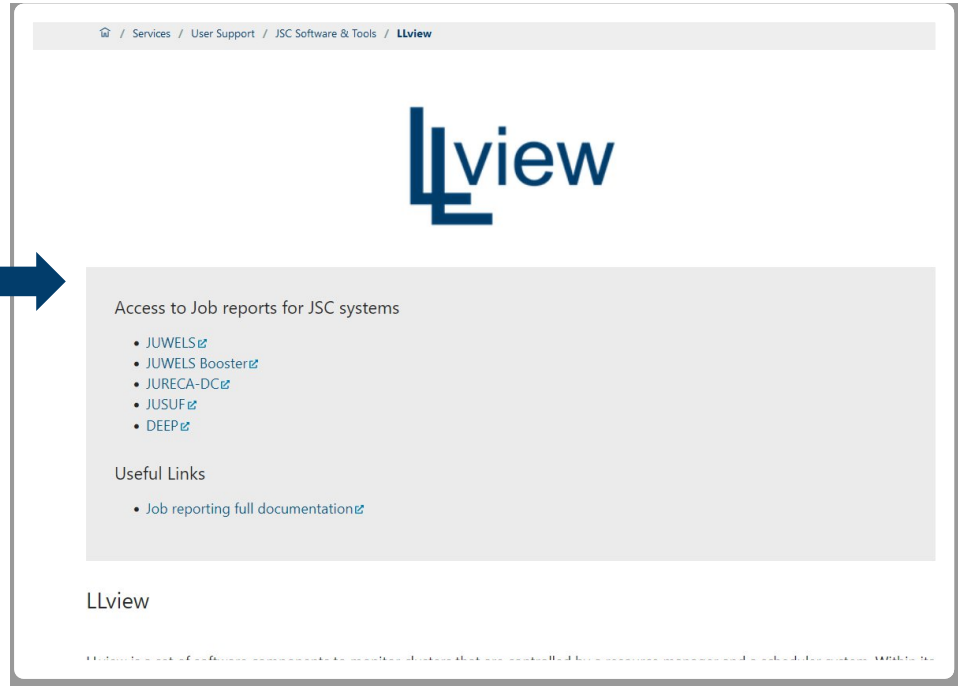
10. Feb. 2022, 12:00:00 - 7. März 2022, 20:14:16

The default software stage has been changed to Stages/2022. If you wish to continue using the previous default stack please load Stages/2020 before any other module. Note that this stage will be deprecated.

Job monitoring & reports: LLview

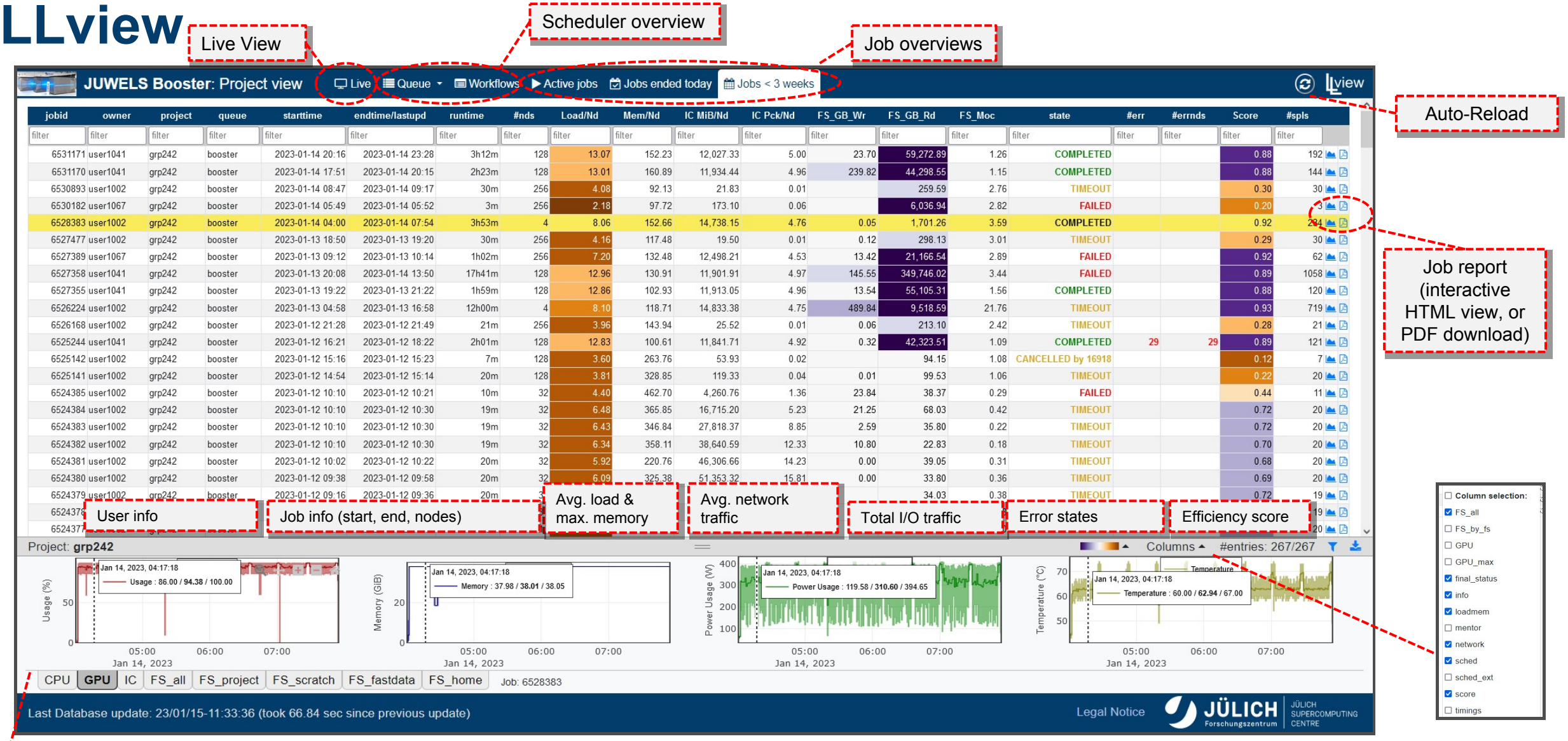


https://llview.fz-juelich.de/<system>



Logindata: JUDOOR username & password

LLview



LLview version 2.0
Dec. 2022

Job reports

Job Runtime: **22h40m** → 94.42% of Wall: 1d00h00m

Job Start Time:	**2021-11-20 23:58:33**	
Job Last Timestamp:	**2021-11-21 22:38:12**	(Running)
Current Time:	2021-11-21 22:38:12	
Job Endtime (Est.):	2021-11-21 23:58:51	

Queue:	**booster**		
Job Size, #Nodes:	**1**	*#Data Points:*	*1147*
Job Size, #GPUs:	**4**	*#Data Points:*	*901*

Job Performance Metrics

	min.	avg.	max.	
Load (CPU-Nodes):	**1.88**	**4.02**	**4.24**	
Memory (CPU-Nodes):	**20532.40**	**26328.19**	**26384.40**	*MiB*
Interconnect Traffic (in):	**0.00**	**12.73**	**7887.81**	*MiB/s*
Interconnect Traffic (out):	**0.00**	**0.08**	**29.35**	*MiB/s*
Interconnect Packets (in):	**0**	**306**	**2328**	*pck/s*
Interconnect Packets (out):	**1**	**76**	**3658**	*pck/s*

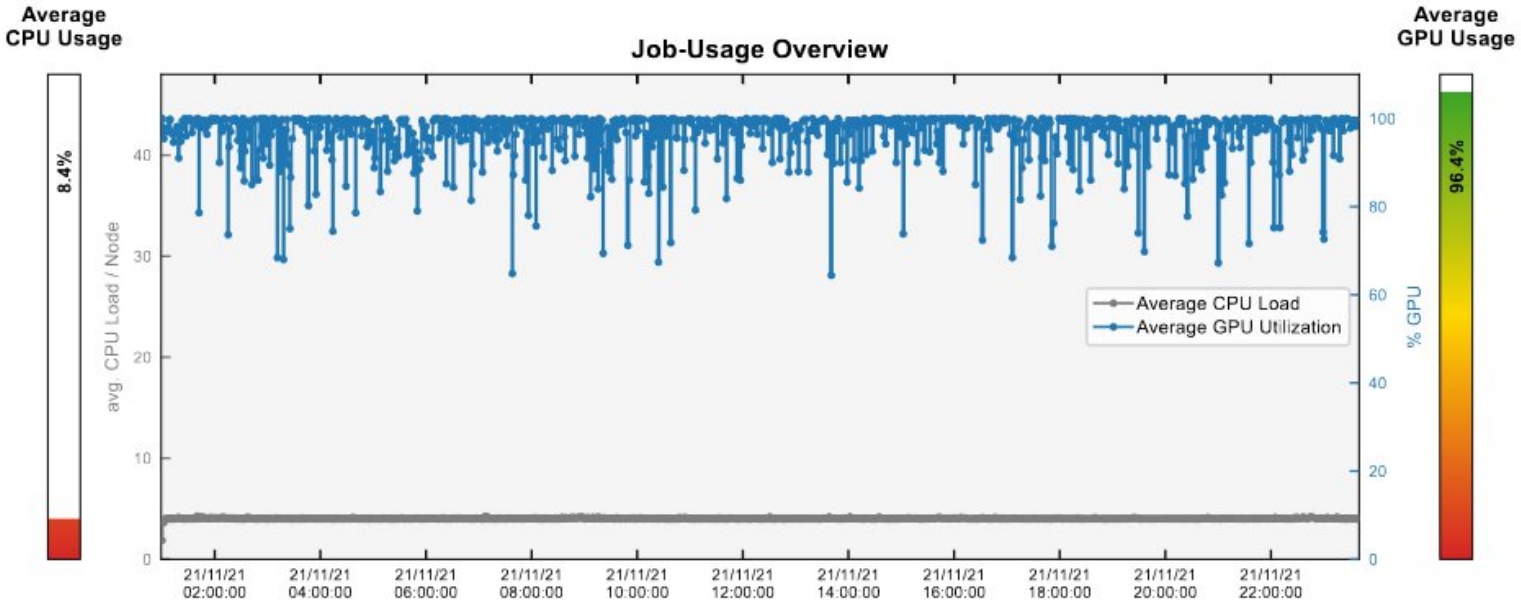
Job I/O Statistics

	Total Data Write	Total Data Read	max. Data Rate/Node Write	max. Data Rate/Node Read	max. Open-Close Rate/Node
$HOME:	**0.00** *MiB*	**0.00** *MiB*	**0.00** *MiB/s*	**0.00** *MiB/s*	**0.00** *op./s*
$PROJECT:	**0.00** *MiB*	**0.00** *MiB*	**0.00** *MiB/s*	**0.00** *MiB/s*	**0.00** *op./s*
$SCRATCH:	**0.00** *MiB*	**0.00** *MiB*	**0.00** *MiB/s*	**0.00** *MiB/s*	**0.00** *op./s*
$FASTDATA:	**0.00** *MiB*	**0.00** *MiB*	**0.00** *MiB/s*	**0.00** *MiB/s*	**0.00** *op./s*

Job GPU Statistics

avg. GPU Usage:	**96.40** %	avg. Mem. Usage Rate:	**13.52** %	avg. GPU Temp.:	**69.03** °C	avg. GPU Power:	**310.22** W
max. Clk Stream/Mem:	**1410/1215** MHz	max. Mem. Usage:	**1738.50** MiB	max. GPU Temp.:	**75.00** °C	max. GPU Power:	**343.43** W

This job will use approximately 1 nodes × 48 cores × 24.000 hours = 1152.00 core-h for the specified walltime (up to now: 1087.68)



Job reports – further job stats

Nodelist

1 jwc07n106 Interconnect group: 88	2 jwc07n107 Interconnect group: 88	3 jwc07n108 Interconnect group: 88	4 jwc07n109 Interconnect group: 88	5 jwc07n110 Interconnect group: 88	6 jwc07n111 Interconnect group: 88	7 jwc07n112 Interconnect group: 88	8 jwc07n113 Interconnect group: 88
			9 jwc07n114 Interconnect group: 88	10 jwc07n115 Interconnect group: 88			

Job Finalization Report

Job State: **FAILED** Job Return Code: **11** Job Signal Number: **0**

Timings (Accounting):

Start Time	**2021-11-20 11:25:20**
End Time	**2021-11-21 10:25:44**
Wall Time	**24.00**
Runtime	**23.00 hours**

Step RCs:

Step: **batch**	RC: **11**	Sig.-Nr: **0**
Step: **0**	RC: **0**	Sig.-Nr: **9**

Node System Error Report

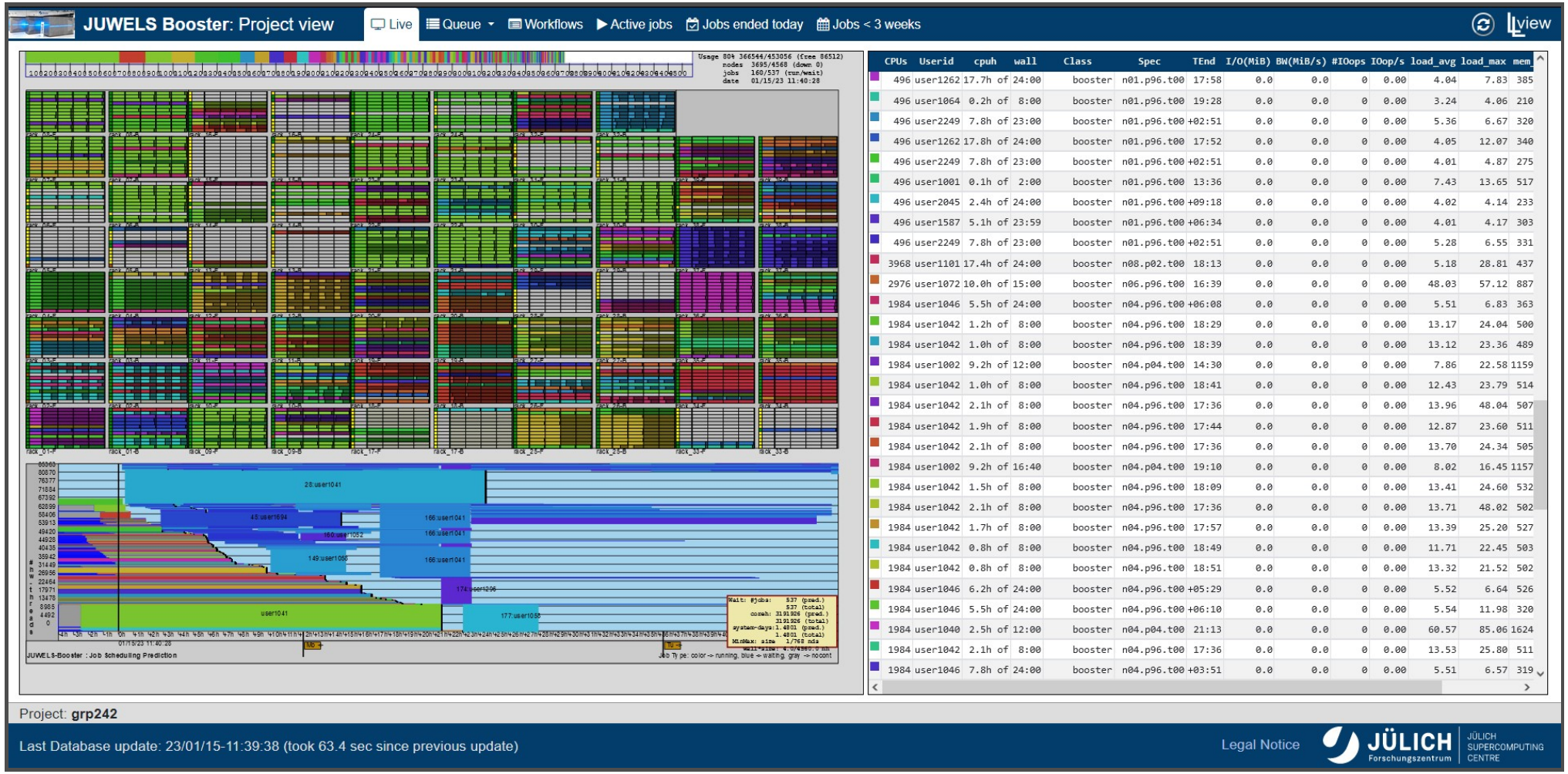
Msgs **1** # Nodes **1**

Error Messages:

```
2021-11-21T10:25:08+0100 jwc07n112.juwels kernel: ramses3d invoked oom-killer: gfp_mask=0x6280ca(GFP_HIGHUSER_MOVABLE|__GFP_ZERO), order=0, oom_
score_adj=0
```

Scheduler overview

- Current usage of system:
  - clickable
  - update 1min
- Mapping of jobs to nodes
- Prediction of system usage using JuFo



JuFo: Simulator for Job Schedulers on HPC Systems, C.Karbach, T.Bauer, JSC

HELP

Contact SC support at sc@fz-juelich.de or your Mentor if you need any help.

- *Which **system** did you use? What is your **user ID**?*
- *If there was an error, what is the **error message**?*
- *Is the error **reproducible**?*
- *If related to a job, what was the **job ID**?*
- *Which **module environment** did you use?*