

First Steps: User Portal and Job Monitoring Webportals and Support-Tools @ JSC

30.05.2023 I Dr. Jolanta Zjupa



Mitglied der Helmholtz-Gemeinschaft





Compute project vs. data project

	Compute project	Data project
Call	Twice per year	Continuously open
Computing time		
Grants system access	JUWELSJURECAJUDAC	• JUDAC
Filesystem access on all systems	PROJECTSCRATCH	 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

JuDoor Login



Portal for managing accounts, projects and resources at JSC.

Login using JSC webservice account	Login with e-mail callback
Username	Login mail address
luehrs2	
Password	A confirmation email to confirm your identity will be sent to this address.
•••••	Send identification mail
Login Register Reset password	

If you are stuck take a look at the 🔁 JuDoor Documentation.

https://judoor.fz-juelich.de



Step 2: Join a project

Two alternatives

Join a project 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

Request access for resources



JUDOOR Overview

An user can be part of multiple compute and data projects





JUDOOR Overview

Project details

Project training2000 **Project Mentor:** Data access is possible up to Project specific permanent contact 3 month after the end of the point at JSC, in addition to **Project title** Parallel I/O project via JUDAC. sc@fz-juelich.de. Computeproject Type The mentor is available for **Principal Investigator** Sebastian Lührs requests concerning further support and training offers by JSC Project Mentor Sebastian Lührs or helps to arrange in-depth code **Project duration:** analyses. 01.01.2020 Start date Job execution is only possible during the runtime of the project More details: End date 29.02.2020 if there is an available budget. https://www.fz-Community juelich.de/en/ias/jsc/services/user-Training support/project-mentoring Address Forschungszentrum Jülich GmbH, JSC Wilhelm-Johnen-Straße 52425 Jülich Germany **Project unix group:** Unix group for project raining2000 Group name



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related top level folders

JUDOOR Overview

Each projects grants access to various systems and partitions.





Step 3: Upload your SSH-key

JULICH JULICH SUPERCOMPUTING SSH keys on jureca orschungszent More details on from-clause Here you can upload an SSH public key to the system. Information on how to create an SSH public key can be found here. handling and key generation It might take up to 15 minutes until the newly added SSH key is activated. Upload SSH public keys To use our systems your public key options have to include a from=-clause to restrict the usage of the key to your personal IP address range. Your current IP address is 134.94.52.69. See the documentation for more information. Your current public Remove all other existing public keys. Your public key and options string from="134.94.52.69" ssh-ed25519 AAAAC3N... Can be a list of static IP, a static Paste the content of your .pub-file here or upload a file below. network range, a static hostname or a hostname suffix using * as a Your public key file Additional public key options wildcard symbol Browse You can specify your from= clause and other public key options here Start upload of SSH-Keys Add additional keys...

Your SSH keys on jureca

sebi@zam495			i 🔟
SHA256:		MD5:	
Options: from="134.94.0.0/16"			





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)



- Setup SSH connection through your favourite editor (VSC, Sublime, Atom, Kate, ... many others)
- Mount the Filesystem to your local machine through a mount point





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

One software toolchain: Intel compiler & ParaStationMPI

	Compiler/GCCcore/8.3.0 [100]	MPI/intel/2019.3.	199-GCC-8.3.0/psm	1pi/5.2.2-1	
	intel/2019.3.199-GCC-8.3 [83]	ABINIT/8.10.2	LAMMPS/12Dec2018	Silo/4.10.2	
Software	intel/2019.3.199 666-8-3 [82]	ARPACK-NG/3.7.0	MUMPS/5.1.2	SuiteSparse/5.4.0-	
toolchains	intel/2019.3.199-GCC-8.3 [79]	ASE/3.17.0-Python-3.6.8	MUST/1.6-rc3-Python-3.6.8	METIS-5.1.0	
	GCC/8.3.0/psmpi/5.2.2-1 [73]	Boost/1.69.0-Python-2.7.16	Meep/1.7.0	Valgrind/3.14.0	
	Core [48]	Boost/1.69.0-Python-3.6.8	NAMD/2.13	VampirServer/9.6.1	
	Compiler/GCC/8.3.0 [14]	CDO/1.9.5	NCL/6.6.2	YAXT/0.6.0	
	Compiler/intel/2019.3.199 [13]	CGAL/4.13.1-Python-2.7.16	NCO/4.7.9	buildenv/intel-para	
	intel/2019.3.199-GCC-8.3 [13]	CGAL/4.13.1-Pvthon-3.6.8	OSPRav/1.8.4	darshan-runtime/3.1.7	
	GCC/8.3.0/MVAPICH2/2.3.2 [9]	CP2K/6.1-plumed-elpa	PETSc/3.11.1	darshan-util/3.1.7	
	GCC/8.3.0/MVAPICH2/2.3.1 [8]	CPMD/4.3	PETSc/3.11.1 complex	ecCodes/2.12.0	
	Compiler/mpi/intel/2019.3[7]	FLPA/2016.05.004	PETSc/3.11.1 int8	h5pv/2.9.0-Python-2.7.16	
	PGI/19.3-GCC-8.3.0/MVAPIC [5]	FLPA/2018.11.001	PLUMED/2.5.1	h5pv/2.9.0-Pvthon-3.6.8	
	PGI/19.3-GCC-8.3.0/MVAPIC[5]	ELPA/2018.11.001-apu	ParMETIS/4.0.3	imkl/2019.3.199	
	Compiler/mpi/GCC/8.3.0 [4]	ELPA/2018.11.001-single	ParMETIS/4.0.3-double	mpi4py/3.0.1-Python-2.7.16	
	Compiler/mpi/PGI/19.3-GCC [2]	ESME/7 1 0r	PyFerret/7 5 0-Python-2 7 16	mpi4py/3.0.1-Python-3.6.8	
	show hidden modules:	Elemental/0.87.7	QuantumESPRESSO/6.4.1	mpiP/3.4.1	Can be loaded on the system by
		Extrae/3.7.0	R/3 5 3	$netCDE_C++4/4 = 0$	using:
		FFTW/3 3.8	R/3 5 3 bak 20190521110136	netCDE-Fertran/4.4.5	module load Intel
		GPAW/1.5.2-Python-3.6.8	RELION/3.0.4	netCDE/4.6.3	module load ParaStationMPI
		GROMACS/2019 1	SCOTCH/6.0.6	netcdt4_nython/1.5.0.1_	module load netCDF
		CROMACS/2019.1	15010Nib/1.7.2	Duthen 2.7.16	
		GROMACS/2019.1.Dak 20190/1218	SLEDC/2 11 1	potodf4 pythop/1 5 0 1	
		UDEE (1 10 E	Scolago /2 F	Duthon 2.6.9	
		HDF5/1.10.5	Scalasca/2.5	Python-3.0.8	
		Harminv/1.4.1	Score-P/S.0	parallel-netcol/1.11.0	
		<u>Hypre/2.15.1</u>	Score-P/6.0	petsc4py/3.11.0-	
		Hypre/2.15.1-Digint	Score-P/default	Python-3.6.8	
lk tomorrow by			<u>Siesta/4.0.2</u>	sprng/1	
				sprng/5-14042019	
Schobel (JSC)				sundials/3.2.1	
	1			sundials/4.1.0	



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Slurm job submission



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 <u>ended</u>
- 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
                                    https://apps.fz-juelich.de/jsc/hps/just/jutil.html
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>]
```



Project quota overview: KontView





3-month window

total quota

used quota

now

Project quota overview: KontView

PI/PA view: display quota per user:







JSC KontView for Juwels and Jureca - Quota view

User Info - Job Info -



project	group	storage	filesystem	P_Leiter	Start	Ende	GBused	%ofSoft	GBsoft	GBsoftPercHard	GBhard	InodeUsage	InodeUsagePercSoft	InodeSoft	InodeUsagePercHard	InodeHard
filter	filter	filter	filter	filter	filter	filter	filter	filter	filter	filter	filter	filter	filter	filter	filter	filter
							∑ 160998.00	Ø 82.49	∑ 209819.00	Ø 75.71	∑ 226705.00	∑ 1037230.00	Ø 9.52	∑ 7100000.00	Ø 8.65	∑ 7810000.00
o_1070008056	o_107000805	6 data	largedata	n_1164480197	01.07.2020	30.06.2021	93880	91.68%	102400	83.35%	112640	2396	2.40%	100000	2.18%	110000
o_2601404513	o_260140451	3 scratch	scratch	n_1164480197	01.04.2020	31.03.2021	51947	56.37%	92160	53.40%	97280	1000158	25.00%	4000000	22.73%	4400000
o_2601404513	o_260140451	3 project	project	t n_1164480197	01.04.2020	31.03.2021	15171	99.42%	15259	90.39%	16785	34676	1.16%	3000000	1.05%	3300000





used quota total

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used quota user

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Documentation

JUWELS

Jülich Wizard for European Leadership Science



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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>)



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Service status



- Support

SC Support

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JUWELS







JUWELS Cluster

The Cluster partition of the JUWELS Supercomputer Z



JUWELS Cluster is currently degraded

Degraded base services

SCSCRATCH Z

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.



Unavailable login nodes • juwelsvis01.fz-juelich.de

Job monitoring & reports: LLview



Logindata: JUDOOR username & password





Job reports

Job Runtime: 22h4	0m → 94.4	42% of Wall:	1d00h00m	Job	Perfor	mance Metrie	s				
Job Start Time: Job Last Timestamp Current Time: Job Endtime (Est.):	2021-11-20 2021-11-21 2021-11-21 2021-11-21	23:58:33 22:38:12 22:38:12 23:58:51	(Running)	L N Ir	oad (CF lemory iterconr	PU-Nodes): (CPU-Nodes) nect Traffic (in nect Traffic (ou	: :): it):	min. 1.88 20532.40 0.00 0.00	avg. 4.02 26328.19 12.73 0.08	ma: 4.2 26384.4 7887.8 29.3	k. 4 0 <i>MiB</i> 1 <i>MiB/s</i> 5 <i>MiB/s</i>
Queue:	booster			Ir	terconr	ect Packets (in):	0	306	232	8 pck/s
Job Size, #Nodes:	1	#Data Points:	1147	Ir	terconr	ect Packets (out):	1	76	365	8 pck/s
Job Size, #GPUs:	4	#Data Points:	901								
Job I/O Statistics \$HOME: \$PROJECT: \$SCRATCH: \$FASTDATA:	Total I	Data Write 0.00 MiB 0.00 MiB 0.00 MiB 0.00 MiB	Total Da 0. 0. 0. 0.	ta Read 00 MiB 00 MiB 00 MiB 00 MiB	max. D	ata Rate/Node 0.00 / 0.00 / 0.00 / 0.00 /	Nrite m: AiB/s AiB/s AiB/s AiB/s	ax. Data Ra	te/Node Read m 0.00 <i>MiB/s</i> 0.00 <i>MiB/s</i> 0.00 <i>MiB/s</i> 0.00 <i>MiB/s</i>	ax. Open-Clos	e Rate/Node 0.00 op./s 0.00 op./s 0.00 op./s 0.00 op./s
Job GPU Statistics avg. GPU Usage: 1 max. Clk Stream/Mem: 1	96.40 % 1410/1215 №	avg. Mem. l IHz max. M	Jsage Rate: lem. Usage:	13.52 % 1738.50	MiB	avg. GPU Ter max. GPU Ter	np.: 69.0 np.: 75.0	3 °C 0 °C	avg. GPU max. GPU	Power: 310.2 Power: 343.4	2 W 3 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								

	Inh Ohnter	EAU ED	1-1	Datura Carda 44	Joh Cincol Murchen 0
	Job State:	FAILED	ol	b Return Code: 11	Job Signal Number: 0
		Timings (Acc	counting):		
		Start Time	2021-11-20 11:25:2	0	
		End Time	2021-11-21 10:25:4	4	
		Wall Time	24.00		
		Runtime	23.00 hours		
	Step RCs:				
	Step:	batch	RC: 11	SigNr: 0	
	Step	0	RC: 0	SigNr: 9	
Node System Error Rep	ort				
	# Msgs	1	# Nodes 1		
Error Messages:					
021-11-21T10:25:08+0100 j	wc07n112.juw	els kernel: r	amses3d invoked com-kill	er: gfp mask=0x628	Oca(GFP HIGHUSER MOVABLE! GFP ZERO), order=(
core adi=0					
ore_an1_n					



Scheduler overview

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

	S Booster : Proje	ct view	ive 🔳 Queue 👻	Workflows	Active jobs	🗇 Jobs ended today 🛗 Jobs	s < 3 weeks							
						Usage 80% 366544/453056 (free 86512)	CPUs Userid cpuh wall	Class	Spec TE	nd I/O(MiB) BW(M	liB/s) #IOops	IOop/s]	oad avg le	oad max mem 🔨
1002003004005006007008009	904200210220220240250250270	1802902002102202302402502	602702802908008108208	130840850860870880890	600610620630640650	0 jobs 160/537 (run/wait) date 01/15/23 11:40:28	496 user1262 17.7h of 24:00	booster	n01.p96.t00 17	:58 0.0	0.0	0.00	4.04	7.83 385
							496 user1064 0.2h of 8:00	booster	n01.p96.t00 19	:28 0.0	0.0	0.00	3.24	4.06 210
							496 user2249 7.8h of 23:00	booster	n01.p96.t00 +02	:51 0.0	0.0	0.00	5.36	6.67 320
		* 15-R	202 218	214 324	rank 32-8		496 user1262 17.8h of 24:00	booster	n01.p96.t00 17	:52 0.0	0.0	0.00	4.05	12.07 340
							496 user2249 7.8h of 23:00	booster	n01.p96.t00 +02	:51 0.0	0.0	0.00	4.01	4.87 275
		15.8 Fact 23.5		201 314	G2CX 314B		496 user1001 0.1h of 2:00	booster	n01.p96.t00 13	:36 0.0	0.0	0.00	7.43	13.65 517
					IBBEB.		496 user2045 2.4h of 24:00	booster	n01.p96.t00 +09	:18 0.0	0.0	0.00	4.02	4.14 233
201 (B.B.				24 W.F	7201 10-B		496 user1587 5.1h of 23:59	booster	n01.p96.t00 +06	:34 0.0	0.0	0.00	4.01	4.17 303
							496 user2249 7.8h of 23:00	booster	n01.p96.t00 +02	:51 0.0	0.0	0.00	5.28	6.55 331
	20112	v 13.8. rank 31.5.	201 21A	ant 20.5	Fact 20.8	et 17.6	3968 user1101 17.4h of 24:00	booster	n08.p02.t00 18	:13 0.0	0.0	0.00	5.18	28.81 437
							2976 user1072 10.0h of 15:00	booster	n06.p96.t00 16	:39 0.0	0.0	0.00	48.03	57.12 887
							1984 user1046 5.5h of 24:00	booster	n04.p96.t00+06	:08 0.0	0.0	0.00	5.51	6.83 363
							1984 user1042 1.2h of 8:00	booster	n04.p96.t00 18	:29 0.0	0.0	0.00	13.17	24.04 500
							1984 user1042 1.0h of 8:00	booster	n04.p96.t00 18	:39 0.0	0.0	0.00	13.12	23.36 489
	an 11-5	9 11-5 Feb	ag 198	arx 27.F	rank 27-8		1984 user1002 9.2h of 12:00	booster	n04.p04.t00 14	:30 0.0	0.0	0.00	7.86	22.58 1159
							1984 user1042 1.0h of 8:00	booster	n04.p96.t00 18	:41 0.0	0.0	0.00	12.43	23.79 514
721 172F	adk 10.7	2 1155 rank 12.5	202 12-8	ack 26-F	rank 26-8. ra	ok M.F. ank M.R.	1984 user1042 2.1h of 8:00	booster	n04.p96.t00 17	:36 0.0	0.0	0.00	13.96	48.04 507
							1984 user1042 1.9h of 8:00	booster	n04.p96.t00 17	:44 0.0	0.0	0.00	12.87	23.60 511
rack_01-F rack_01-8	aa_0?₹ a	x_09-8 rack_17-F	rack_17-8	ack_25-P	rack_25-B ra	ICK_33.F RCK_33.6	1984 user1042 2.1h of 8:00	booster	n04.p96.t00 17	:36 0.0	0.0	0.00	13.70	24.34 505
80870	-						1984 user1002 9.2h of 16:40	booster	n04.p04.t00 19	:10 0.0	0.0	0.00	8.02	16.45 1157
76377 71884		28:user10.41					1984 user1042 1.5h of 8:00	booster	n04.p96.t00 18	:09 0.0	0.0	0.00	13.41	24.60 532
6/392 62899 58406			100-100-001				1984 user1042 2.1h of 8:00	booster	n04.p96.t00 17	:36 0.0	0.0	0.00	13.71	48.02 502
53913 49420		160:user1052	166:user1041				1984 user1042 1.7h of 8:00	booster	n04.p96.t00 17	:57 0.0	0.0	0.00	13.39	25.20 527
44928						*	1984 user1042 0.8h of 8:00	booster	n04.p96.t00 18	:49 0.0	0.0	0.00	11.71	22.45 503
# 31449 h 26956		149.05611000	166:user1041				1984 user1042 0.8h of 8:00	booster	n04.p96.t00 18	:51 0.0	0.0	0.00	13.32	21.52 502
. 22464 t 17971			174:0 6011296				1984 user1046 6.2h of 24:00	booster	n04.p96.t00 +05	:29 0.0	0.0	0.00	5.52	6.64 526
r 8985 • 4492	usert	041		177:user105		Walt: #jdba: 537 (pred.) 537 (total) comeh: 3191926 (pred.)	1984 user1046 5.5h of 24:00	booster	n04.p96.t00+06	:10 0.0	0.0	0.00	5.54	11.98 320
a 0 4 1 - 13 - 12 - 11 - 11 - 11 - 11	42h 43h 44h 45h 46h 47h 48h 49h 410	h411h4 2h413h414h415h416h417h418	sh 419 h 420h 421 h 422h 42 3h 424h 42	5n 4 26 n 42 7n 4 28 h 42 9n 4 30 h 43 1h	1432h/433h/434h/435h/4 <mark>8</mark> 6h/43	3191926 (total) aystam-days:1.4801 (pred.) 7n438h439h440 1.4801 (total)	1984 user1040 2.5h of 12:00	booster	n04.p04.t00 21	:13 0.0	0.0	0.00	60.57	85.06 1624
01/15/23 1 JUWELS-Booster : Job Scheduling Pr	11:40:28 Prediction	1 <u>10</u> -			Job Ty	MinNax: size 1/768 nis wall*size: 4.0/4560.0 nh pe: color -> running, blue -> waiting, gray -> no cont	1984 user1042 2.1h of 8:00	booster	n04.p96.t00 17	:36 0.0	0.0	0.00	13.53	25.80 511
							1984 user1046 7.8h of 24:00	booster	n04.p96.t00+03	:51 0.0	0.0	0.00	5.51	6.57 319 🗸
							<							>
Project: grp242														
_ast Database updat	te: 23/01/15-11:39:38	(took 63.4 sec sind	ce previous upda	ite)						Legal Notice	J.	JÜL	CH	JÜLICH SUPERCOMPUTING CENTRE

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



30.05.2023





Contact SC support at <u>sc@fz-juelich.de</u> 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?



