

## Agenda:

- WEXAC Fast track: Wiki and useful links page.
- WEXAC real time monitor tool: RTM
- WEXAC Best Practices and our recommendations.
- WEXAC LSF Explorer, Grafana.
- WEXAC new tools: PAC, Jupytherhub, Rstudio, etc.
- WEXAC Private cloud options.
- WEXAC and Public cloud integration (AWS).





# Ways to contact HPC people:

- Email: <a href="mailto:hpc@weizmann.ac.il">hpc@weizmann.ac.il</a>
- Mailing list: wexac-news@weizmann.ac.il
- WhatsApp Channel: https://chat.whatsapp.com/05qVVCCcR8v9234vit28gc
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Yaron Weitz HPC Expert

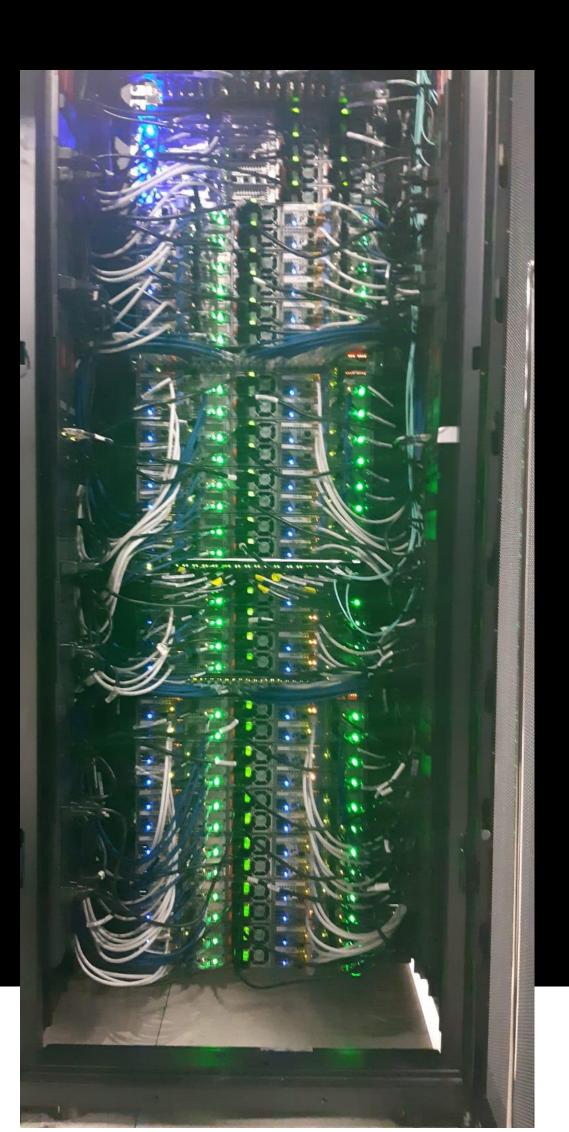


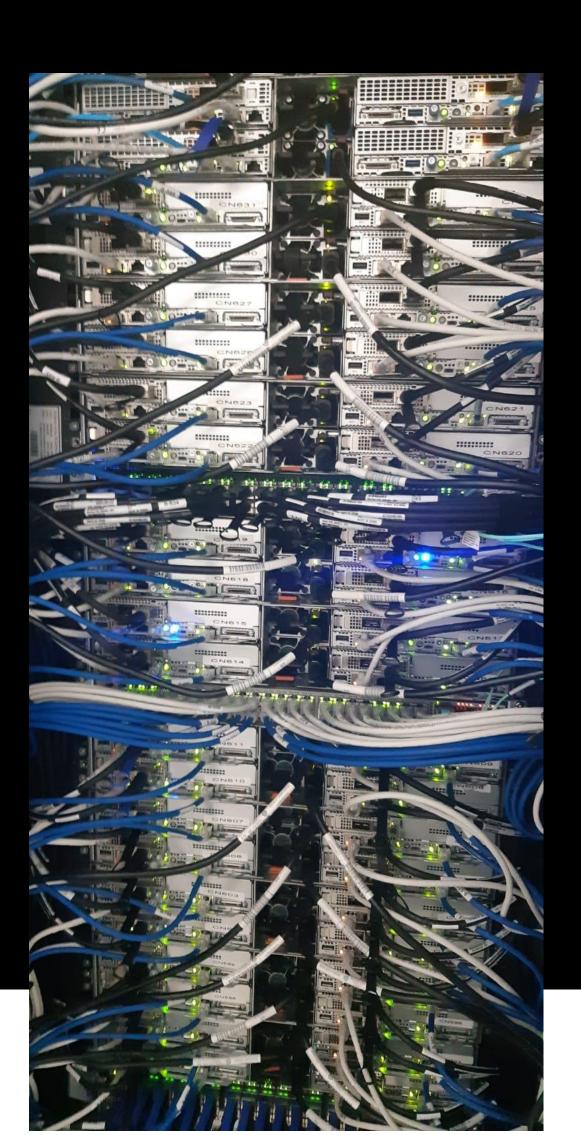
Jerry Mersel Programmer

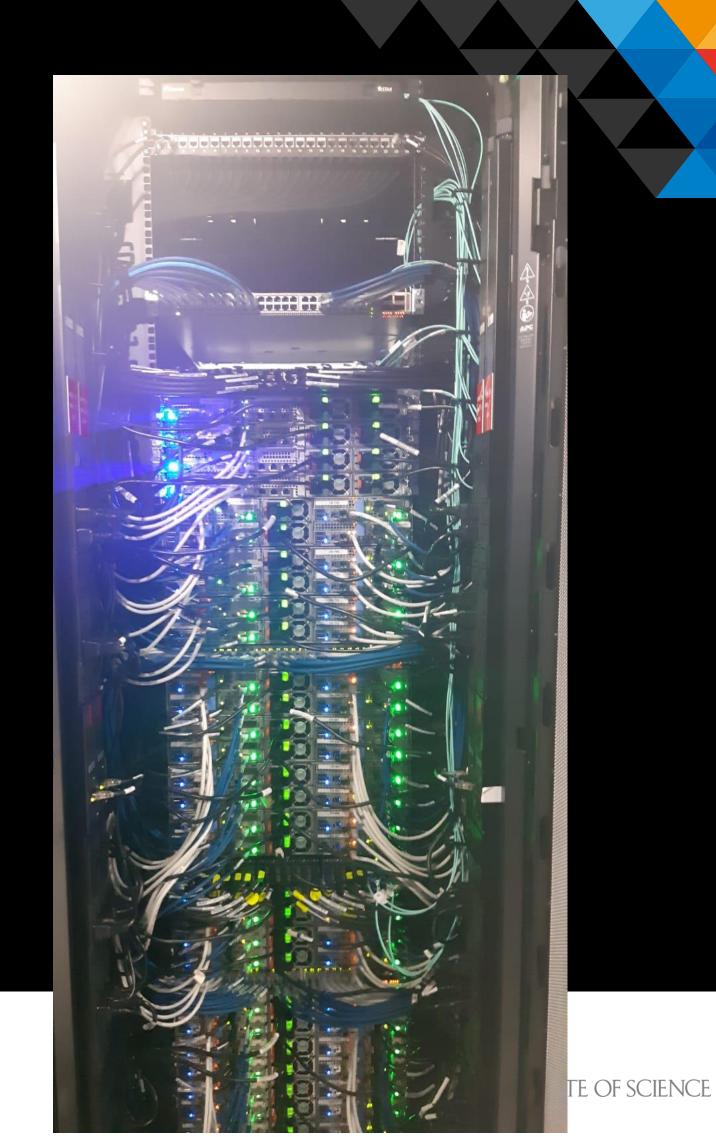


## People behind WEXAC:









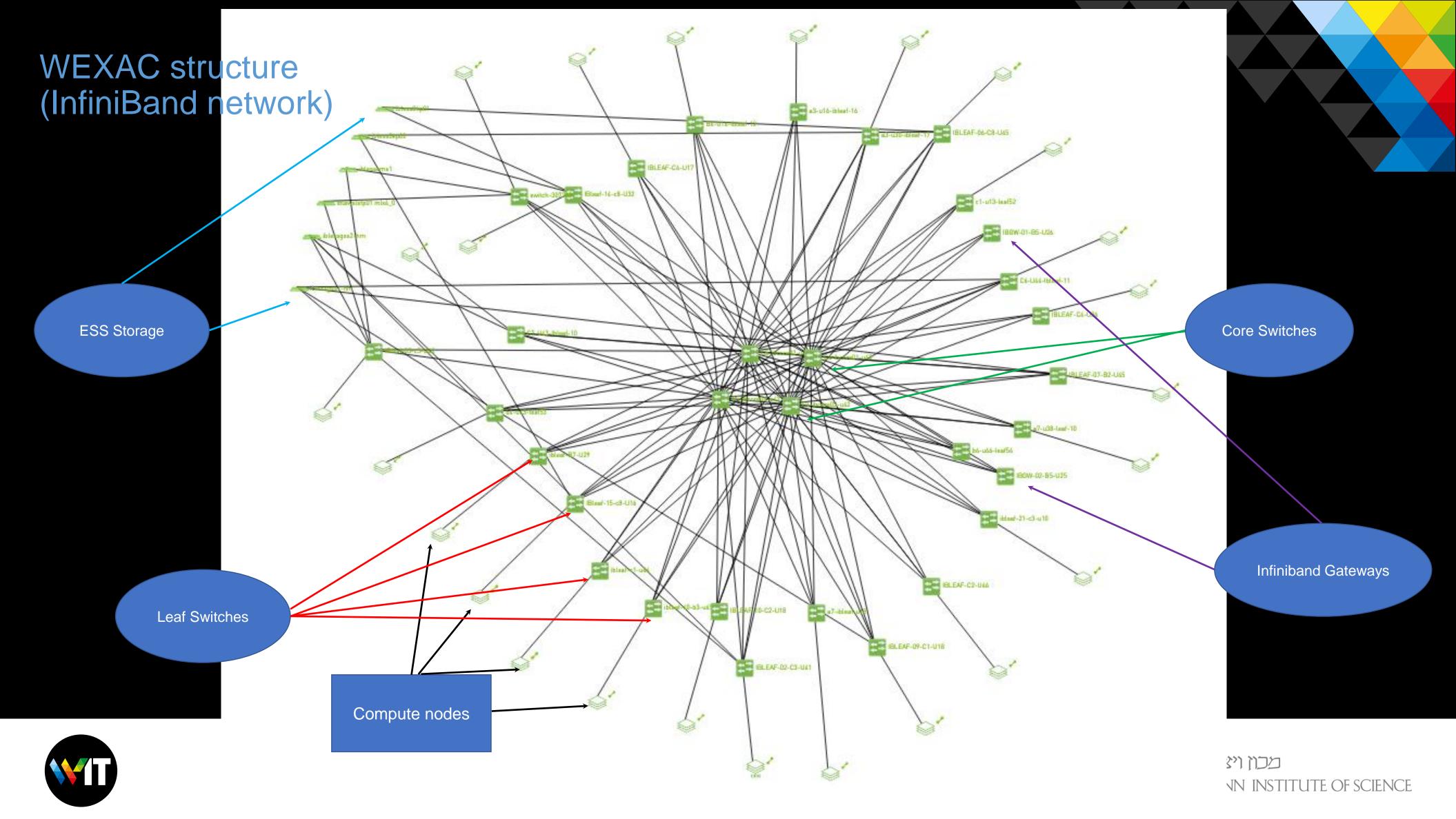




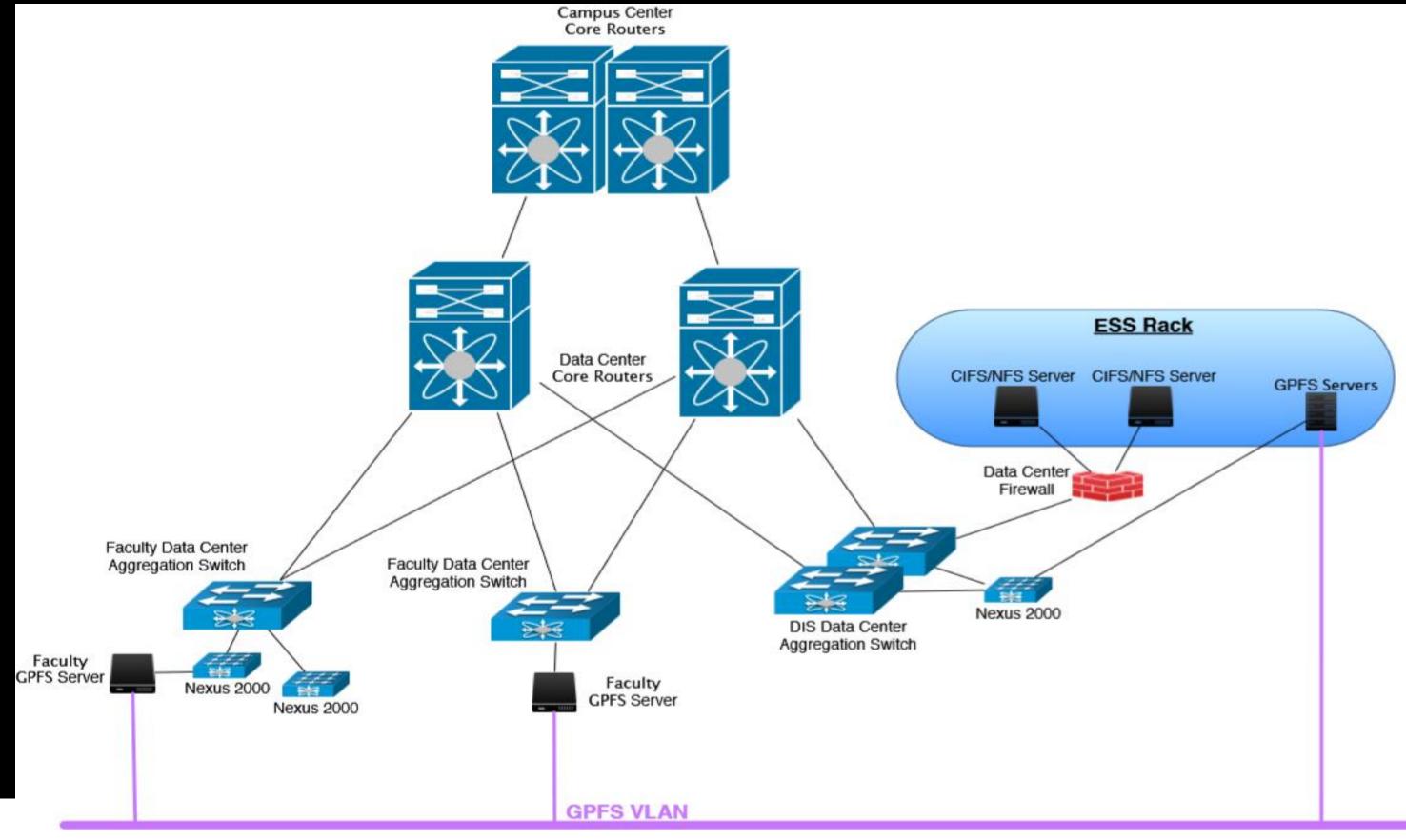








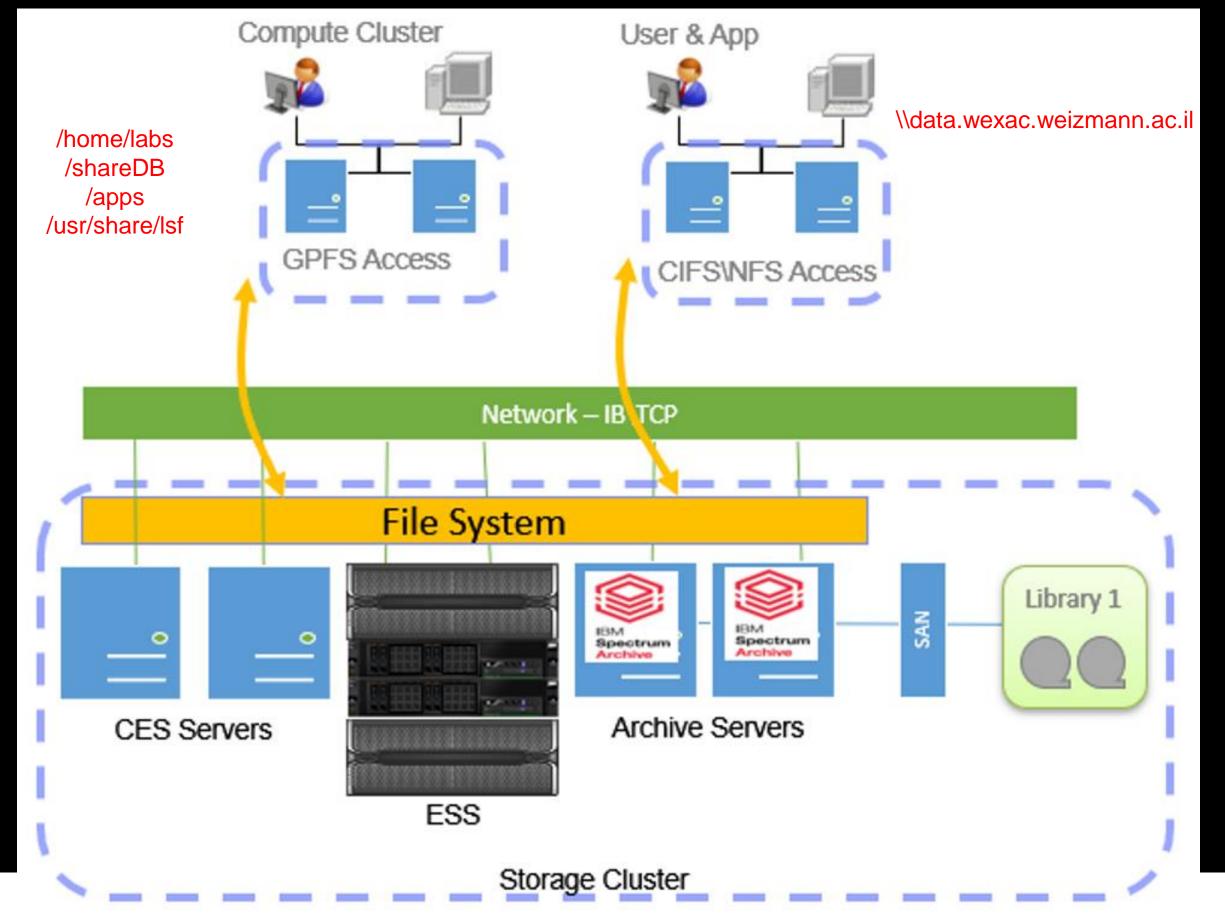
#### WEXAC structure (Ethernet network)







#### WEXAC structure (IBM storage):







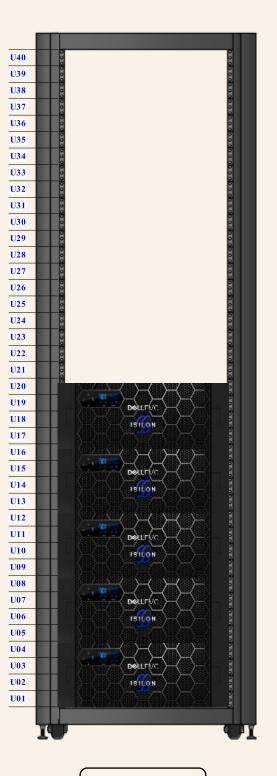
#### WEXAC structure (Isilon storage):

Single File System With two storage pools:

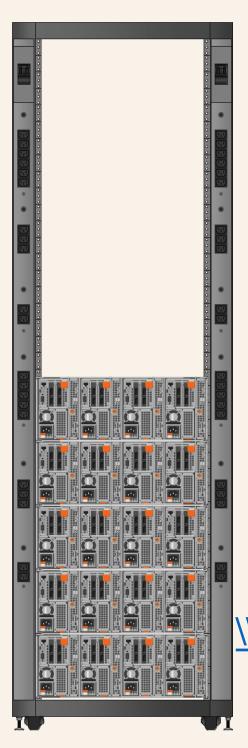
- 8 x F800
- 12 x A2000

Each pool will serve different use case :

- F800 for AI and HPC workloads
- A2000 as NL400 replacement for StorWIS service



Front View



Standard File Sharing Services

12 X A2000 ~2,163TIBU

12 x A2000, 240TB, 64GB, 2X10GbE + 2X8G FC W/ OPTICS

\\\isi.storwis.weizmann.ac.il\\labs\\\isi.storwis.weizmann.ac.il\\users

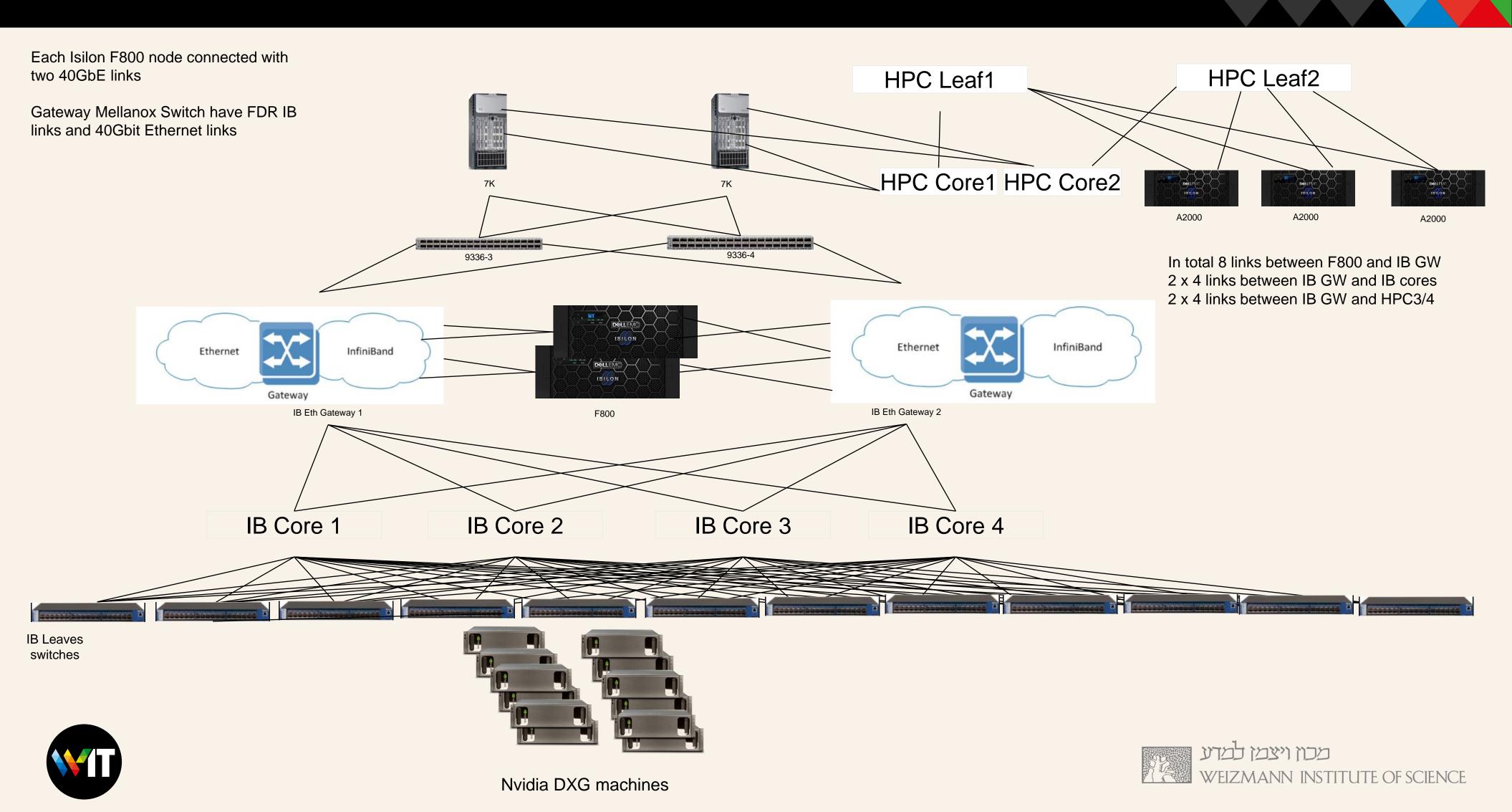
HPC and DL/AI
8 X F800 ~302TIBU 5Y
8 x F800, 48TB, 256GB, 2x40GbE (QSFP+) F800
Backend Network
2 x 36 x Ports QDR Mellanox Switch

\\isi.bigdata.weizmann.ac.il\projects

Rear View







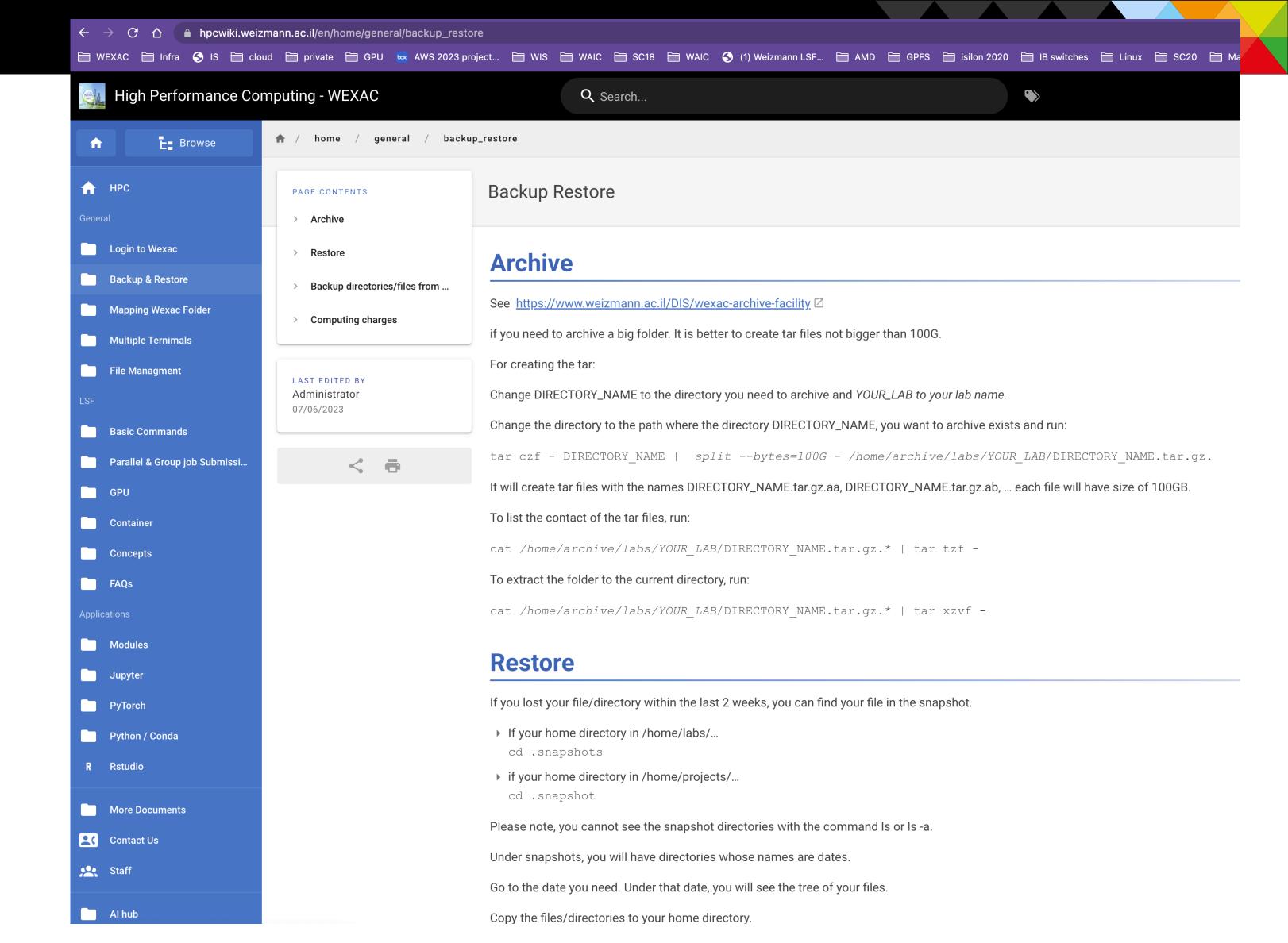
#### WEXAC fast track

- Wiki <a href="https://hpcwiki.weizmann.ac.il/">https://hpcwiki.weizmann.ac.il/</a>
- Useful links <a href="https://appsrv.wexac.weizmann.ac.il/">https://appsrv.wexac.weizmann.ac.il/</a>













#### **WEXAC Application Server**

Software name	URLs						
Rstudio Server	rstudio rstudio2						
Jupytherhub	<u>access compute</u> <u>access1 compute</u> <u>access2</u> <u>access3</u> <u>access4</u>						
RTM	IBM Spectrum LSF RTM						
Platform Application Center	<u>PAC</u>						
Access servers Monitoring	<u>Monitoring</u>						
LSF Explorer	<u>Explorer</u>						
Ganglia	<u>Compute nodes</u> <u>Access servers</u>						
Wexac DOCS	<u>Docs</u>						
Wexac Workshops	Oct 2020: mp4 timestamps pdf July 19, 2021: mp4-beginners pdf-beginners July 26, 2021: mp4-advanced pdf-advanced pdf-nvidia July 19, 2022: presentation slides						



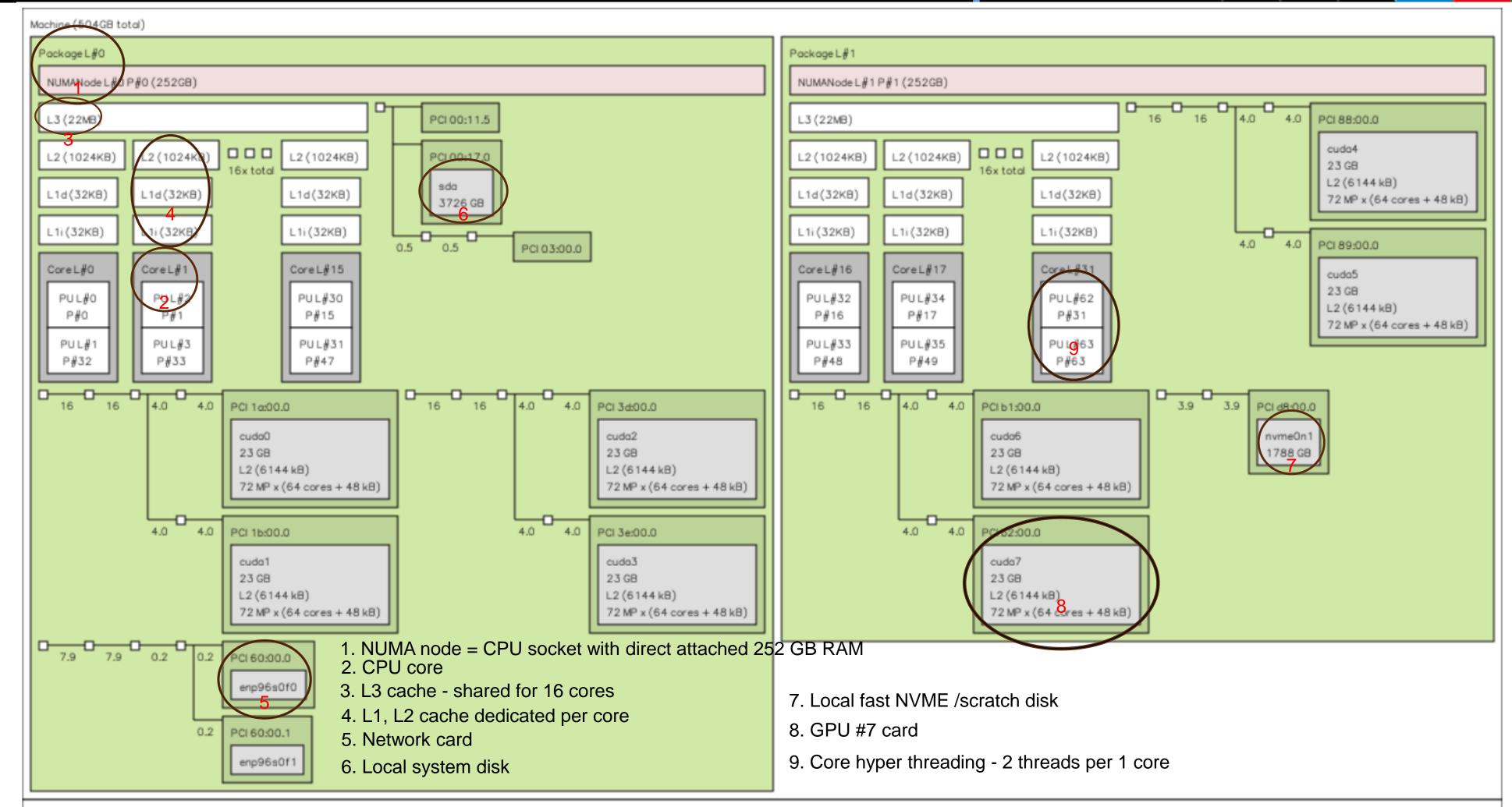




- Memory: 2 types
  - CPU memory defined by -R "rusage[mem=1024]" in case of 1GB required
  - GPU memory defined as a part og GPU resources -gpu num=1:gmem=1000 means 1GB GPU RAM
- Memory allocated as # of cores multiply requested memory
- Tasks: multiply all resources. -n 4 -R "rusage[mem=1024]" -gpu num=1 means 4 cores, 4 GB CPU RAM, 4 GPU









Host: etc-lambda-01 Date: Tue 25 Feb 2020 09:57:37 AMPST

- Affinity awareness: NUMA nodes, sockets, cores, threads resources are not multiplied all other resources
  - bsub -n 2 -q gpu-short -gpu num=2:gmem=1000:aff=yes -R"span[hosts=1]
     rusage[mem=100]affinity[core(3,same=numa,exclusive=(numa,injob)):cpubind=numa:membind=loc alonly]" yourcode
  - This bsub command means to start 2 independent tasks when both tasks locality will be on the same execution host and each task will use 2 GPU with strict affinity CPU - GPU. Each task will use 3 cores on same NUMA level using exclusively NUMA during job execution when CPU bind is on NUMA level as well and use only memory attached locally to specific NUMA
  - bsub -q gpu-short -gpu num=4:gmem=1000:aff=yes -R"span[hosts=1] rusage[mem=100]affinity[core(6,same=numa,exclusive=(numa,injob)):cpubind=numa:membind=loc alonly]"yourcode
  - In this case the same 4 GPU's and 6 CPU cores will act together in the same NUMA binding.
     Important for tightly coupled CPU/GPU workloads
- Bottom line: if you are using tasks with -n flag your code must be aware of it and spread independent tasks to different resources allocated by LSF. Otherwise, it will be just resources wasting.





```
EXTERNAL MESSAGES:
MSG_ID FROM
                  POST_TIME
                                  MESSAGE
                                                                       ATTACHMENT
       vadimm
                                  hgn07:gpus=3,1,5,7;
                  Jul 23 12:40
RESOURCE REQUIREMENT DETAILS:
Combined: select[(type = any ) && (type == any)] order[-slots:-ngpus_physical]
                     rusage[mem=100.00] span[hosts=1] affinity[core(3,same=num
                    a,exclusive=(numa,injob))*1:cpubind=numa:membind=localonly
Effective: select[(((type = any ) && (type == any))) && (ngpus>0)] order[-slot
                    s:-ngpus_physical] rusage[mem=100.00,ngpus_physical=2.00:g
                    mem=1000.00] span[hosts=1] affinity[core(3,same=numa,exclu
                    sive=(numa,injob))*1:cpubind=numa:membind=localonly]
AFFINITY:
                    CPU BINDING
                                                           MEMORY BINDING
                                                                 NUMA SIZE
HOST
                                   EXCL
                                          IDS
                           LEVEL
                                                           POL
                    TYPE
                                                          local 0
hgn07
                                          /0/0/3
                                                                      100.0MB
                                   numa
                    core
                           numa
                                           /A /A /A
                                          / 0/ 0/ 0
                                                           local 1
                                          /1/1/0
                                                                      100.0MB
hgn07
                    core
                                   numa
                           numa
                                          /1/1/1
                                          /1/1/2
```

#### GPU REQUIREMENT DETAILS:

Combined: num=2:mode=shared:mps=no:j\_exclusive=no:gmem=1000.00:gvendor=nvidia Effective: num=2:mode=shared:mps=no:j\_exclusive=no:gmem=1000.00:gvendor=nvidia



```
EXTERNAL MESSAGES:
MSG_ID FROM
                                 MESSAGE
                  POST_TIME
                                                                      ATTACHMENT
                  Jul 23 12:55
                                 hgn05:gpus=5,6,4,7;
       vadimm
RESOURCE REQUIREMENT DETAILS:
Combined: select[(type = any ) && (type == any)] order[-slots:-ngpus_physical]
                     rusage[mem=100.00] span[hosts=1] affinity[core(6,same=num
                    a,exclusive=(numa,injob))*1:cpubind=numa:membind=localonly
Effective: select[(((type = any ) && (type == any))) && (ngpus>0)] order[-slot
                    s:-ngpus_physical] rusage[mem=100.00,ngpus_physical=4.00:g
                    mem=1000.00] span[hosts=1] affinity[core(6,same=numa,exclu
                    sive=(numa,injob))*1:cpubind=numa:membind=localonly]
AFFINITY:
                    CPU BINDING
                                                          MEMORY PINDING
HUST
                                                                NUMA SIZE
                    TYPE
                           LEVEL
                                  EXCL
                                         IDS
                                                          P0L
                                                          local 1
hgn05
                                                                     100.0NB
                                         /1/1/0
                                  numa
                    core
                           numa
                                         /1/1/1
                                         /1/1/2
                                         /1/1/3
                                         /1/1/4
                                         /1/1/8
```

#### GPU REQUIREMENT DETAILS:

Combined: num=4:mode=shared:mps=no:j\_exclusive=no:gmem=1000.00:gvendor=nvidia Effective: num=4:mode=shared:mps=no:j\_exclusive=no:gmem=1000.00:gvendor=nvidia



- Memory overall job memory reservation calculated as # of cores \* required memory. Example if you asked for 4 cores and 4 GB RAM 16 GB RAM will be allocated for this job. So if only 4 GB RAM required for 4 cores jobs ask for 1GB RAM and 4 cores.
- bsub –q new-short –n 4 –R "rusage[mem=1024]" yourscript

```
[vadimm@access4 ~]$ bsub -q new-short -n 4 -R "rusage[mem=1024]" sleep 999
Memory reservation is (MB): 1024
Memory Limit is (MB): 1024
Amount of tasks (-n X) reserved: 4
=== Your total amount of memory reservation for this job is (MB): 4096 ===
Job <875152> is submitted to queue <new-short>.
[vadimm@access4 ~]$ bsub -q new-short -n 4 -R "rusage[mem=4096]" sleep 999
Memory reservation is (MB): 4096
Memory Limit is (MB): 4096
Amount of tasks (-n X) reserved: 4
=== Your total amount of memory reservation for this job is (MB): 16384 ===
Job <875459> is submitted to queue <new-short>.
```





- GPU allocated as # of tasks \* requested GPU. For instance if you ask for 4 tasks and 2 GPU system will try to assign 8 GPU for your task causing extreme pending time and resources wasting! Please use cores instead fo tasks.
- bsub -q gpu-short -n 4 -gpu num=2:j\_exclusive=yes -o ~/output-%J.out -e ~/error-%J.err
   nvidia-smi [vadimm@access4 ~]\$ bjobs -1 879732

```
Job <879732>, User <vadimm>, Project <default>, User Group <testing-wx-grp-lsf>
                     , Status <DONE>, Queue <gpu-short>, Job Priority <50>, Com
                     mand <nvidia-smi>, Share group charged </vadimm>, Esub <me
                    m nonre group gpu>
Thu Jul 20 16:31:52: Submitted from host <access4>, CWD <$HOME>, Output File <o
                     utput 879732.out>, Error File <error-879732.err>, Re-runna
                     ble, 4 Task(s), Requested GPU <====2:j_exclasive-yes>;
Thu Jul 20 16:31:53: Started 4 Task(s) on Host(s) <1*ibdgx005> <2*hgn01> (<1*gac)
                     cess06>, Allocated 4 Slot(s) on Host(s) <1" Lougx005> <2"iig
                     n01> <1*gaccess06>, Execution Home </home/labs/testing/vad
                     imm>, Execution CWD </home/labs/testing/vadimm>;
Thu Jul 20 16:31:55: Done successfully. The CPU time used is 0.3 seconds.
                     HOST: ibdgx005; CPU_TIME: 0 seconds
```





```
EXTERNAL MESSAGES:
MSG_ID FROM
                                                                      ATTACHMENT
                  POST_TIME
                                 MESSAGE
                                 gacces: 96; gpus=2,1 hgn01: gpus=6,2,1
                  Jul 20 16:31
      vadimm
RESOURCE REQUIREMENT DETAILS:
Combined: select[(type = any ) && (type == any)] order[-slots:-ngpus_physical]
                     affinity[core(1)*1]
Effective: select[((type = any ) && (type == any)) && (ngpus>0)] order[-slots:
                    -ngpus_physical] rusage[ngpus_physical=2.00:gmem=6248.00]
                    affinity[core(1)*1]
GPU REQUIREMENT DETAILS:
Combined: num=2:mode=shared:mps=no:j_exclusive=yes:gmem=6248.00:aff=no:gvendor
                    =nvidia
Effective: num=2:mode=shared:mps=no:j_exclusive=yes:gmem=6248.00:aff=no:gvendo
                    r=nvidia
```





```
Sender: LSF System <lsfadmin@weizmann.ac.il>
```

Subject: Job 879732: <nvidia-smi> in cluster <wexac> Done

Job <nvidia-smi> was submitted from host <access4> by user <vadimm> in cluster <wexac> at Thu Jul 20 16:31:52 2023
Job was executed on host(s) <1\*ibdgx005>. in queue <gpu-short>, as user <vadimm> in cluster <wexac> at Thu Jul 20 16:3
1:53 2023

```
<2*han01>
<1*gaccess06>
```

</home/labs/testing/vadimm> was used as the home directory.

```
[vadimm@access4 ~]$ cat output-879732.out
Thu Jul 20 16:31:55 2023
 NVIDIA-SMI 525.60.13 Driver Version: 525.60.13
                                                     CUDA Version: 12.0
                                              Disp.A | Volatile Uncorr. ECC
                  Persistence-MI Bus-Id
 Fan Temp Perf Pwr:Usage/Capl
                                        Memory-Usage | GPU-Util Compute M.
      Tesla V100-SXM2... On
                                 00000000:0A:00.0 Off
                    42W / 300W L
                                     75MiB / 32768MiB
                                                                    Default
   1 Tesla V100-SXM2... On 1
                                00000000:86:00.0 Off
                                    109MiB / 32768MiB |
                                                                    Default
 Processes:
  GPU
        {\sf GI}
            CI
                                                                 GPU Memory
                                   Process name
  No running processes found
```





• GPU – allocated as # of tasks \* requested GPU. For instance, if you ask for 4 tasks and 2 GPU system will try to assign 8 GPU for your task causing extreme pending time and resources wasting! Please use cores instead fo tasks.

• bsub -q gpu-short -gpu num=2:j\_exclusive=yes -R affinity[core\*4] -o ~/output-%J.out -e ~/error-%J.err nvidia-smi

```
[[vadimm@access4 ~]$ bjobs -l 880501
Job <880501>, User <vadimm>, Project <default>, User Group <testing-wx-grp-lsf>
                     , Status <DONE>, Queue <gpu-short>, Job Priority <50>, Com
                     mand <nvidia-smi>, Share group charged </vadimm>, Esub <me
                     m nonre group gpu>
Thu Jul 20 16:47:10: Submitted from host <access4>, CWD <$HOME>, Output File <o
                     utput-880501.out>, Error File <error-880501.err>, Re-runna
                     ble, Requested Resources <affinity[core*4]>, Requested GPU
                     <num=2:j_exclusive=yes>;
Thu Jul 20 16:47:11: Started i Task(s) on Host(s) <hgn01>, Allocated 4 Slot(s)
                     on Host(s) <4*hgn01>) Execution Home </home/labs/testing/v
                     adimm>, Execution CWD </home/labs/testing/vadimm>;
Thu Jul 20 16:47:12: Done successfully. The CPU time used is 0.2 seconds.
                     HOST: hgn01; CPU_TIME: 0 seconds
```





```
EXTERNAL MESSAGES:
MSG_ID FROM
                  POST_TIME
                                 MESSAGE
                                                                     ATTACHMENT
                  Jul 20 16:47 (hgn01:gpus=0,1;
0
       vadimm
                                                                         Ν
RESOURCE REQUIREMENT DETAILS:
Combined: select[(type = any ) && (type == any)] order[-slots:-ngpus_physical]
                    affinity[core(1)*4]
Effective: select[(((type = any ) && (type == any))) && (ngpus>0)] order[-slot
                    s:-ngpus_physical] rusage[ngpus_physical=2.00:gmem=6248.00
                    ] affinity[core(1)*4]
GPU REQUIREMENT DETAILS:
Combined: num=2:mode=shared:mps=no:j_exclusive=yes:gmem=6248.00:aff=no:gvendor
                    =nvidia
Effective: num=2:mode=shared:mps=no:j_exclusive=yes:gmem=6248.00:aff=no:gvendo
                    r=nvidia
```





- GPU allocated as # of tasks \* requested GPU. For instance, if you ask for 4 tasks and 2 GPU system will try to assign 8 GPU for your task causing extreme pending time and resources wasting! Please use cores instead fo tasks.
- bsub -q gpu-short -gpu num=2:gmem=1000:aff=yes -R affinity[core\*4] -o ~/output-%J.out -e ~/error-%J.err nvidia-smi

```
EXTERNAL MESSAGES:
MSG_ID FROM POST_TIME
                                MESSAGE
                                                                   ATTACHMENT
                 Jul 20 17:17
      vadimm
                                hgn05:gpus=1,2;
0
RESOURCE REQUIREMENT DETAILS:
Combined: select[(type = any ) && (type == any)] order[-slots:-ngpus_physical]
                    affinity[core(1)*4]
Effective: select[(((type = any ) && (type == any))) && (ngpus>0)] order[-slot
                    s:-ngpus_physical] rusage[ngpus_physical=2.00:gmem=1000.00
                   ] affinity[core(1)*4]
GPU REQUIREMENT DETAILS:
Combined: num=2:mode=shared:mps=no:j_exclusive=no:gmem=1000.00:gvendor=nvidia
Effective: num=2:mode=shared:mps=no:j_exclusive=no:gmem=1000.00:gvendor=nvidia
```



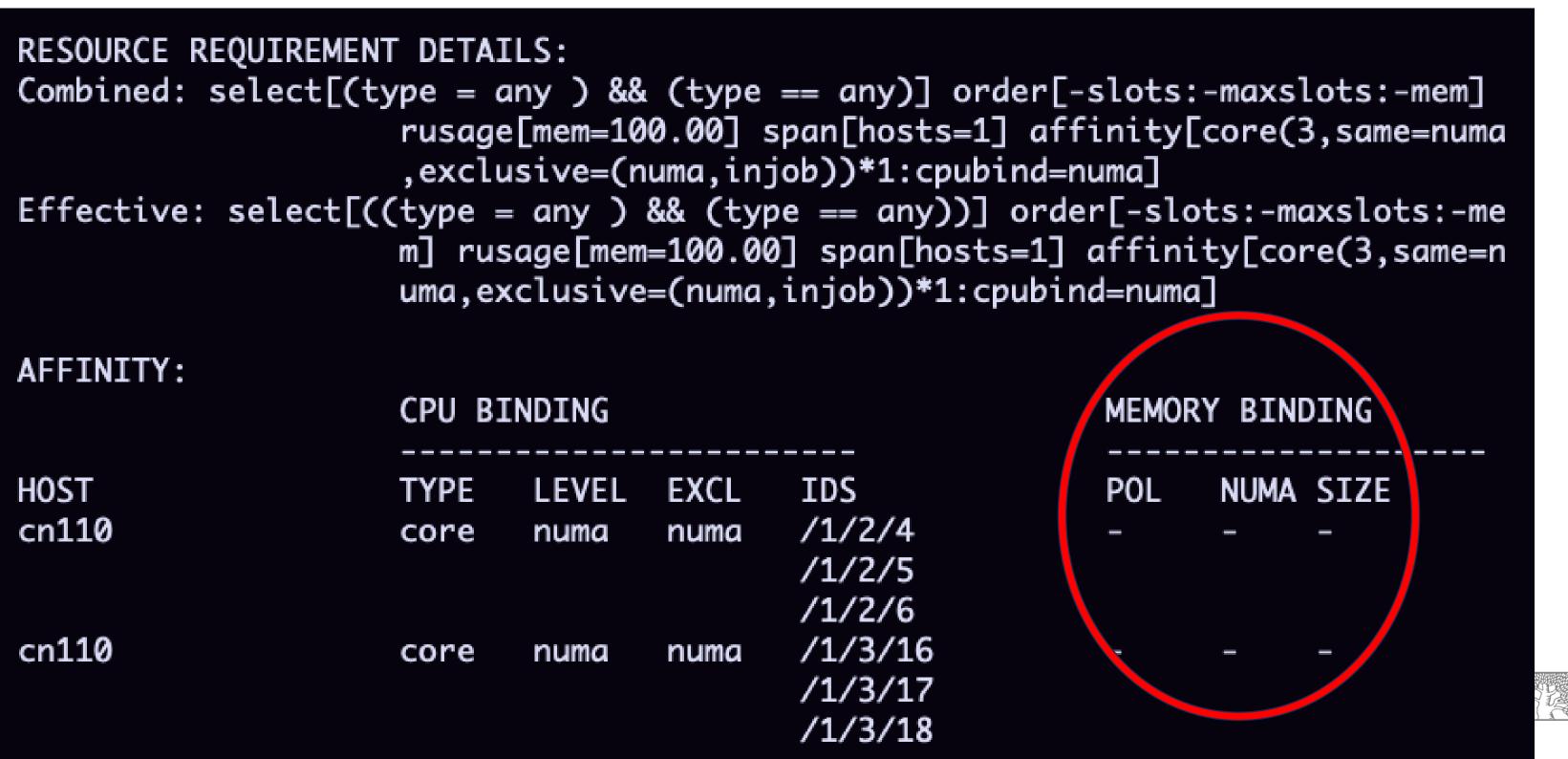


```
[[vadimm@access4 ~]$ cat output-881819.out
Thu Jul 20 17:17:48 2023
 NVIDIA-SMI 525.60.13 Driver Version: 525.60.13 CUDA Version: 12.0
 GPU Name Persistence-MI Bus-Id Disp.A | Volatile Uncorr. ECC |
 Fan Temp Perf Pwr:Usage/Capl Memory-Usage | GPU-Util Compute M. |
                                                            MIG M.
   0 Quadro RTX 6000 On | 00000000:15:00.0 Off |
                                                               Off I
 33%
     26C
            P8 13W / 260W I
                              3949MiB / 24576MiB | 0%
                                                           Default |
                                                               N/A I
   1 Quadro RTX 6000 On | 000000000:39:00.0 Off |
                                                              Off I
 33% 25C P8 15W / 260W | 3917MiB / 24576MiB | 0% Default |
                                                               N/A
 Processes:
  GPI CI CI
                    PID Type Process name
                                                         GPU Memory
       ID ID
                                                         Usage
      N/A N/A
                   2515
                                                            164MiB
                               python
                  7.8899
       N/A N/A
                            C python
                                                            164MiB
                  33083
                            C python
       N/A N/A
                                                            164MiB
                  76287
       N/A N/A
                           C python
                                                            164MiB
```





- Other affinity job CPU only NUMA binding, memory relaxed to any available place:
  - bsub -n 2 -R"span[hosts=1] rusage[mem=100]affinity[core(3,same=numa,exclusive=(numa,injob)):cpubind=numa]" yourcode





- Other affinity job involving both CPU and GPU with only NUMA binding, memory aligned to task NUMA level:
  - bsub -n 2 -q gpu-short -gpu num=2:gmem=1000:aff=yes -R"span[hosts=1] rusage[mem=100]affinity[core(3,same=numa):cpubind=numa:membind=localonly]"

```
EXTERNAL MESSAGES:
                  POST_TIME
MSG_ID FROM
                                 MESSAGE
                                                                      ATTACHMENT
                                 hgn13:gpus=2,3,5,6;
       vadimm
                  Jul 23 12:39
RESOURCE REQUIREMENT DETAILS:
Combined: select[(type = any ) && (type == any)] order[-slots:-ngpus_physical]
                     rusage[mem=100.00] span[hosts=1] affinity[core(3,same=num
                    a)*1:cpubind=numa:membind=localonly]
Effective: select[(((type = any ) && (type == any))) && (ngpus>0)] order[-slot
                    s:-ngpus_physical] rusage[mem=100.00,ngpus_physical=2.00:g
                    mem=1000.00] span[hosts=1] affinity[core(3,same=numa)*1:cp
                    ubind=numa:membind=localonly]
AFFINITY:
                    CPU BINDING
                                                          MEMORY BINDING
HOST
                                  EXCL
                                         IDS
                                                               NUMA SIZE
                           LEVEL
                                         /0/0/17
hgn13
                                                          local 0
                                                                     100.0MB
                    core
                           numa
                                         /0/0/18
                                          /0/0/19
hgn13
                                                                    100.0MB
                                                          local i
                                          /1/1/9
                    core
                           numa
                                         /1/1/10
                                         /1/1/11
GPU REQUIREMENT DETAILS:
Combined: num=2:mode=shared:mps=no:j_exclusive=no:gmem=1000.00:gvendor=nvidia
Effective: num=2:mode=shared:mps=no:j_exclusive=no:gmem=1000.00:gvendor=nvidia
```



## WEXAC basic concepts - summary

- LSF tasks multiply all other resources
- Affinity threads doesn't multiple all other resources
- Pickup of right job size in terms of CPU cores, CPU memory, GPU memory, GPU setup is crucial for effective jobs, pending time reduction and achieve high fair share score.

SHARE_INFO_FO	R: new-s	hort/						
USER/GROUP	SHARES	PRIORITY	STARTED	RESERVED	CPU_TIME	RUN_TIME	<b>ADJUST</b>	GPU_RUN_TIME
aihubadm	100	33.333	0	0	0.0	0	0.000	0
nirc	100	33.333	0	0	0.0	0	0.000	0
leep	100	33.333	0	0	0.0	0	0.000	0
tomerant	100	33.333	0	0	0.0	0	0.000	0
alexkon	100	33.331	0	0	1.2	0	0.000	0
gabril	100	33.330	0	0	1.3	0	0.000	0
vitalyg	100	33.324	0	0	4.6	0	0.000	0
golann	100	33.220	0	0	52.8	0	0.000	0
amy	100	32.390	0	0	449.4	0	0.000	0
eliranso	100	27.668	0	0	3159.0	0	0.000	0
vadimm	100	6.665	4	0	0.0	1	0.000	0
nathanl	100	2.281	10	0	23.8	3902	0.000	0
fabrizio	100	1.495	0	0	328540.8	0	0.000	0
nachumn	100	1.425	1	0	20135.1	21695	0.000	0
saarsh	100	1.414	10	0	56.6	13578	0.000	0
efratw	100	1.351	4	0	20688.3	19802	0.000	0
angolo	100	1.141	10	0	2597.9	19496	0.000	0
arielo	100	1.106	4	0	1914.7	27025	0.000	0
tamark	100	0.885	10	0	32.8	28780	0.000	0
adiwi	100	0.399	10	0	1597.2	78341	0.000	0
yufei	100	0.362	1	0	90156.7	91113	0.000	0

SHARE_INFO_FO	R: gpu-s	hort/						
USER/GROUP	SHARES	PRIORITY	STARTED	RESERVE	D CPU_TIME	RUN_TIME	<b>ADJUST</b>	GPU_RUN_TIME
vadimm	1	0.953	0	0	0.9	0	0.000	17
alexkon	1	0.952	0	0	1.7	0	0.000	17
vitalyg	1	0.569	0	0	4198.2	0	0.000	0
nancyy	1	0.218	0	0	1525.6	0	0.000	1190
nathanl	1	0.055	6	0	12.9	3637	0.000	3637
angolo	1	0.036	0	0	3600.7	0	0.000	9384
sagima	1	0.016	8	0	6744.6	17459	0.000	17459
karbati	1	0.008	36	0	443903.3	43030	0.000	0
dijin18	1	0.006	40	0	594210.6	30814	0.000	0
gavriel	1	0.002	6	0	150993.3	1358807	0.000	0
saurabhm	1	0.002	1	0	19129.8	4639	0.000	176274
erezy	1	0.002	77	0	1330228.1	1196698	0.000	0
yuril	1	0.001	4	0	220667.3	219886	0.000	219905
sagyk	1	0.001	2	0	378272.8	262115	0.000	262363
joel	1	0.001	21	0	3757288.8	637295	0.000	0
ronsar	1	0.001	8	0	245799.0	466469	0.000	466469
dekely	1	0.000	12	0	244582.0	815497	0.000	815498
jonasm	1	0.000	9	0	923955.8	190838	0.000	1717542
guylu	1	0.000	468	0	1840099.9	78374	0.000	1622840
yaelami	1	0.000	157	0	112651.7	1148122	0.000	2005626
jonatham	1	0.000	187	0	8395377.0	8530559	0.000	8534280



#### Platform RTM

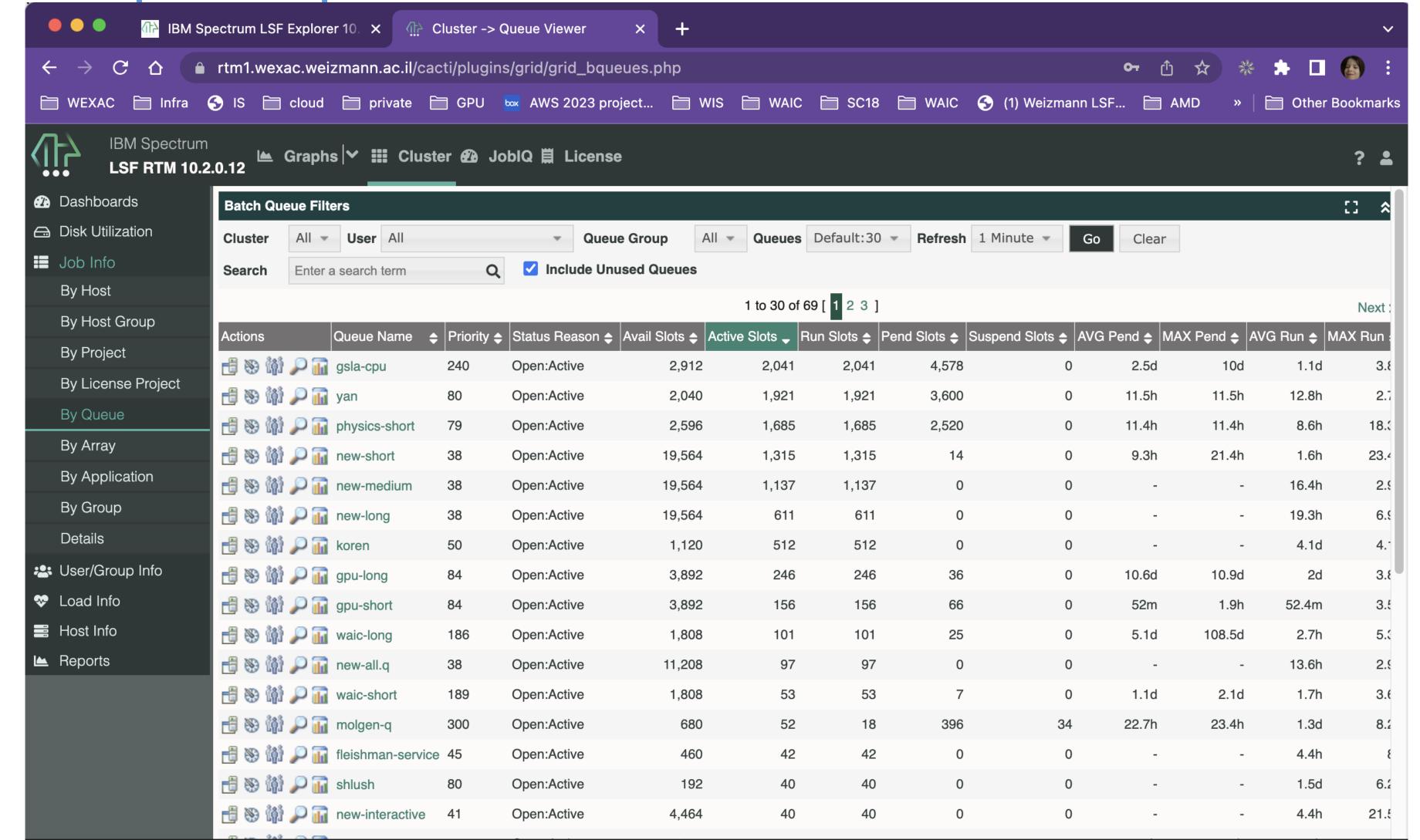
- Can be used to monitor and manage LSF jobs in real-time
- https://rtm1.wexac.weizmann.ac.il/ WEXAC's RTM





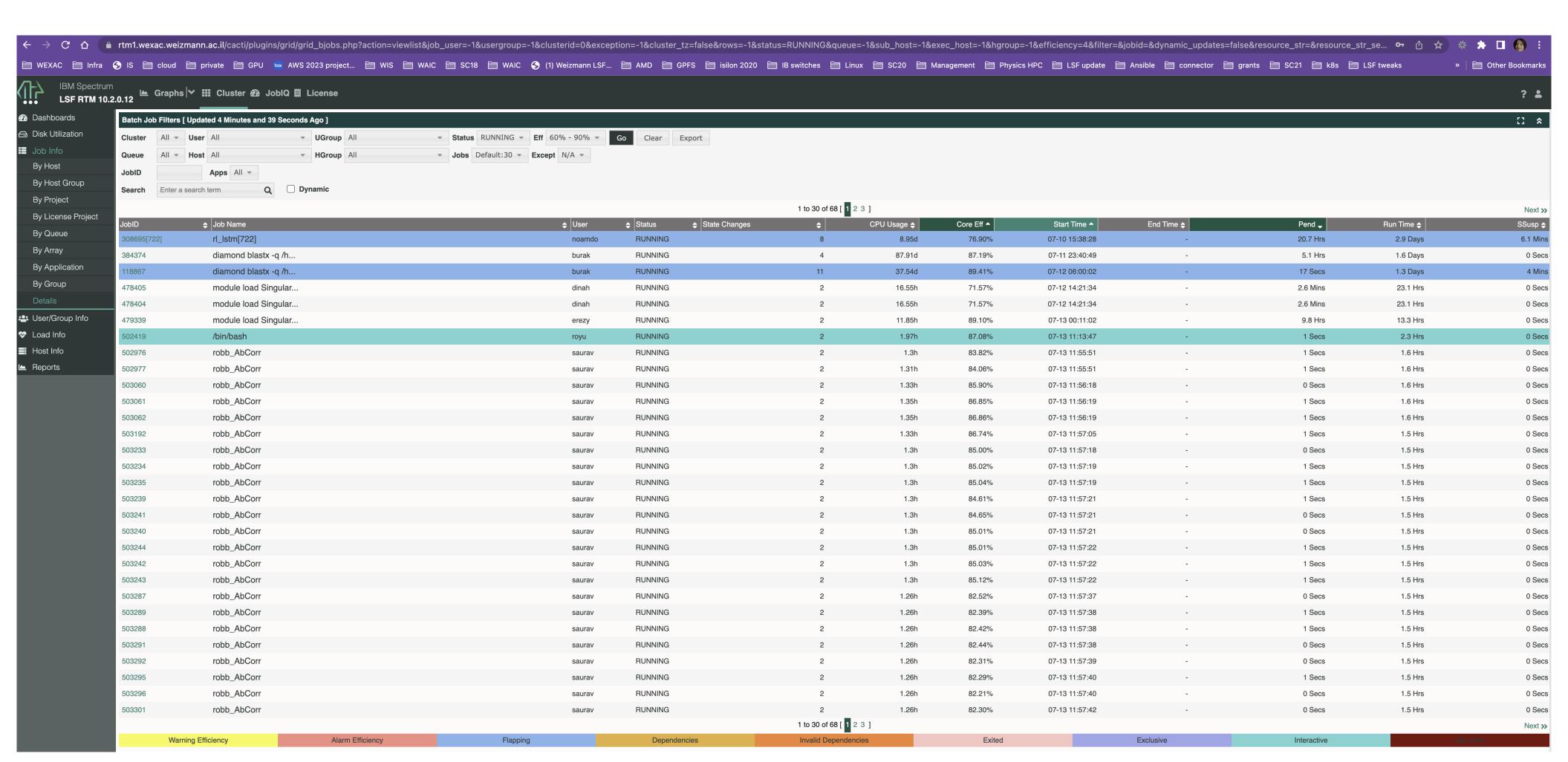


#### RTM Graphs https://rtm1.wexac.weizmann.ac.il



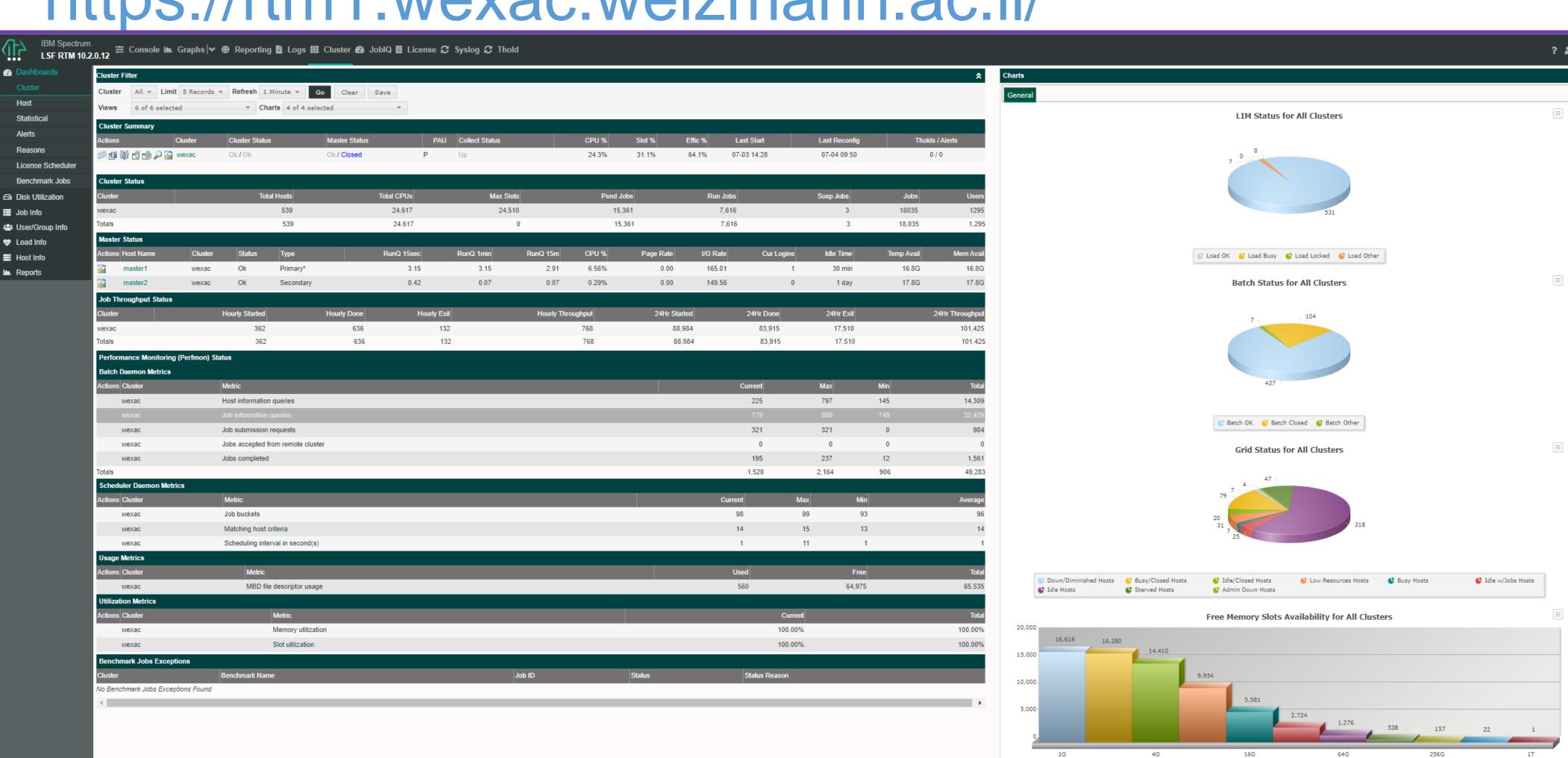


#### RTM Graphs https://rtm1.wexac.weizmann.ac.il

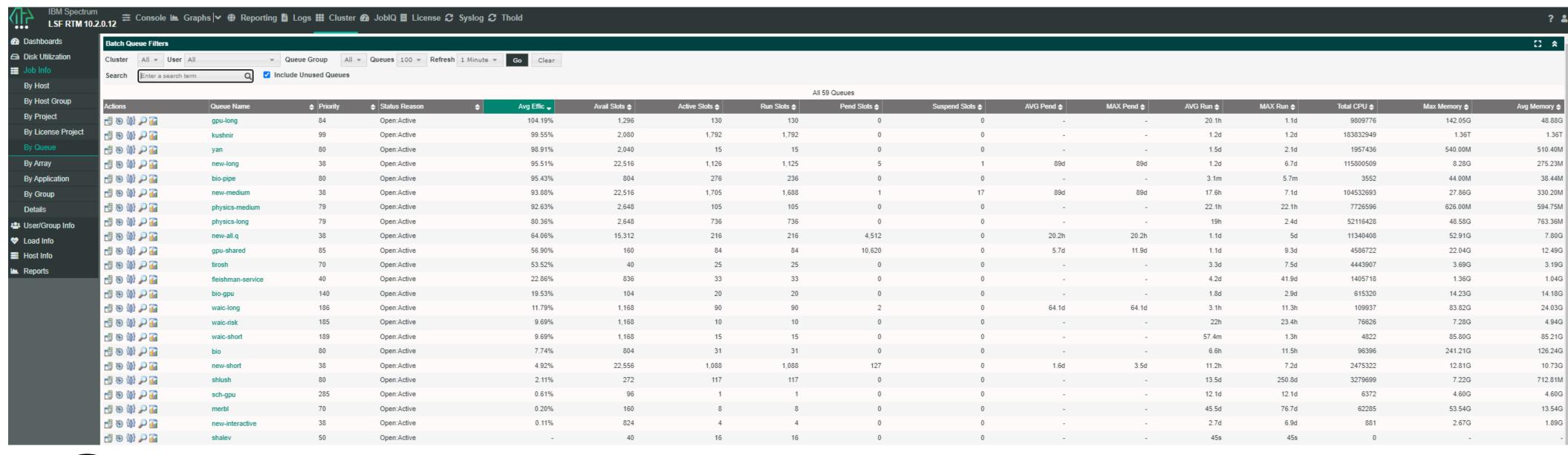


## RTM – Real Time Monitoring

### https://rtm1.wexac.weizmann.ac.il/



# RTM Queues status







## RTM - Bad job resource allocation example #1

Job Graphs	Host Graphs	License Usage					
Show User Jobs General Information							
Jobid:		47604			Status:	DONE	
Jobname:		HLA-A01; 0	01 3.txt			20.12	
Project:		default			License Project:	-	
Queue:		gpu-medium	m		Cluster Name:	wexac	
User:					User Group:		
Charged SAAP:					·		
Submission Details							
Submit Time:		2021-05-18	3 11:34:13		Number of CPUs:	12	
Submit Host:		access3					
Asked Hosts/Groups:		-			Runtime Estimate:	-	
Combined ResReq:		select[((type	e = any ) && (ngpus>0)) && (type == any)] order[gpu_maxfact	tor] rusage[mem=2000.00:ngpus_physical=1.00] affinity[thread(1)*1]			
Submit Command:			pan-4.0/netMHCpan -a	a HLA-A01: 01 -I 8,9,10,11,12,13,14 -f "HLA-A01; 01_3.txt" >/netMHCp	an_output/HLA-A01; 01_3.txt*		
Submit Dir:		\$HOME/TC	GA-Data driven approach/TCGA HLA-I/_4_netMHCpan/fasta	2			
Resource Requirements:		rusage[men	m=2000]				
Output File:		/parallel_c	output/HLA-A01;01_3.txt-%J.o				
Error File:		/parallel_c	output/HLA-A01;01_3.txt-%J.e				
Execution Environment							
Ex Host:		12*hgn02 (	(6*hgn02, 6*hgn11)				
Start Time:		2021-05-18	3 11:34:23				
Username:					UID String:	42234	
User Home:					Working Dir:		n approach/TCGA HLA-I/_4_netMHCpan/fasta2
Max Processors:		(12)			Max Allocated Slots:	12	
CPU Limit:					Run Time Limit:	12 Hours	
Memory Limit:		1.953G			Swap Limit:	0.000M	
Effective ResReq:		select[(((typ	pe = any ) && (type == any))) && (ngpus>0)] order[gpu_maxfa	actor] rusage[mem=2000.00,ngpus_physical=1.00] affinity[thread(1)*1]			
Current/Last Status							
PGIDS:		64330					
PIDS:		46739,	46740, 46741, 64330, 64371, 64373, 64380				
Threads:		8					
Pend Time:		10 Sec	conds	PROV Time:		Run Time:	4.47 Hours
Effective Pending Time Limit:							
PSUSP Time:		-		USUSP Time:		SSUSP Time	•
Unknown Time		-					
Cumulative CPU:		4.46 Ho		System Time:		User Time:	4.46 Hours
Cur Mem Used:		38.000		Max Mem Used:	38.000M	Job Efficiency:	8.31%
Cur V.Memory Size:		0.000M	M.	Max V.Memory Size:	M000.0		
Exit Code:		0		End Time:	2021-05-18 16:02:23		



# RTM - Bad job resource allocation example #1

- In the above example, we see job's detailed information.
   This can help us identify jobs that was submitted with wrong resource allocation.
- We can see that job was executed on a gpu queue while this program using only cpu power
- We can see that this job was submitted with 12 cores allocation while the job was really using only 1 core (look job efficency parameter)
- We can see that 24GB of memory was requested for job, while only 38MB(!) was actually used
- Understanding the most optimal resource requirements for programs is very important for jobs and overall system usage efficency.
- Our recommendation prior massive array or MPI job submission just run 1-2 jobs to understand the actual resources demands.



## RTM - Bad job resource allocation example #2

JobID	Job Name	Queue	User	UGroup	JGroup	Status	State Changes	Mem Request	Mem Wasted ▼ 1×	Max	x Memory	CPU Usage	CPU Effic	Num Nodes	Num CPUs	<b>Execution Host</b>
950371	ciwd		the barrie	landaria granto	-	DONE	2	-	4611.72G	638.	3.28G	4442.81d	99.65%	32	896	896*cn462

- In the above job details table, we can see a parallel mpi job that requested 896 CPU's per job and more than 5TB of RAM memory.
- While we can see that CPU efficiency of the job is very good, we can see that there are more than 4.6TB(!) of memory was completely wasted.
- Always check your jobs real resource usage in order to prevent such big resource waste.



#### RTM - Bad job resource allocation example #3

JobID Job Name	Queue	User	UGroup	JGroup	Status	State Changes	Mem Request	Mem Wasted	Max Memory	CPU Usage /	CPU Effic ▼ 1×	Num Nodes	Num CPUs	Execution Host
144643 module load matlab/R	gpu-short	CETTOTAL .	Lyo. wx-gro-lsf	-	DONE	2	-	4.79G	3.02G	3.97d	2481.48%	1	1	ibdgx001

- In the above job details table, we can see the opposite situation comparing to other examples.
- Here we can see a job that has over efficency rate of 2481%
- What does it mean? It means that the requested resources for that job was significantly smaller than was really needed for that job.
- In this case, we see that CPU request for that job is only one single CPU, while the job was actually using almost 25 CPU's.
- This situation is bad too because user is taking more resources than was requested and it affect badly on the LSF scheduler performance and resource calculations.



#### WEXAC Best practicies and recommendations

- Minimal Linux knowledge required
- Load only essential modules
- Don't mix different toolchains (for instance gcc/10.3.0 with gcc/8.3.0)
- If you must have multiple modules loaded make sure they belong to same toolchain (example: foss/2021b)
- You should plan which 1 environment type you want to use out of below 3 options (don't mix them!):
  - Conda
  - Modules
  - Containers



### WEXAC Best practicies and recommendations

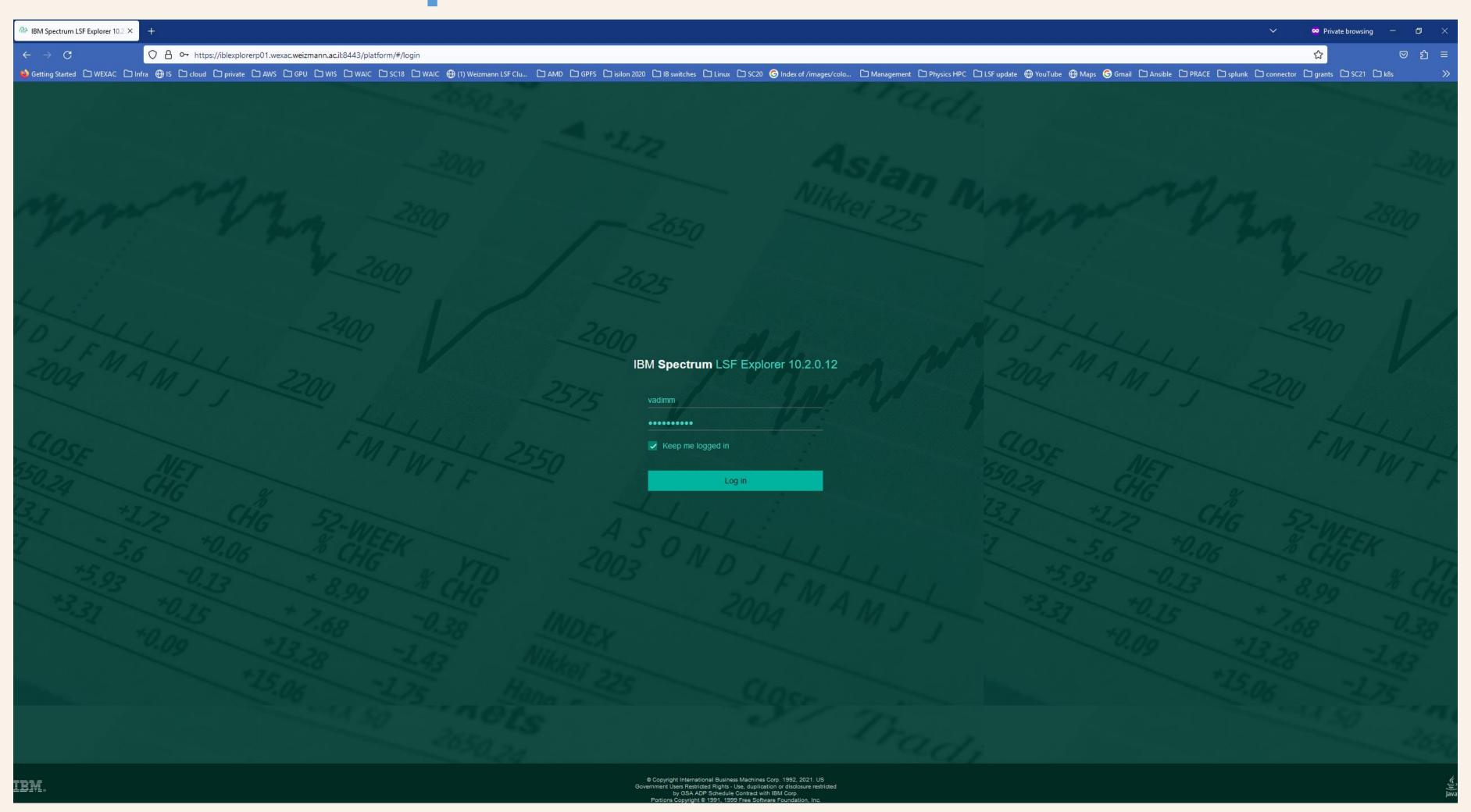
- If you are using container all your environment for current job should be inside the container!
- In case of modules usage don't use conda!
- Conda users don't use containers neither modules!
- Make sure you have clean environment and clean ~/.bashrc to avoid compatibility issues.
- Pipelines involves multiple environment types should be separated to different job types or including sterilization between different environment types switching like module purge or conda deactivate commands between different pipelines steps.



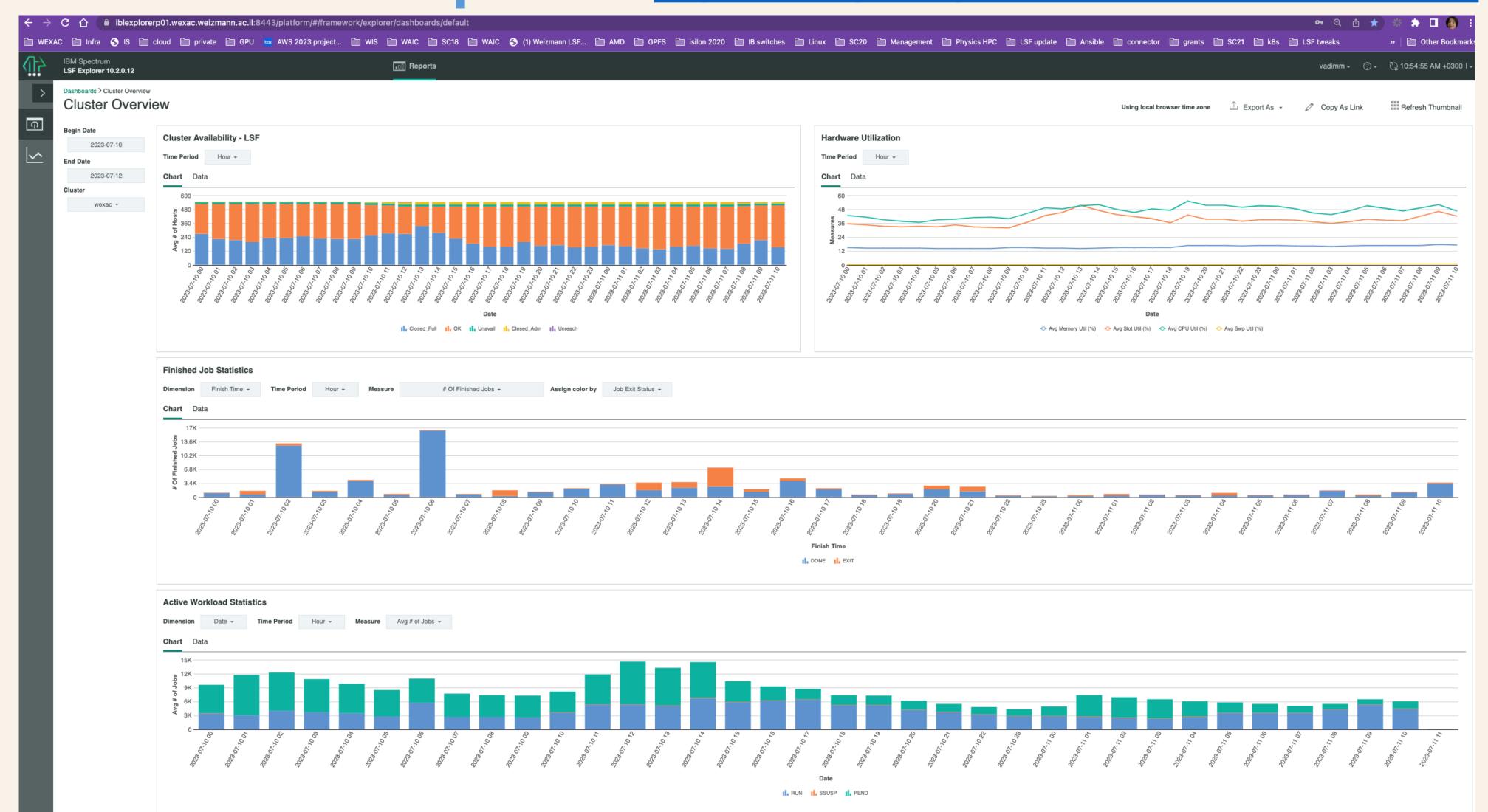
## WEXAC Best practicies and recommendations

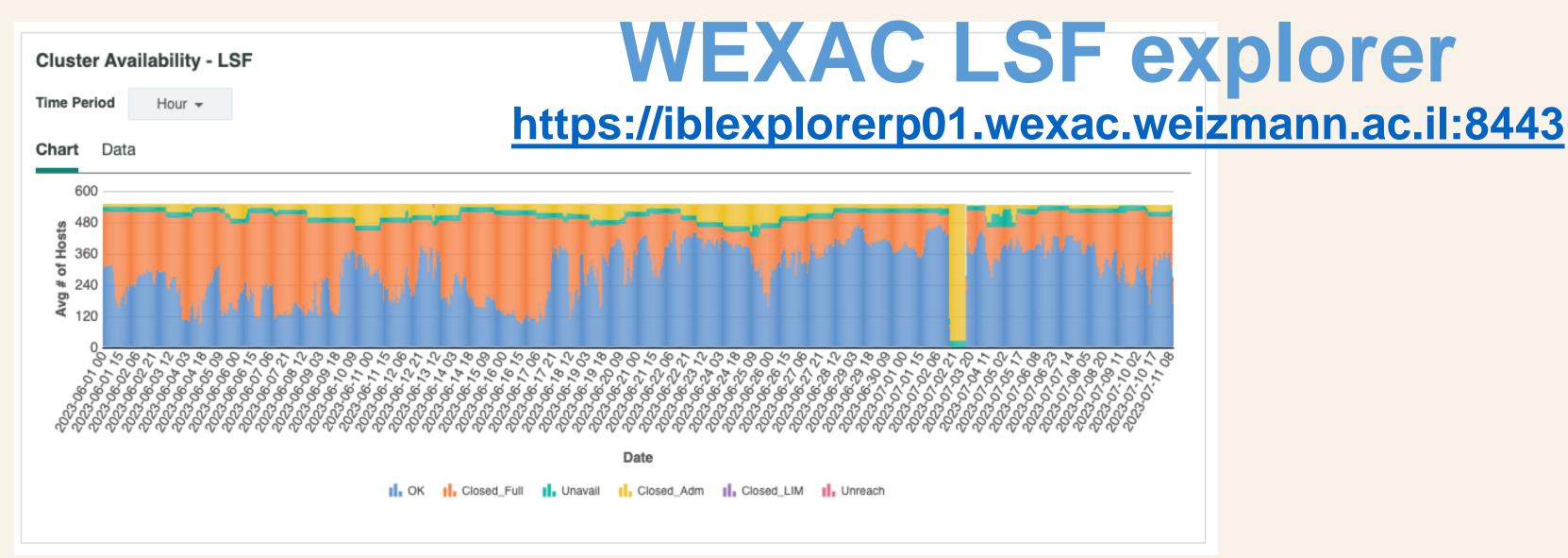
```
[vadimm@access4 ~]$ ml
No modules loaded
[vadimm@access4 ~]$ ml foss/2021b
「vadimm@access4 ~]$ ml
Currently Loaded Modules:
                                    5) numactl/2.0.14-GCCcore-11.2.0
 1) GCCcore/11.2.0
    9) hwloc/2.5.0-GCCcore-11.2.0
                                       13) PMIx/4.1.0-GCCcore-11.2.0
 17) gompi/2021b
 2) zlib/1.2.11-GCCcore-11.2.0
                                    6) XZ/5.2.5-GCCcore-11.2.0
                                       14) OpenMPI/4.1.1-GCC-11.2.0
  10) OpenSSL/1.1
 18) FFTW/3.3.10-gompi-2021b
 3) binutils/2.37-GCCcore-11.2.0
                                    7) libxml2/2.9.10-GCCcore-11.2.0
   11) libevent/2.1.12-GCCcore-11.2.0
                                       15) OpenBLAS/0.3.18-GCC-11.2.0
 19) ScaLAPACK/2.1.0-gompi-2021b-fb
                                    8) libpciaccess/0.16-GCCcore-11.2.
 4) GCC/11.2.0
 12) UCX/1.11.2-GCCcore-11.2.0
                                       16) FlexiBLAS/3.0.4-GCC-11.2.0
 20) foss/2021b
```

## WEXAC LSF explorer <a href="https://iblexplorerp01.wexac.weizmann.ac.il:8443">https://iblexplorerp01.wexac.weizmann.ac.il:8443</a>

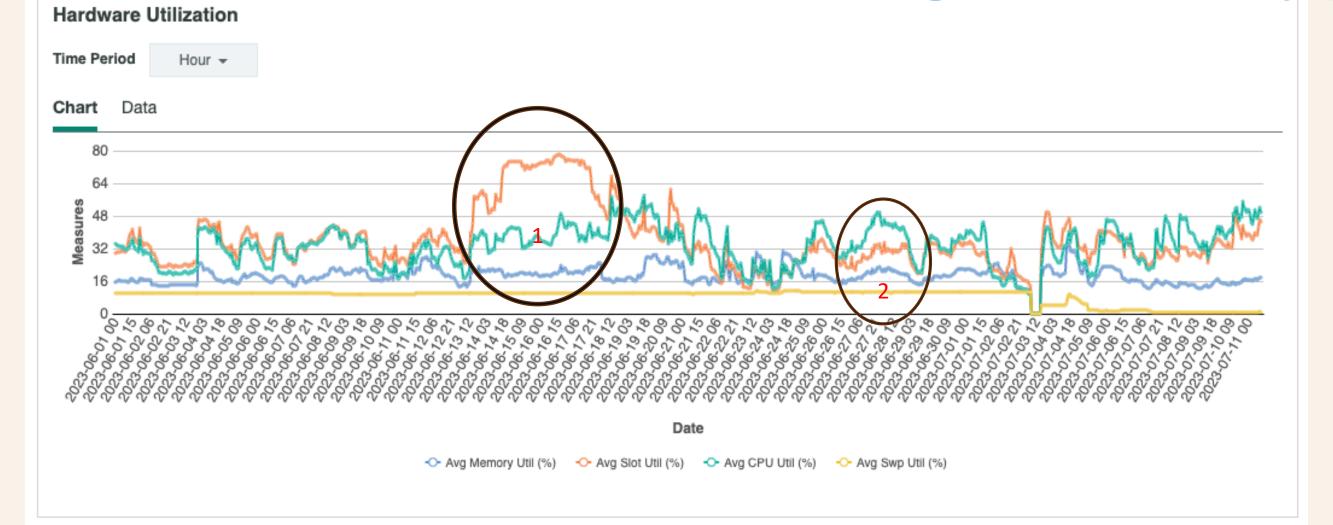


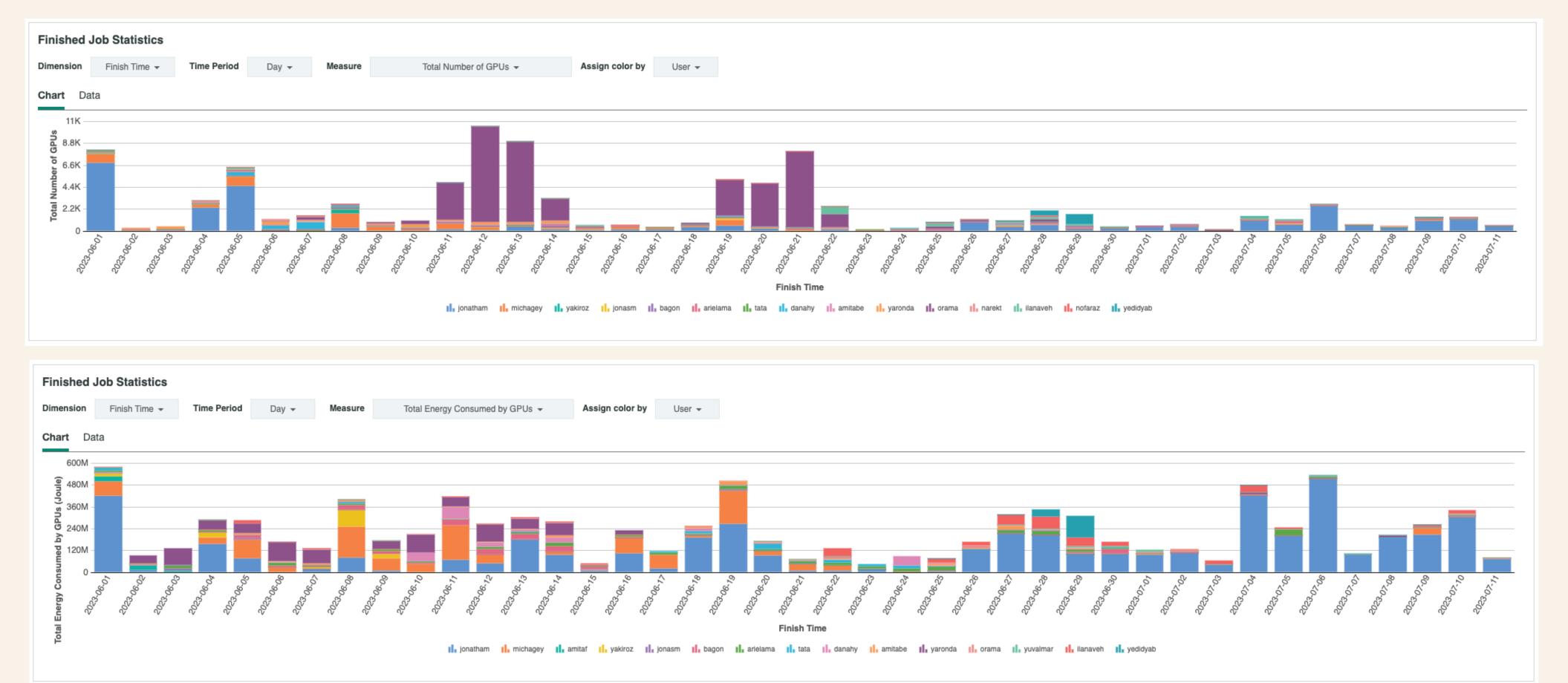
### WEXAC LSF explorer <a href="https://iblexplorerp01.wexac.weizmann.ac.il:8443">https://iblexplorerp01.wexac.weizmann.ac.il:8443</a>



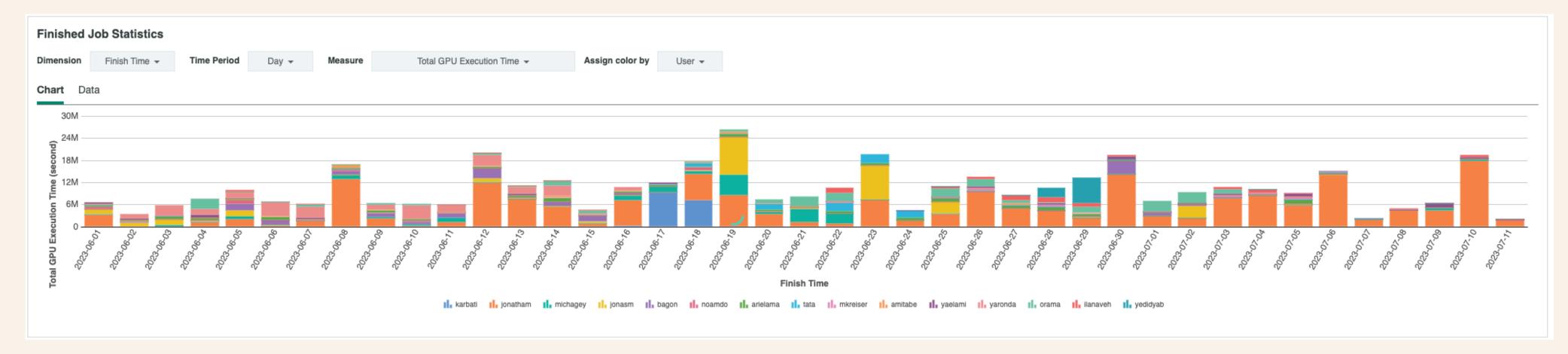


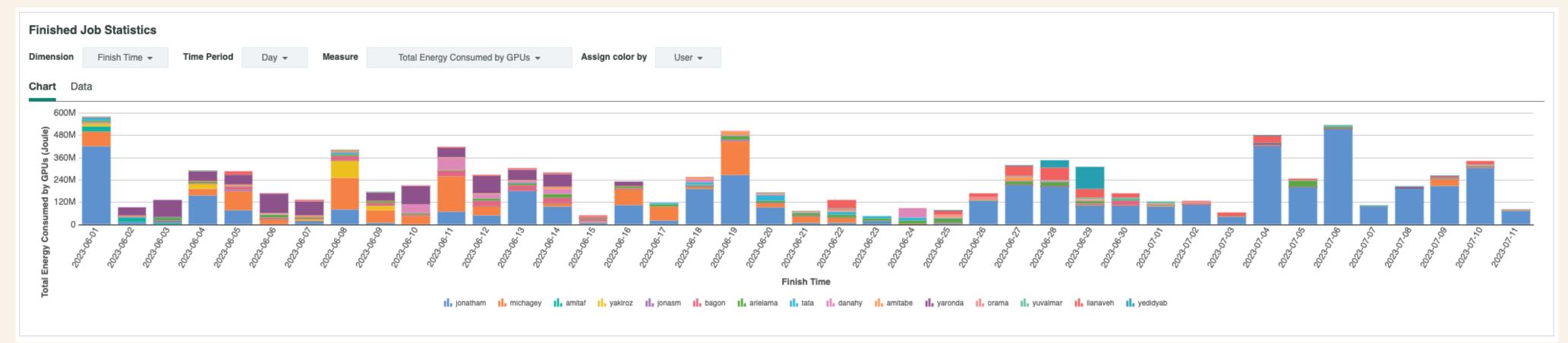
High delta between CPU util and Slot util – bad sign of efficiency problems

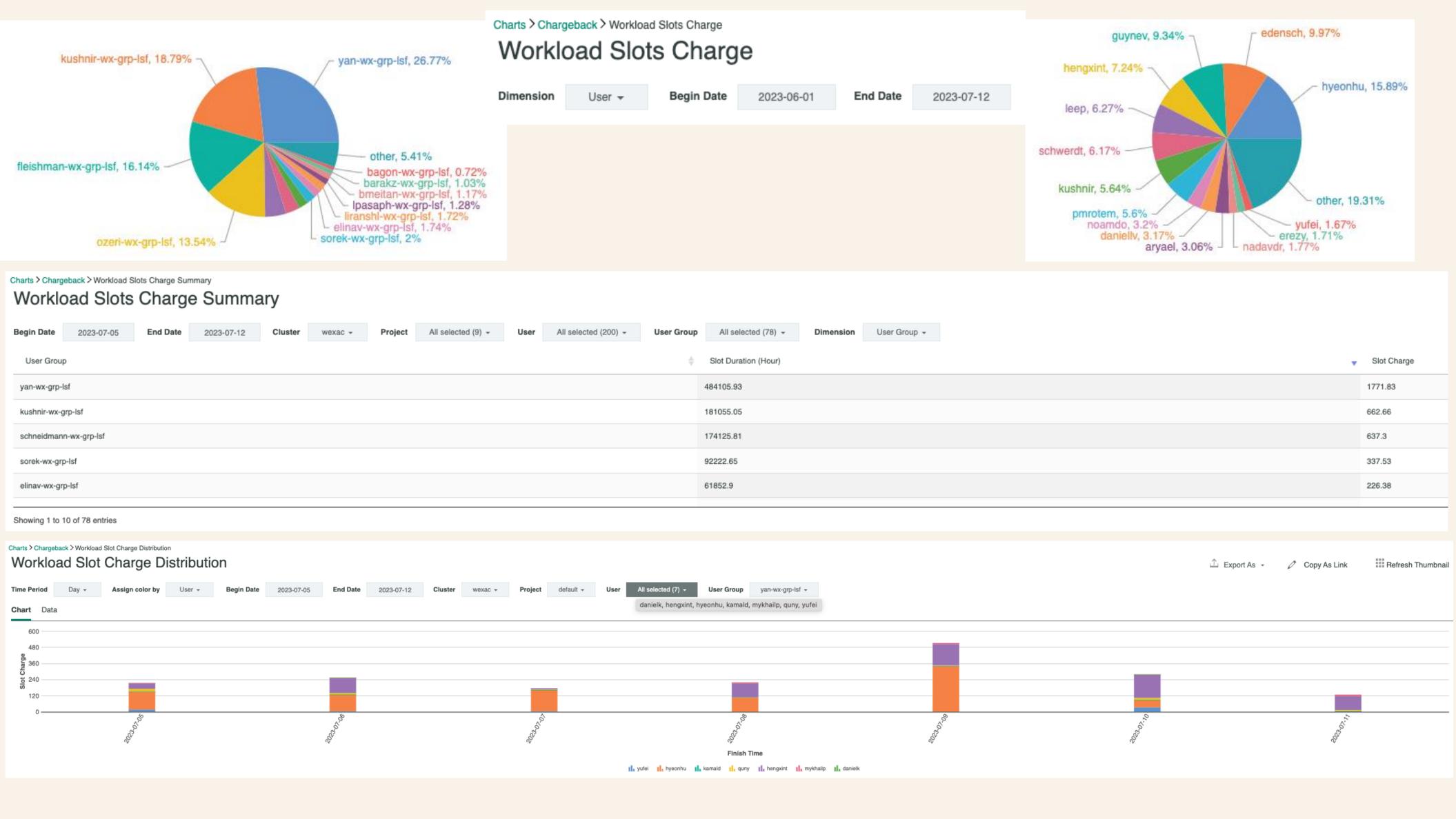




Looking for correlation between GPU allocation and energy consumption



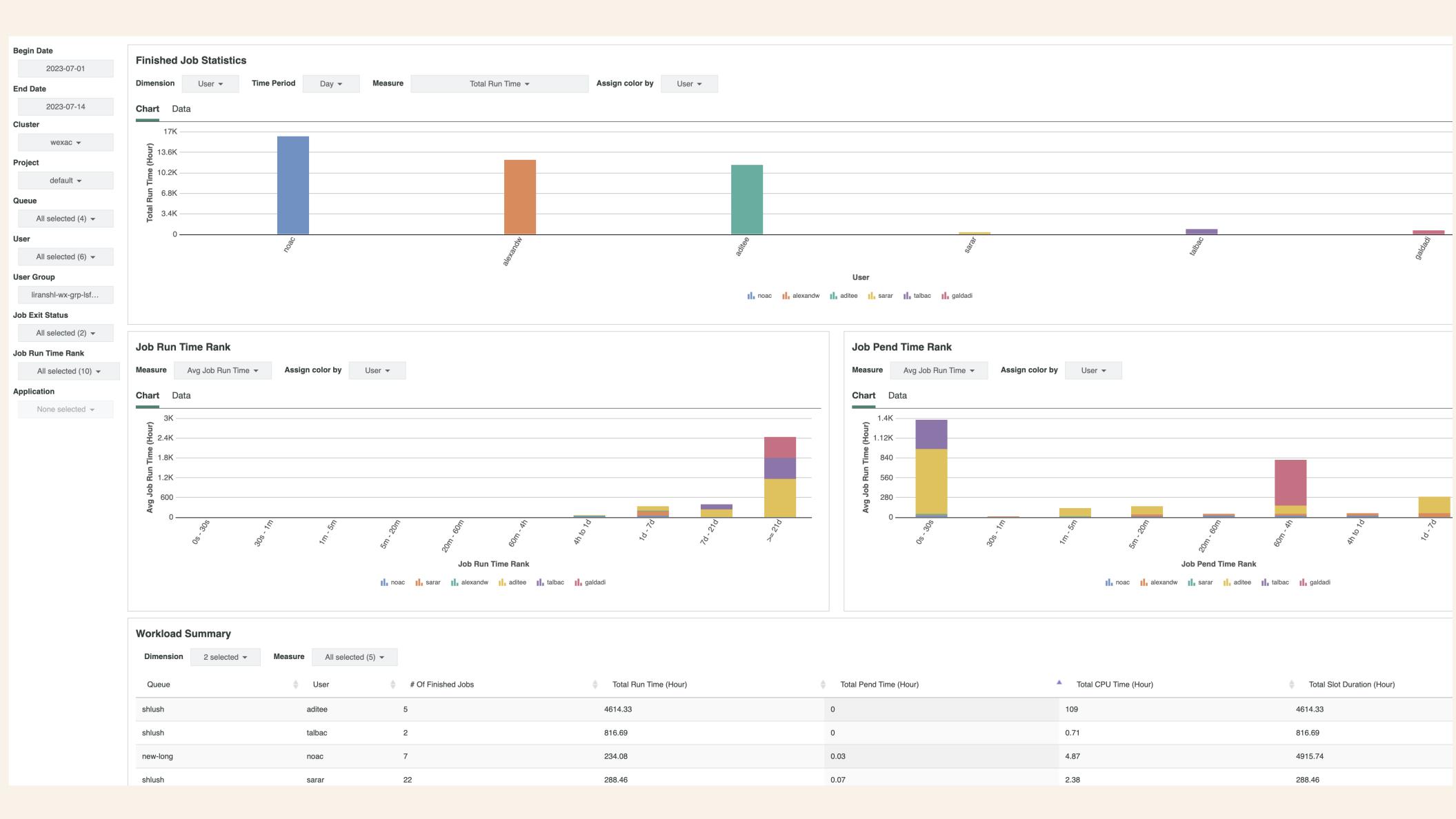




## LSF explorer dashboards



Dashboards > Workload Accounting **Workload Accounting** Refresh Thumbnail Using local browser time zone Copy As Link Begin Date **Finished Job Statistics** 2023-07-07 Hour ▼ Total Run Time ▼ Assign color by End Date 2023-07-14 Chart Data Cluster 20K wexac ▼ 후 16K **Project** 2 12K All selected (7) ▼ All selected (45) ▼ User All selected (185) ▼ User Group All selected (76) ▼ 👖 erezy 👖 noamdo 👖 jonatham 👖 yufei 👖 noac 👖 uripatis 👖 yuvalw 👖 pmrotem 👖 guynev 👖 hyeonhu 👖 yotamco 👖 amy 👖 omrile 👖 alexandw 👖 karbati Job Exit Status All selected (2) ▼ **Job Run Time Rank Job Pend Time Rank** Job Run Time Rank Assign color by User ▼ Assign color by User ▼ Measure Avg Job Run Time ▼ Avg Job Run Time ▼ All selected (10) ▼ Chart Data Chart Data None selected ▼ 2K -<u> 후</u> 1.6K **윈** 1.04K 1.2K 800 520 400 260 👖 pmrotem 👖 eliranso 👖 jeremyg 👖 edensch 👖 hyeonhu 👖 sarar 👖 reutsh 👖 aditee 👖 burak 👖 dormats 👖 jiayiy 👖 rvaldes 👖 divaf 👖 nofaraz 👖 talbac 👖 guynev 👖 alexandw 👖 hyeonhu 👖 eliranso 👖 yuvalw 👖 galv 👖 reutsh 👖 aditee 👖 dormats 👖 jiayiy 👖 rvaldes 👖 talbac 👖 burak 👖 divaf 👖 nofaraz **Workload Summary** Measure All selected (5) ▼ Queue ▼ Total CPU Time (Hour) # Of Finished Jobs Total Run Time (Hour) Total Pend Time (Hour) Total Slot Duration (Hour) User 21267 13907.42 1096248.4 13365.43 13907.42 sorek-gpu erezy 169463.36 11.57 3918 11.62 6.12 new-short avnim new-medium noamdo 5292 55482.69 82309.41 185072.8 55482.69 44431.36 549.31 550.76 sch-gpu 827 550.76



## Pending jobs troubleshooting

First, use bjobs -l yourjobid command

Then add bjobs -I -p1 yourjobid or bjobs -I -p2 yourjobid or bjobs -I -p3 yourjobid

bjobs -l -p1 53690

```
[vadimm@ibdgxa01 ~]$ bjobs 53690

JOBID USER STAT QUEUE FROM_HOST EXEC_HOST JOB_NAME SUBMIT_TIME
53690 amy PEND new-medium access *_fcgrH_16 Jul 23 11:09

[vadimm@ibdgxa01 ~]$ bjobs -l 53690

PENDING REASONS:

Job requirements for reserving resource (mem) not satisfied: 55 hosts;
```

#### PENDING REASONS:

```
Job's requirements for resource reservation not satisfied (Resource: mem): cn6 53, cn652, cn651, cn650, cn789, cn788, cn787, cn784, cn783, cn782, cn781, cn780, cn779, cn778, cn773, cn770, cn110, cn769, cn769, cn767, cn109, cn766, cn106, cn763, cn105, cn762, cn 102, cn100, cn759, cn758, cn757, cn754, cn753, cn751, cn74 9, cn748, cn747, cn746, cn745, cn743, cn742, cn741, cn098, cn097, cn096, cn095, cn094, cn093, cn092, cn091, cn088, c n087, cn710, cn086, cn084;
```

#### bjobs -l -p2 53690

```
PENDING REASONS:

Candidate host pending reasons (85 of 545 hosts):

Job's requirements for resource reservation not satisfied (Resource: mem): c

n653, cn652, cn651, cn650, cn789, cn788, cn787, cn784, cn7

83, cn782, cn781, cn780, cn779, cn778, cn773, cn770, cn110

, cn769, cn767, cn109, cn766, cn106, cn763, cn105, cn762,

cn102, cn100, cn759, cn758, cn757, cn754, cn753, cn751, cn

749, cn748, cn747, cn746, cn745, cn743, cn742, cn741, cn09

8, cn097, cn096, cn095, cn094, cn093, cn092, cn091, cn088,

cn087, cn086, cn084;

Job slot limit reached: cn752, cn108, cn750, cn765, cn709, cn107, cn262, cn7

64, cn774, cn055, cn744, cn772, cn771, cn104, cn739, cn099

, cn103, cn760, cn184, cn101, cn183, cn786, cn768, cn785,

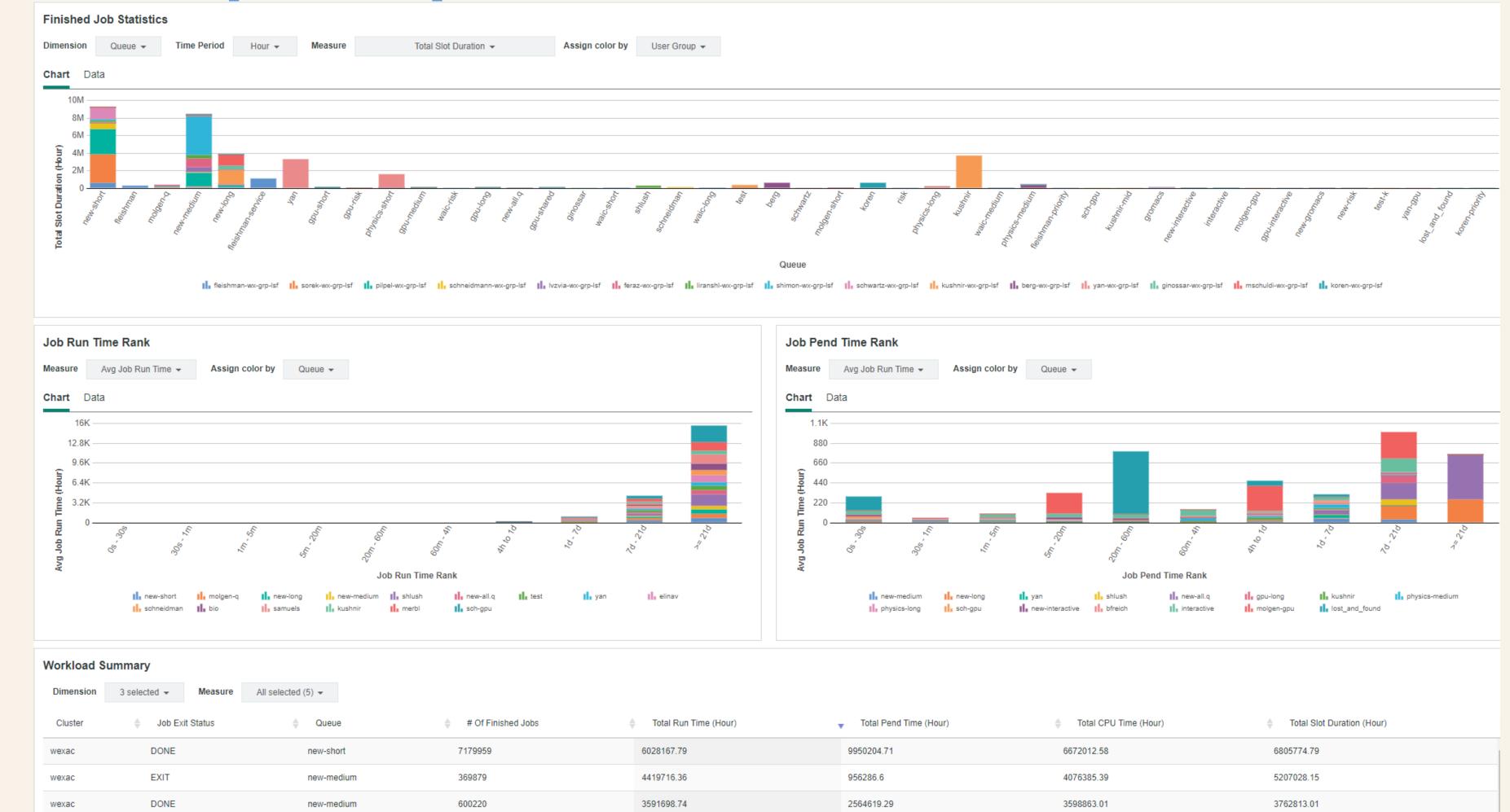
cn090, cn089, cn756, cn755, cn710, cn180, cn085, cn775;
```

#### bjobs -l -p3 53690

```
PENDING REASONS:
Candidate host pending reasons (85 of 545 hosts):
 Job's requirements for resource reservation not satisfied (Resource: mem): c
                   n653, cn652, cn651, cn650, cn789, cn788, cn787, cn784, cn7
                   83, cn782, cn781, cn780, cn779, cn778, cn773, cn770, cn110
                    , cn769, cn767, cn109, cn766, cn106, cn763, cn105, cn762,
                    cn102, cn100, cn759, cn758, cn757, cn754, cn753, cn751, cn
                   749, cn748, cn747, cn746, cn745, cn743, cn742, cn741, cn09
                   7, cn096, cn095, cn094, cn093, cn092, cn091, cn088, cn087,
                    cn086, cn084;
 Job slot limit reached: cn775, cn752, cn108, cn750, cn765, cn709, cn107, cn2
                   62, cn764, cn774, cn055, cn744, cn772, cn771, cn104, cn739
                    , cn099, cn098, cn103, cn760, cn184, cn101, cn183, cn786,
                    cn768, cn090, cn089, cn785, cn756, cn710, cn755, cn085, cn
Non-candidate host pending reasons (460 of 545 hosts):
 Not specified in job submission: cn561, cn232, cn718, cn562, cn233, hgn30, c
                   n719, cn563, cn234, hgn31, cn564, cn235, hgn32, cn565, cn2
                    36, cn080, hgn33, cn566, cn237, cn081, hgn34, cn567, cn238
```

```
hgn04, cn381, cn208, cn053, hgn05, cn382, cn209, hgn06, c
n383, hgn08, hgn07, cn384, cn056;
Load information unavailable: cn082, ibdgx001, cn273, cn279, cn432, cn761, c
n601, cn602, cn457, ops, cn463, cn162, iblpacp02, cn668, c
n044, cn054;
Closed by LSF administrator: cn078, dgxws01, dgxws02, hgn44, hgn45, hgn47, c
n433, cn451, cn456, iblpacp01, cn182, cn186;
```

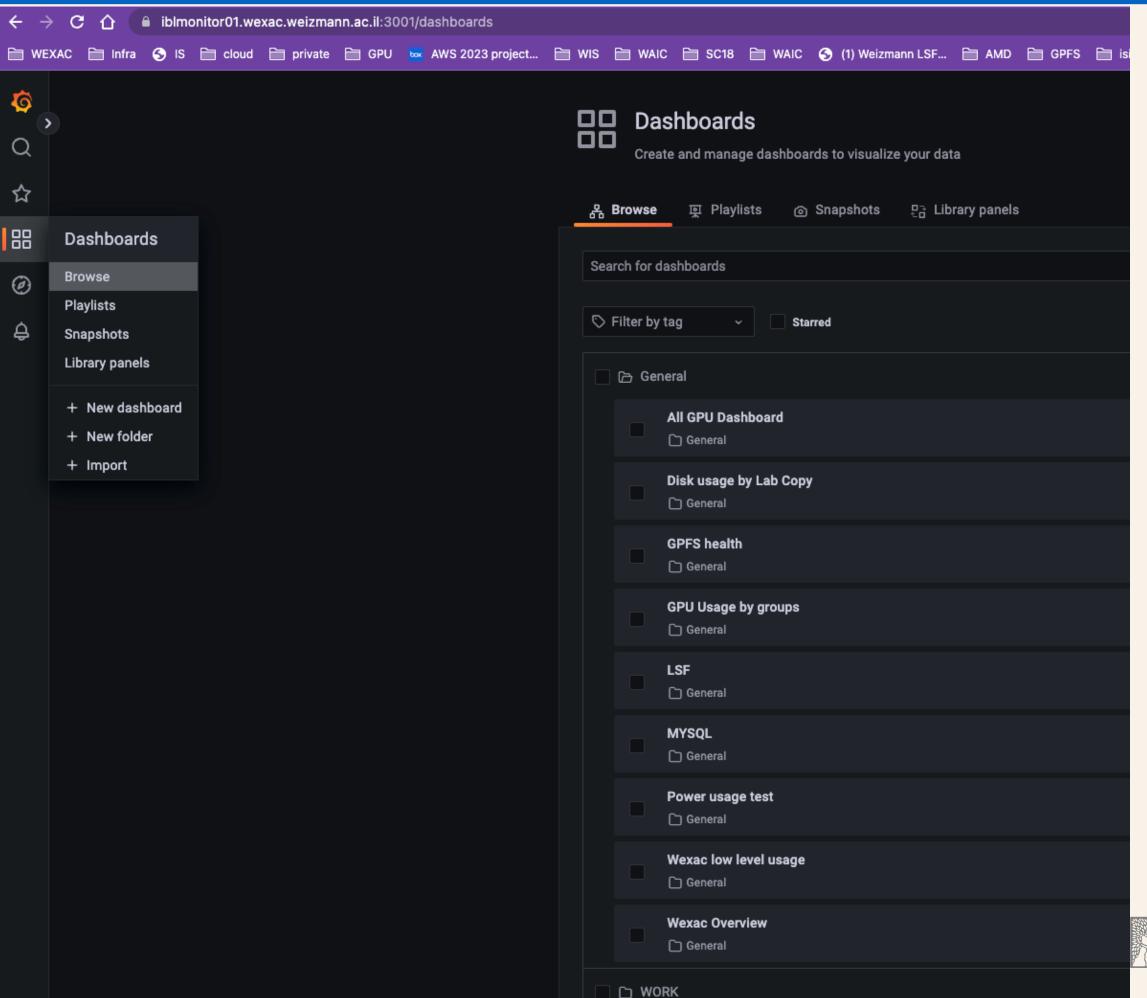
## LSF Explorer - Workload insights and statistics https://iblexplorerp01.wexac.weizmann.ac.il:8443





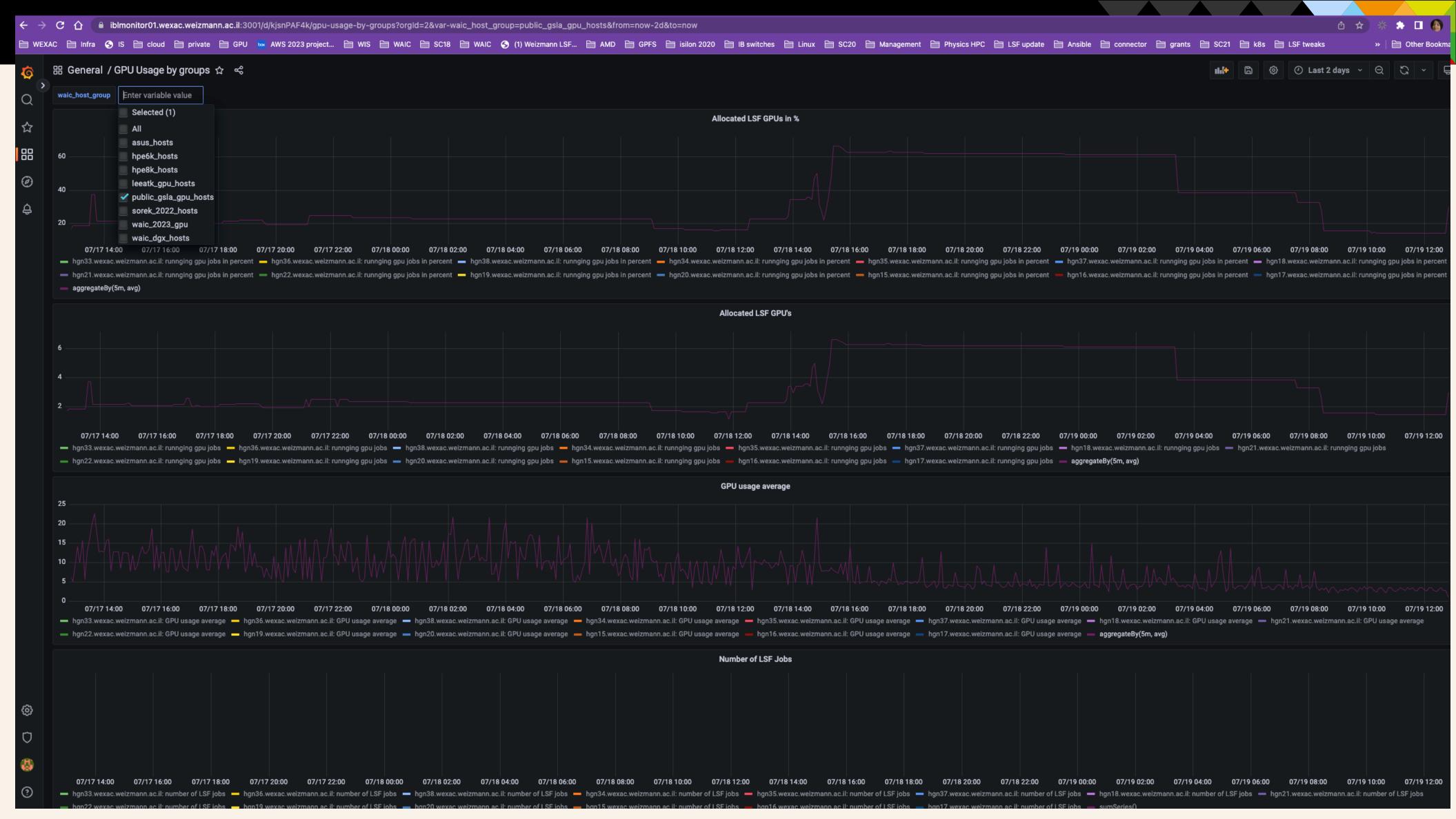
#### WEXAC Grafana

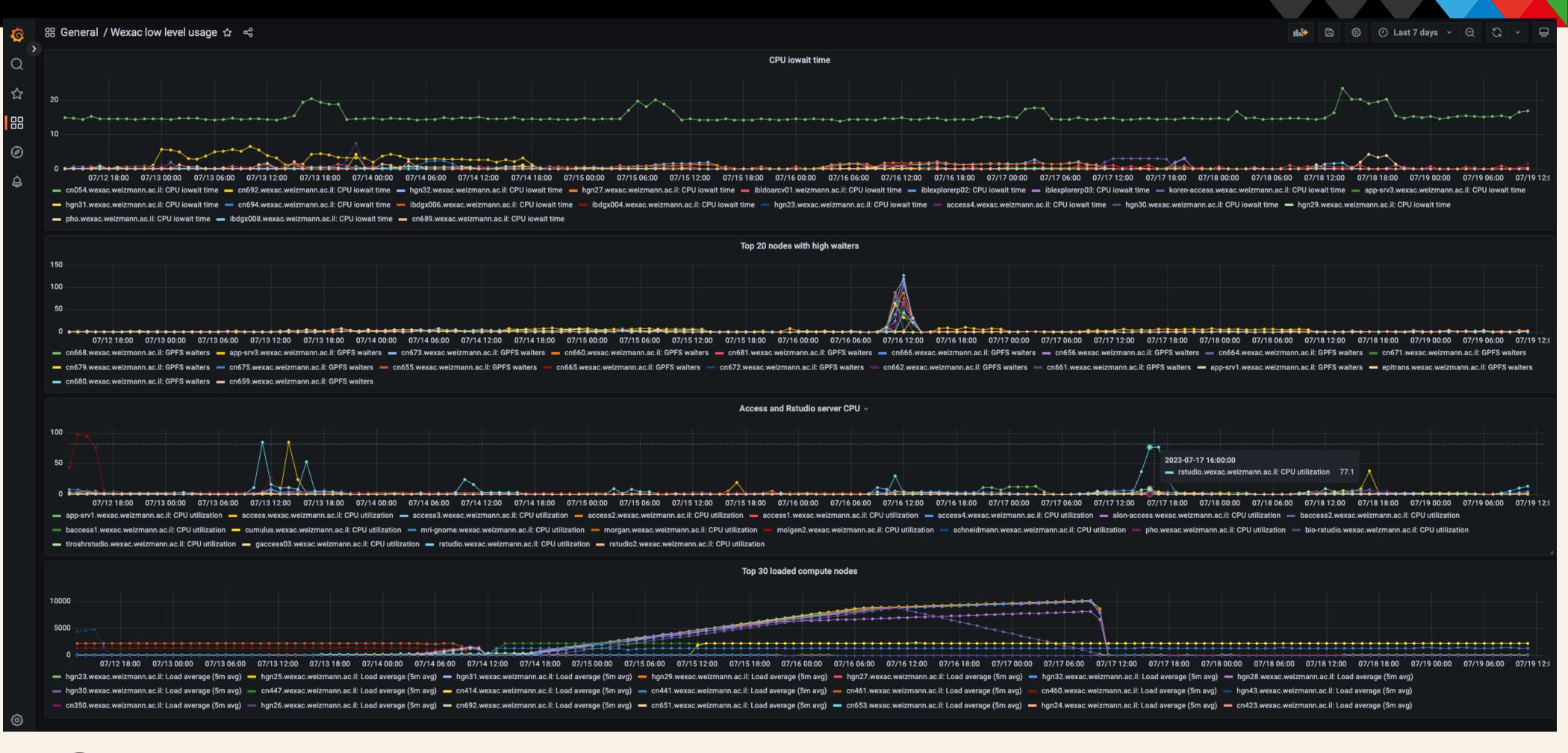
## https://iblmonitor01.wexac.weizmann.ac.il:3001



WEIZMANN INSTITUTE OF SCIENCE

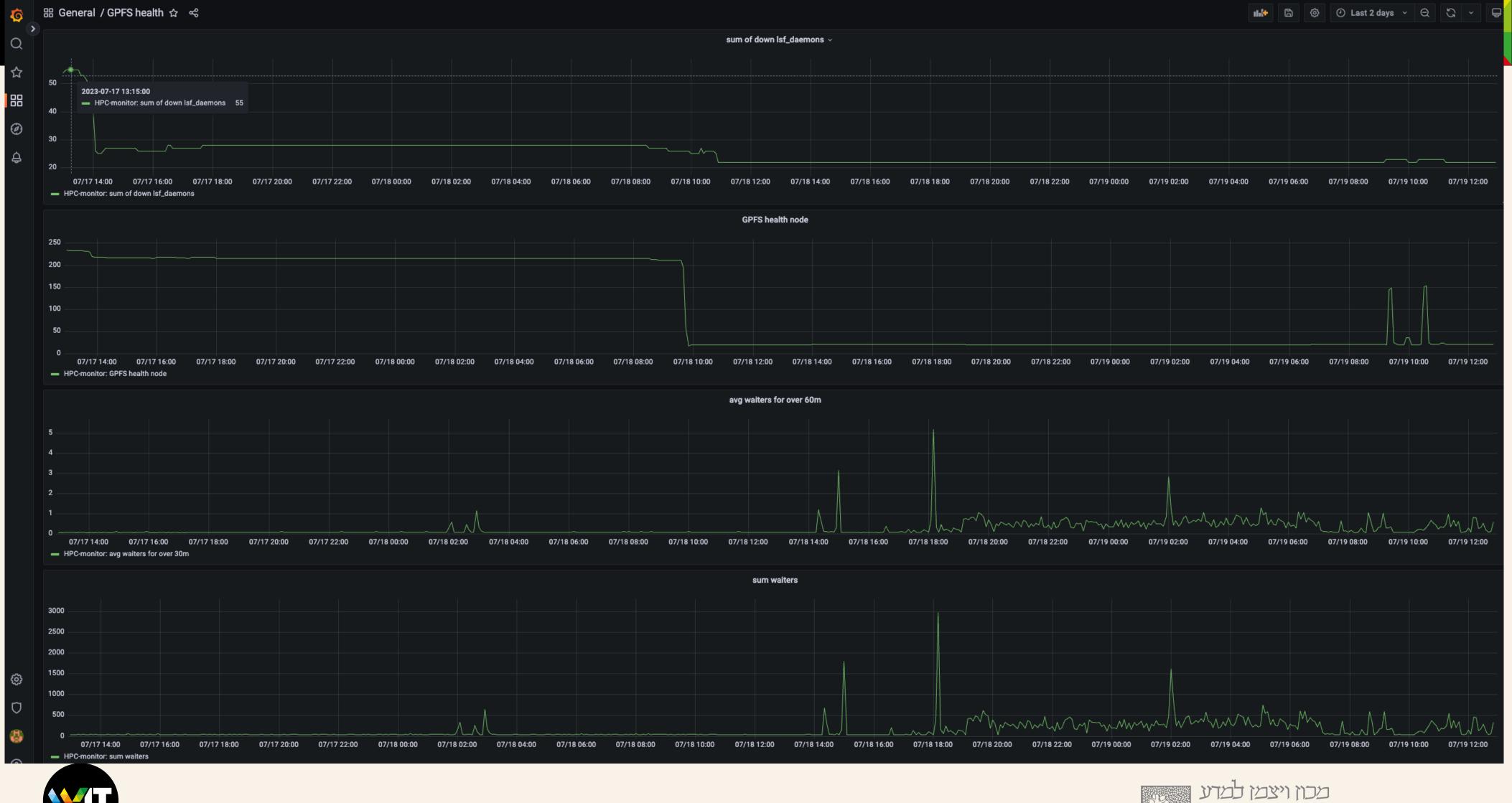






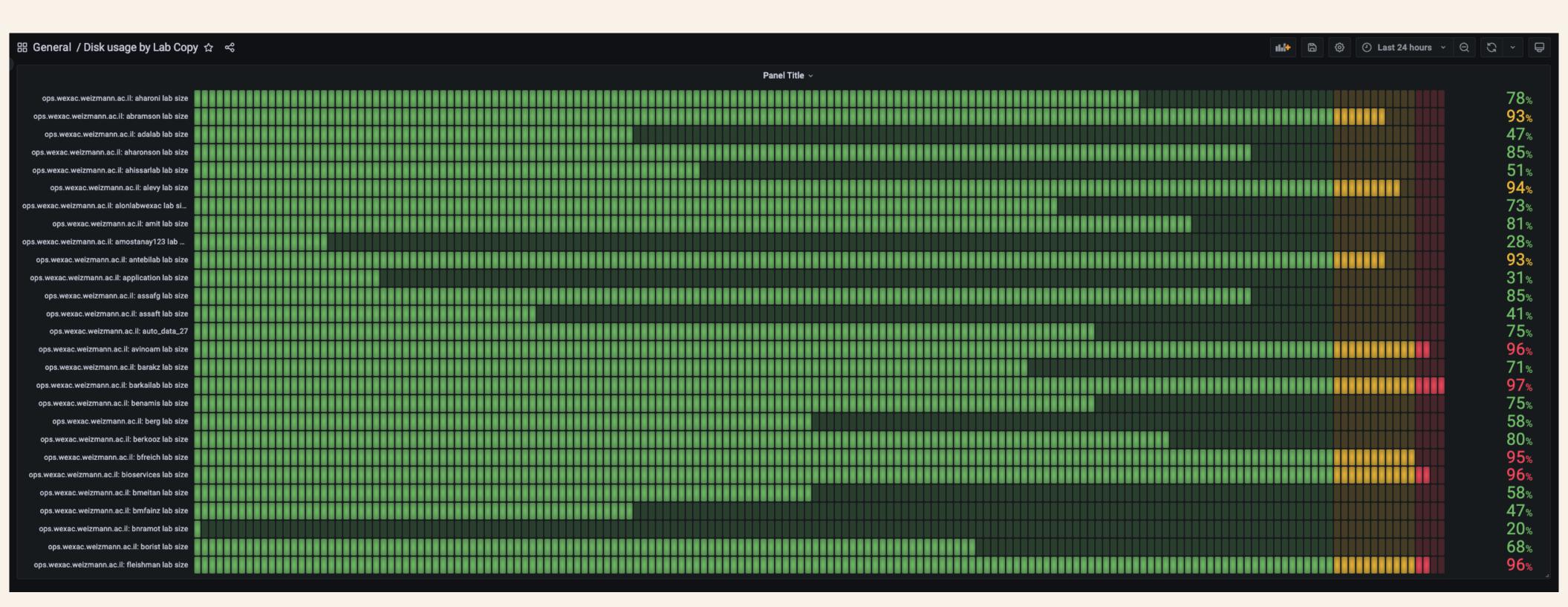






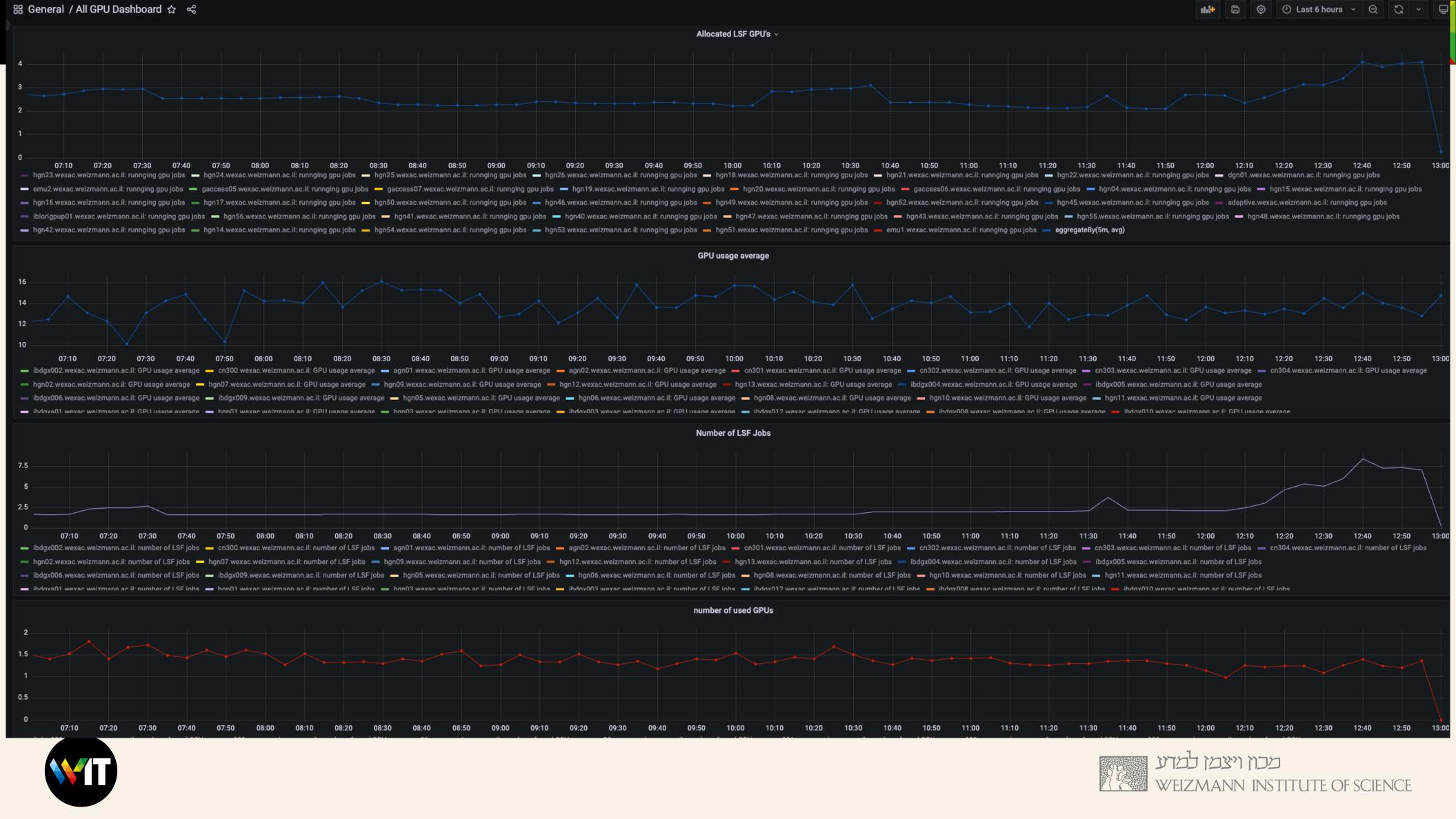


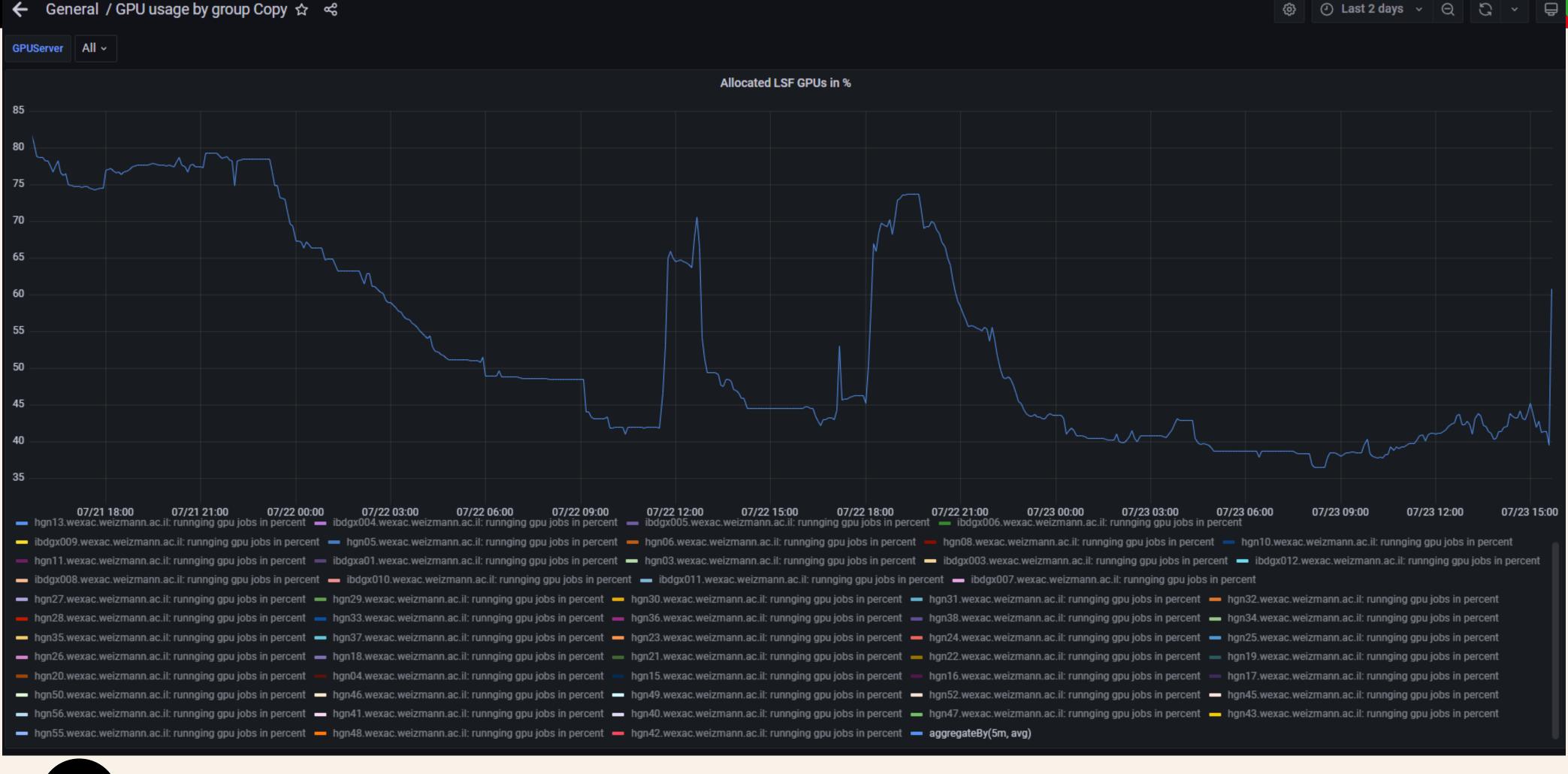






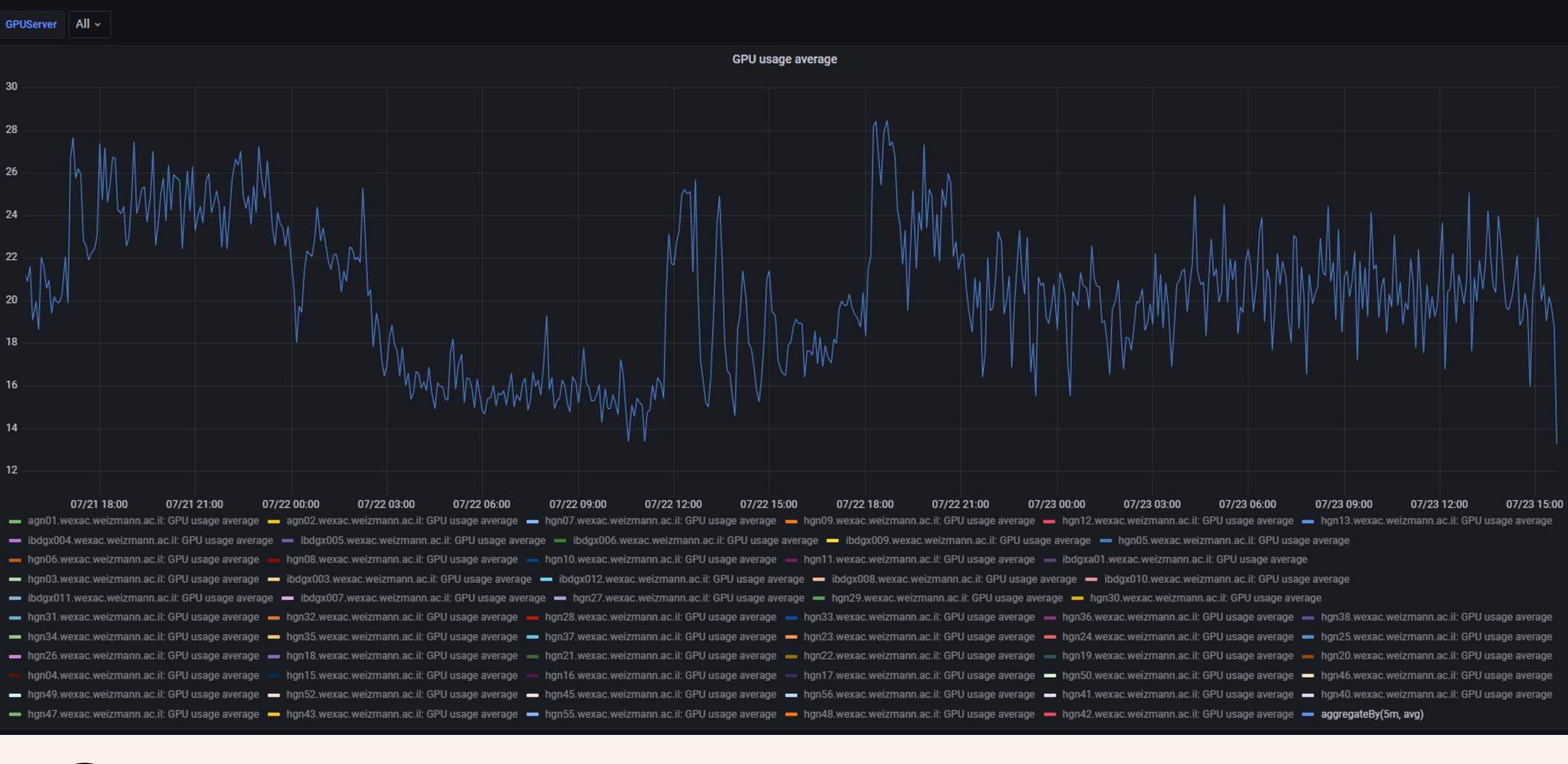












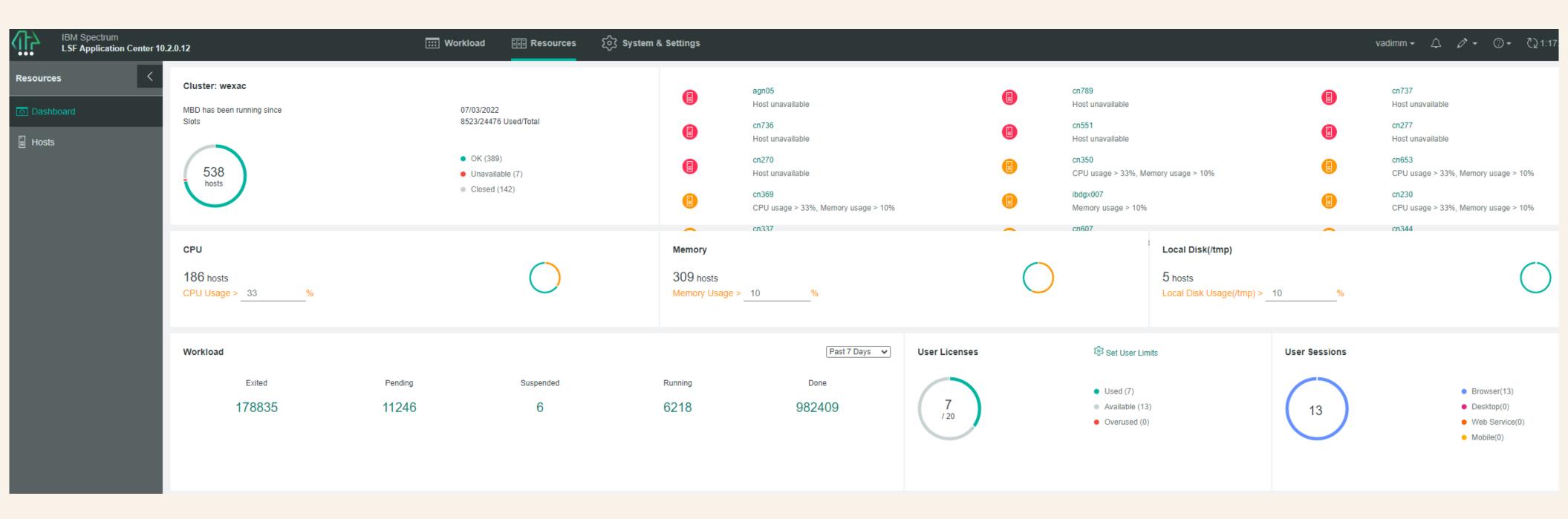


← General / GPU usage by group Copy ☆ ペ



② Last 2 days ∨ Q 😋 ∨ 💂

## LSF PAC - Platform Application Center https://iblpacp01.wexac.weizmann.ac.il:8443/

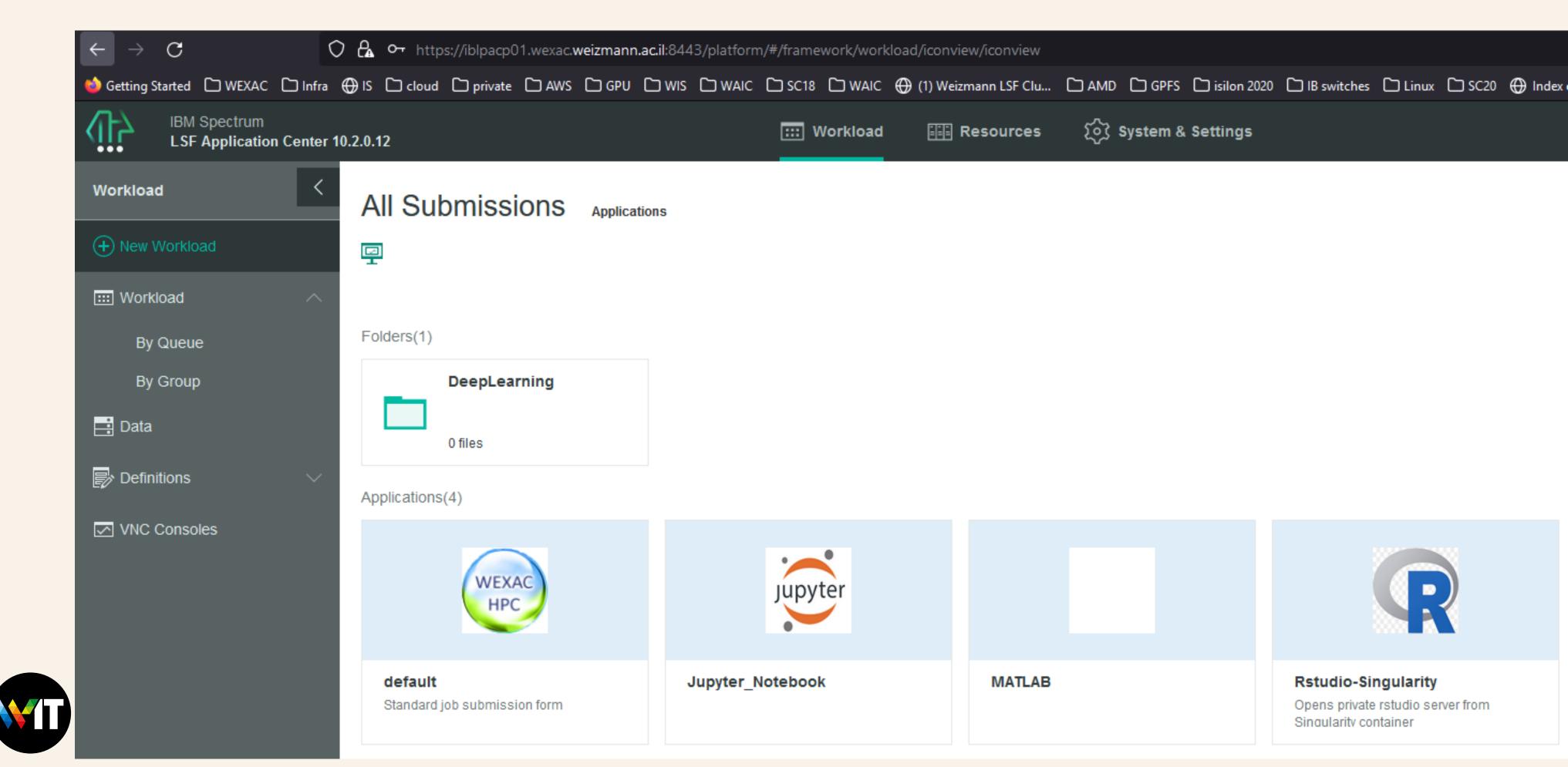






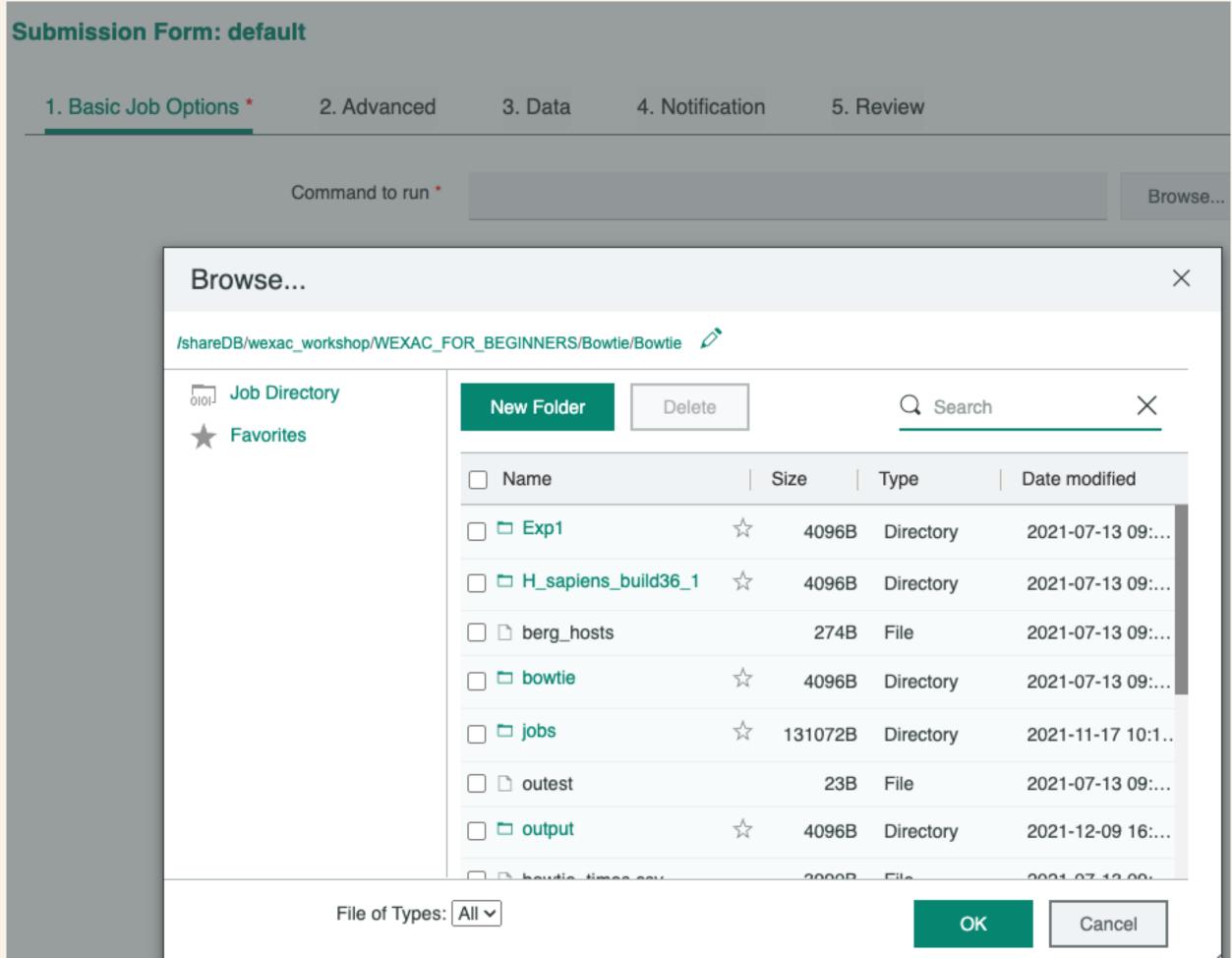
## LSF PAC - Platform Application Center

## https://iblpacp01.wexac.weizmann.ac.il:8443/



## LSF PAC - Platform Application Center

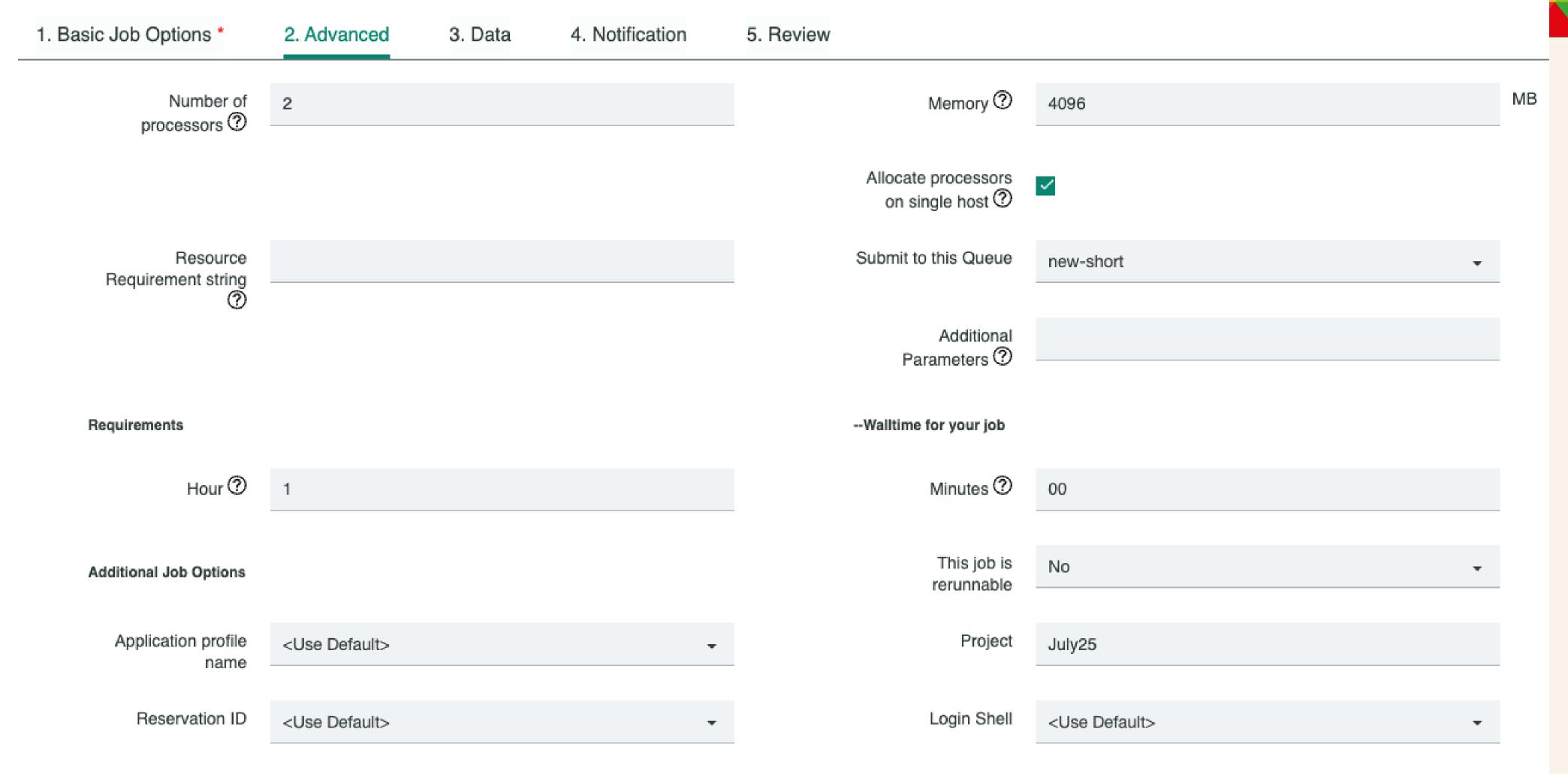
## https://iblpacp01.wexac.weizmann.ac.il:8443/







#### Submission Form: default







asic Job Options *	2. Advanced 3. Data 4. Notif	fication 5. Review			
Input file	Drag here or browse to upload local file	Add Server File			
Delete    File Name	Move to   ✓ Open with   ✓	↑   Type	Size	Actions	
☐ ☐/shareDB/we	exac_workshop/WEXAC_FOR_BEGINNERS/Bow	rtie/Bowtie/Exp1 Server	4096B		
Output file	Enter the file path				Brov
Error file	Enter the file path				





#### **Submission Form: default**

- Basic Job Options \*
- Advanced

Data

4. Notification

Review

Specify when you want to be notified about your workload.



- When workload starts
- When workload ends
- If workload exits
- If workload is suspended

#### Notify via:













#### **Submission Form: default**



Memory reservation is (MB): 4096Memory Limit is (MB): 4096 Amount of tasks (-n X) reserved: 2 === Your total amount of memory reservation for this job is (MB): 8192 === Job <561894> is submitted to queue <new-short>.

#### **Basic Job Options**

Command to run \*:

/shareDB/wexac\_workshop/WEXAC\_FOR\_BEGINNERS/Bowtie/Bowtie//benchm\_bowtie.sh Job Name :

bowtie July25

#### Advanced

Number of processors :

2

Allocate processors on

single host:

Yes

00

Memory: Submit to this Queue:

new-short

4096 MB

Hour:

This job is rerunnable: No

Minutes: Project:

July25

#### Data

Input file:

/shareDB/wexac\_workshop/WEXAC\_FOR\_BEGINNERS/Bowtie/Bowtie/Exp1

#### Notification



When workload starts

When workload ends

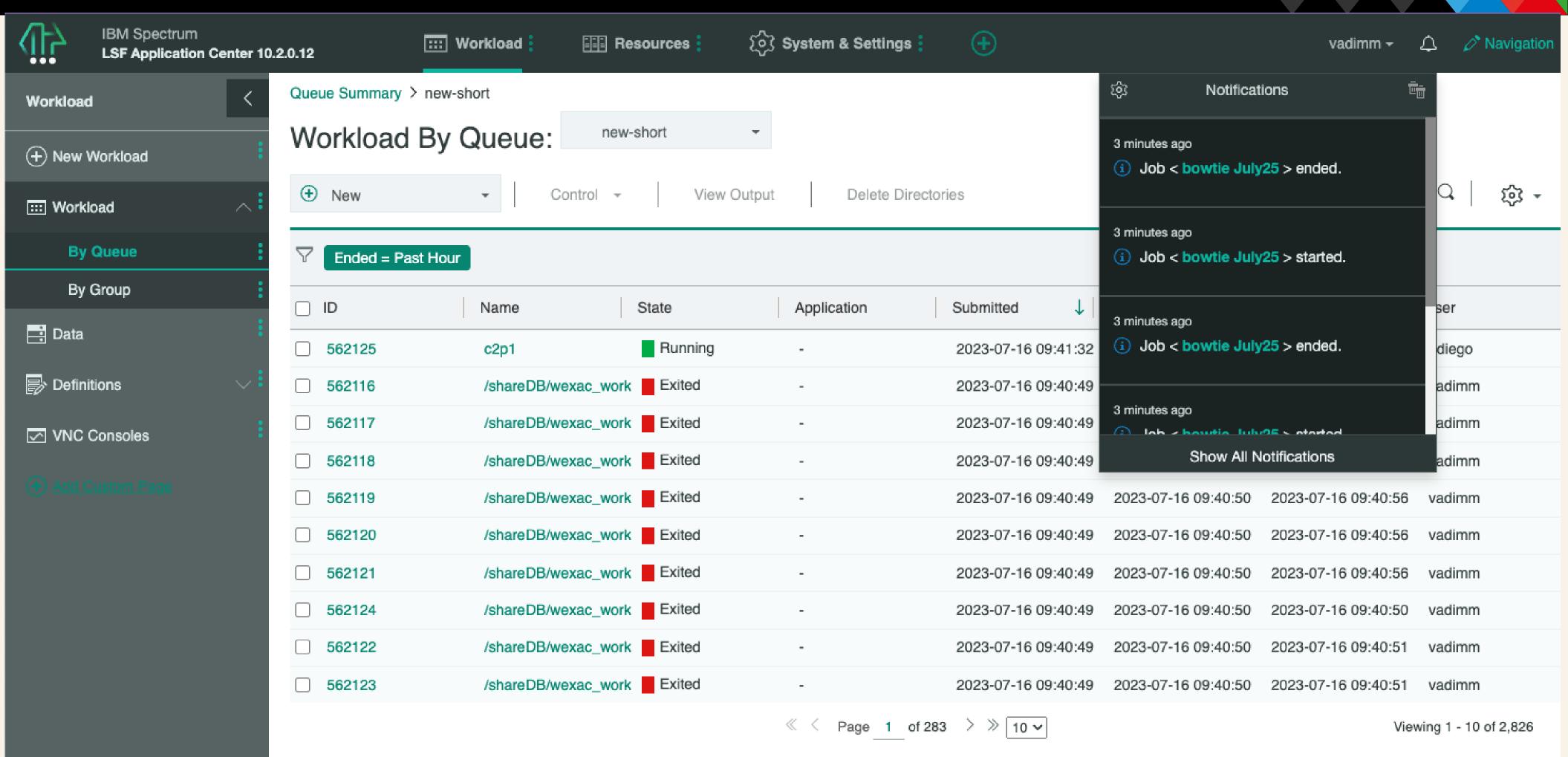
If workload exits

If workload is suspended

Notify via:

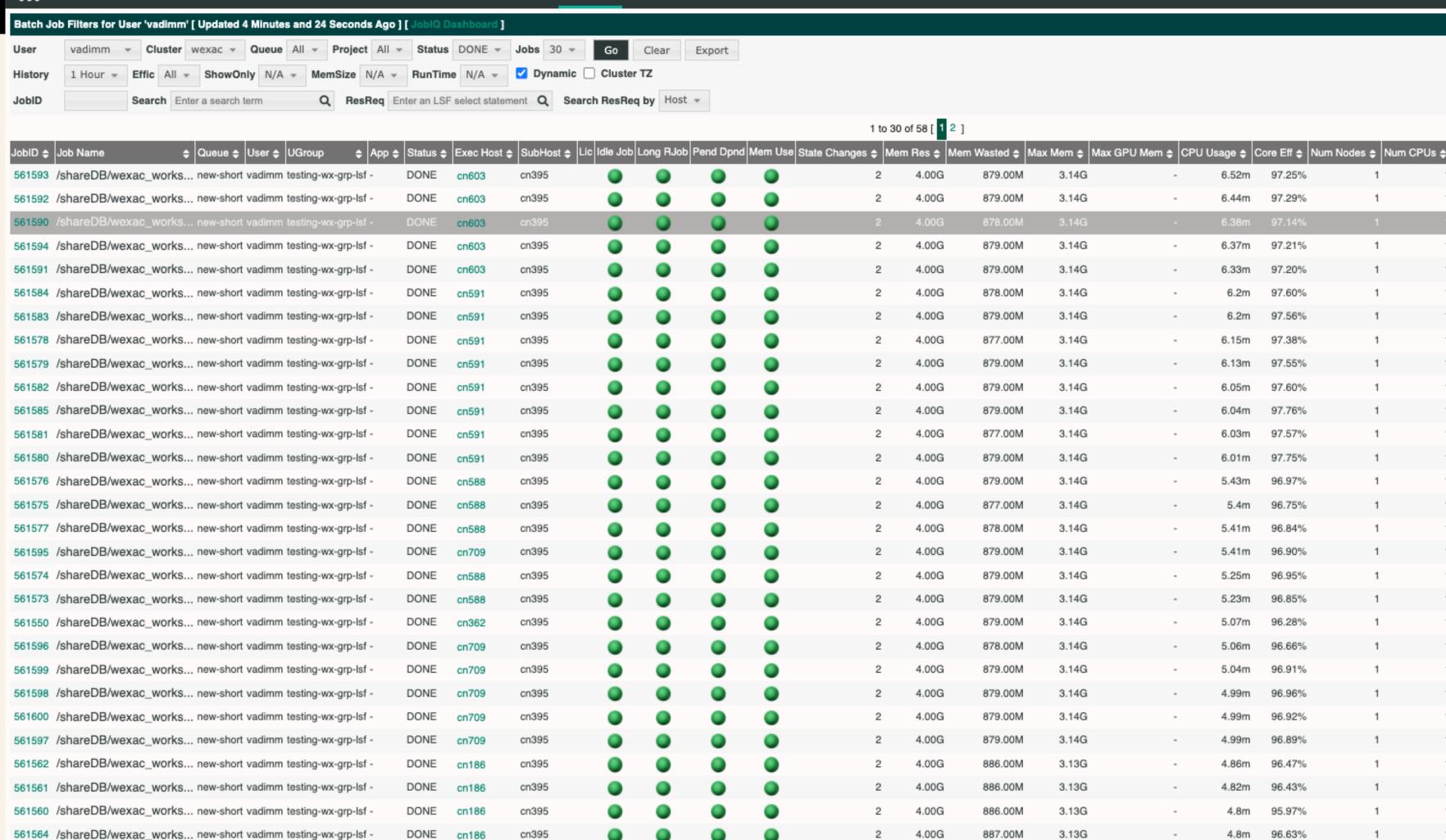












4.79m

96.51%

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מכון וי י

561563 /shareDB/wexac\_works... new-short vadimm testing-wx-grp-lsf

cn186

DONE

cn395

3.13G

886.00M

4.00G

1 to 30 of 58 [ 1 2 ]

2

Batch Job 561592 for User All Users [ Jo	blQ Dashboard ] [ JoblQ Jobs ]					
Job Detail Job Graphs Host Graphs	License Usage					
General Information						
Job ID	561592		Status	DONE		1
Job Name	/shareDB/wexac_workshop/Bowtie/bowtie2-2.0.5_x86/bowtie2 -x /shareDB/wexac_workshop/Bowtie/H_sapiens_build36_1/b					
Project	default		License Project			
Queue	new-short		Cluster Name	wexac		
User	vadimm		User Group	testing-wx-grp-lsf		
Charged SAAP	/vadimm					
Mail User			Job Priority	50		
Submission Details						
Submit Time	2023-07-16 09:17:06		Number of CPUs	1		
Submit Host	cn395					
Asked Hosts/Groups	-		Runtime Estimate	-		
Combined ResReq	select[(type = any ) && (type == any)] order[-slots:	maxslots:-mem] rusage[mem=4096.00] affinity[thr	ead(1)*1]			
Submit Command	/shareDB/wexac_workshop/Bowtie/bowtie/bowtie2 1-outbr.sam	-2.0.5_x86/bowtie2 -x /shareDB/wexac_workshop/	Bowtie/H_sapiens_build36_1/build36.1end-to-en	ndsensitive -U /shareDB/wexac_workshop/Bow	tie/Exp1/Inputbr -S /sha	
Submit Directory	/shareDB/wexac_workshop/Bowtie					
Resource Requirements	rusage[mem=4096]					
Output File	/shareDB/wexac_workshop/Bowtie/jobs/out.%J					
Error File	/shareDB/wexac_workshop/Bowtie/jobs/err.%J					
Execution Environment						
Exec Host	cn603					
Start Time	2023-07-16 09:17:07					
Username	vadimm		UID String	25003		
User Home	/home/labs/testing/vadimm		Working Dir	/shareDB/wexac_workshop/Bowtie		
Max Processors	1		Max Allocated Slots	1		
CPU Limit			Run Time Limit	1 Days		
Memory Limit	4.000G		Swap Limit	-		
Effective ResReq	select[((type = any ) && (type == any))] order[-slots	:-maxslots:-mem] rusage[mem=4096.00] affinity[th	nread(1)*1]			
Current/Last Status						
PGIDS	10755					
PIDS	10755, 10783, 10796, 10803					
Threads	5					
Pend Time	1 Seconds	PROV Time		Run Time	6.62 Minutes	
Effective Pending Time Limit	-					
PSUSP Time	-	USUSP Time	•	SSUSP Time	-	
Unknown Time	-					
Cumulative CPU	6.44 Minutes	System Time	•	User Time	6.43 Minutes	233333344544
Cur Memory Used	3.142G	Max Memory Used	3.142G	Job Efficiency	97.29%	RIS
Cur V.Memory Size		Max V.Memory Size				
Exit Code	0	End Time	2023-07-16 09:23:44			



#### **Submission Form: test**



Memory reservation is (MB): 3080Memory Limit is (MB): 3080 Amount of tasks (-n X) reserved: 2 === Your total amount of memory reservation for this job is (MB): 6160 === Job <562127> is submitted to queue <new-short>.

Form Name: test ▼

1. Basic Job Options \*

Advanced

4. Notification

Data

5. Review

#### **Basic Job Options**

Command to run \*:

/shareDB/wexac\_workshop/WEXAC\_FOR\_BEGINNERS/Bowtie/Bowtie/benchm\_bbw\tiensen:

Bowtie July 25 - test2

3080 MB

No

#### Advanced

Number of processors :

Allocate processors on

2

single host:

Yes

Hour:

Memory:

30 Minutes:

Project: bowtie5 Submit to this Queue: new-short

0

This job is rerunnable:

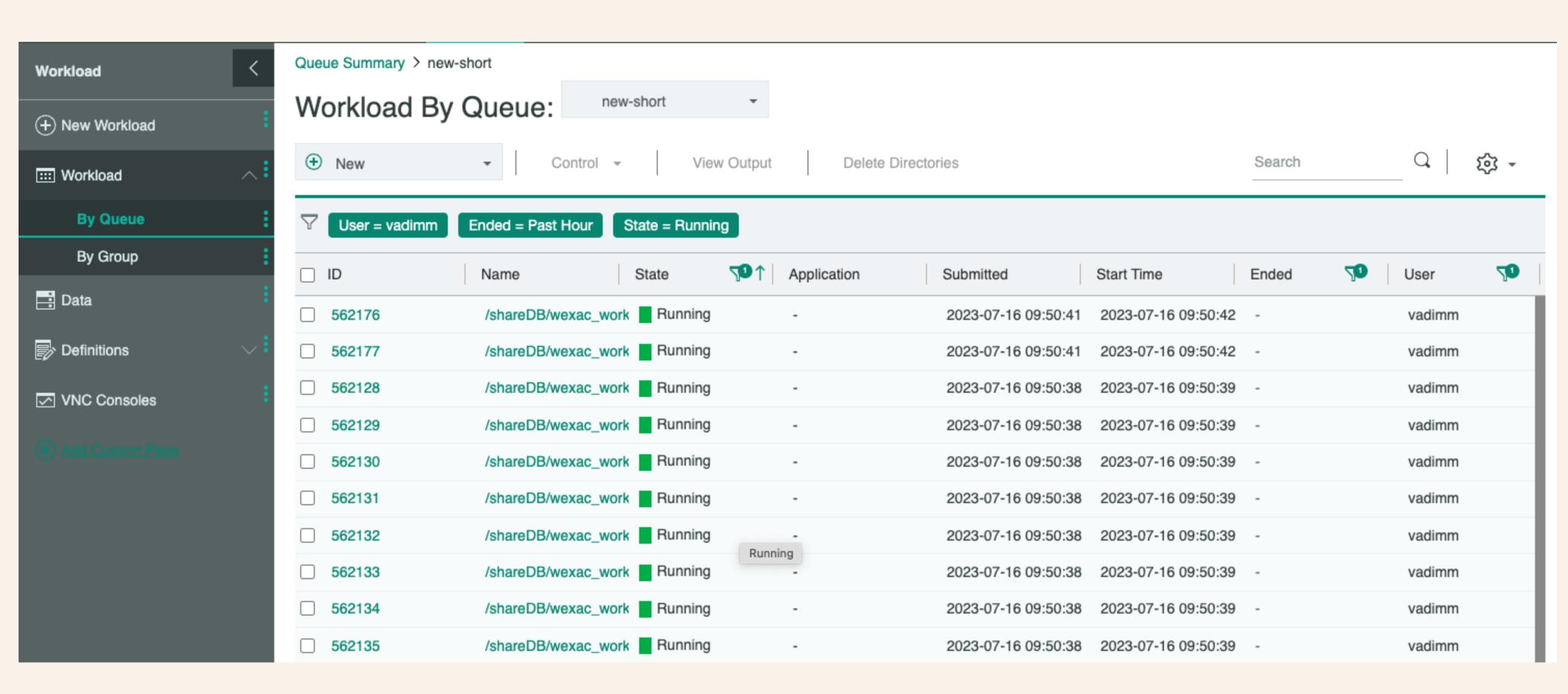
#### Notification



- When workload starts
- When workload ends
- If workload exits
- If workload is suspended

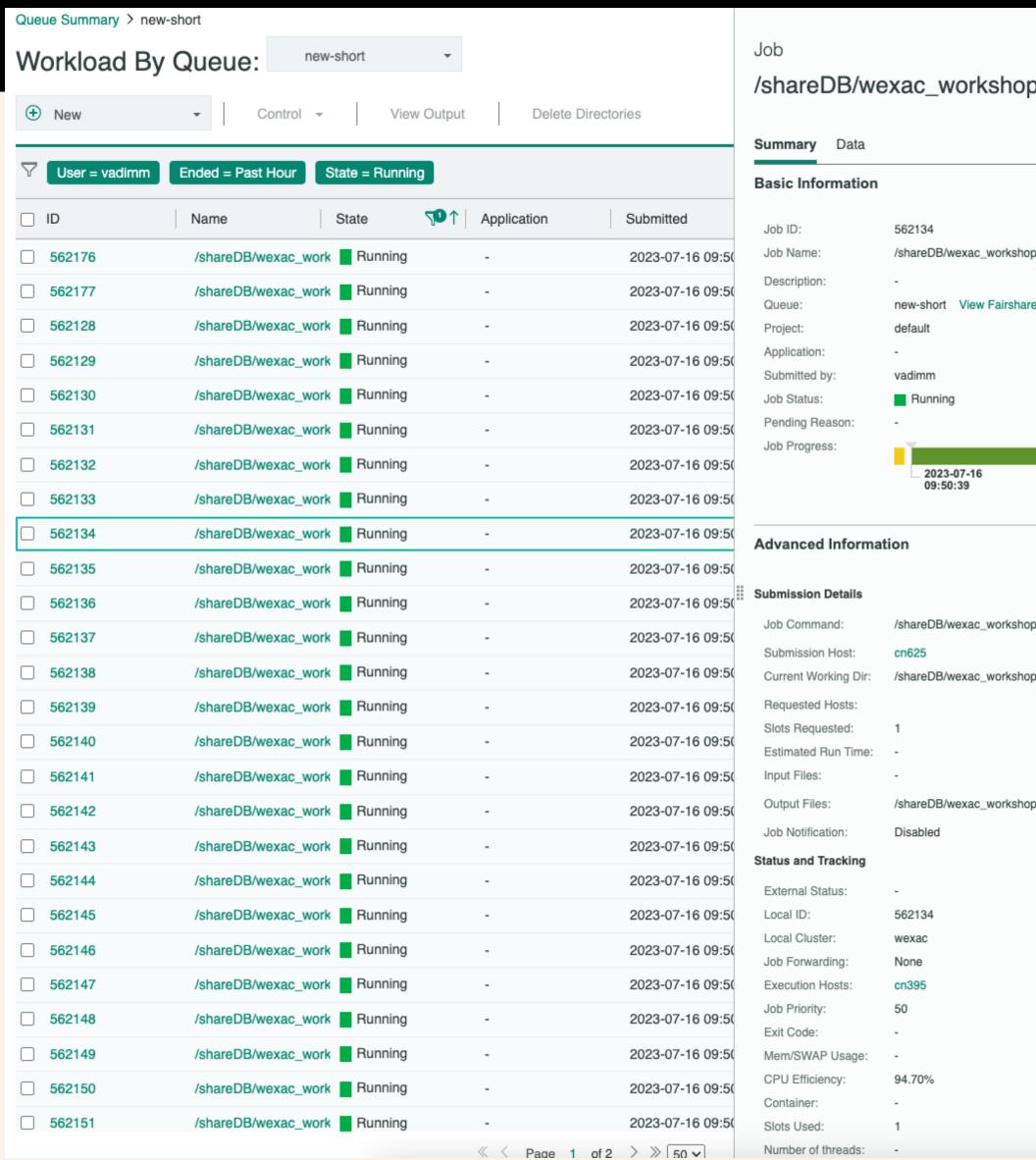
Notify via:











/shareDB/wexac\_workshop/Bo...

X

/shareDB/wexac\_workshop/Bowtie...

new-short View Fairshare Information

2023-07-16 09:53:30

/shareDB/wexac\_workshop/Bowtie...

/shareDB/wexac\_workshop/Bowtie

/shareDB/wexac\_workshop/Bowtie...





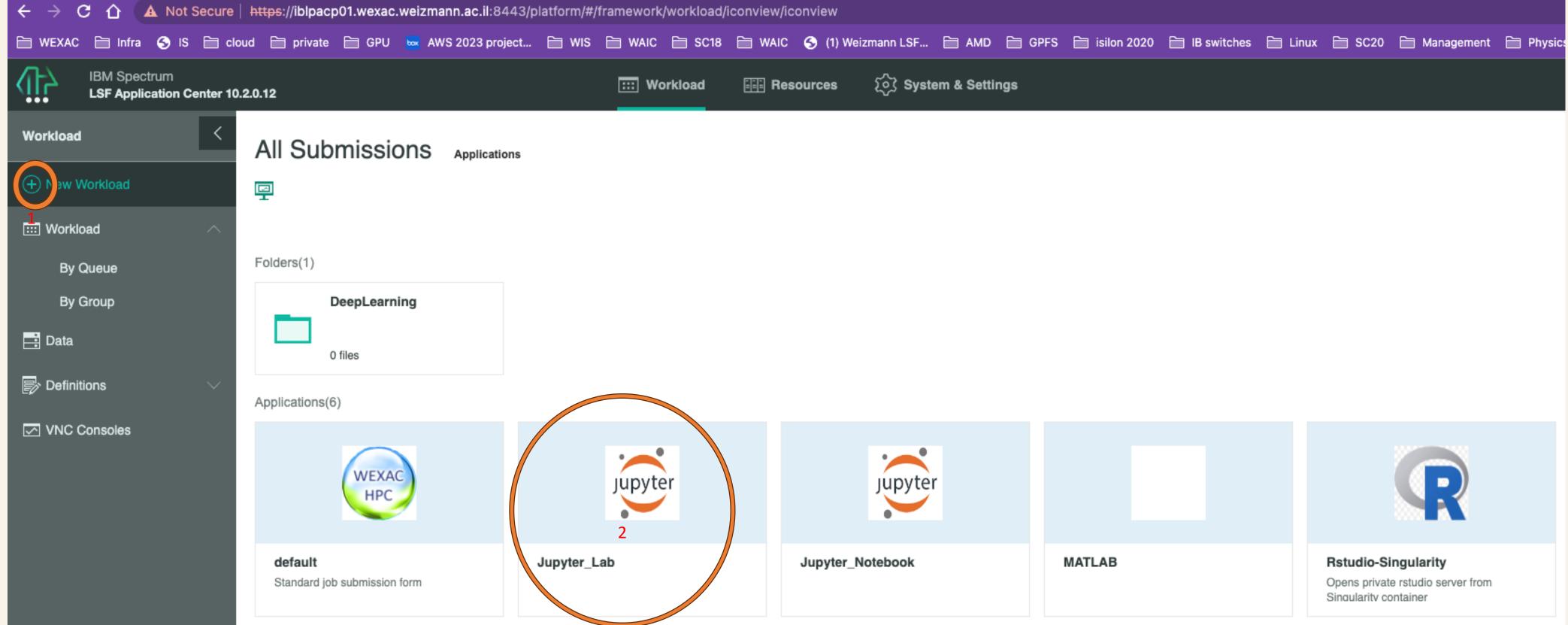


#### LSF PAC - Platform Application Center

```
[vadimm@access output]$ ls -la
total 20930720
drwxrwxrwx 2 root
                                        8192 Jul 16 09:17
                    root
                                       16384 Jun 13 11:29
drwxrwxrwx 7 root
                    root
-rw-r--r-- 1 vadimm testing-wx-grp 759274937 Jul 16 09:23 Exp1-outbe.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759495212 Jul 16 09:23 Exp1-outbf.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759293416 Jul 16 09:23 Exp1-outbg.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759344489 Jul 16 09:23 Exp1-outbh.sam
-rw-r--r-- 1 vadimm testing-wx-grp 760894038 Jul 16 09:23 Exp1-outbi.sam
-rw-r--r-- 1 vadimm testing-wx-grp 760653451 Jul 16 09:23 Exp1-outbj.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759836464 Jul 16 09:23 Exp1-outbk.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759183533 Jul 16 09:21 Exp1-outbl.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759169655 Jul 16 09:21 Exp1-outbm.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759138626 Jul 16 09:21 Exp1-outbn.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759582466 Jul 16 09:22 Exp1-outbo.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759170838 Jul 16 09:23 Exp1-outbp.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759237494 Jul 16 09:23 Exp1-outbq.sam
-rw-r--r-- 1 vadimm testing-wx-grp 760350597 Jul 16 09:23 Exp1-outbr.sam
-rw-r--r-- 1 vadimm testing-wx-grp 761008311 Jul 16 09:23 Exp1-outbs.sam
-rw-r--r-- 1 vadimm testing-wx-grp 760287262 Jul 16 09:23 Exp1-outbt.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759705155 Jul 16 09:22 Exp1-outbu.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759567102 Jul 16 09:22 Exp1-outbv.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759252744 Jul 16 09:22 Exp1-outbw.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759232941 Jul 16 09:22 Exp1-outbx.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759656301 Jul 16 09:22 Exp1-outby.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759269421 Jul 16 09:22 Exp1-outbz.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759701559 Jul 16 09:21 Exp1-outca.sam
-rw-r--r-- 1 vadimm testing-wx-grp 761172986 Jul 16 09:21 Exp1-outcb.sam
-rw-r--r-- 1 vadimm testing-wx-grp 760700650 Jul 16 09:21 Exp1-outcc.sam
-rw-r--r-- 1 vadimm testing-wx-grp 759748746 Jul 16 09:21 Exp1-outcd.sam
-rw-r--r-- 1 vadimm testing-wx-grp 186778087 Jul 16 09:18 Exp1-outce.sam
```



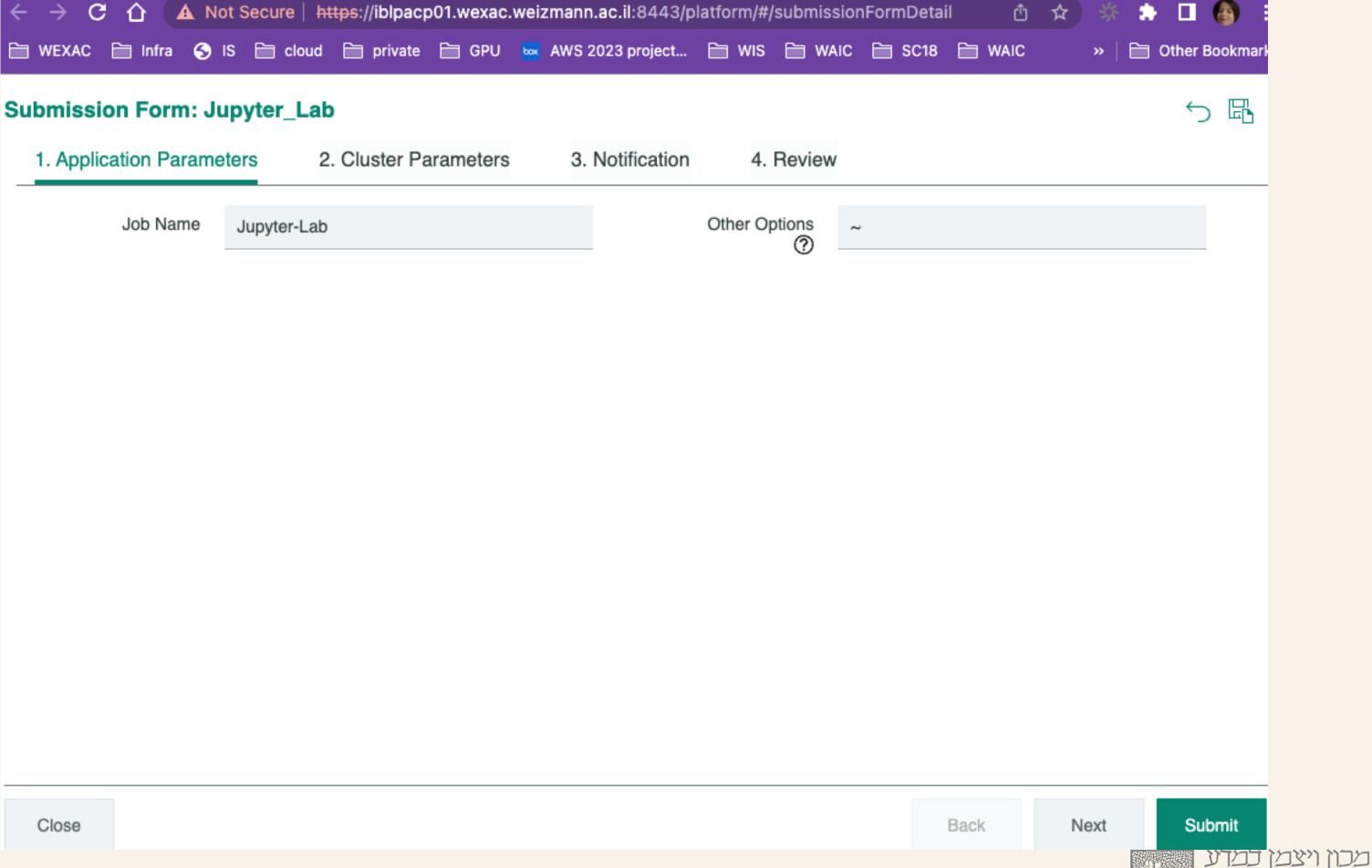








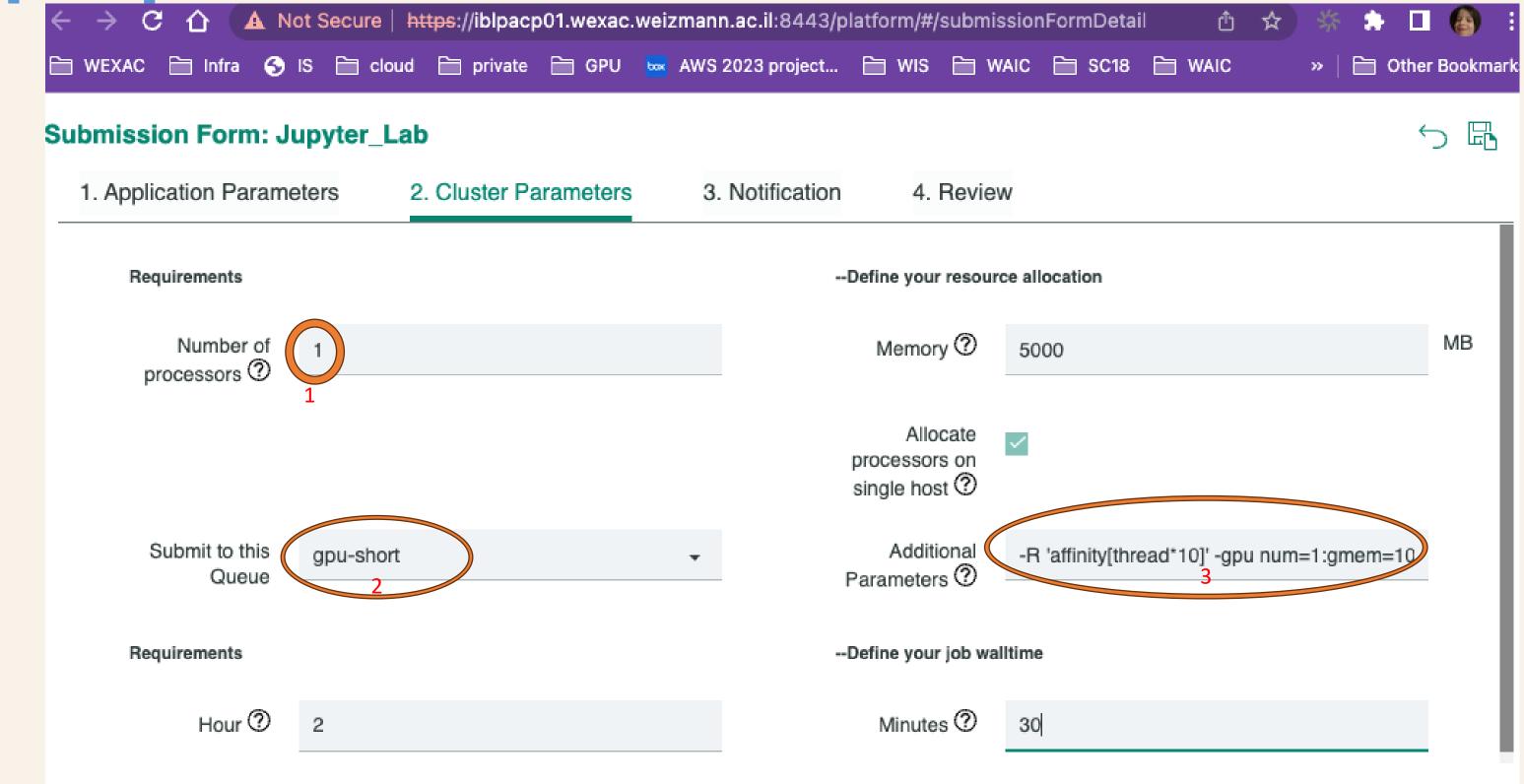
https://iblpacp01.wexac.weizmann.ac.il:8443/



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https://iblpacp01.wexac.weizmann.ac.il:8443/

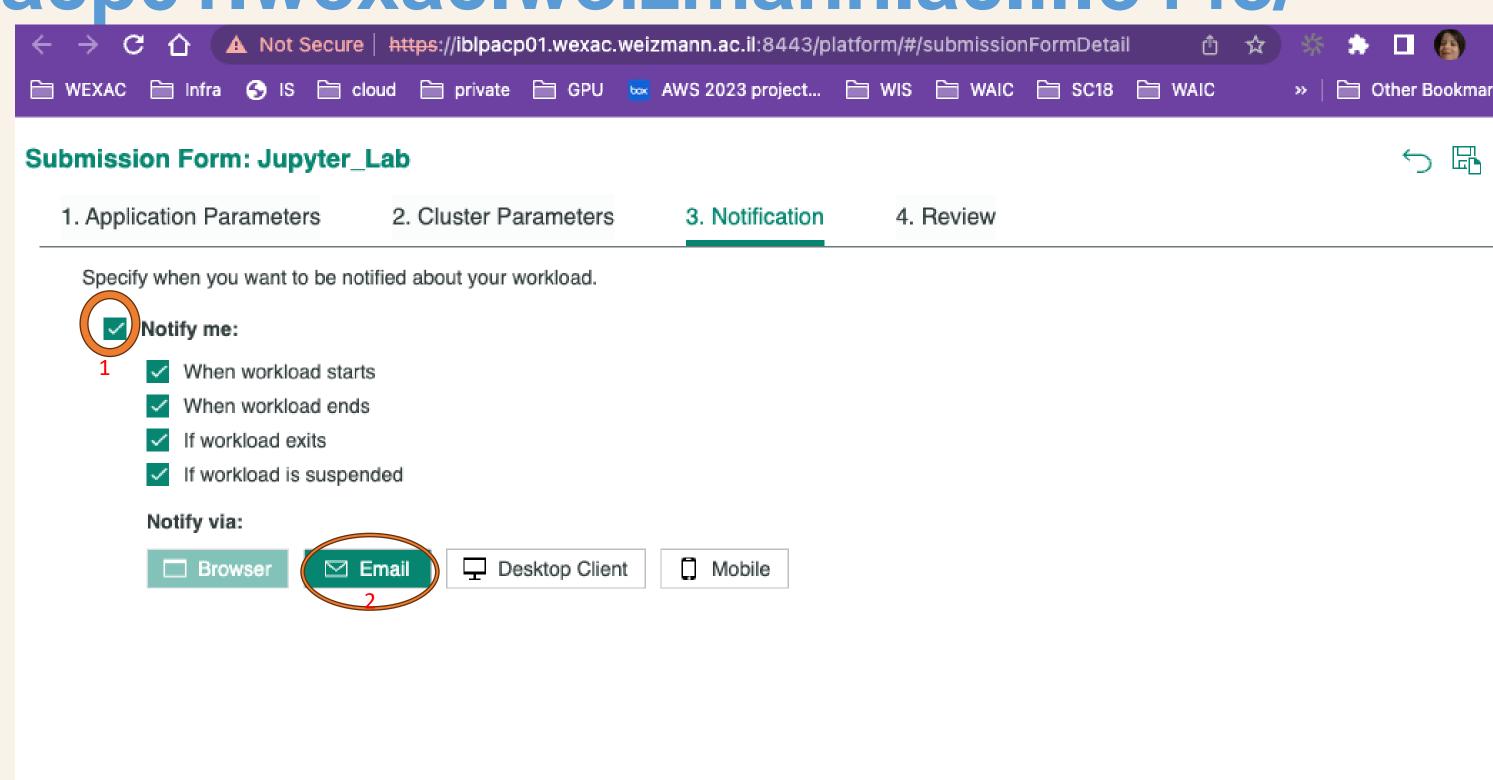




Back

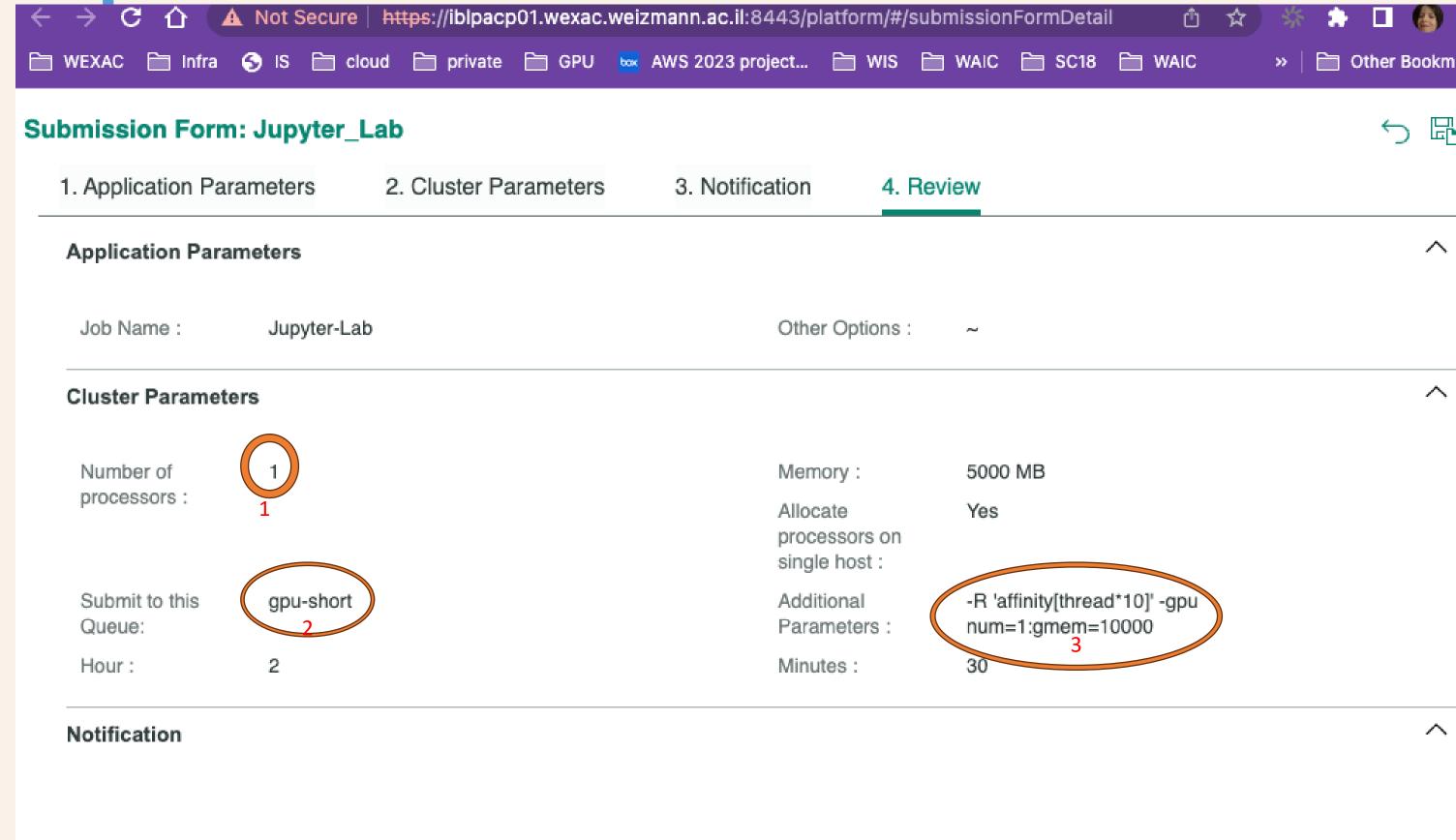
Next

Submit





https://iblpacp01.wexac.weizmann.ac.il:8443/





Submit

Close

## https://iblpacp01.wexac.weizmann.ac.il:8443/

Submission Form: Jupyter\_Lab







Please note that memory reconstion is per task (-n X)Memory reservation is (MB): 5000 Amount of tasks (-n X) reserved: 1 === Your total amount of memory reservation for this X job is (MB): 5000 === (Job <671710>) is submitted to queue <gpu-short>.

- 1. Application Parameters
- 2. Cluster Parameters
- Notification
- 4. Review

#### **Application Parameters**

Job Name:

Jupyter-Lab

gpu-short

Other Options : ~

#### **Cluster Parameters**

Number of

processors:

1

2

Memory :

Allocate

Yes

5000 MB

processors on single host :

Submit to this Queue:

Additional Parameters : -R 'affinity[thread\*10]' -gpu num=1:gmem=10000

Hour:

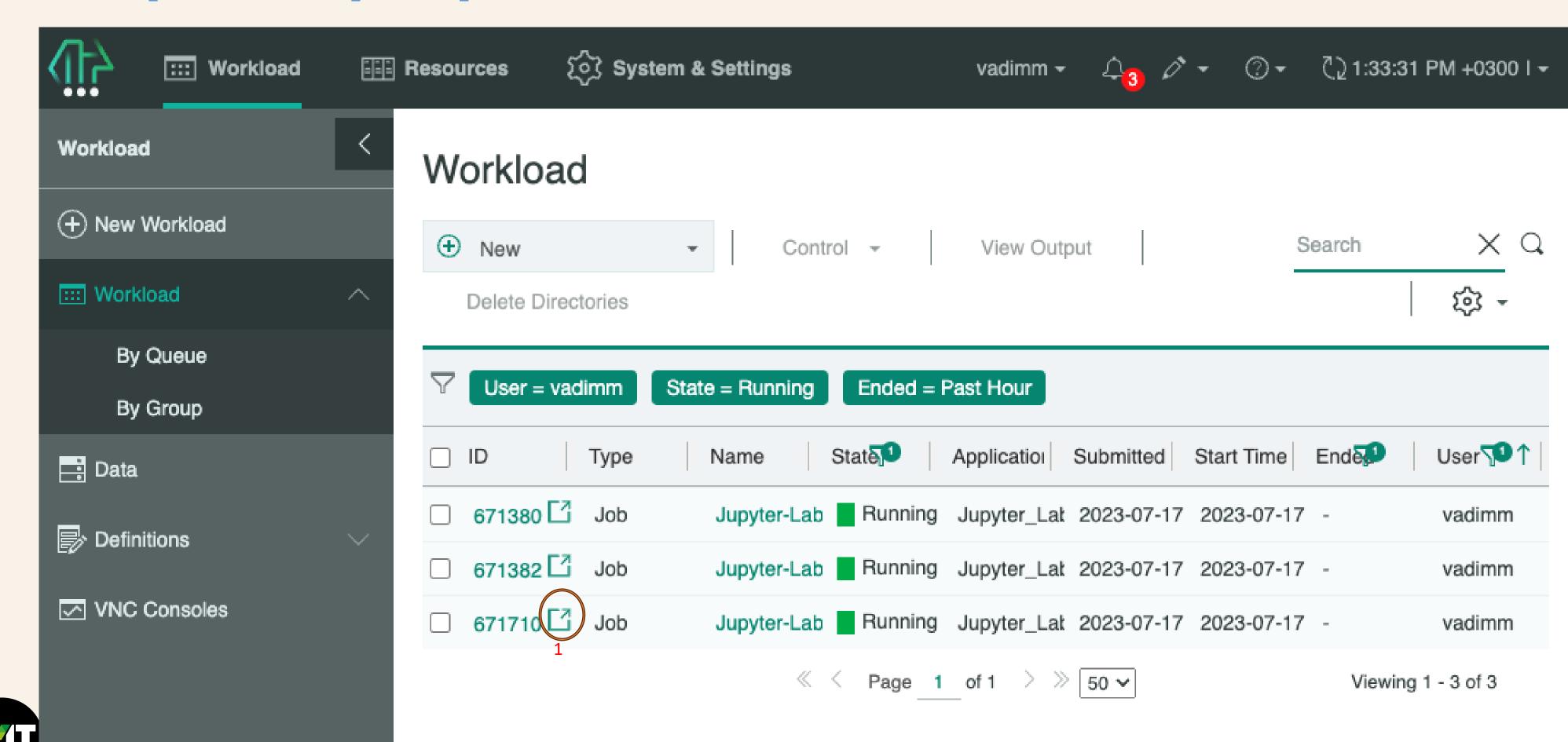
Minutes:

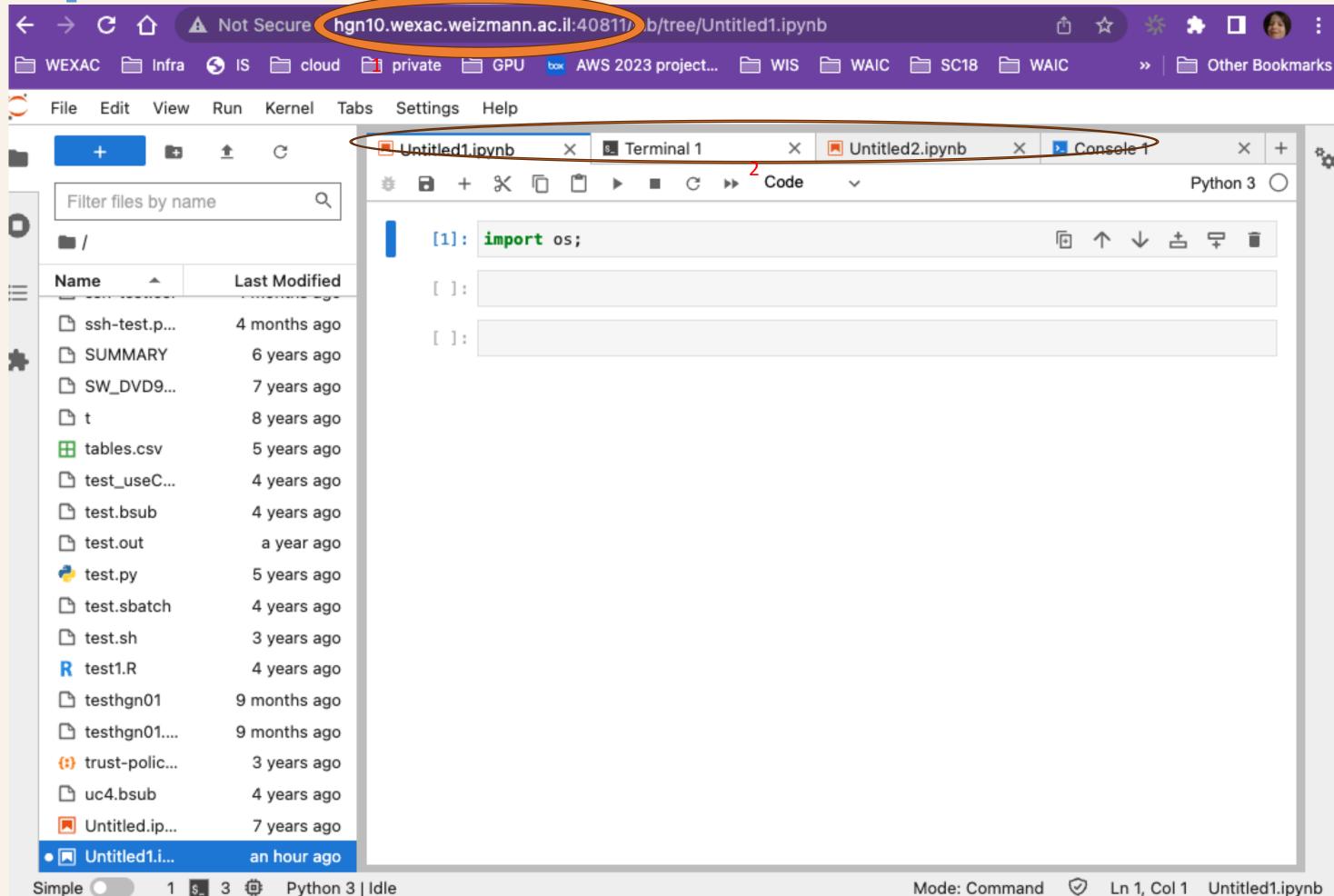
30

#### Notification

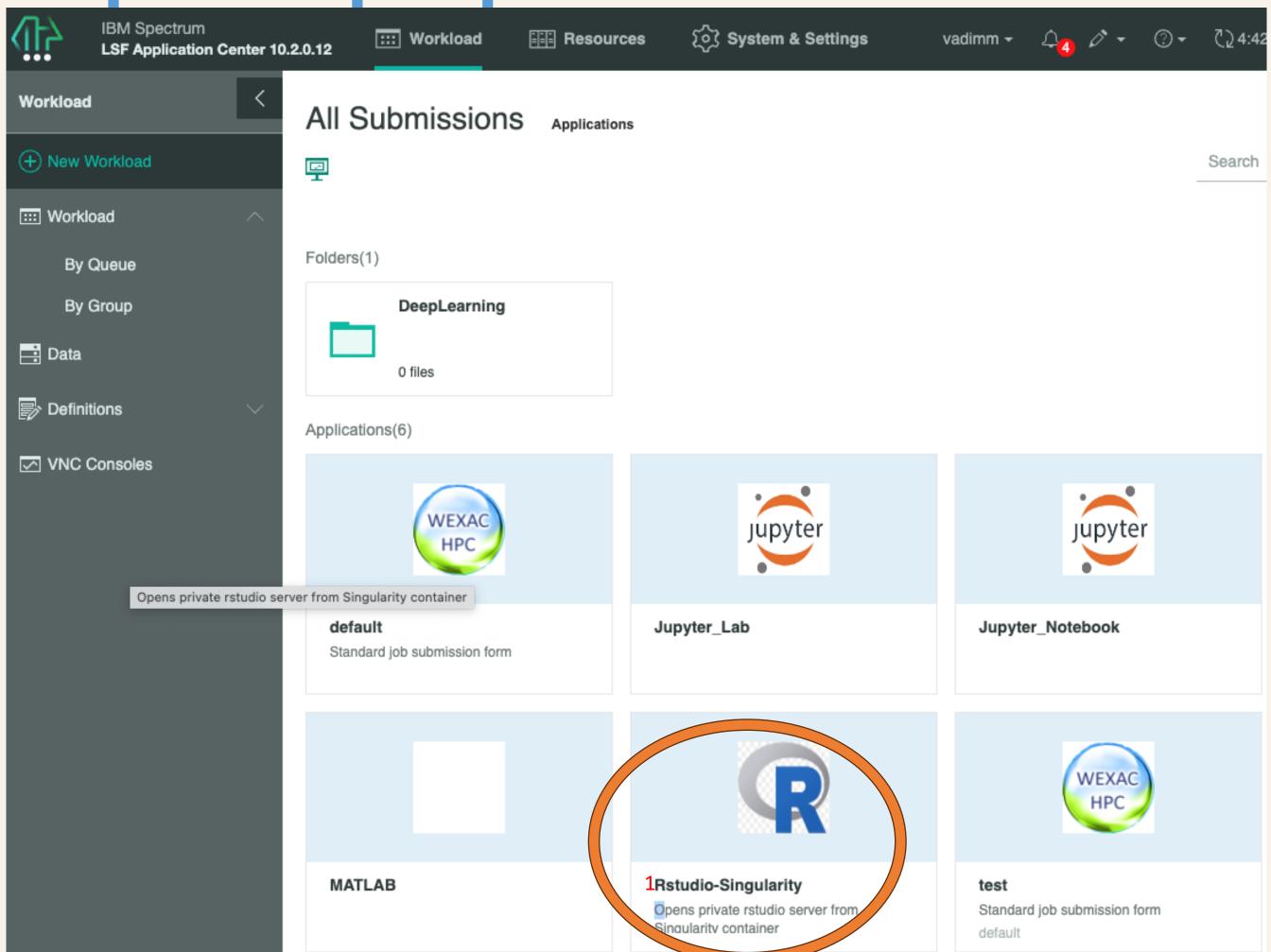


 $\wedge$ 



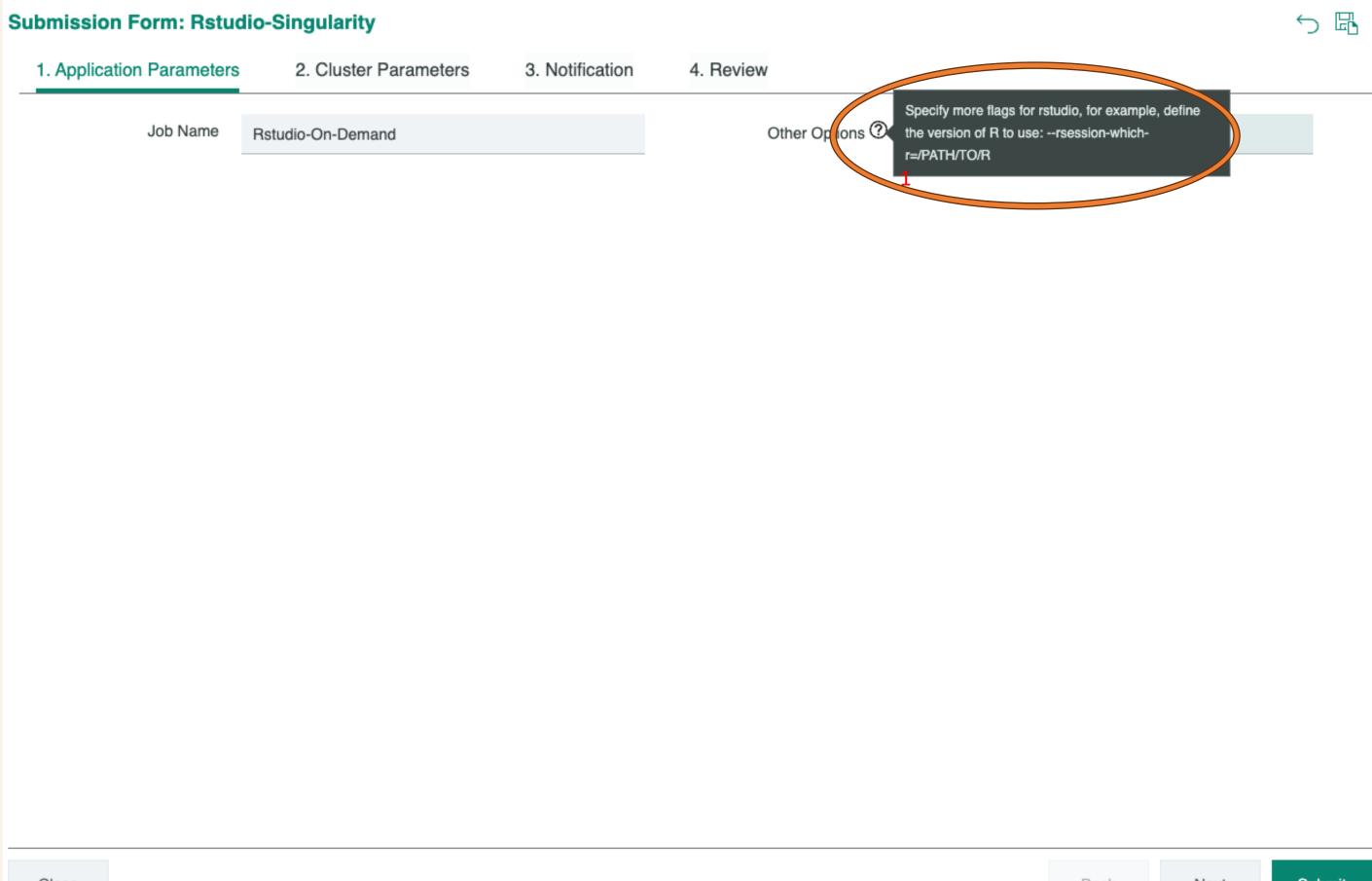






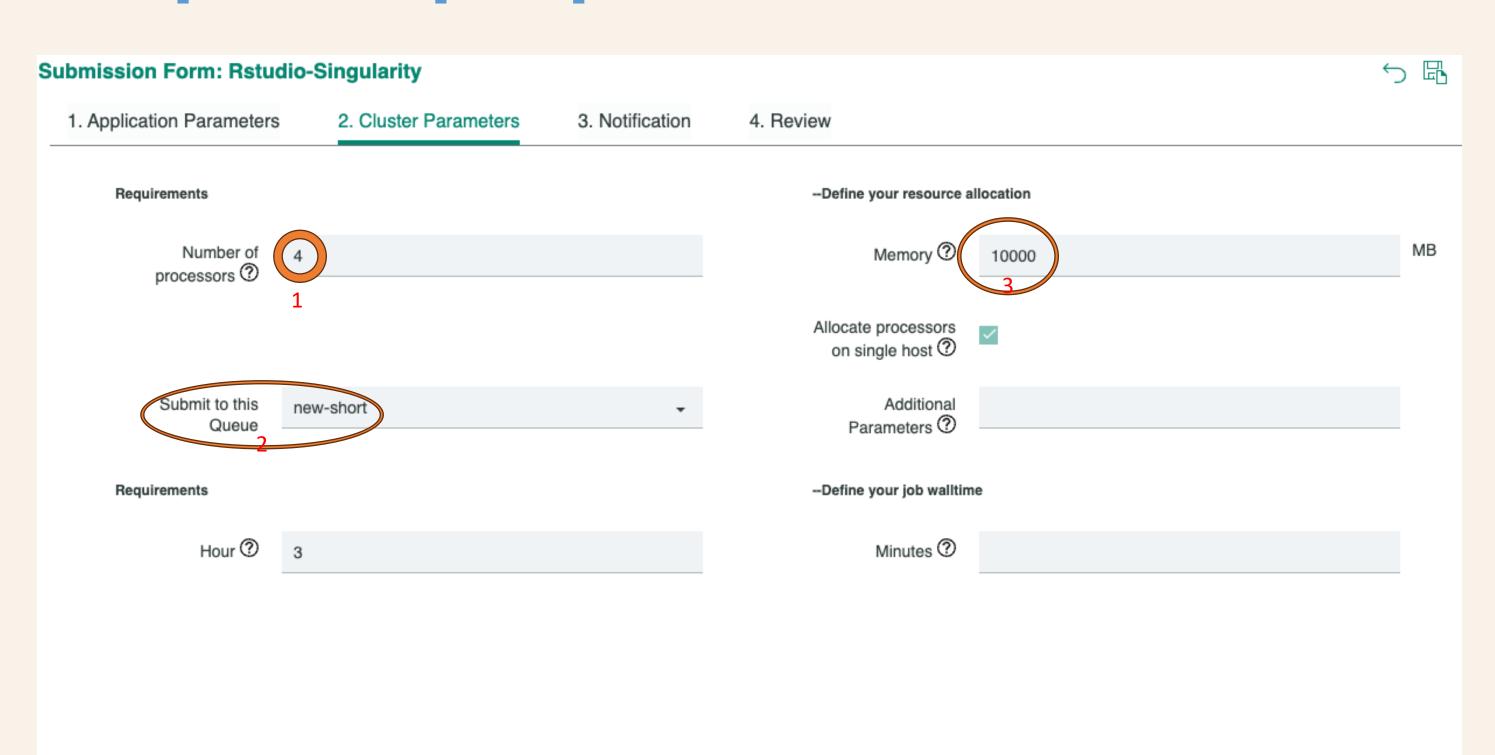








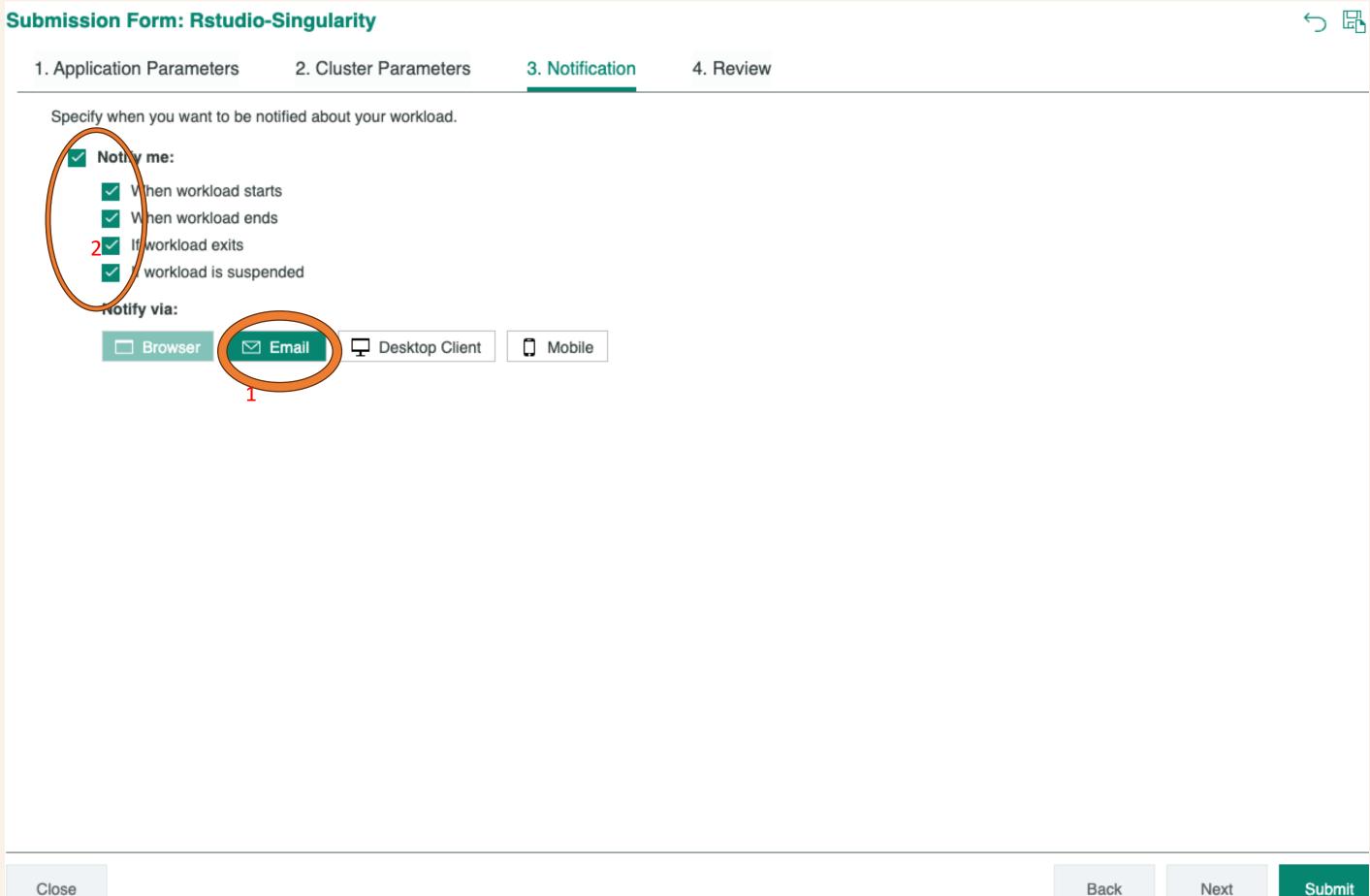
#### https://iblpacp01.wexac.weizmann.ac.il:8443/



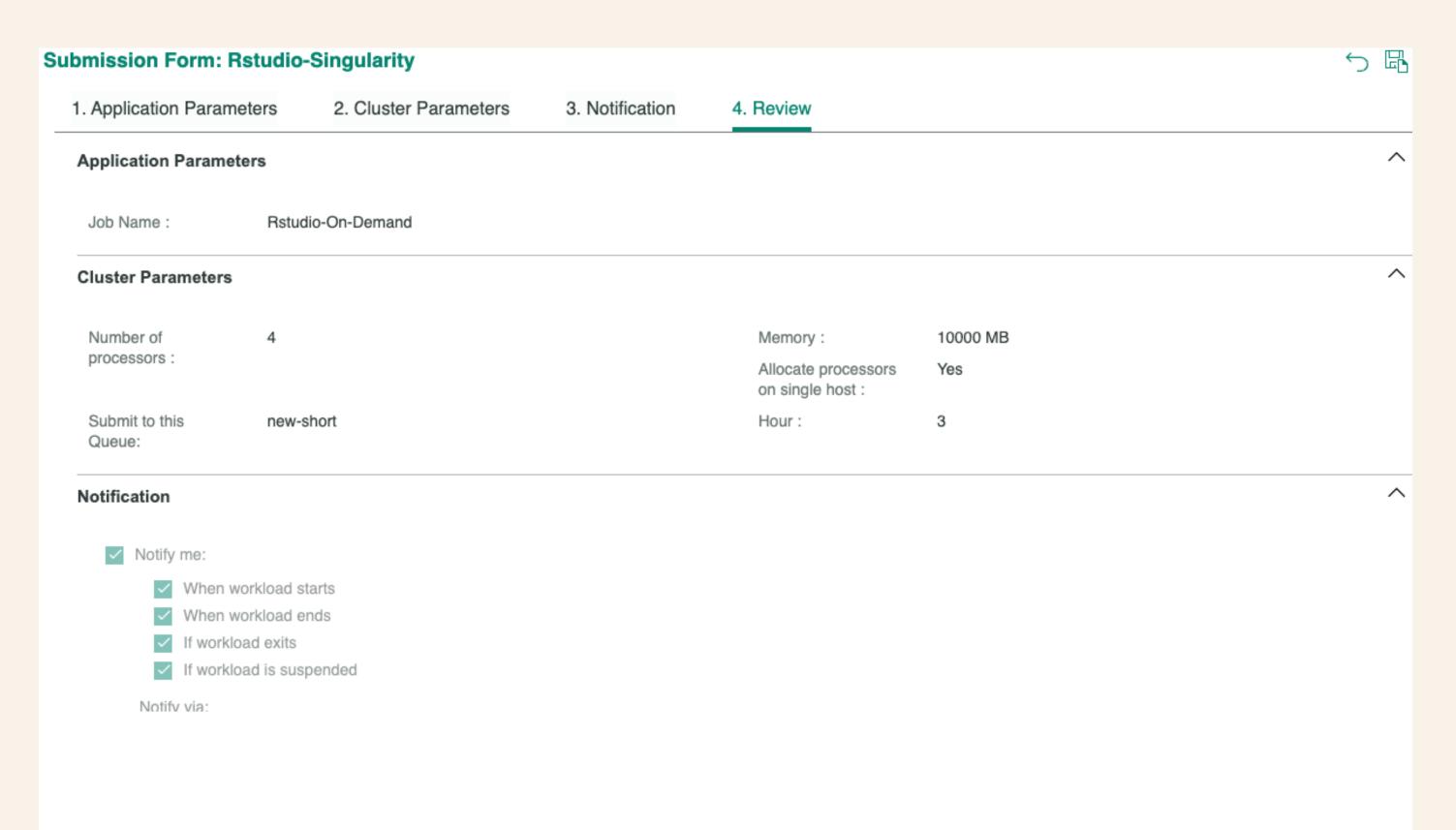




Next

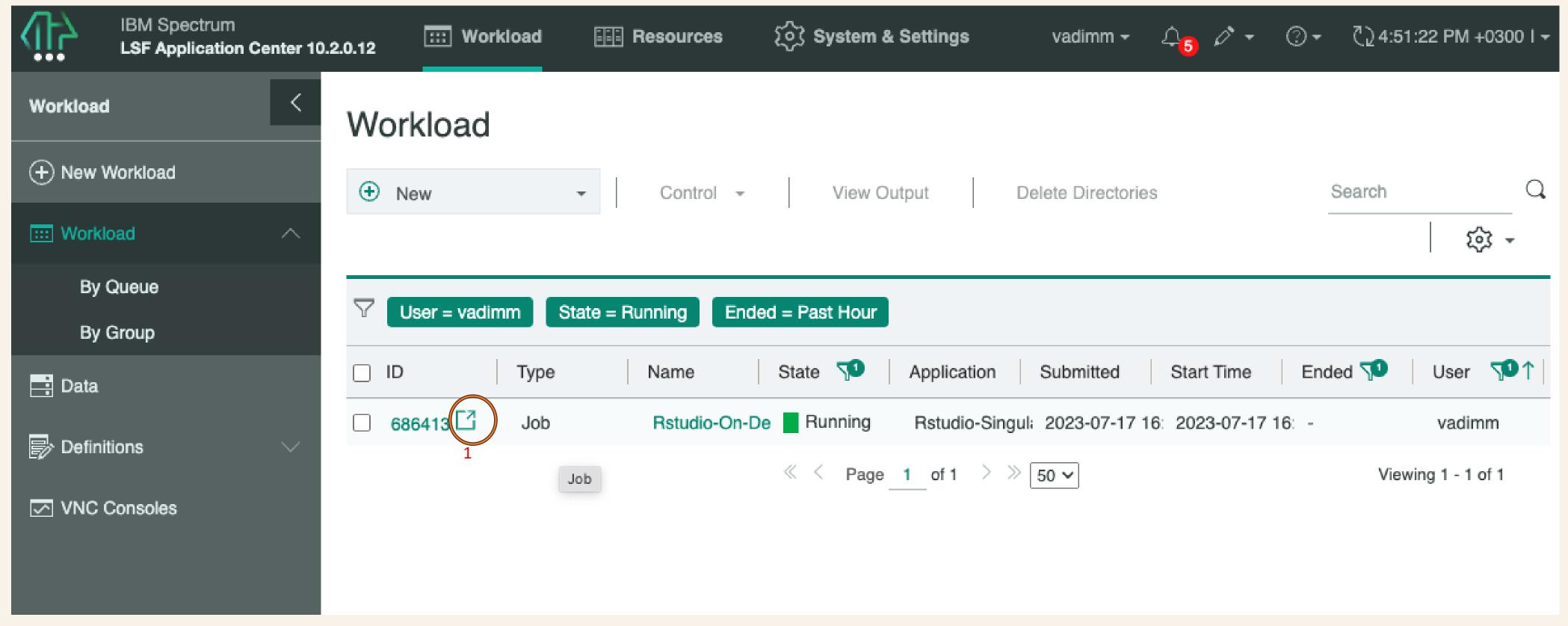
















#### Example of Rstudio application

This will open the RSTUDIO login page. Use your username and TEMPORARY PASSWORD received in the rstudio.log file.



To open rstudio.log file you can press the JOBID and then choose the rstudio.log file and press OPEN:

D - 4 1	:- O- D	E 4004	\	
rstud	io-On-Demand (4	54021	_ائا (	Actions +
Summary	Data			
	_			
Directory:	Remote Job Directory(access4)	*		
Location:	/home/labs/testing/igorc/.pac/igorc			
	-Demand_1656406124778ujllG			
Tail	Open	Search		C
11441	Оран			
Downl	oad			
More	Actions +			
Oper	n with applications =			
	lame			File Size
File N				4 1479
	studio.log			1 KB
✓ □ n	studio.log utput.igorc.txt			3 KB
✓ □ n				
✓ □ n	utput.igorc.txt	«	Page	3 KB
✓ □ n	utput.igorc.txt	«	< Page	3 KB





#### Example of Rstudio application - Summary

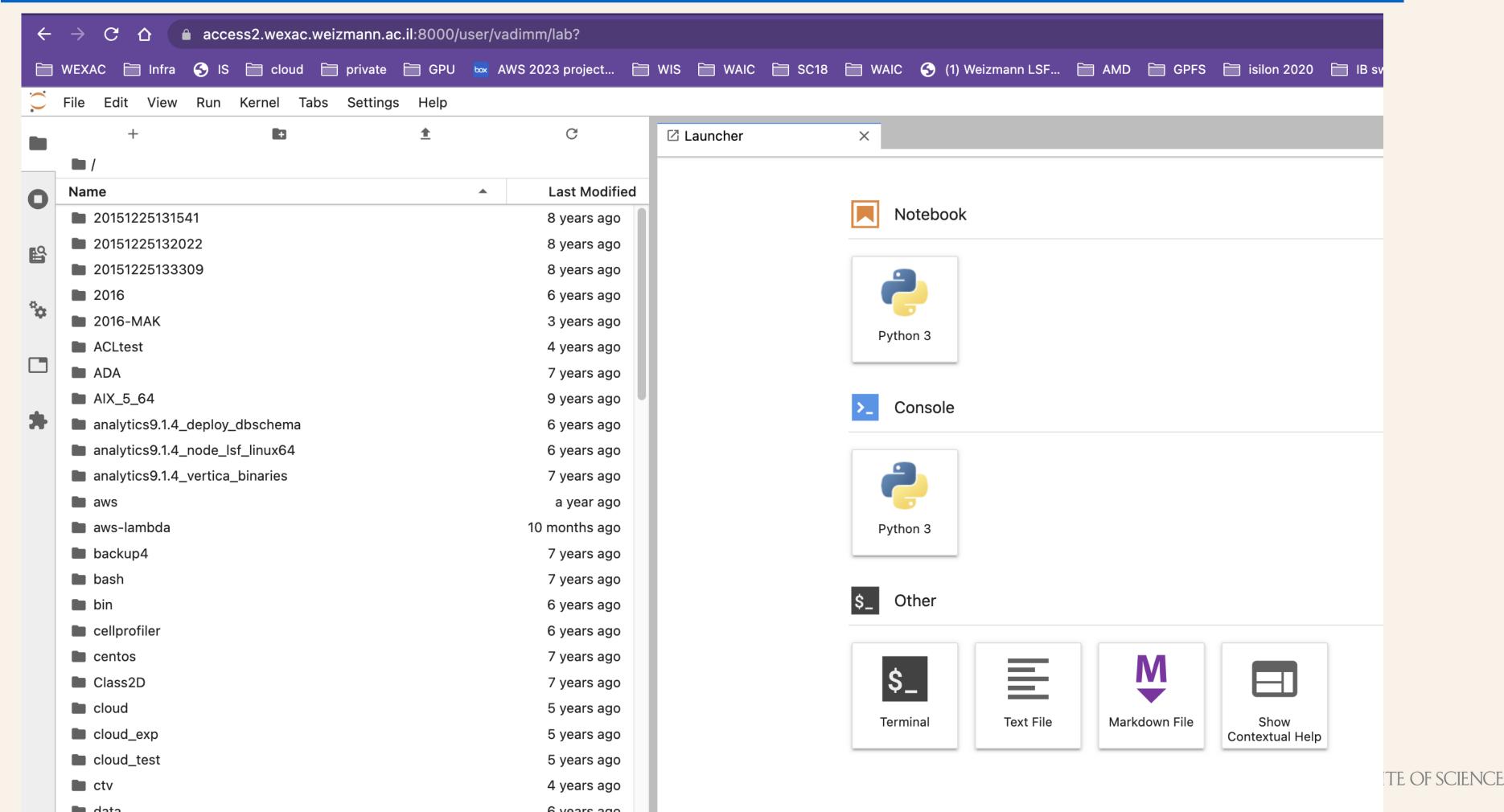
- Visit the LSF PAC web interface: <a href="https://iblpacp01.wexac.weizmann.ac.il:8443/">https://iblpacp01.wexac.weizmann.ac.il:8443/</a>
- Login with your wexac username and password.
- On the RESOURCE TAB you may overview cluster statistics such as amount of available and closed nodes.
- In order to run an interactive job, navigate to WORKLOAD tab.
- On the NEW WORKLOAD page, you can execute available applications.
- On the WORKLOAD page you may overview details of your jobs.





#### WEXAC Jupyterhub

#### https://access2.wexac.weizmann.ac.il:8000/hub/login





WEXAC members have private access nodes.

WEXAC members have private compute nodes.

WEXAC members uses only their own private hosts in private queues.

WEXAC guests and members use both public and private resources.







A lot of guest's jobs preempted due to high priority members starting in the middle of guest's jobs.

Significant overhead in management and maintenance of >20 private access servers.

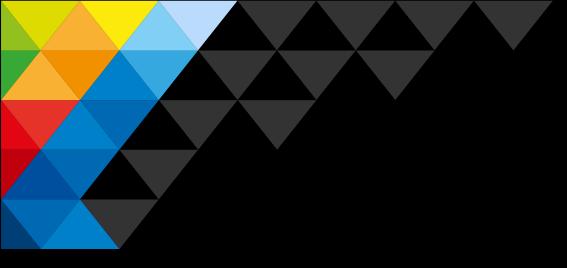
Silos of compute power: >20 different hardware configurations use different WEXAC members queues.

Couldn't tackle the low cluster utilization due to straight connection between private queues and specific HW configuration.

No overprovisioning option







## Current hosts groups Design

#### Multiple heterogeneous hosts groups

Tirosh\_hosts = tirosh queues

Schwartz\_hosts = schwartz queues

Bio\_hosts = bio queues

Kushnir\_hosts = kushnir queues

hpc@weizmann.ac.il





# GSLA Queue Conceptual Design

Single homogeneous host group

Single GSLA hosts group
Will serve Schwartz, bio, Tirosh
and kushnir queues

hpc@weizmann.ac.il





### The goals:

Replace private compute servers with GSLA hardware pool.

Reduce amount of cluster queues.

Reduce preemption percentage of WEXAC guests and members.

Introduce overprovisioning option.





## How we plan to achieve these goals (Phase I):

In phase 1 we'll introduce shared GSLA hardware pool.

2 new GSLA queues deployment replacing existing member queues.

Low priority GSLA queue will be deployed for member risk and all public users. Deploy policy of low slot guarantee per user. 2 nopreemption duration GSLA risk queues: gsla-risk-short and gsla-risk-long, 4 hours and 7 days respectfully, based on fair share policy.

High priority GSLA queue for members only will be deployed. 30% oversubscription of selected GSLA resources.

Each group will have his own maximum slot allocation in shared GSLA pool







#### Phase I benefits:

Reduce public workloads preemption percentage.

Increase hardware utilization by unification of cluster hardware.

Old members servers' hardware refresh.



### Example of HPC available resources

	Resource type	Billing type	Minimum allocation	Price (NIS) Given 5 years lifecycle
1	Interactive CPU physical server 52 cores, 256 GB RAM	Reserved	1 day	17.71
2	CPU cores – single CPU core 2 GHz frequency *, 4GB RAM	Reserved	1 day	0.34
3	GPU cards – single A40, 12 cores, 80 GB RAM	Reserved	1 day	16.05
4	Interactive GPU server	Reserved	1 day	160.47

<sup>\*</sup> We commit to 2 GHz frequency, but CPU might belong to different generations







#### Storage available resources and costs

	Resource type	Billing type	Minimum allocation	Monthly price Given 5 years lifecycle
1	GPFS storage	Actual usage	1 month*	60 NIS per 1TB**
2	StorWIS	Actual usage	1 month	10 NIS per 1TB**
3	Archive	Actual usage	1 month	15 NIS per 1TB

<sup>\* 1</sup> month equal system price divide by 60 months

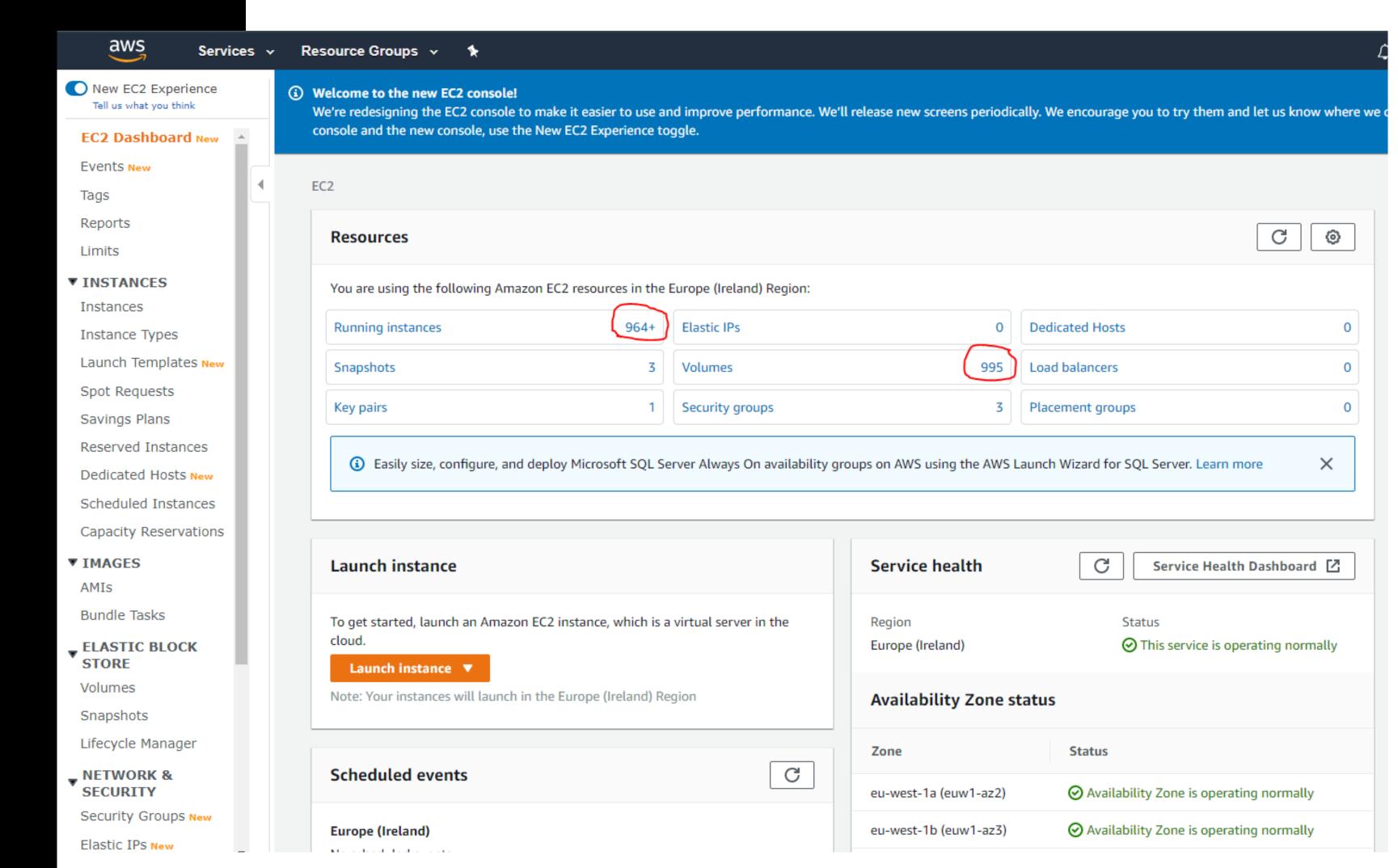






<sup>\*\*</sup> Backup charged separately

## WEXAC and AWS cloud integration



#### The AWS HPC Platform

The HPC (High Performance Computing) section's objective is to speed up your scientific work and make it more efficient. This includes making AWS (Amazon Web Services) resources easy for you to utilize for HPC workloads.

To that end, we have established a AWS service platform facilitating easy onboarding of scientists to the WIS network-integrated AWS resources.

#### Service benefits include:

- Easy registration through Internal Services
- Billing via internal WIS systems
- The ability to specify a monthly budget, to control AWS resources assigned to your account
- DevOps services deployment of your scientific solutions on the cloud



#### The AWS HPC Platform

AWS provides the most elastic and scalable cloud infrastructure for execution of your HPC applications. With virtually unlimited capacity, researchers and HPC system owners can innovate without being burdened by the limitations of on-premises HPC infrastructure.

- The platform delivers an integrated suite of services providing everything required to quickly and easily build and manage HPC clusters on the cloud.
- These workloads span traditional HPC applications, such as genomics, computational chemistry and weather prediction, as well as such emerging applications as machine learning/deep learning.
- Flexible configuration and practically unlimited scalability allow you to grow or scale back your infrastructure as per workload requirements, rather than the other way around.
- Additionally, WEXAC integration allows you to easily migrate data back and forth between WEXAC and AWS infrastructures.



#### WEXAC Web Resources

https://hpcwiki.weizmann.ac.il/

https://appsrv.wexac.weizmann.ac.il/

https://www.weizmann.ac.il/hpc

https://www.weizmann.ac.il/DIS/sites/DIS/files/uploads/it/wexac\_training\_session.pdf

https://insightiq.weizmann.ac.il

https://wiki.weizmann.ac.il/ai\_wiki/index.php/WAIC\_cluster

https://iblmonitor01.wexac.weizmann.ac.il:3001/d/kjsnPAF4k/gpu-usage-by-groups?orgId=2

Join the WEXAC WhatsApp group!

https://chat.whatsapp.com/05qVVCCcR8v9234vit28gc

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#### Questions?



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July 2023 WEXAC workshop

#### Thank you

