אגף מערכות מידע
DIVISION OF InformationSystems

מכון ויצמן למדע
WEIZMANN INSTITUTE OF SCIENCE

Information Technology
Infrastructure Branch

WAIC workshop

Presented by: Vadim Malkin

June 25, 2019

Agenda

- Brief Introduction
- Monitoring
- Accessing the System
- Submitting Jobs
- Introduction to Docker
- Use Cases
- Question

Back to the Future: From WEIZAC to WEXAC

USERS TRAINING

hpc@weizmann.ac.il

Current WEXAC Status

- Computing power : more than 300 servers , above 7000 cores – the biggest Weizmann Institute of Science campus cluster
- Storage capacity : 2 PByte total capacity, about 1 PByte in use
  - 1.6 Pbyte of additional storage for StorWIS, about 0.9 PByte in use
- Modules : more than 600 scientific applications with different versions installed in WEXAC.
- Nvidia NGC repository integration.
- Containerized ready environment

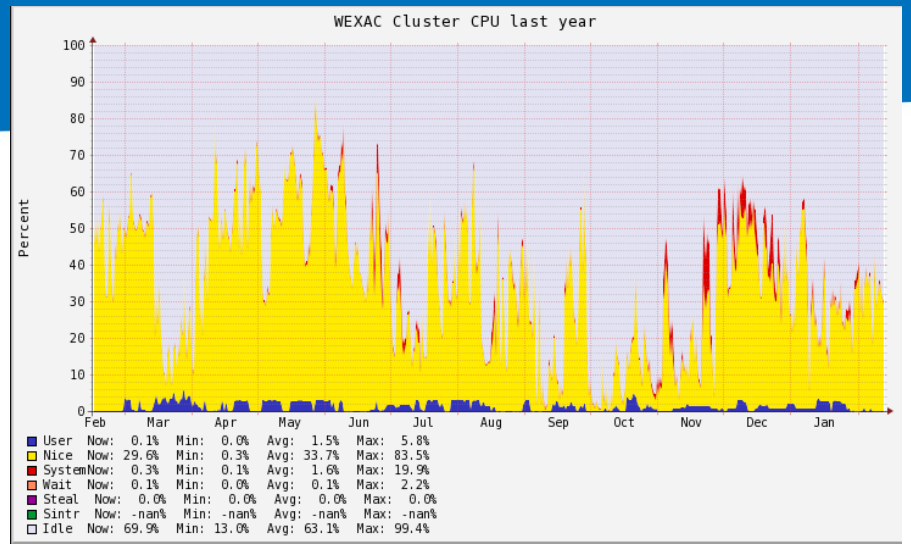
Best practices to compile serial and parallel applications.

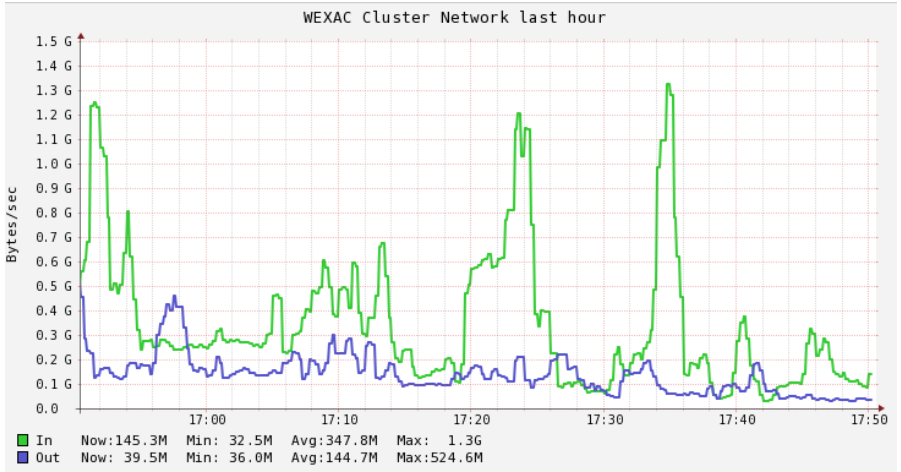
- Use Latest Compilers and frameworks
- Use the relevant servers for compilation
- Use a fast interconnect (Infiniband)
- In parallel application cases use a MPI library with good collectiveness (MVAPICH2 or Intel MPI)
- Don’t re-invent the wheel – use optimized libraries , like NetCDF , HDF5 , Intel MKL, Nvidia NGC
- Use a last FFT library (FFTW or Intel FFTW wrappers)
- Use productivity tools like DDT , mpiP , OpenMPI , STAT, Nvidia profilers for debugging and application profiling

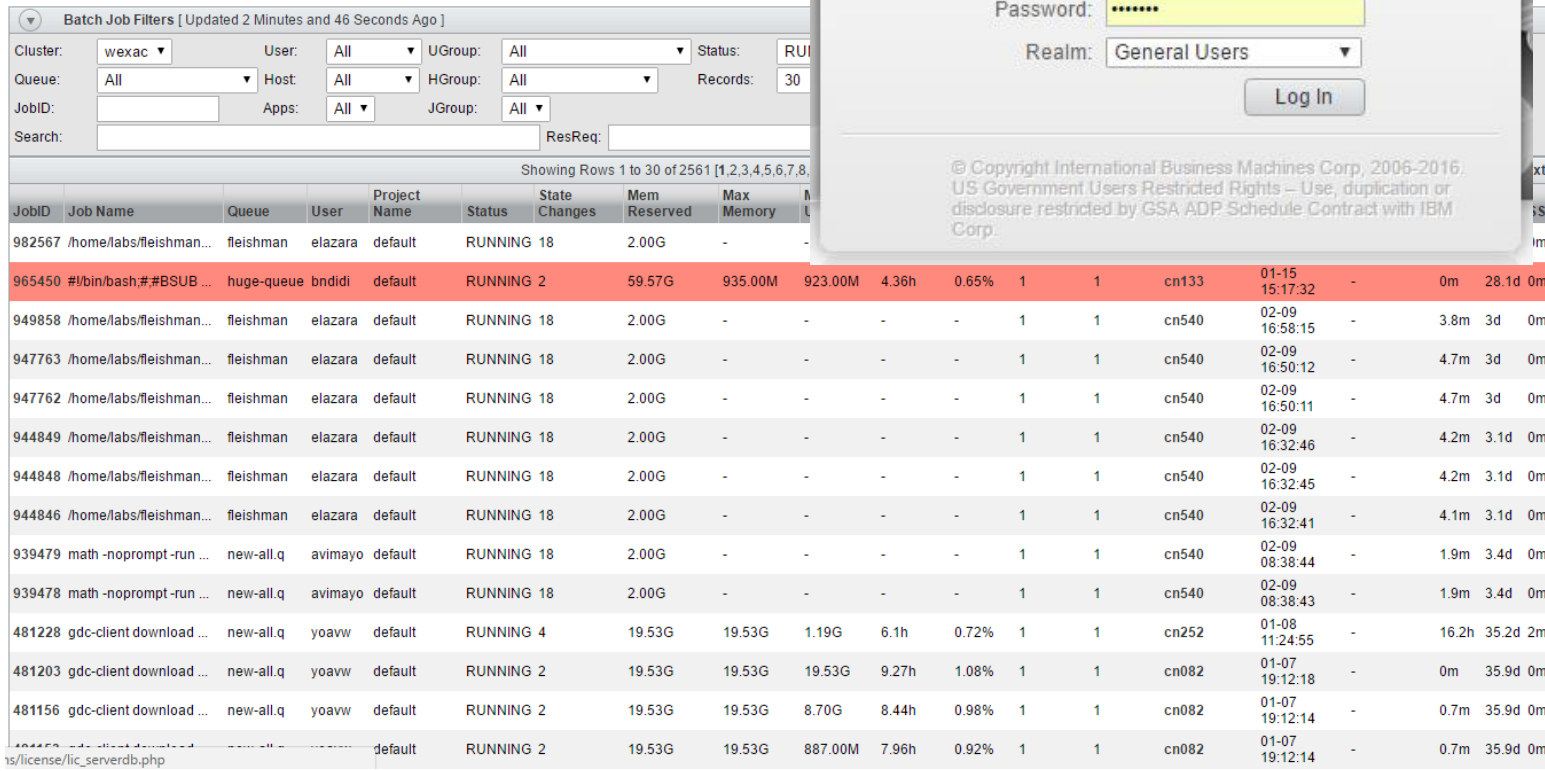
Ganglia Monitoring and Graphics Tool

- Ganglia monitoring tool is primary built for monitoring clusters of servers, and it does its job at the best.
- It represents the overall performance of a cluster of servers in an overview
- Suppose you have multiple clusters in a datacenter, then in that case you can arrange them and call it as a grid and have an overall performance overview of that grid.
- Performance monitoring to the base machine of a collection of virtual machines, can be done using ganglia monitoring tool.

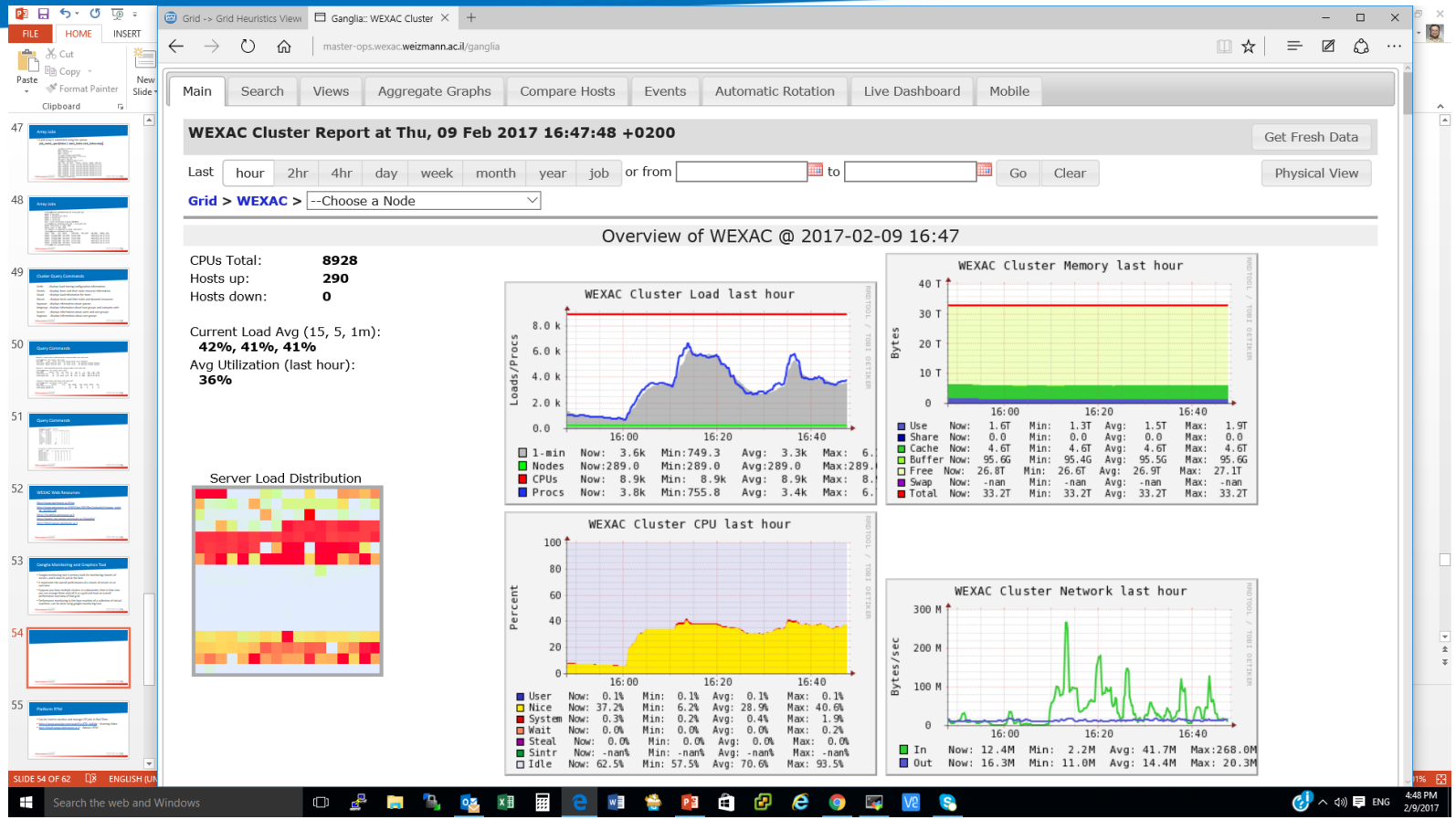
WEXAC real-time monitor: Ganglia and RTM







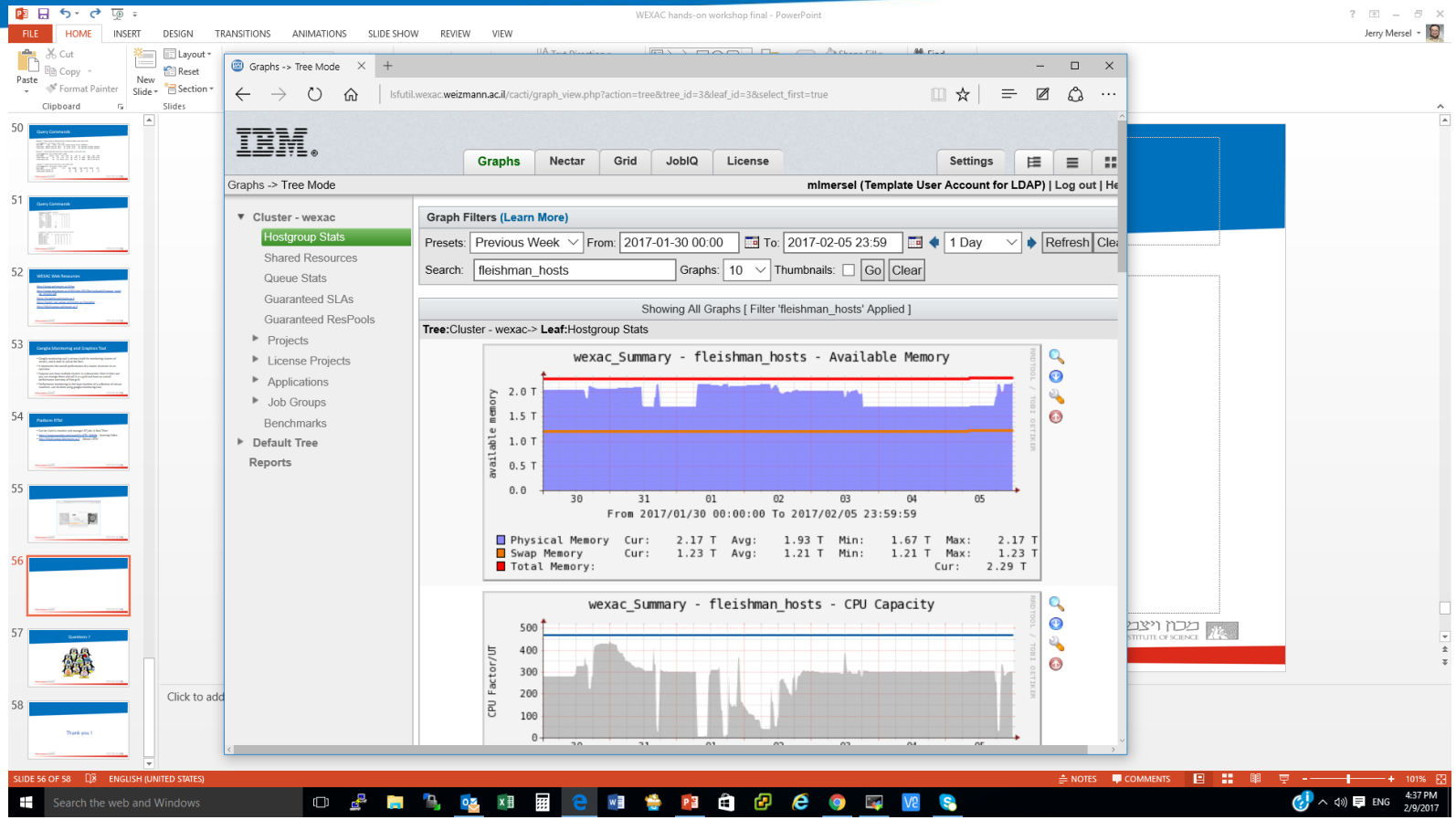
Ganglia Grid Overview



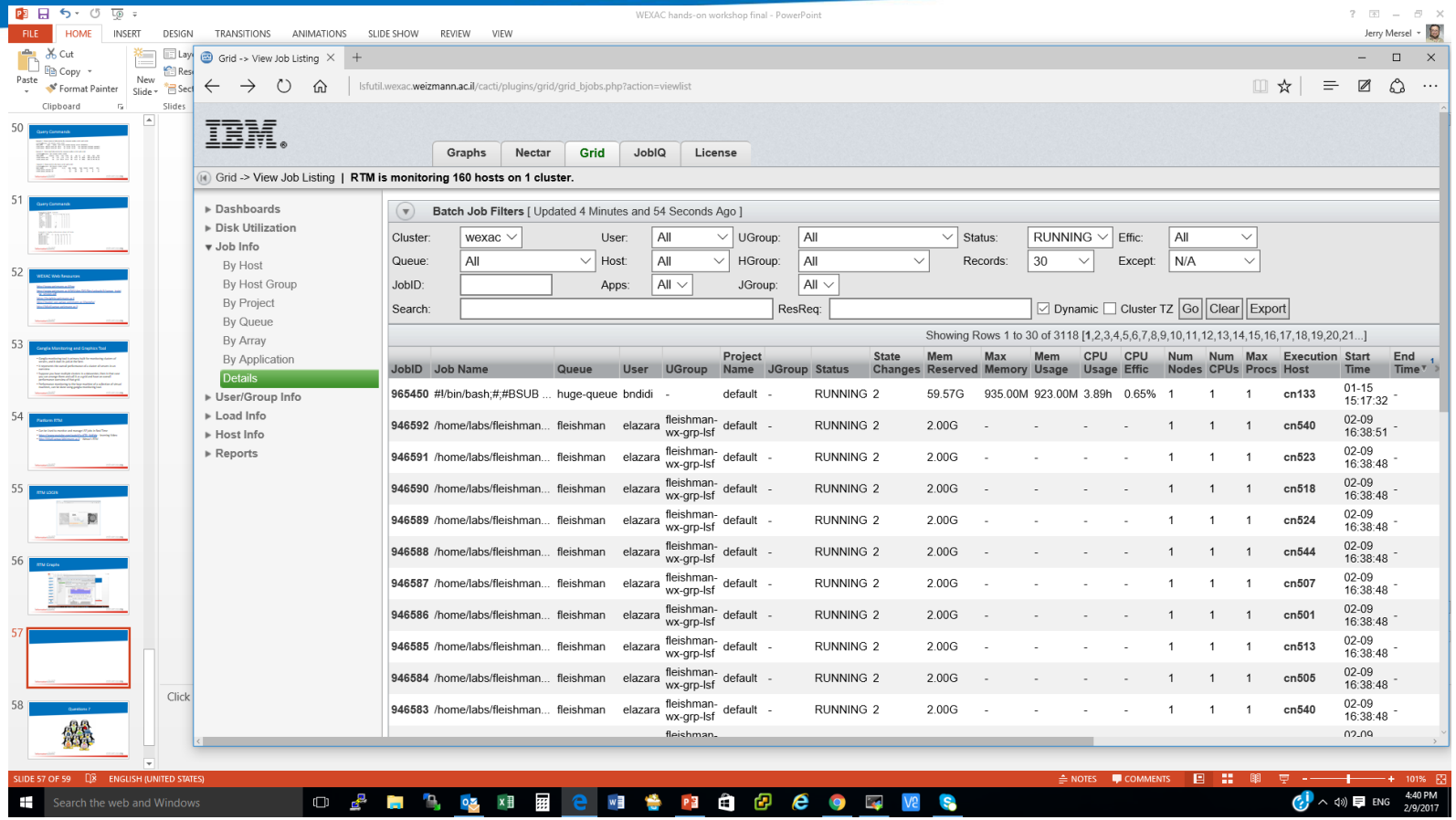
Platform RTM

- Can be Used to monitor and manage LSF jobs in Real Time
- https://www.youtube.com/watch?v=if7R_IId4Wg – learning Video
- http://rtm.wexac.weizmann.ac.il – WEXAC's RTM

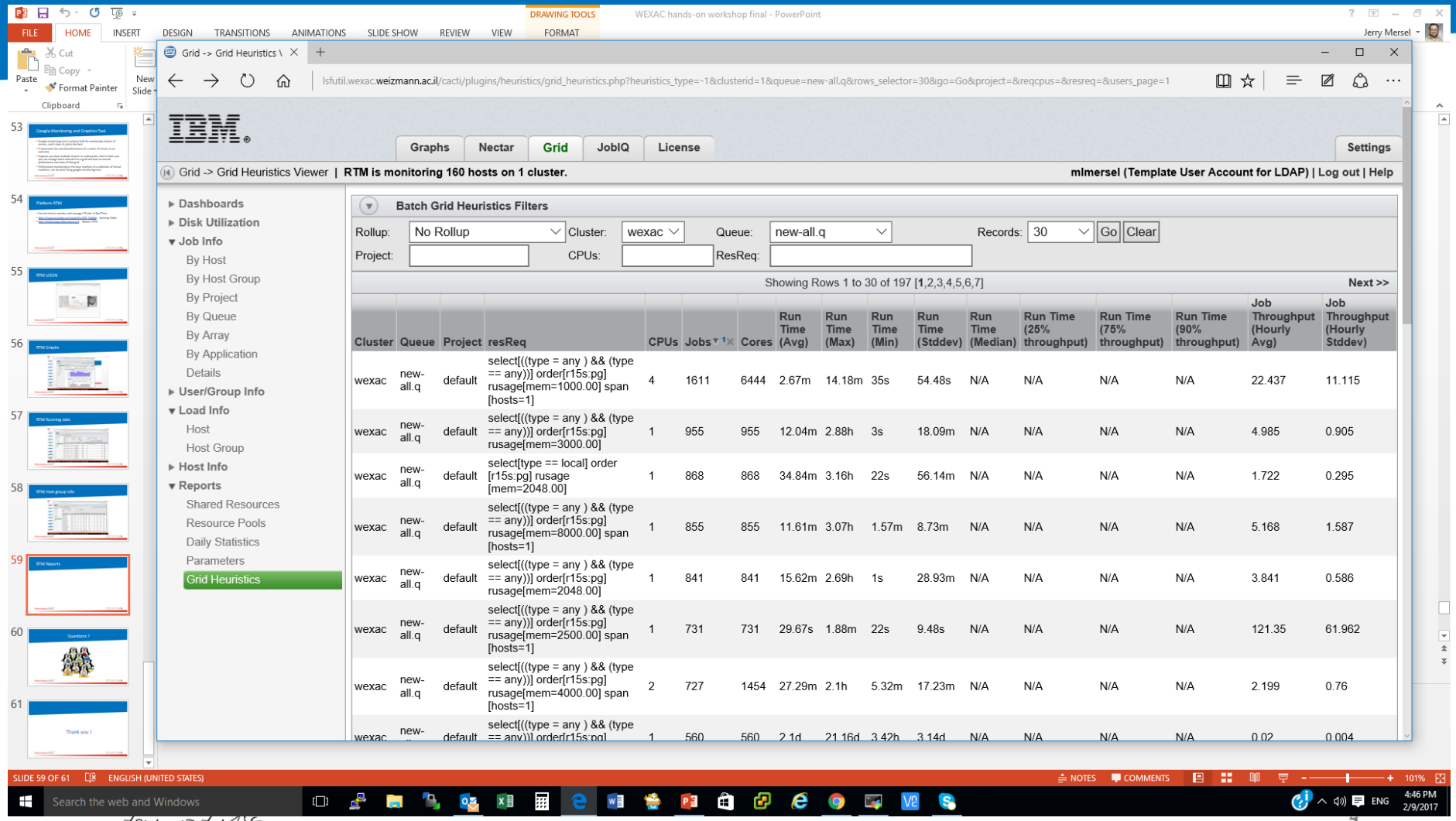
RTM Graphs


WEXAC hands-on workshop final - PowerPoint
Graphs -> Tree Mode
lsfutil.wexac.weizmann.ac.il/cacti/graph_view.php?action=tree&tree_id=3&leaf_id=3&select_first=true
IBM
Graphs
Nectar
Grid
JobIQ
License
Settings
Graphs -> Tree Mode
mlmersel (Template User Account for LDAP) | Log out
Cluster - wexac
Hostgroup Stats
Shared Resources
Queue Stats
Guaranteed SLAs
Guaranteed ResPools
Projects
License Projects
Applications
Job Groups
Benchmarks
Default Tree
Reports
Graph Filters (Learn More)
Presets: Previous Week From: 2017-01-30 00:00 To: 2017-02-05 23:59 1 Day Refresh
Search: fleishman_hosts Graphs: 10 Thumbnails: Go Clear
Showing All Graphs [Filter 'fleishman_hosts' Applied]
Tree:Cluster - wexac-> Leaf:Hostgroup Stats
wexac_Summary - fleishman_hosts - Available Memory
available memory
From 2017/01/30 00:00:00 To 2017/02/05 23:59:59
Physical Memory Cur: 2.17 T Avg: 1.93 T Min: 1.67 T Max: 2.17 T
Swap Memory Cur: 1.23 T Avg: 1.21 T Min: 1.21 T Max: 1.23 T
Total Memory: Cur: 2.29 T
wexac_Summary - fleishman_hosts - CPU Capacity
CPU Factor/UT

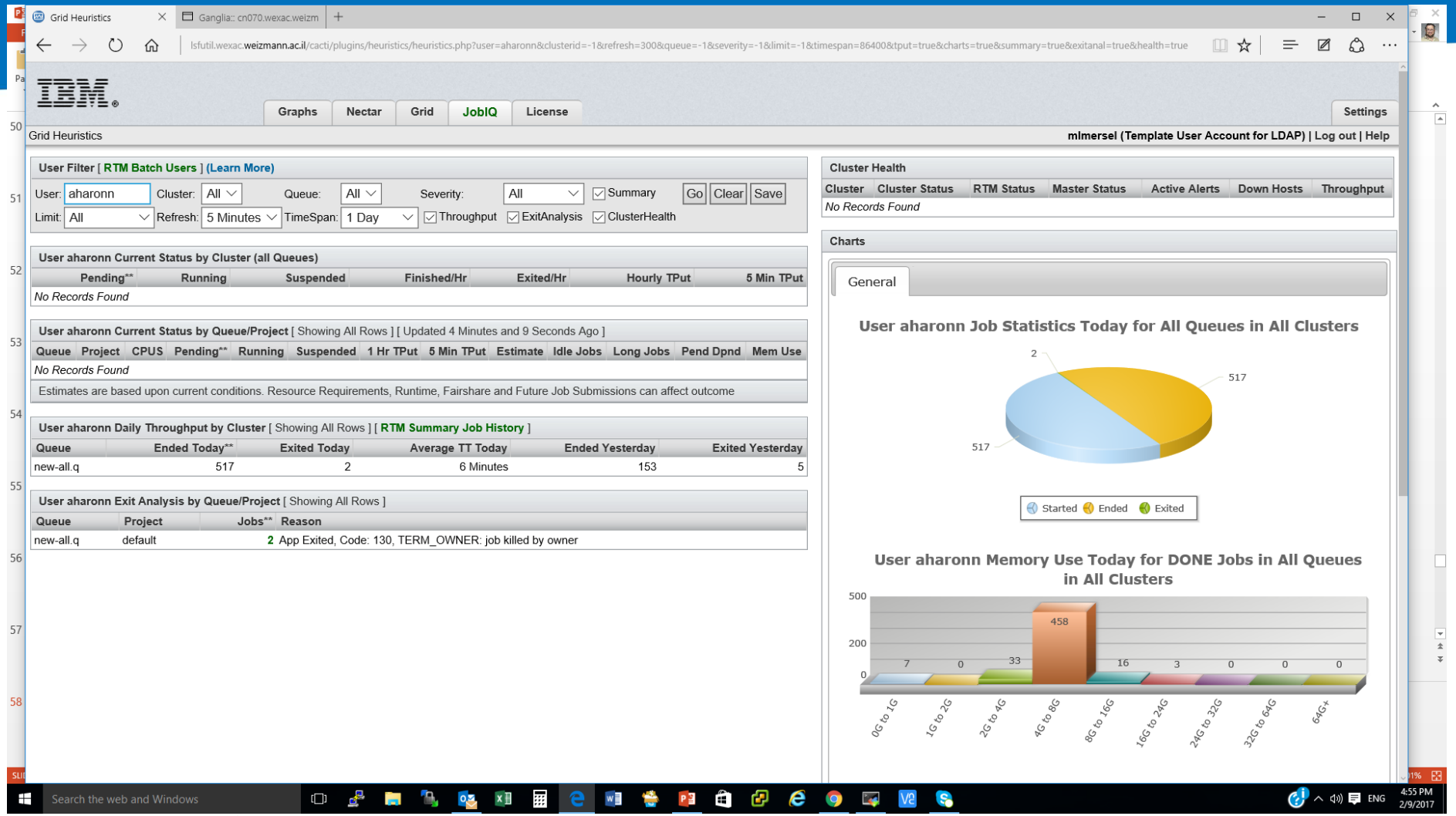
RTM Running Jobs



RTM Reports


WEXAC hands-on workshop final - PowerPoint
Grid -> Grid Heuristics
lsfutil.wexac.weizmann.ac.il/cacti/plugins/heuristics/grid_heuristics.php?heuristics_type=-1&clusterid=1&queue=new-all.q&rows_selector=30&go=Go&project=&reqcpus=&resreq=&users_page=1
IBM
Graphs
Nectar
Grid
JobIQ
License
Settings
Grid -> Grid Heuristics Viewer | RTM is monitoring 160 hosts on 1 cluster.
mlmersel (Template User Account for LDAP) | Log out | Help
Dashboards
Disk Utilization
Job Info
By Host
By Host Group
By Project
By Queue
By Array
By Application
Details
User/Group Info
Load Info
Host
Host Group
Host Info
Reports
Shared Resources
Resource Pools
Daily Statistics
Parameters
Grid Heuristics
Batch Grid Heuristics Filters
Rollup: No Rollup
Cluster: wexac
Queue: new-all.q
Records: 30
Go
Clear
Project:
CPUs:
ResReq:
Showing Rows 1 to 30 of 197 [1,2,3,4,5,6,7]
Next >>
Cluster | Queue | Project | resReq | CPUs | Jobs | Cores | Run Time (Avg) | Run Time (Max) | Run Time (Min) | Run Time (Stddev) | Run Time (Median) | Run Time (25% throughput) | Run Time (75% throughput) | Run Time (90% throughput) | Job Throughput (Hourly Avg) | Job Throughput (Hourly Stddev)
wexac | new-all.q | default | select[((type = any) && (type == any))] order[r15s:pg] rusage[mem=1000.00] span[hosts=1] | 4 | 1611 | 6444 | 2.67m | 14.18m | 35s | 54.48s | N/A | N/A | N/A | N/A | 22.437 | 11.115
wexac | new-all.q | default | select[((type = any) && (type == any))] order[r15s:pg] rusage[mem=3000.00] | 1 | 955 | 955 | 12.04m | 2.88h | 3s | 18.09m | N/A | N/A | N/A | N/A | 4.985 | 0.905
wexac | new-all.q | default | select[type == local] order[r15s:pg] rusage[mem=2048.00] | 1 | 868 | 868 | 34.84m | 3.16h | 22s | 56.14m | N/A | N/A | N/A | N/A | 1.722 | 0.295
wexac | new-all.q | default | select[((type = any) && (type == any))] order[r15s:pg] rusage[mem=8000.00] span[hosts=1] | 1 | 855 | 855 | 11.61m | 3.07h | 1.57m | 8.73m | N/A | N/A | N/A | N/A | 5.168 | 1.587
wexac | new-all.q | default | select[((type = any) && (type == any))] order[r15s:pg] rusage[mem=2048.00] | 1 | 841 | 841 | 15.62m | 2.69h | 1s | 28.93m | N/A | N/A | N/A | N/A | 3.841 | 0.586
wexac | new-all.q | default | select[((type = any) && (type == any))] order[r15s:pg] rusage[mem=2500.00] span[hosts=1] | 1 | 731 | 731 | 29.67s | 1.88m | 22s | 9.48s | N/A | N/A | N/A | N/A | 121.35 | 61.962
wexac | new-all.q | default | select[((type = any) && (type == any))] order[r15s:pg] rusage[mem=4000.00] span[hosts=1] | 2 | 727 | 1454 | 27.29m | 2.1h | 5.32m | 17.23m | N/A | N/A | N/A | N/A | 2.199 | 0.76
wexac | new-all.q | default | select[((type = any) && (type == any))] order[r15s:pg] | 1 | 560 | 560 | 2.1d | 21.16d | 3.42h | 3.14d | N/A | N/A | N/A | N/A | 0.02 | 0.004
SLIDE 59 OF 61
ENGLISH (UNITED STATES)
Search the web and Windows
4:46 PM
2/9/2017

RTM Batch Users



GPU monitoring tools

- http://waicmgmt01.wexac.weizmann.ac.il:30200/
- Grafana monitoring tool allow to visualize DGX machines utilization

GUI portal for GPU status

MobaXterm for Windows users

- Enhanced terminal for Windows with X11 server, tabbed SSH client, network tools and much more
- **Download:** **http://mobaxterm.mobatek.net/download.html**

WEXAC Access Servers

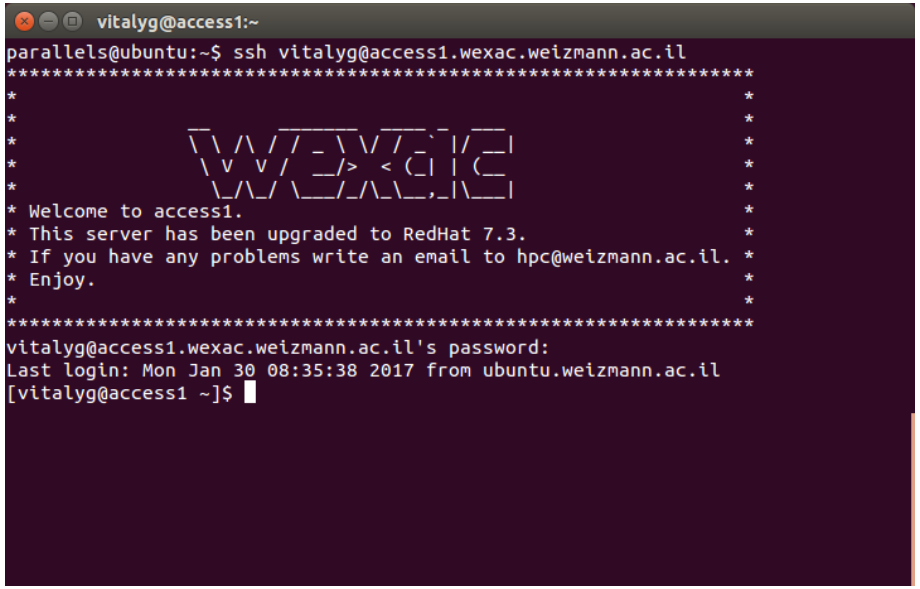
access.wexac.weizmann.ac.il

access2.wexac.weizmann.ac.il

access3.wexac.weizmann.ac.il

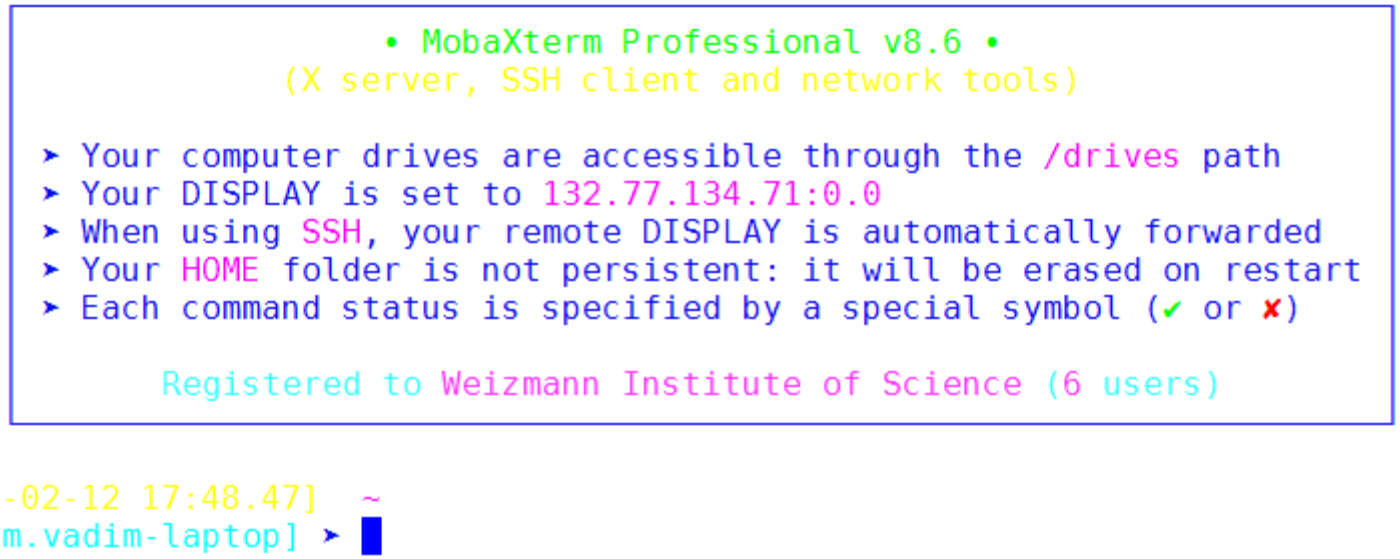
access4.wexac.weizmann.ac.il

waiclogin01.wexac.weizmann.ac.il

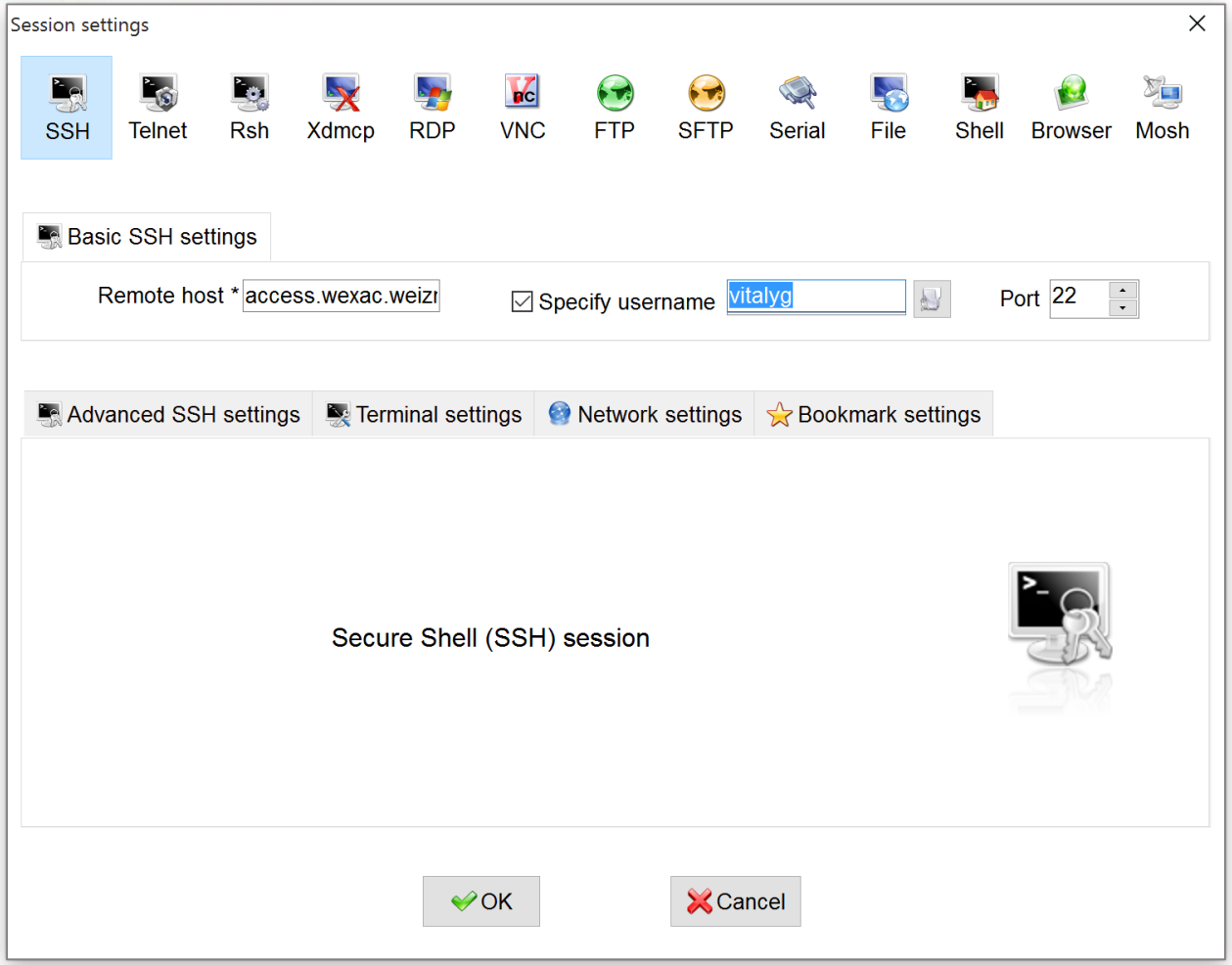


hpc@weizmann.ac.il

MobaXterm User Interface



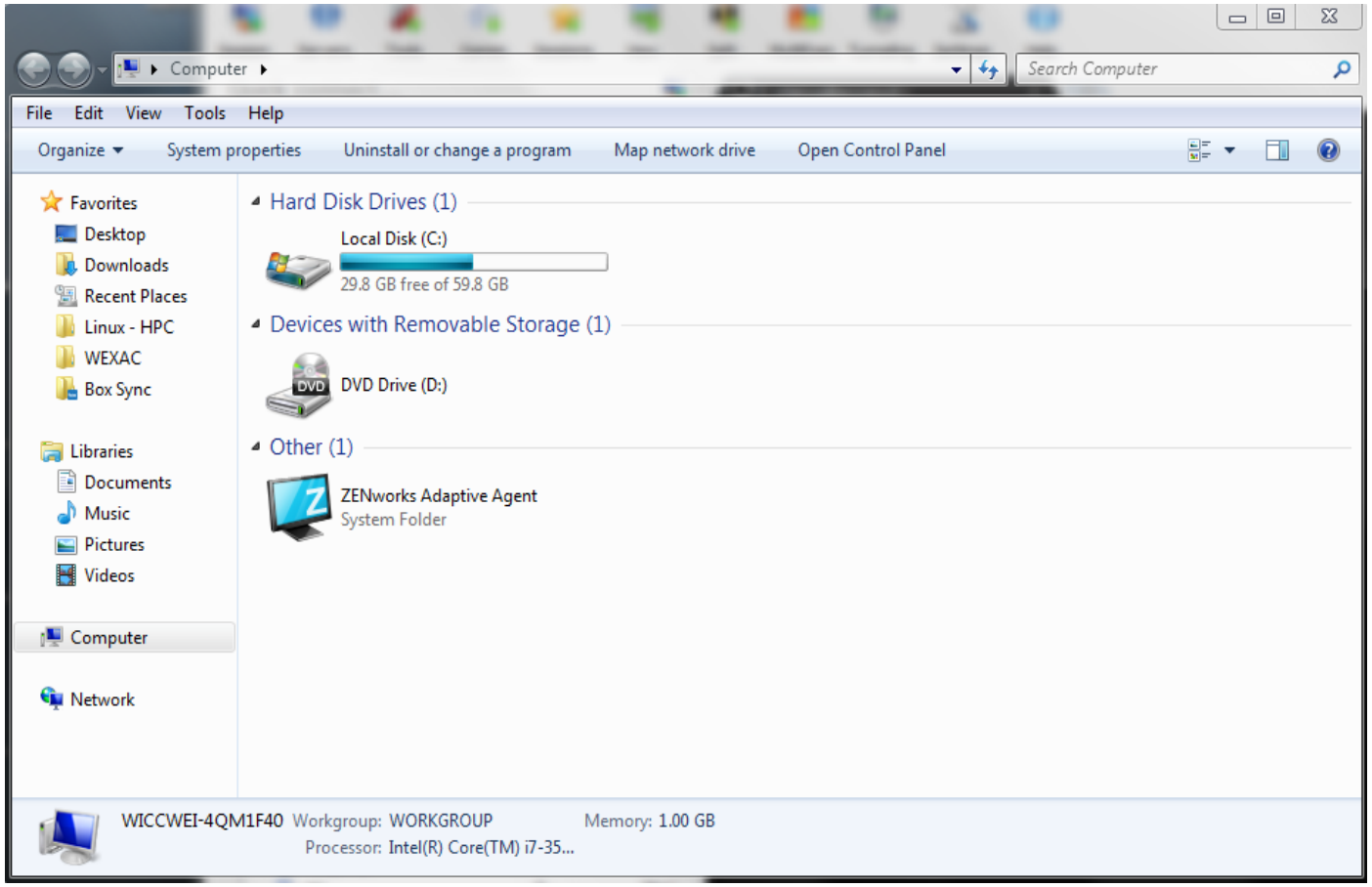
MobaXterm – Create SSH session



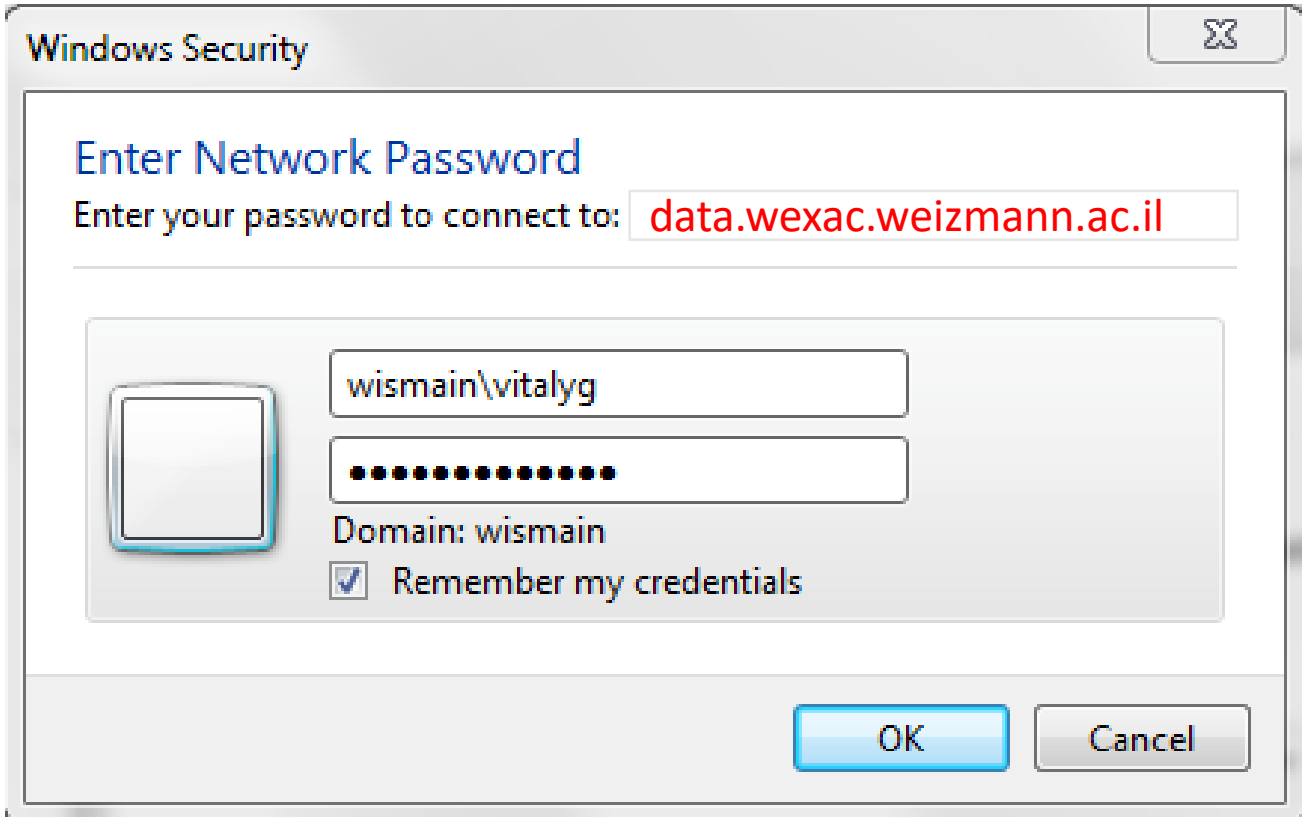
MobaXterm – WEXAC prompt

```
[vadim.vadim-laptop] ➤ ssh vadimm@access.wexac.weizmann.ac.il
*************************************************************************
*                                                                       *
*                                                                       *
*                __        _______  ____ _  ___                        *
*               \ \ /\ / / _ \ \/ / _` |/ __|                           *
*                \ V  V /  __/>  < (_| | (__                            *
*                 \_/\_/ \___/_/\_\__,_|\___|                           *
* Welcome to access.                                                    *
* This server has been upgraded to RedHat 7.3.                          *
* If you have any problems write an email to hpc@weizmann.ac.il.        *
* Enjoy.                                                                *
*                                                                       *
*************************************************************************
Last login: Sun Feb 12 17:48:00 2017 from v-lap.weizmann.ac.il
[vadimm@access ~]$
```

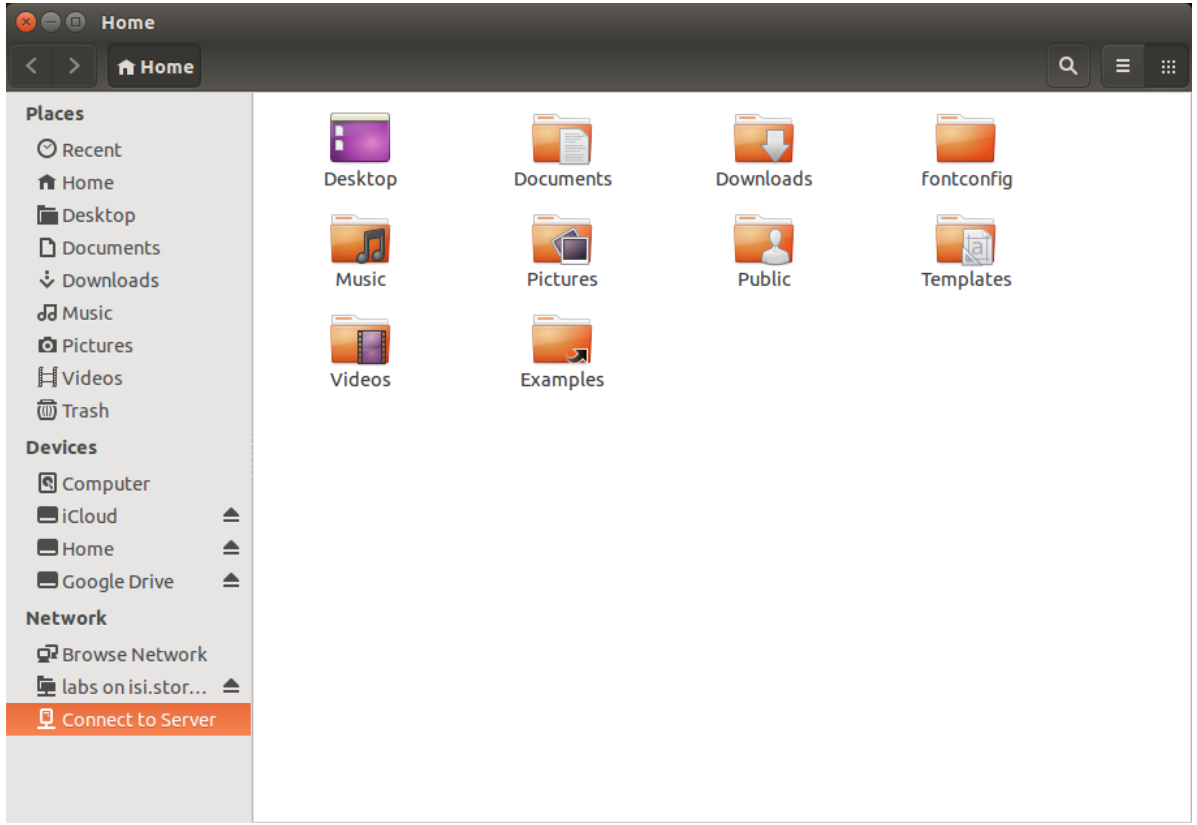
Map Network Drive – Windows workstation \\data.wexac.weizmann.ac.il



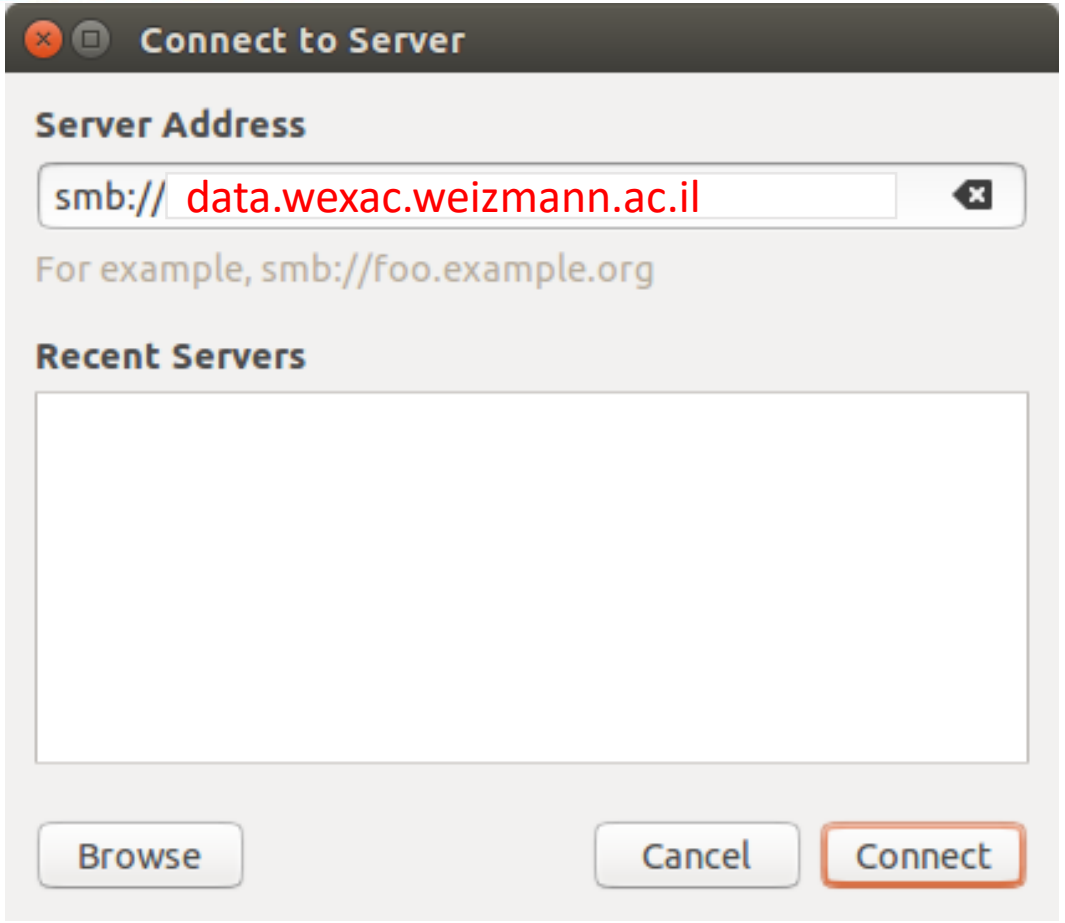
Universal WIS credentials



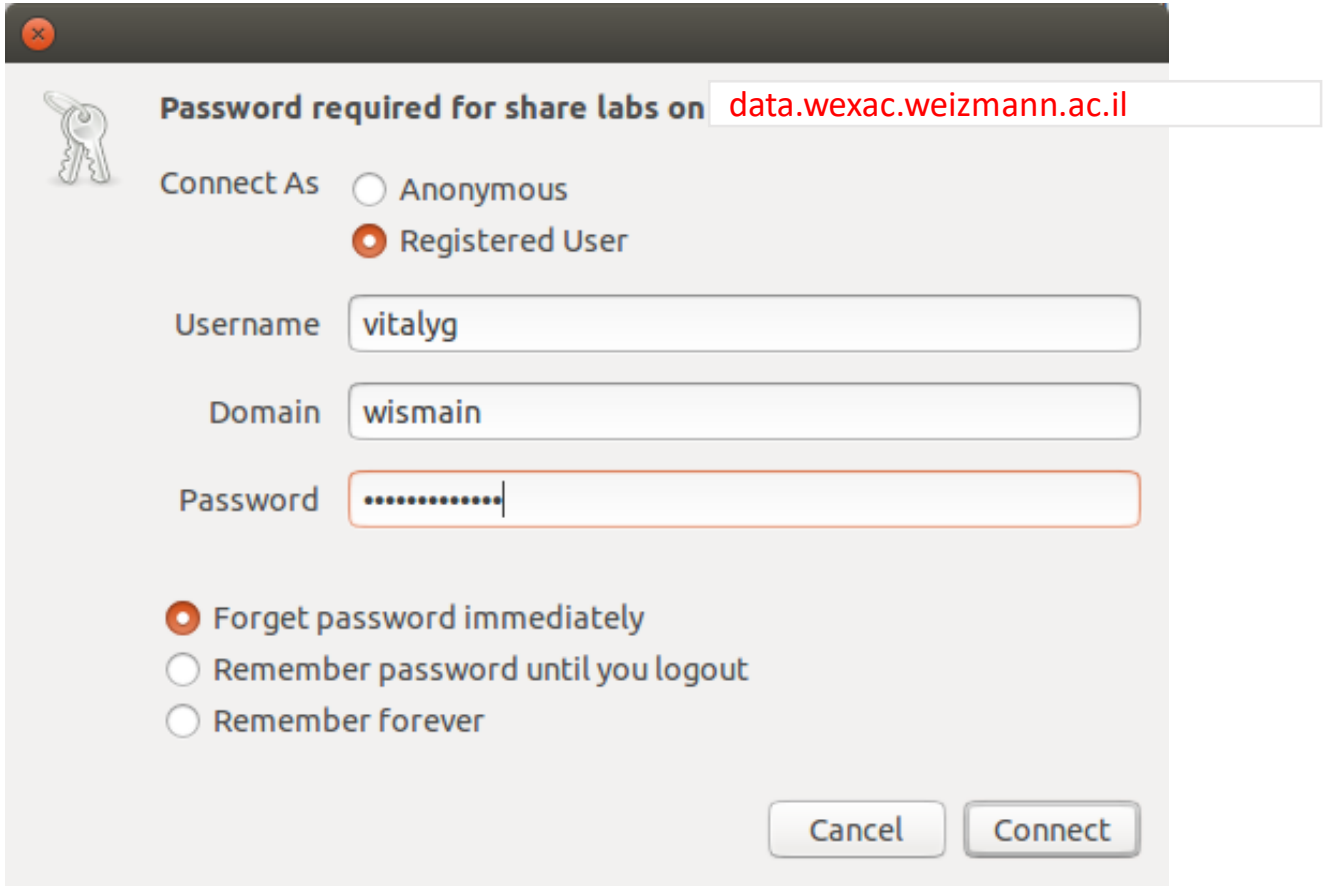
Access WEXAC from Ubuntu
\\data.wexac.weizmann.ac.il



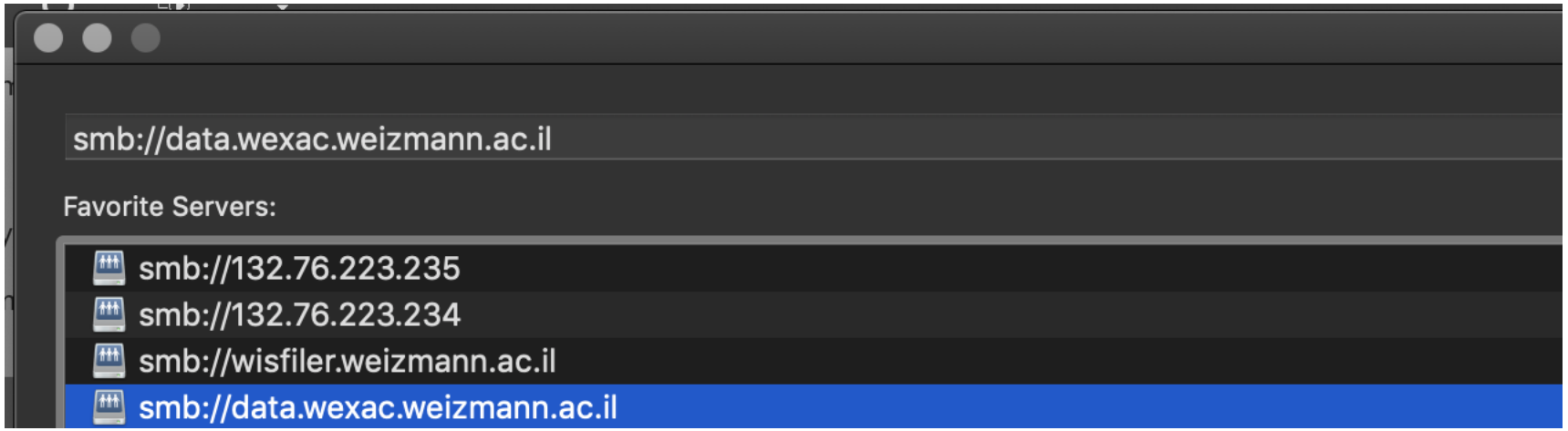
Access WEXAC from Ubuntu



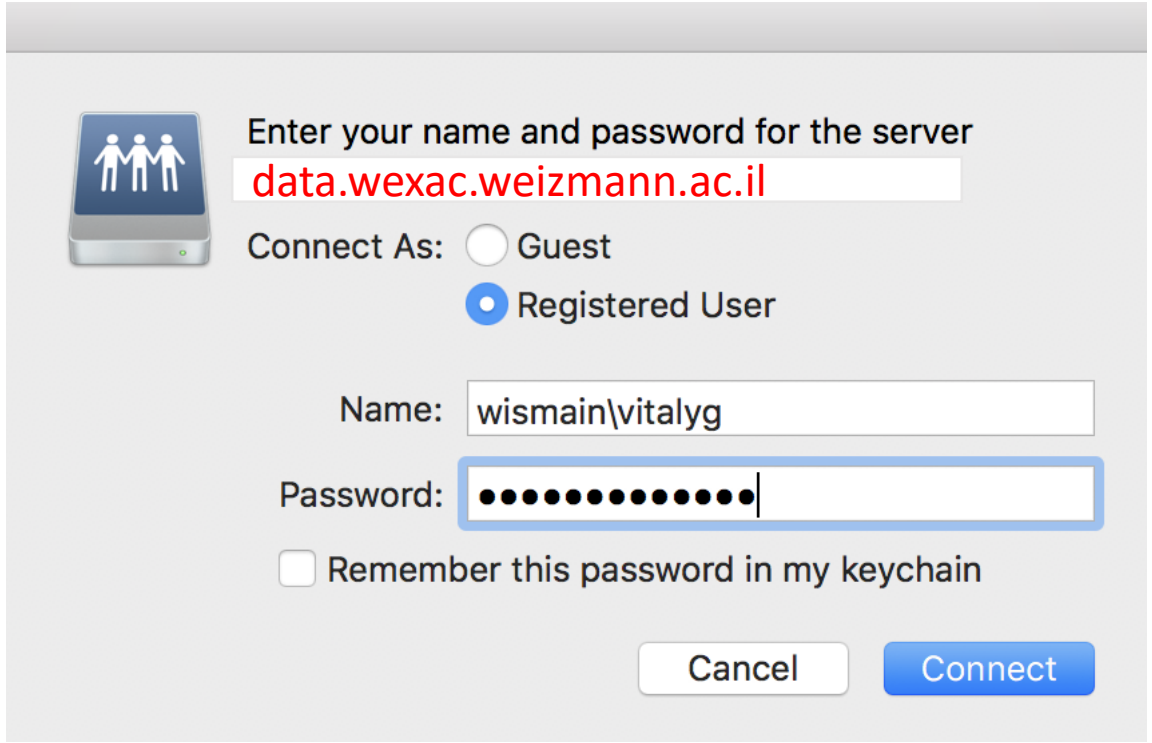
Universal DIS credentials used to access WEXAC from Ubuntu



Access WEXAC from MAC



Access WEXAC from MAC using universal DIS credentials



WEXAC Modules

```
[vitalyg@access ~]$ module avail

------------------------------ /apps/RH7U2/Modules/default/modulefiles/general -----------------------
annovar/2016Feb01            homer/4.8                    namd/2.12b1/multicore-CUDA
artemis/1.47                 icompiler/2015               namd/2.9/ibverbs-smp-CUDA
aspera/3.5.4                 icompiler/2016               namd/2.9/multicore-CUDA
assemblytics/2016Dec11       icompiler/2017               ngsplot/2.61
barcomb/1                    IGV/2.3.88                   pacbio/Jan-2017
blast/2.2.26                 IMOD/4.7.15                  prinseq/0.20.4
cap3/0.1                     jdk/8.111                    RepeatMasker/4.0.6
cellranger/1.2.1             jre/8.111                    resmap/1.1.4
chimera/1.11.2               kallisto/0.43.0              SeqMonk/1.36.0
circos/0.69-3                mathematica/11.0(default)    snpEff/3.0
cuda/7.5                     mathematica/8.0              spider/23.03
cuda/8.0.44(default)         matlab/R2016b                svtyper/0.1.1
cytoscape/3.4.0              MotionCor2/10-19-2016        tablet/1.16.09.06
eigen/3.3.0                  namd/2.12b1/ibverbs          trf/4.09
fastqc/0.11.5                namd/2.12b1/ibverbs-smp      trimmomatic/0.36
fastq_screen/0.9.5           namd/2.12b1/ibverbs-smp-CUDA unblur/1.02
GATK/3.7                     namd/2.12b1/KNL-multicore    weblogo/2.8.2

------------------------------ /apps/RH7U2/Modules/default/modulefiles/intel -----------------------
bedtools/2.26.0              koren/intel-2017/hdf5/1.8.12  pigz/2.3.4
blat/35                      koren/intel-2017/hdf5/1.8.16  python/2.7(default)
bowtie/1.1.2                 koren/intel-2017/netcdf/4.1.3 python/3.5
bowtie2/2.2.9                kushnir/hdf5-2016/1.10.0      relion/1.4
bwa/0.7.15                   ldhat/1.0                     samtools/1.3.1
fftw/3.3.5                   lumpy/0.2.13                  shrimp/2.2.3
fltk/1.3.4                   moreutils/0.6                 stringtie/1.3.0
hdf5/1.10.0                  parallel-netcdf/1.7.0         vcftools/0.1.15
htslib/1.3.1                 pear/0.9.10

------------------------------ /apps/RH7U2/Modules/default/modulefiles/gnu -------------------------
abyss/2.0.2          cufflinks/2.2.1      hmmer/3.1b1          ncbi-blast+/2.5.0    sqlite/3.15.2
bamtools/2.4.1       delly/0.7.6          jemalloc/4.4.0       openblas/0.2.19      sra-tools/2.8.0
bazel/0.4.2          delly_parallel/0.7.6 KaKs_Calculator/2.0  openmpi/2.0.1        stampy/1.0.31
bcftools/1.3.1       detonate/1.11        kentUtils            pandoc/1.18          star/2.5.2b
bcl2fastq/2.17.1.14  dos2unix/7.3.4       lapack/3.7.0         pdsh/2.29            tabix/0.2.6
bedtools-gnu/2.26.0  ea-utils/1.1.2       libgd/2.2.2          perl/5.24.0          texlive/2016
bioawk/1.0           eig/6.1.3            libgsl/2.3           perl/5.24.0_2        tiff/4.0.7
boost/1.55.0         emboss/6.6.0         libgtextutils/0.7    primer3/2.3.7        tophat/2.1.1
boost/1.62.0         expander/7.11        libxml2/2.9.4        python/2.7.12        trinity/2.3.2
breakdancer/1.4.5    falcon/0.3.0         libxslt/1.1.29       python/3.5.2         vcflib/1.0.0
breseq/0.29.0        fasta/36.3.8d        lynx/2.8.3           R/3.3.2              velvet/1.2.10
bwa-gnu/0.7.15       fastx/0.0.14         mafft/7.305          relion/2.0           ViennaRNA/2.3.1
bzip2/1.0.6          fftw/3.3.4           meme/4.11.2          rmblast/2.2.8        wxwidgets/3.1.0
cd-hit/4.6.6         file/5.29            mipgen/22-Dec-2016   rsem/1.3.0           zlib/1.2.8
clustalw/2.1         freebayes/1.1.0      miRDeep/2.0.0.8      samtools/0.1.19      zsh/5.2
cmake/3.7.1          gcc/5.4.0            motioncorr/2.1       samtools/1.3.1a
CORTEX/1.0.5.21      git/2.11.0           mummer/3.23          sga/0.10.15
cortex_con/0.05      graphviz/2.38.0      mvapich2/2.2         sickle/1.33
ctffind/4.1.5        hisat/2.0.5          mysql/5.7.16         sparsehash/2.0.3
```

Modules (contd.)

```
[vitalyg@access ~]$ module --help

  Modules Release 3.2.10 2012-12-21 (Copyright GNU GPL v2 1991):

  Usage: module [ switches ] [ subcommand ] [subcommand-args ]

Switches:
        -H|--help                   this usage info
        -V|--version                modules version & configuration options
        -f|--force                  force active dependency resolution
        -t|--terse                  terse    format avail and list format
        -l|--long                   long     format avail and list format
        -h|--human                  readable format avail and list format
        -v|--verbose                enable  verbose messages
        -s|--silent                 disable verbose messages
        -c|--create                 create caches for avail and apropos
        -i|--icase                  case insensitive
        -u|--userlvl <lvl>          set user level to (nov[ice],exp[ert],adv[anced])
  Available SubCommands and Args:
        + add|load                  modulefile [modulefile ...]
        + rm|unload                 modulefile [modulefile ...]
        + switch|swap               [modulefile1] modulefile2
        + display|show              modulefile [modulefile ...]
        + avail                     [modulefile [modulefile ...]]
        + use [-a|--append]         dir [dir ...]
        + unuse                     dir [dir ...]
        + update
        + refresh
        + purge
        + list
        + clear
        + help                      [modulefile [modulefile ...]]
        + whatis                    [modulefile [modulefile ...]]
        + apropos|keyword           string
        + initadd                   modulefile [modulefile ...]
        + initprepend               modulefile [modulefile ...]
        + initrm                    modulefile [modulefile ...]
        + initswitch                modulefile1 modulefile2
        + initlist
        + initclear
```

Modules (contd.)

```
[vitalyg@access ~]$ module list
Currently Loaded Modulefiles:
  1) matlab/R2016b      2) mathematica/11.0   3) R/3.3.2           4) python/2.7
[vitalyg@access ~]$ module load bowtie2/2.2.9
[vitalyg@access ~]$ module list
Currently Loaded Modulefiles:
  1) matlab/R2016b      3) R/3.3.2           5) bowtie2/2.2.9
  2) mathematica/11.0   4) python/2.7
[vitalyg@access ~]$ module load samtools/1.3.1
[vitalyg@access ~]$ module list
Currently Loaded Modulefiles:
  1) matlab/R2016b      3) R/3.3.2           5) bowtie2/2.2.9      7) samtools/1.3.1
  2) mathematica/11.0   4) python/2.7        6) icompiler/2017
[vitalyg@access ~]$
```

WEXAC Job Submission & Control commands

`bsub` - submits a batch job to LSF

`bjobs` - displays information about LSF jobs

`bhist` - displays historical information about jobs

`bkill` - sends signals to kill, suspend, or resume unfinished jobs

`bmod` - modifies job submission options of a job

`bpeek` - displays the stdout and stderr output of an unfinished job

`bstop` - suspends unfinished jobs

`bresume` - resumes unfinished jobs

`bswitch` - switches jobs from one queue to another

bsub – Commonly Used Options

`-q` *qname*	submits the job to the specified queue
`-o` *file*	redirect stdout, stderr and resource usage information of the job to the specified *output file*
`-e` *file*	redirect stderr to the specified error file
`-oo/-eo` *file*	same as -o/-e, but overwrite file if it exists
`-i` *filename*	use the specified file as standard input for the job
`-n` number	specify number of job slots
`-g` *jobgroup*	submit job to specified group
`-J` *jobname*	assigns the specified name to the job
`-R` res_req	runs job on a host that meets the specified resource requirements
`-L` *shell*	Initializes the execution environment using the specified login shell

bsub – Methods for Submitting Jobs

- By script or command
```
$ bsub -q new-new-all.q -J example -o example-%J.o -e
example-%J.e date
```

- By job spooling
```
$ bsub < job_file
```

job_file example:
```
#BSUB -q new-all.q
#BSUB -J example
#BSUB -o example-%J.o
#BSUB -e example-%J.e
date
```

bsub – Methods for Submitting Jobs

Interactively

```
$ bsub
bsub> #BSUB -q new-all.q
bsub> #BSUB -J example
bsub> #BSUB -o example-%J.o
bsub> #BSUB -e example-%J.e
bsub> date
bsub> ^D
Job <2387> is submitted to queue <new-all.q>.
```

Resource Requirements (-R)

Resource requirement string is divided into following sections:

Selection	-	**select[*selection_string*]**
Usage	-	**rusage[*rusage_string*]**
Ordering	-	**order[*order_string*]**
Locality	-	**span[*span_string*]**
Same	-	**same[*same_string*]**
CU	-	**cu[*cu_string*]**

Span and same sections are used for parallel jobs

Resource Requirements Examples

Example 1. Select execution host candidates that have at least 2GB free RAM

```
$ bsub -R "select[mem>2GB]" myJob
```

Example 2. Select execution host candidates with Infiniband interconnect

```
$ bsub -R "defined(ib)" myJob
```

Example 3. Select candidate hosts that have 1000MB free swap and order by amount of available memory

```
$ bsub -R "select[swp>1000] order[mem]" myJob
```

Resource Requirements Examples – Parallel jobs example of usage

Example 4. Candidate hosts should have min 500MB free RAM, job will reserve 400MB RAM.

```
$ bsub -n 4 -R "select[mem>500] rusage[mem=400]" myJob
```

Example 5. All slots required for a parallel job should reside on the same host

```
$ bsub -n 4 -R "span[hosts=1]" parallelJob
```

Example 6. 12-CPU parallel job should run on up to 4 CPUs per host , all candidate hosts must have the same CPU model

```
$ bsub -n 12 -R "span[ptile=4] same[model]" parallelJob
```

Array Jobs – example of usage

- A job array is submitted using the syntax:
  job_name_spec[index | start_index-end_index:step]

```
[vitalyg@access mathematica]$ cat array_math.job
#BSUB -q new-short
#BSUB -J mathematica[1-10]
#BSUB -o results.%J
#BSUB -e results.%J
math -script fullCluster.m ${LSB_JOBINDEX}
[vitalyg@access mathematica]$ bsub < array_math.job
Memory reservation is (MB): 2048
Memory Limit is (MB): 2048
Job <618114> is submitted to queue <new-short>.
[vitalyg@access mathematica]$ bjobs
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
618114  vitalyg RUN   new-short  access.wexa cn145.wexac *matica[1] Jan 22 13:22
618114  vitalyg RUN   new-short  access.wexa cn145.wexac *matica[2] Jan 22 13:22
618114  vitalyg RUN   new-short  access.wexa cn145.wexac *matica[3] Jan 22 13:22
618114  vitalyg RUN   new-short  access.wexa cn145.wexac *matica[4] Jan 22 13:22
618114  vitalyg RUN   new-short  access.wexa cn145.wexac *matica[5] Jan 22 13:22
618114  vitalyg RUN   new-short  access.wexa cn145.wexac *matica[6] Jan 22 13:22
618114  vitalyg RUN   new-short  access.wexa cn145.wexac *matica[7] Jan 22 13:22
618114  vitalyg RUN   new-short  access.wexa cn145.wexac *matica[8] Jan 22 13:22
618114  vitalyg RUN   new-short  access.wexa cn145.wexac *matica[9] Jan 22 13:22
618114  vitalyg RUN   new-short  access.wexa cn145.wexac *atica[10] Jan 22 13:22
[vitalyg@access mathematica]$
```

Array Jobs

```
[vitalyg@access mathematica]$ cat array_math.job
#BSUB -q new-short
#BSUB -J mathematica[1-10:2]
#BSUB -o results.%J
#BSUB -e results.%J
math -script fullCluster.m ${LSB_JOBINDEX}
[vitalyg@access mathematica]$ bsub < array_math.job
Memory reservation is (MB): 2048
Memory Limit is (MB): 2048
Job <618115> is submitted to queue <new-short>.
[vitalyg@access mathematica]$ bjobs
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
618115  vitalyg PEND  new-short  access.wexa             *matica[1] Jan 22 13:27
618115  vitalyg PEND  new-short  access.wexa             *matica[3] Jan 22 13:27
618115  vitalyg PEND  new-short  access.wexa             *matica[5] Jan 22 13:27
618115  vitalyg PEND  new-short  access.wexa             *matica[7] Jan 22 13:27
618115  vitalyg PEND  new-short  access.wexa             *matica[9] Jan 22 13:27
[vitalyg@access mathematica]$
```

bjobs – View Jobs

-a	Display information about jobs in all states, including recently finished jobs
-A	Displays summarized information about job arrays
-d	Display information about jobs that finished recently
-l|-w	Display information in long or wide format
-p	Display information about pending jobs
-r	Display information about running jobs
-g `job_group`	Display information about jobs in specified group
-J `job_name`	Display information about specified job or array
-q `queue`	Display information about jobs in specified queue
-u `user`	Display information about jobs for specified users/groups

bjobs – Example 1

```
[vitalyg@access ~]$ bjobs
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
478504  vitalyg RUN   short      access.wexa cn165.wexac example3   Jan 17 10:47
478502  vitalyg RUN   new-all.q  access.wexa cn165.wexac example1   Jan 17 10:47
478503  vitalyg USUSP new-all.q  access.wexa cn165.wexac example2   Jan 17 10:47
478505  vitalyg RUN   short      access.wexa cn160.wexac example4   Jan 17 10:48
478506  vitalyg RUN   short      access.wexa cn160.wexac example5   Jan 17 10:48
478507  vitalyg RUN   short      access.wexa cn160.wexac example6   Jan 17 10:48
478509  vitalyg PEND  short      access.wexa               example7   Jan 17 10:50
[vitalyg@access ~]$
```

bjobs – Example 2 : detailed job view

```
[vitalyg@access ~]$ bjobs -l 478509

Job <478509>, Job Name <example7>, User <vitalyg>, Project <default>, Status <P
                     END>, Queue <short>, Command <sleep 999>
Tue Jan 17 10:50:42: Submitted from host <access.wexac.weizmann.ac.il>, CWD <$H
                     OME>, Output File </dev/null>, Re-runnable, Requested Reso
                     urces <rusage[mem=2048]>, Specified Hosts <cn149>;

 MEMLIMIT
      2 G
 PENDING REASONS:
 There are no suitable hosts for the job;

 SCHEDULING PARAMETERS:
            r15s   r1m  r15m   ut      pg     io    ls    it    tmp    swp    mem
 loadSched   -     -     -     -       -      -     -     -     -      -      -
 loadStop    -     -     -     -       -      -     -     -     -      -      -

             ngpus ngpus_shared ngpus_excl_t ngpus_excl_p ngpus_prohibited
 loadSched       -            -            -            -                 -
 loadStop        -            -            -            -                 -

          gpu_temp0 gpu_ecc0 gpu_temp1 gpu_ecc1 gpu_temp2 gpu_ecc2    nmics
 loadSched        -         -         -         -         -         -        -
 loadStop         -         -         -         -         -         -        -

          mic_temp0 mic_temp1 mic_freq0 mic_freq1 mic_power0 mic_power1
 loadSched        -         -         -         -          -          -
 loadStop         -         -         -         -          -          -

          mic_freemem0 mic_freemem1 mic_util0 mic_util1 mic_ncores0 mic_ncores1
 loadSched           -            -         -         -           -           -
 loadStop            -            -         -         -           -           -

 RESOURCE REQUIREMENT DETAILS:
 Combined: select[(type = any ) && (type == any)] order[r15s:pg] rusage[mem=204
                     8.00]
 Effective: -
```

bhist – Jobs History options

-a Display information about all jobs

-b|-l|-w Display information in brief, long, or wide format

-d Display information about finished jobs

-p Display information about pending jobs

-s Display information about suspended jobs

-t Display job events chronologically

-C|-D|-S|-T *start_time,end_time*

Display information about completed, dispatched, submitted, or all jobs in specified time window

-q *queue* Display information about jobs submitted to specified queue

-u *username|all* Display information about jobs submitted by user or all users

bhist – Example 1

```
[vitalyg@access ~]$ bhist
Summary of time in seconds spent in various states:
JOBID   USER    JOB_NAME  PEND    PSUSP   RUN     USUSP   SSUSP   UNKWN   TOTAL
478502  vitalyg example1  0       0       539     0       0       0       539
478503  vitalyg example2  1       0       46      486     0       0       533
478504  vitalyg example3  1       0       520     0       0       0       521
478505  vitalyg example4  0       0       471     0       0       0       471
478506  vitalyg example5  1       0       467     0       0       0       468
478507  vitalyg example6  0       0       464     0       0       0       464
478509  vitalyg example7  342     0       0       0       0       0       342

[vitalyg@access ~]$
```

bhist – Example 2 : detailed job information

```
[vitalyg@access ~]$ bhist -l 478502

Job <478502>, Job Name <example1>, User <vitalyg>, Project <default>, Command <
                     sleep 999>
Tue Jan 17 10:47:25: Submitted from host <access.wexac.weizmann.ac.il>, to Queu
                     e <new-all.q>, CWD <$HOME>, Output File </dev/null>, Re-ru
                     nnable, Requested Resources <rusage[mem=2048]>;

 MEMLIMIT
      2 G
Tue Jan 17 10:47:25: Dispatched 1 Task(s) on Host(s) <cn165.wexac.weizmann.ac.i
                     l>, Allocated 1 Slot(s) on Host(s) <cn165.wexac.weizmann.a
                     c.il>, Effective RES_REQ <select[((type = any ) && (type =
                     = any))] order[r15s:pg] rusage[mem=2048.00] >;
Tue Jan 17 10:47:25: Starting (Pid 13646);
Tue Jan 17 10:47:25: Running with execution home </home/labs/training/vitalyg>,
                      Execution CWD </home/labs/training/vitalyg>, Execution Pi
                     d <13646>;

Summary of time in seconds spent in various states by  Tue Jan 17 10:58:15
  PEND     PSUSP    RUN      USUSP    SSUSP    UNKWN    TOTAL
  0        0        650      0        0        0        650
```

Manipulating Jobs

bkill - send signals to kill, suspend, or resume unfinished jobs

Tip: use JobID 0 to kill all your jobs

bmod - modify job submission options of a job

bpeek - display the stdout and stderr output of an unfinished job

bstop - suspend unfinished jobs

bresume - resume unfinished jobs

bswitch - switch jobs from one queue to another

Manipulating Jobs

```
[vitalyg@access ~]$ bsub -q new-all.q -oo output -eo error -J example sleep 999
Memory reservation is (MB): 2048
Memory Limit is (MB): 2048
Job <478532> is submitted to queue <new-all.q>.
[vitalyg@access ~]$ bjobs 478532
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
478532  vitalyg RUN   new-all.q  access.wexa cn169.wexac example    Jan 17 12:54
[vitalyg@access ~]$ bstop 478532
Job <478532> is being stopped
[vitalyg@access ~]$ bjobs 478532
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
478532  vitalyg USUSP new-all.q  access.wexa cn169.wexac example    Jan 17 12:54
[vitalyg@access ~]$ bresume 478532
Job <478532> is being resumed
[vitalyg@access ~]$ bjobs 478532
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
478532  vitalyg SSUSP new-all.q  access.wexa cn169.wexac example    Jan 17 12:54
[vitalyg@access ~]$ bjobs 478532
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
478532  vitalyg RUN   new-all.q  access.wexa cn169.wexac example    Jan 17 12:54
```

Manipulating Jobs

Example 2

```
[vitalyg@access ~]$ bjobs
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
478529  vitalyg RUN   new-all.q  access.wexa cn146.wexac example    Jan 17 12:41
478530  vitalyg PEND  new-all.q  access.wexa             example    Jan 17 12:43
[vitalyg@access ~]$ bmod -q new-short 478530
Parameters of job <478530> are being changed
[vitalyg@access ~]$ bjobs
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
478530  vitalyg RUN   new-short  access.wexa cn146.wexac example    Jan 17 12:43
478529  vitalyg RUN   new-all.q  access.wexa cn146.wexac example    Jan 17 12:41
[vitalyg@access ~]$
```

Cluster Query Commands

lsinfo - displays load sharing configuration information

lshosts - displays hosts and their static resource information

lsload - displays load information for hosts

bhosts - displays hosts and their static and dynamic resources

bqueues - displays information about queues

bmgroup - displays information about host groups and compute units

busers - displays information about users and user groups

bugroup - displays information about user groups

Query Commands

Example 1. Show resource information for compute nodes cn141 and cn142

```
[vitalyg@access ~]$ lshosts cn141 cn142
HOST_NAME      type    model  cpuf ncpus maxmem maxswp server RESOURCES
cn141.wexac  X86_64 Intel_EM  60.0    16  63.8G  23.4G    Yes (mpichp4 intelmpi openmpi)
cn142.wexac  X86_64 Intel_EM  60.0    16  63.8G  23.4G    Yes (mpichp4 intelmpi openmpi)
```

Example 2 . Show load information for compute nodes cn141 and cn142

```
[vitalyg@access ~]$ lsload cn141 cn142
HOST_NAME       status  r15s   r1m  r15m   ut    pg  ls    it   tmp   swp   mem
cn142.wexac.wei     ok   1.0   1.0   1.0   3%   0.0   0  3834   18G 23.4G 54.3G
cn141.wexac.wei     ok   2.0  20.0  14.0   9%   0.0   0  3862   18G 23.4G 58.1G
```

Example 3. Show statistics for hosts cn141 and cn142

```
[vitalyg@access ~]$ bhosts cn141 cn142
HOST_NAME          STATUS       JL/U    MAX  NJOBS    RUN  SSUSP  USUSP    RSV
cn141.wexac.weizma ok              -     32     20     20      0      0      0
cn142.wexac.weizma ok              -     32     10     10      0      0      0
```

Query Commands

Example 4. Show queues

```
[vitalyg@access ~]$ bqueues
QUEUE_NAME      PRIO STATUS          MAX JL/U JL/P JL/H NJOBS  PEND   RUN  SUSP
bio-mem           85  Open:Active      -    -    -    -     0     0     0     0
sorek-high-prio   80  Open:Active      -    6    -    -     0     0     0     0
bio               80  Open:Active      -    -    -    -     0     0     0     0
schwartz          80  Open:Active      -    -    -    -     0     0     0     0
feulf             80  Open:Active      -    -    -    -     1     1     0     0
bio-smrt          75  Open:Active      -    -    -    -     0     0     0     0
bio-guest         70  Open:Active      -    -    -    -     0     0     0     0
wicc-priority     65  Open:Active      -    -    -    -     0     0     0     0
fleishman-prior   60  Open:Active      -   40    -    -     0     0     0     0
hanna-priority    60  Open:Active      -    6    -    -     0     0     0     0
koren-priority    60  Open:Active      -    -    -    -     0     0     0     0
lancet-priority   60  Open:Active      -    6    -    -     0     0     0     0
schneidman-prio   60  Open:Active      -   60    -    -     0     0     0     0
all-high          60  Open:Active      - 1000    -    -     0     0     0     0
new-short         60  Open:Active      - 1024    -    -     0     0     0     0
```

Example 5. Display information about all hosts

```
[vitalyg@access ~]$ bhosts
HOST_NAME          STATUS       JL/U    MAX  NJOBS    RUN  SSUSP  USUSP    RSV
cn080.wexac.weizma ok              -     24     10     10      0      0      0
cn081.wexac.weizma ok              -     24     20     20      0      0      0
cn083.wexac.weizma unavail         -     32      0      0      0      0      0
cn084.wexac.weizma ok              -     32     30     30      0      0      0
cn103.wexac.weizma ok              -     24     20     20      0      0      0
cn104.wexac.weizma ok              -     24     20     20      0      0      0
cn105.wexac.weizma ok              -     24     20     20      0      0      0
cn106.wexac.weizma ok              -     24     20     20      0      0      0
cn107.wexac.weizma ok              -     24      0      0      0      0      0
cn108.wexac.weizma closed          -     24     20     20      0      0      0
```

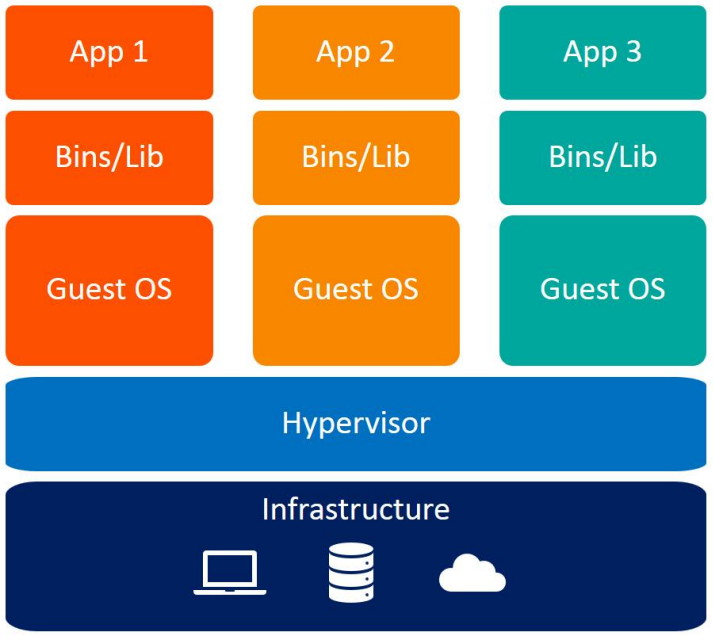
What Is A Docker Container?

- A Docker container is a mechanism for bundling a Linux application with all of its libraries, data files, and environment variables so that the execution environment is always the same, on whatever Linux system it runs and between instances on the same host.
- Unlike a VM which has its own isolated kernel, containers use the host system kernel. Therefore, all kernel calls from the container are handled by the host system kernel. DGX systems
uses Docker containers as the mechanism for deploying deep learning frameworks.

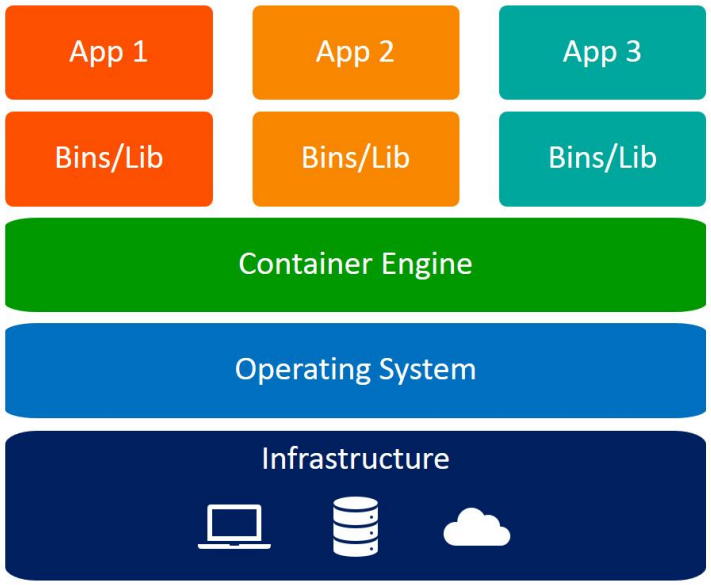
Why Use A Container?

- One of the many benefits to using containers is that you can install your application, dependencies and environment variables one time into the container image; rather than on each system you run on. In addition, the key benefits to using containers also include:
- Install your application, dependencies and environment variables one time into the container image; rather than on each system you run on.
- There is no risk of conflict with libraries that are installed by others.
- Containers allow use of multiple different deep learning frameworks, which may have conflicting software dependencies, on the same server.
- After you build your application into a container, you can run it on lots of other places, especially servers, without having to install any software.
- Legacy accelerated compute applications can be containerized and deployed on newer systems, on premise, or in the cloud.
- Specific GPU resources can be allocated to a container for isolation and better performance.
- You can easily share, collaborate, and test applications across different environments.
- Multiple instances of a given deep learning framework can be run concurrently with each having one or more specific GPUs assigned.
- Containers can be used to resolve network-port conflicts between applications by mapping container-ports to specific externally-visible ports when launching the container.

Virtual Machines vs. Containers



Virtual Machines



Containers

Docker Lifecycle

- DGXWS01 is used to build custom Docker images
- An image can be pulled and manipulated as required or built from a Dockerfile created by a user
- The image can be manipulated and then pushed to a private repository

Docker Cheat Sheet

ORCHESTRATE

Initialize swarm mode and listen on a specific interface
```
docker swarm init --advertise-addr 10.1.0.2
```

Join an existing swarm as a manager node
```
docker swarm join --token <manager-token> 10.1.0.2:2377
```

Join an existing swarm as a worker node
```
docker swarm join --token <worker-token> 10.1.0.2:2377
```

List the nodes participating in a swarm
```
docker node ls
```

Create a service from an image exposed on a specific port and deploy 3 instances
```
docker service create --replicas 3 -p 80:80 --name web nginx
```

List the services running in a swarm
```
docker service ls
```

Scale a service
```
docker service scale web=5
```

List the tasks of a service
```
docker service ps web
```

BUILD

Build an image from the Dockerfile in the current directory and tag the image
```
docker build -t myapp:1.0 .
```

List all images that are locally stored with the Docker engine
```
docker images
```

Delete an image from the local image store
```
docker rmi alpine:3.4
```

SHIP

Pull an image from a registry
```
docker pull alpine:3.4
```

Retag a local image with a new image name and tag
```
docker tag alpine:3.4 myrepo/myalpine:3.4
```

Log in to a registry (the Docker Hub by default)
```
docker login my.registry.com:8000
```

Push an image to a registry
```
docker push myrepo/myalpine:3.4
```

RUN

```
docker run
          --rm  remove container automatically after it exits
            -it  connect the container to terminal
     --name web  name the container
      -p 5000:80  expose port 5000 externally and map to port 80
-v ~/dev:/code  create a host mapped volume inside the container
    alpine:3.4  the image from which the container is instantiated
       /bin/sh  the command to run inside the container
```

Stop a running container through SIGTERM
```
docker stop web
```

Stop a running container through SIGKILL
```
docker kill web
```

Create an overlay network and specify a subnet
```
docker network create --subnet 10.1.0.0/24 --gateway 10.1.0.1 -d overlay mynet
```

List the networks
```
docker network ls
```

List the running containers
```
docker ps
```

Delete all running and stopped containers
```
docker rm -f $(docker ps -aq)
```

Create a new bash process inside the container and connect it to the terminal
```
docker exec -it web bash
```

Print the last 100 lines of a container's logs
```
docker logs --tail 100 web
```

www.docker.com/getdocker

How to pull a prebuilt docker image from a repository

- https://ngc.nvidia.com/
- Pull the Docker image from NVIDIA NGC repository:

```
docker pull nvcr.io/nvidia/tensorflow:19.05-py3
```

```
root@dgxws01:~# docker pull nvcr.io/nvidia/tensorflow:19.05-py2
19.05-py2: Pulling from nvidia/tensorflow
7e6591854262: Already exists
089d60cb4e0a: Already exists
9c461696bc09: Already exists
45085432511a: Already exists
6ca460804a89: Already exists
2631f04ebf64: Already exists
86f56e03e071: Already exists
234646620160: Already exists
7f717cd17058: Already exists
e69a2ba99832: Already exists
bc9bca17b13c: Already exists
1870788e477f: Already exists
603e0d586945: Already exists
717dfedf079c: Already exists
1035ef613bc7: Already exists
c5bd7559c3ad: Already exists
d82c679b8708: Already exists
059d4f560014: Already exists
f3f14cff44df: Already exists
96502bde320c: Already exists
bc5bb9379810: Already exists
e4d8bb046bc2: Already exists
4e2187010a7c: Already exists
9d62684b94c3: Already exists
e70e61e48991: Already exists
67f66c5c2dbf: Downloading [==================>                                ]  26.99MB/76.22MB
a290186bda3b: Download complete
74711a0ac24c: Download complete
a2fff41d0a70: Downloading [============>                                      ]  1.182MB/5.352MB
30b0cf6a53e9: Downloading [=>                                                 ]  1.617MB/52.75MB
787fc5f5c80a: Waiting
```

```
root@dgxws01:~# docker images
REPOSITORY                  TAG                 IMAGE ID            CREATED             SIZE
nvcr.io/nvidia/pytorch      19.05-py3           7e98758d4777        4 weeks ago         7.55GB
nvcr.io/nvidia/tensorflow   19.05-py2           5ce2c011e671        4 weeks ago         6.76GB
root@dgxws01:~#
```

Build an image from a dockerfile

A dockerfile is a script that contains instructions to customize and configure a container from a base image

Here are some common commands:

- FROM is Mandatory as the first instruction. It denotes the base image to be built from. Use a tag to specify the image.
- RUN = runs commands after Docker image has been created.
- CMD = Run any command when Docker image is started. Use only one CMD instruction in a Dockerfile.
- ENV = Set container environment variables.
- WORKDIR = Sets the working directory for any RUN, CMD, ENTRYPOINT, COPY and ADD instructions.

Instructions can be found here: https://docs.nvidia.com/ngc/ngc-user-guide/custcontfrm.html#custcontfrm

Example using horovod and creating an image from a dockerfile (file is located in slide notes):

```
mkdir horovod-docker
cp /shareDB/wexac_workshop/Dockerfiles/Horovod/Dockerfile horovod-docker/Dockerfile
docker build -t horovod:latest horovod-docker
```

How to modify a docker image

There are two main ways to edit a docker image.

1. The best practice is to modify a dockerfile to include any changes you would require. This approach is preferred as one can easily document changes and better maintain the image.

2. Alternatively, one can use `docker commit` to create a new image from a currently open container.

```
root@ibdgx001:~# docker ps
CONTAINER ID        IMAGE               COMMAND             CREATED             STATUS              PORTS                     NAMES
6ac93b585313        horovod:latest      "/bin/bash"         8 days ago          Up 8 days           0.0.0.0:32768->22/tcp     horovod_master
```

```
root@ibdgx001:~# docker commit 6ac93b585313 ibdgx001:5000/horovod_master
sha256:bf79c96f812e1c71c75dc7bb1cb4cf0ee8e9040238841e9b51a321e1332e55b9
root@ibdgx001:~# docker images
REPOSITORY                          TAG                 IMAGE ID            CREATED             SIZE
ibdgx001:5000/horovod_master        latest              bf79c96f812e        11 seconds ago      8.95GB
horovod                             latest              ffe80b4ddef7        12 days ago         7.91GB
```

How to push an image to the local repository

- Tag the docker image:

  ```
  docker tag pytorch:19.05-py3 ibdgx001:5000/tensorflow-test
  ```

- Push the tagged docker image to the local repository:

  ```
  docker push ibdgx001:5000/tensorflow-test
  ```

```
root@dgxws01:~# docker images
REPOSITORY                  TAG                 IMAGE ID            CREATED             SIZE
nvcr.io/nvidia/pytorch      19.05-py3           7e98758d4777        4 weeks ago         7.55GB
nvcr.io/nvidia/tensorflow   19.05-py2           5ce2c011e671        4 weeks ago         6.76GB
root@dgxws01:~# docker tag nvcr.io/nvidia/tensorflow:19.05-py2 ibdgx001:5000/tensorflow-test
root@dgxws01:~# docker push ibdgx001:5000/tensorflow-test
The push refers to repository [ibdgx001:5000/tensorflow-test]
84ac6b166875: Pushed
805629a17ac4: Pushed
```

- Check:

  ```
  Docker images
  ```

- You should see both the original image as well as the tagged image

```
REPOSITORY                          TAG                 IMAGE ID            CREATED             SIZE
nvcr.io/nvidia/pytorch              19.05-py3           7e98758d4777        4 weeks ago         7.55GB
ibdgx001:5000/tensorflow-test       latest              5ce2c011e671        4 weeks ago         6.76GB
nvcr.io/nvidia/tensorflow           19.05-py2           5ce2c011e671        4 weeks ago         6.76GB
root@dgxws01:~#
```

How to run an interactive job

Run an interactive job by using the -Is option:

```
bsub -q waic-interactive -gpu num=1:j_exclusive=yes -Is /bin/bash
```

Opening an IDE:

```
bsub -q waic-interactive -gpu num=1:j_exclusive=yes -Is /bin/bash
source /etc/profile
module load anaconda
export DISPLAY=<your local computer ip here>:0
spyder
```

How to run a job using a pulled image

Create a file to run the job:

```
cat useCase1
#BSUB -J useCase1
#BSUB -env LSB_CONTAINER_IMAGE=ibdgx001:5000/tensorflow-test
#BSUB -app nvidia-gpu
#BSUB -gpu num=2:j_exclusive=yes
#BSUB -q waic-short
#BSUB -oo test_useCase_out.log
#BSUB -eo test_useCase_err.log
mpiexec -np 2 python /workspace/nvidia-examples/cnn/resnet.py --layers=50 --
precision=fp16 --log_dir=output/resnet50_useCase1
```

How to run a job using a pulled image

Run the job:

```
cat useCase1 | bsub
```

You can check the job using bjobs/bpeek:

```
bjobs -q waic-short -J useCase1

bpeek -f -J test_useCase
```

```
[adamma@access ~]$ cat useCase1 | bsub
Memory reservation is (MB): 1024
Memory Limit is (MB): 1024
Job <401028> is submitted to queue <waic-short>.
[adamma@access ~]$ bpeek -f -J useCase1
<< output from stdout >>
================

NVIDIA Release 19.05 (build 6390159)
TensorFlow Version 1.13.1

Container image Copyright (c) 2019, NVIDIA CORPORATION.  All rights reserved.
Copyright 2017-2019 The TensorFlow Authors.  All rights reserved.

Various files include modifications (c) NVIDIA CORPORATION.  All rights reserved.
NVIDIA modifications are covered by the license terms that apply to the underlying project or file.

NOTE: Legacy NVIDIA Driver detected.  Compatibility mode ENABLED.

NOTE: Detected MOFED driver 4.0-1.0.1; version automatically upgraded.

NOTE: MOFED driver was detected, but nv_peer_mem driver was not detected.
      Multi-node communication performance may be reduced.

('PY', '2.7.12 (default, Nov 12 2018, 14:36:49) \n[GCC 5.4.0 20160609]')
('TF', '1.13.1')
('PY', '2.7.12 (default, Nov 12 2018, 14:36:49) \n[GCC 5.4.0 20160609]')
('TF', '1.13.1')
Script arguments:
  --layers 50
  --predict False
  --precision fp16
  --batch_size 256
  --log_dir output/resnet50_useCase01
  --iter_unit epoch
  --num_iter 90
  --use_xla False
  --display_every 10
Training
Training
  Step Epoch Img/sec   Loss  LR
     1   1.0    47.5  7.589  8.559 2.00000
    10  10.0   627.8  4.946  5.918 1.62000
    20  20.0  1457.6  0.338  1.314 1.24469
    30  30.0  1467.3  0.056  1.037 0.91877
    40  40.0  1470.8  0.065  1.047 0.64222
    50  50.0  1466.6  0.045  1.027 0.41506
    60  60.0  1429.0  0.013  0.995 0.23728
    70  70.0  1454.5  0.001  0.982 0.10889
    80  80.0  1494.3  0.000  0.980 0.02988
    90  90.0  1157.7  0.000  0.980 0.00025
[adamma@access ~]$
```

Submitting an array job

Array Script:

```
./seq_arr.sh -f c.sh -e 10
```

The `-e` must match the elements in the array. In this case (c.sh) there are ten, "`#BSUB -J test[1-10]`".

bsub file(c.sh):

```
#BSUB -q new-short
#BSUB -J test[1-10]
#BSUB -o out/out.%J
#BSUB -e err/err.%J
#BSUB -H
sleep 5
```

The `-H` option is very important!

(Holds the job in the PSUSP state when the job is submitted).

```
Usage:
    seq_arr.sh -f bsub_file -e max_element -c bsub_command

Examples:

Send bsub file with sequence array:
    seq_arr.sh -f my_bsub.sh -e 4

Send the submit in the command line:
    seq_arr.sh -e 5 -c "bsub -H -J "test[1-5]" sleep 5"

[adamma@access4 ~]$ ./seq_arr.sh -f c.sh -e 10

NOTE: the bsub command must have the -H option!!!


c.sh
Job 130511
Parameters of job <130511[2]> are being changed
Parameters of job <130511[3]> are being changed
Parameters of job <130511[4]> are being changed
Parameters of job <130511[5]> are being changed
Parameters of job <130511[6]> are being changed
Parameters of job <130511[7]> are being changed
Parameters of job <130511[8]> are being changed
Parameters of job <130511[9]> are being changed
Parameters of job <130511[10]> are being changed
Job <130511>: Operation is in progress
[adamma@access4 ~]$ bjobs
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
130511  adamma  PSUSP new-short  access4.wex              test[1]    Jun 13 13:53
130511  adamma  PSUSP new-short  access4.wex              test[2]    Jun 13 13:53
130511  adamma  PSUSP new-short  access4.wex              test[3]    Jun 13 13:53
130511  adamma  PSUSP new-short  access4.wex              test[4]    Jun 13 13:53
130511  adamma  PSUSP new-short  access4.wex              test[5]    Jun 13 13:53
130511  adamma  PSUSP new-short  access4.wex              test[6]    Jun 13 13:53
130511  adamma  PSUSP new-short  access4.wex              test[7]    Jun 13 13:53
130511  adamma  PSUSP new-short  access4.wex              test[8]    Jun 13 13:53
130511  adamma  PSUSP new-short  access4.wex              test[9]    Jun 13 13:53
130511  adamma  PSUSP new-short  access4.wex              test[10]   Jun 13 13:53
[adamma@access4 ~]$ bjobs
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
130511  adamma  RUN   new-short  access4.wex cn293.wexac test[2]    Jun 13 13:53
130511  adamma  PEND  new-short  access4.wex              test[3]    Jun 13 13:53
130511  adamma  PEND  new-short  access4.wex              test[4]    Jun 13 13:53
130511  adamma  PEND  new-short  access4.wex              test[5]    Jun 13 13:53
130511  adamma  PEND  new-short  access4.wex              test[6]    Jun 13 13:53
130511  adamma  PEND  new-short  access4.wex              test[7]    Jun 13 13:53
130511  adamma  PEND  new-short  access4.wex              test[8]    Jun 13 13:53
130511  adamma  PEND  new-short  access4.wex              test[9]    Jun 13 13:53
130511  adamma  PEND  new-short  access4.wex              test[10]   Jun 13 13:53
[adamma@access4 ~]$ bjobs
JOBID   USER    STAT  QUEUE      FROM_HOST   EXEC_HOST   JOB_NAME   SUBMIT_TIME
130511  adamma  RUN   new-short  access4.wex cn442.wexac test[5]    Jun 13 13:53
130511  adamma  PEND  new-short  access4.wex              test[6]    Jun 13 13:53
130511  adamma  PEND  new-short  access4.wex              test[7]    Jun 13 13:53
130511  adamma  PEND  new-short  access4.wex              test[8]    Jun 13 13:53
130511  adamma  PEND  new-short  access4.wex              test[9]    Jun 13 13:53
130511  adamma  PEND  new-short  access4.wex              test[10]   Jun 13 13:53
[adamma@access4 ~]$
```

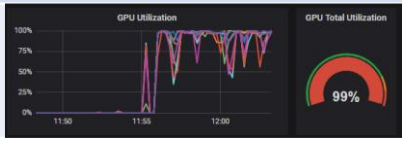
UseCase1 + Grafana

```
cat << EOF_useCase1 > ~/useCase1
#BSUB -J useCase1
#BSUB -env LSB_CONTAINER_IMAGE=nvcr.io/nvidia/tensorflow:19.03-py3
#BSUB -app nvidia-gpu
#BSUB -gpu num=2:j_exclusive=yes
#BSUB -q waic-short
#BSUB -oo useCase1_out.log
#BSUB -eo useCase1_err.log
mpiexec -np 2 python \
/workspace/nvidia-examples/cnn/resnet.py \
--layers=50 \
--precision=fp16 \
--log_dir=output/resnet50_useCase1
EOF_useCase1
```

UseCase1 + Grafana

Instructions	Commands	Expected Results
Submit a job	`bsub < ~/useCase1`	Job is submitted to queue `waic-short`
Verify the job is enqueued and starts running	`bjobs -q waic-short -J useCase1`	Job `useCase1` appears in the output, the job state is RUN
Verify the job is running correctly	`bpeek -f -J useCase1`	Job progresses as expected

Verify the job executed correctly	Inspect file `useCase1_out.log`	File contains lines:
		`Step Epoch Img/sec Loss LR`
		`1 1.0 156.8 7.726 8.697 2.00000`
		`10 10.0 1289.8 5.758 6.729 1.62000`
		`20 20.0 4417.6 2.035 3.010 1.24469`
		`30 30.0 6297.6 0.010 0.991 0.91877`
		`40 40.0 6303.1 0.000 0.976 0.64222`
		`50 50.0 6339.3 0.000 0.968 0.41506`
		Average `Img/Sec` value for steps 30+ should be above 6200

Navigate to Grafana UI	`Navigate to http://waicmgmt01.wexac.weizmann.ac.il:30200`	Successful navigation to Grafana Home Dashboard
Navigate to GPU Nodes dashboard and select the node running . Check node utilization		Per-GPU utilization and Total GPU utilization is above 90% 

UseCase2

```
cat << EOF_useCase2 > ~/useCase2
#BSUB -J useCase2
#BSUB -env "LSB_CONTAINER_IMAGE=ibdgx001:5000/usecase2_1"
#BSUB -app nvidia-gpu
#BSUB -gpu num=1:j_exclusive=yes
#BSUB -q gpu-short
#BSUB -oo useCase2_out.log
#BSUB -eo useCase2_err.log
export MLM_LICENSE_FILE=1700@license.weizmann.ac.il
cd /shareDB/Wexac_workshop/useCase2_code/usecase2/Matlab/exp_code
echo; echo; echo "Running MATLAB"
echo "Test 2.1.1:"
/usr/local/bin/matlab -nodisplay -nosplash -nodesktop -r
"eval_validation_set_exact('0', 0, 1); exit"
echo "Test 2.1.2:"
/usr/local/bin/matlab -nodisplay -nosplash -nodesktop -r
"eval_validation_set_exact('0', 16, 1); exit"
echo "Test 2.1.3:"
/usr/local/bin/matlab -nodisplay -nosplash -nodesktop -r
"eval_validation_set_exact('16', 0, 1); exit"
echo "Test 2.1.4:"
/usr/local/bin/matlab -nodisplay -nosplash -nodesktop -r
"eval_validation_set_exact('16', 16, 1); exit"
echo "Test 2.1.5:"
/usr/local/bin/matlab -nodisplay -nosplash -nodesktop -r
"eval_validation_set_exact('64_32_16_8_4_0', 0, 1); exit"
echo "Test 2.1.6:"
/usr/local/bin/matlab -nodisplay -nosplash -nodesktop -r
"eval_validation_set_exact('64_32_16_8_4_0', 16, 1); exit"
echo; echo; echo "Running PYTHON CONVERT"
echo "Test 2.2.1:"
cd /home/labs/testing/class5/Documents/MATLAB/usecase2/python
python3 convert_columbiagaze_imdb_mat_to_pkl.py
echo; echo; echo "Running PYTHON Imagenet ResNet50"
echo "Test 2.3.1:"
python3 imagenet_resnet50_readout.py --train-res 'hi' --test-blur 0 --cond
'eyes' --layer 3 --input-type 'face_wo_chinrest' --gpu 1 --batch-size 10
echo "Test 2.3.2:"
python3 imagenet_resnet50_readout.py --train-res 'hi' --test-blur 0 --cond
'head' --layer 3 --input-type 'face_wo_eyes' --gpu 1 --batch-size 10
echo "Test 2.3.3:"
python3 imagenet_resnet50_readout.py --train-res 'low' --test-blur 0 --cond
'eyes' --layer 3 --input-type 'face_wo_eyes' --gpu 1 --batch-size 10
echo "Test 2.3.4:"
python3 imagenet_resnet50_readout.py --train-res 'low' --test-blur 16 --cond
'head' --layer 3 --input-type 'eyes' --gpu 1 --batch-size 10
EOF_useCase2
```

UseCase2 - Matlab and PyTorch under a common environment

Instructions	Commands	Expected results
Verify custom image exists	`docker image ls testing:usecase2`	Image `testing:usecase2` exists
Tag image for upload to repository	`docker tag testing:usecase2 ibdgx001:5000/usecase2_1`	Successful execution
Upload image to cloud repository	`docker push ibdgx001:5000/usecase2_1`	All layers are pushed successfully

UseCase2 - Matlab and PyTorch under a common environment

Instructions	Commands	Expected results	

Submit a job	`bsub < ~/useCase2`	Job is submitted to queue waic-short	`[06-May-2019 10:45:08] Evaluating 168 trials (3 batches, 60 images per batch)`
			`[06-May-2019 10:45:08] Running batch #1`
			`[06-May-2019 10:45:10] Running batch #2`
			`[06-May-2019 10:45:11] Running batch #3`
			`Mean classification (LEFT/RIGHT) eyes accuracy is 98.21%`
			`[06-May-2019 10:45:12] Evaluating 168 trials (3 batches, 60 images per batch)`
			`[06-May-2019 10:45:12] Running batch #1`
			`[06-May-2019 10:45:13] Running batch #2`
			`[06-May-2019 10:45:14] Running batch #3`
			`Mean classification (LEFT/RIGHT) head accuracy is 100.00%`
			`Accuracy for sub-tests is:`
			`2.1.1 - 100%`
			`2.1.2 - above 70%`
			`2.1.3 - above 80%`
			`2.1.4 - above 95%`
			`2.1.5 - 100%`
			`2.1.6 - 100%`

Verify the job is enqueued and starts running	`bjobs -q waic-short -J useCase2`	Job useCase2 appears in the output, the job state is RUN	
Verify the job is running correctly	`bpeek -f -J useCase2`	Job progresses as expected	
Verify Matlab part of the job executed correctly	Inspect `useCase2_out.log` file	Matlab runs with outputs similar to the following: →	

Verify "python convert" part of the job executed successfully	Inspect `useCase2_out.log` file	Log contains following output:
		`Running PYTHON CONVERT`
		`Test 2.2.1:`
		`convert_columbiagaze_imdb_mat_to_pkl SUCCESSFUL!`	

Verify "python imagenet resnet50" part of the job executed successfully			

UseCase3 - Intensive I/O – video dataset

```
cat << EOF_useCase3 > ~/useCase3
#BSUB -J useCase3
#BSUB -env LSB_CONTAINER_IMAGE=nvcr.io/weizmann1/waic:usecase3
#BSUB -app nvidia-gpu
#BSUB -gpu num=2:j_exclusive=yes
#BSUB -q gpu-short
#BSUB -oo useCase3_out.log
#BSUB -eo useCase3_err.log
export
PATH=/opt/conda/bin:/usr/local/mpi/bin:/usr/local/nvidia/bin:/usr/local/cuda/bi
n:/usr/local/sbin:/usr/local/bin:${PATH}
cd useCase3_code
/opt/conda/bin/python train.py --t_win 31 --epochs 2 --tag useCase3 -b 8
EOF_useCase3
```

UseCase3 - Intensive I/O – video dataset

Instructions	Commands	Expected results
First copy code to home directory: cp -R /shareDB/wexac_workshop/useCase3_code/ ~/		
Submit a job	bsub < ~/useCase3	Job is submitted to queue waic-short
Verify the job is enqueued and starts running	bjobs -q waic-short -J useCase3	Job useCase3 appears in the output, the job state is RUN
Verify the job is running correctly	bpeek -f -J useCase3	Job progresses as expected. After running for about 5 minutes useCase3_err.log file's last line looks like: train 0: 1%| | 8/1000 [05:21<7:24:43, 26.90s/it]
Verify the job executed correctly	Wait till the job finishes running (should take about 6-7 hours). Inspect useCase3_*.log files	useCase3_err.log file doesn't contain any significant errors. Any errors related to qsub can be ignored. useCase2_out.log file contains expected job execution logs

Troubleshooting for usecases

For the use cases we need to copy the code to our home directory (run from your specific home directory):

```
cp -R /shareDB/wexac_workshop/useCase3_code/ ~/
```

If output/ exists after running useCase1 remove it and try running useCase1 again

```
rm -R output/
```

WEXAC Web Resources

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

http://www.weizmann.ac.il/DIS/sites/DIS/files/uploads/it/wexac_training_session.pdf

https://insightiq.weizmann.ac.il

http://master-ops.wexac.weizmann.ac.il/ganglia/

http://lsfutil.wexac.weizmann.ac.il

https://www.facebook.com/HpcAtWeizmann/

http://wiki.weizmann.ac.il/ai_wiki/index.php/WAIC_cluster

Join the WhatsApp group!

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

Questions ?

Thank you !

hpc@weizmann.ac.il