

Matlab on the Biowulf Cluster

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High Performance Computing Services

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Download these slides from:

<https://hpc.nih.gov/training/handouts/matlab4biowulf.pdf>

Outline

- Motivation
- Quick review of the Biowulf cluster
- Matlab Institute Wide License
- Running Matlab scripts interactively
- Running Matlab scripts as batch jobs
 - Running single job with *sbatch*
 - Running job array with *swarm*
 - Monitoring jobs
 - Limits, pitfalls and caveats
- Conclusion

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- We have implemented a new licensing model for Matlab
- This new model gives Biowulf users access to virtually UNLIMITED Matlab licenses and ALL toolboxes
- Users do not need to compile their Matlab code to submit batch jobs to the cluster

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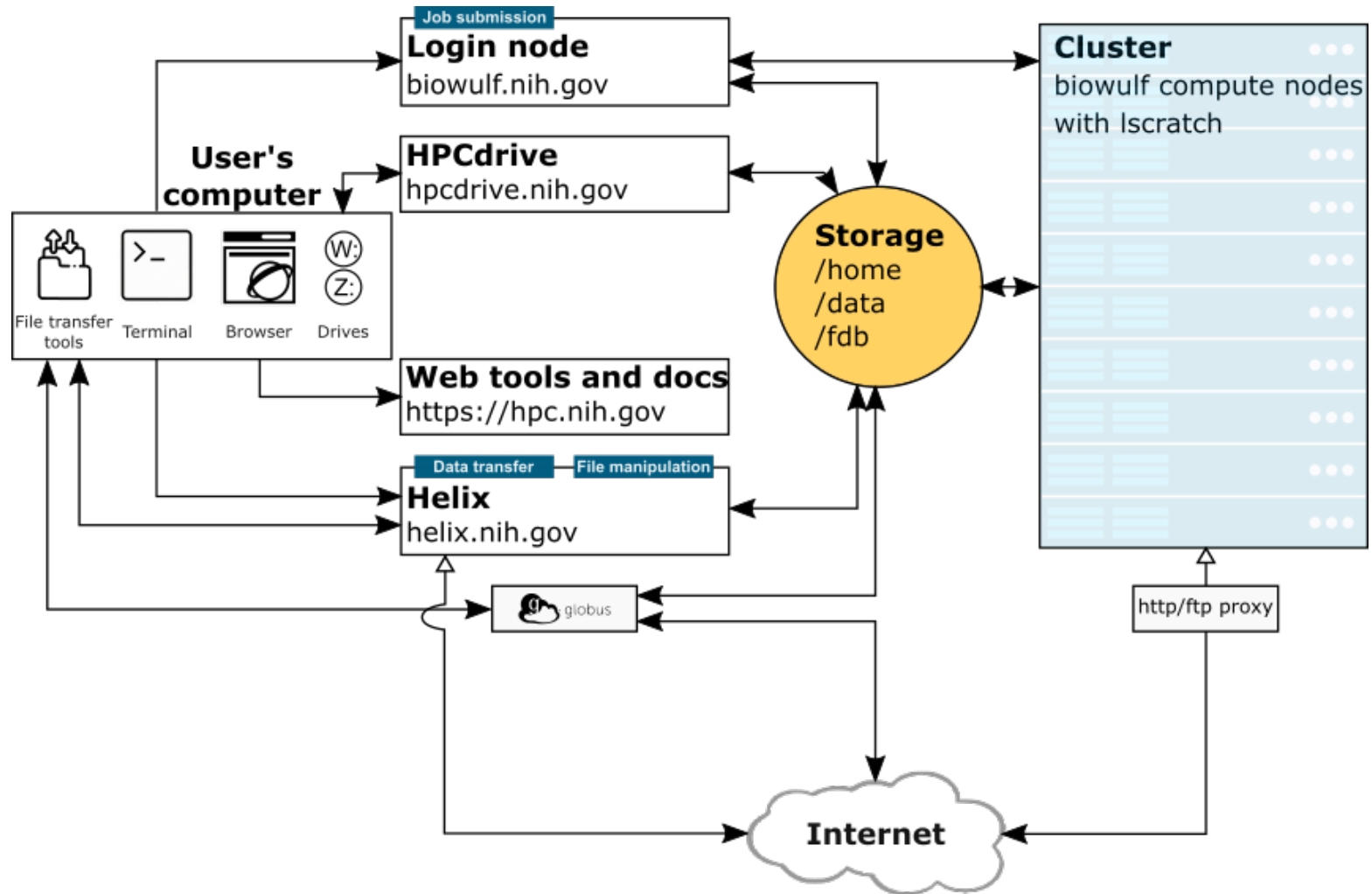
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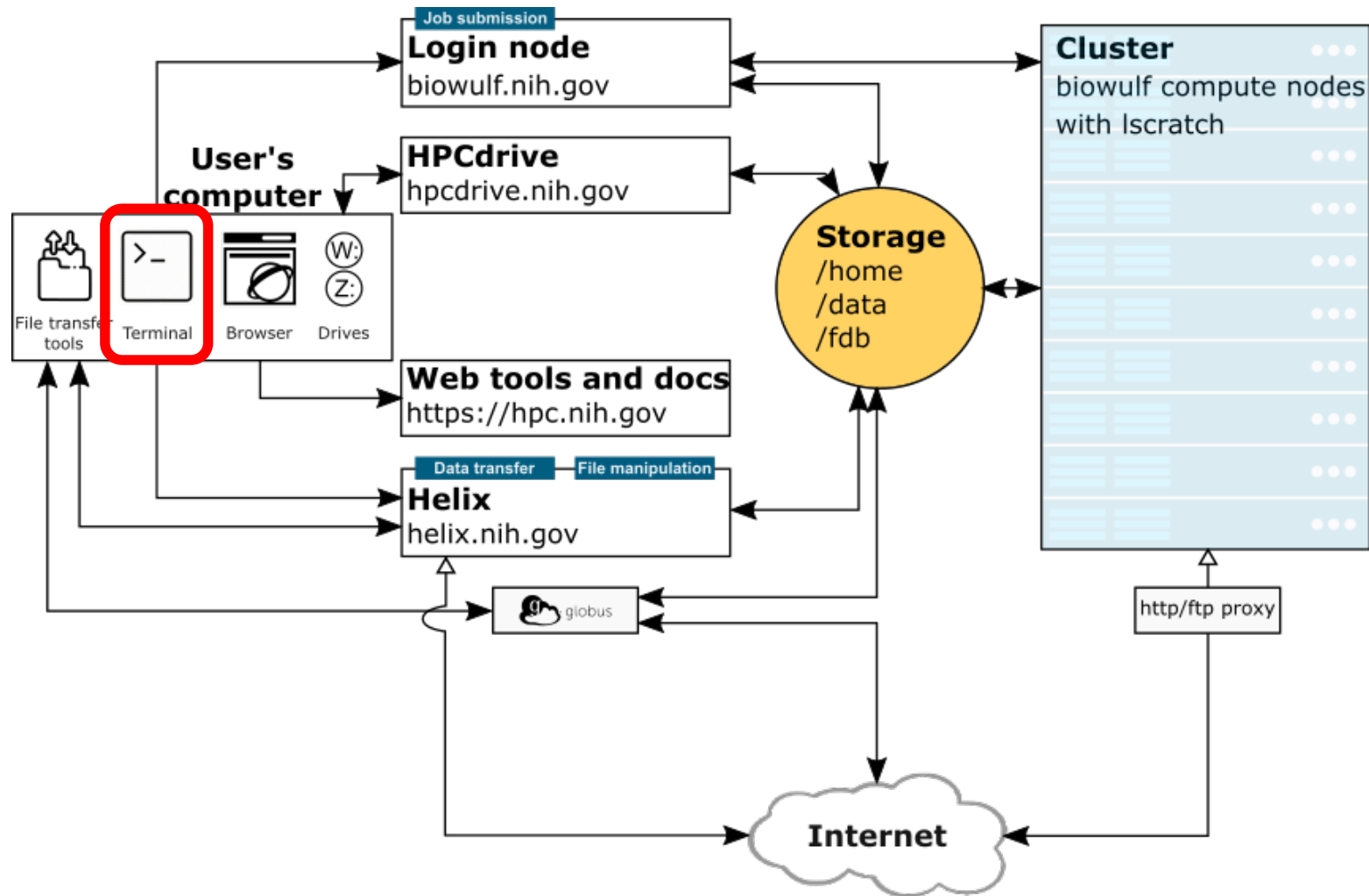
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Quick review of Biowulf cluster



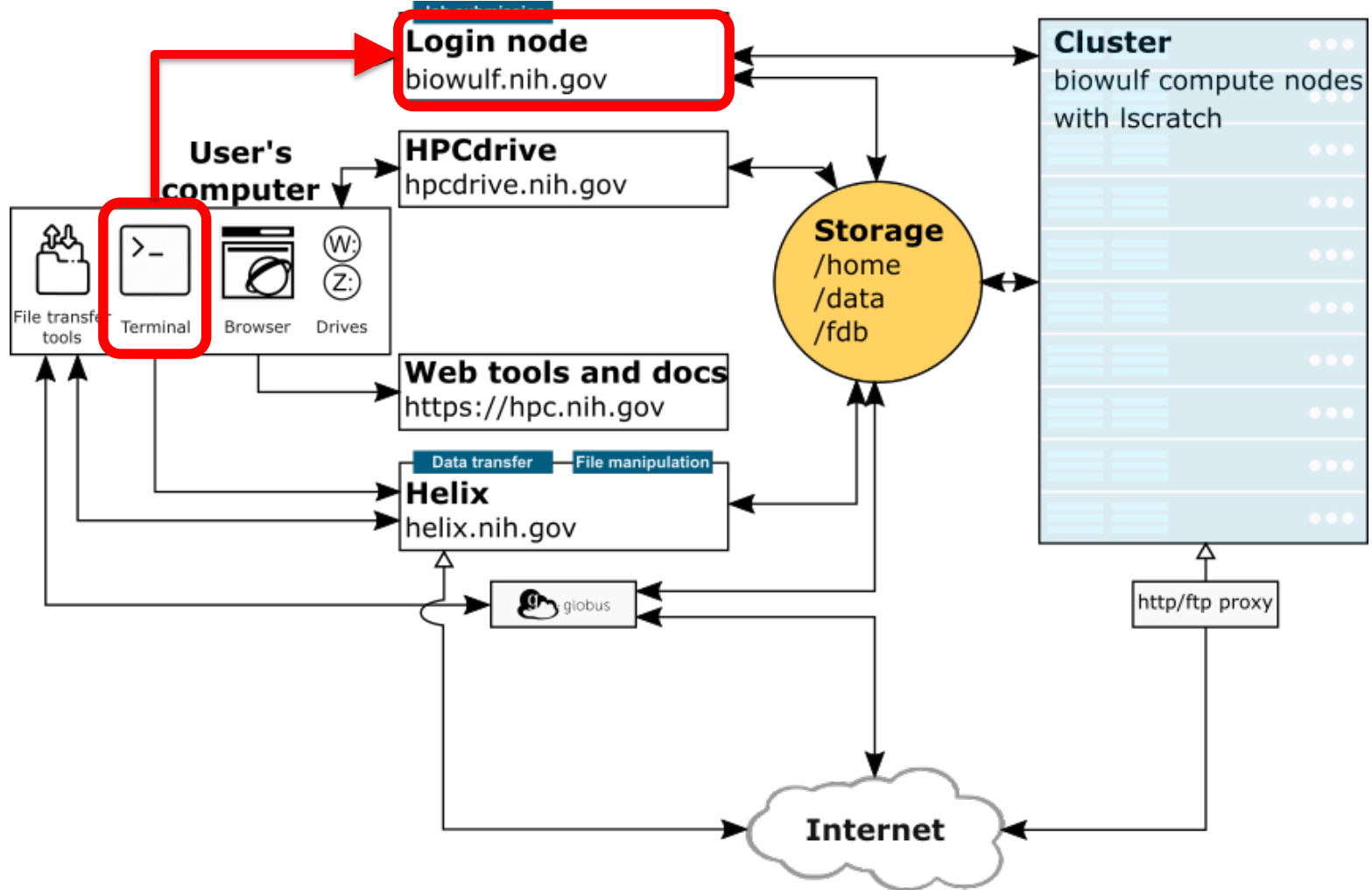
Source: <https://hpc.nih.gov/systems>

Quick review of Biowulf cluster



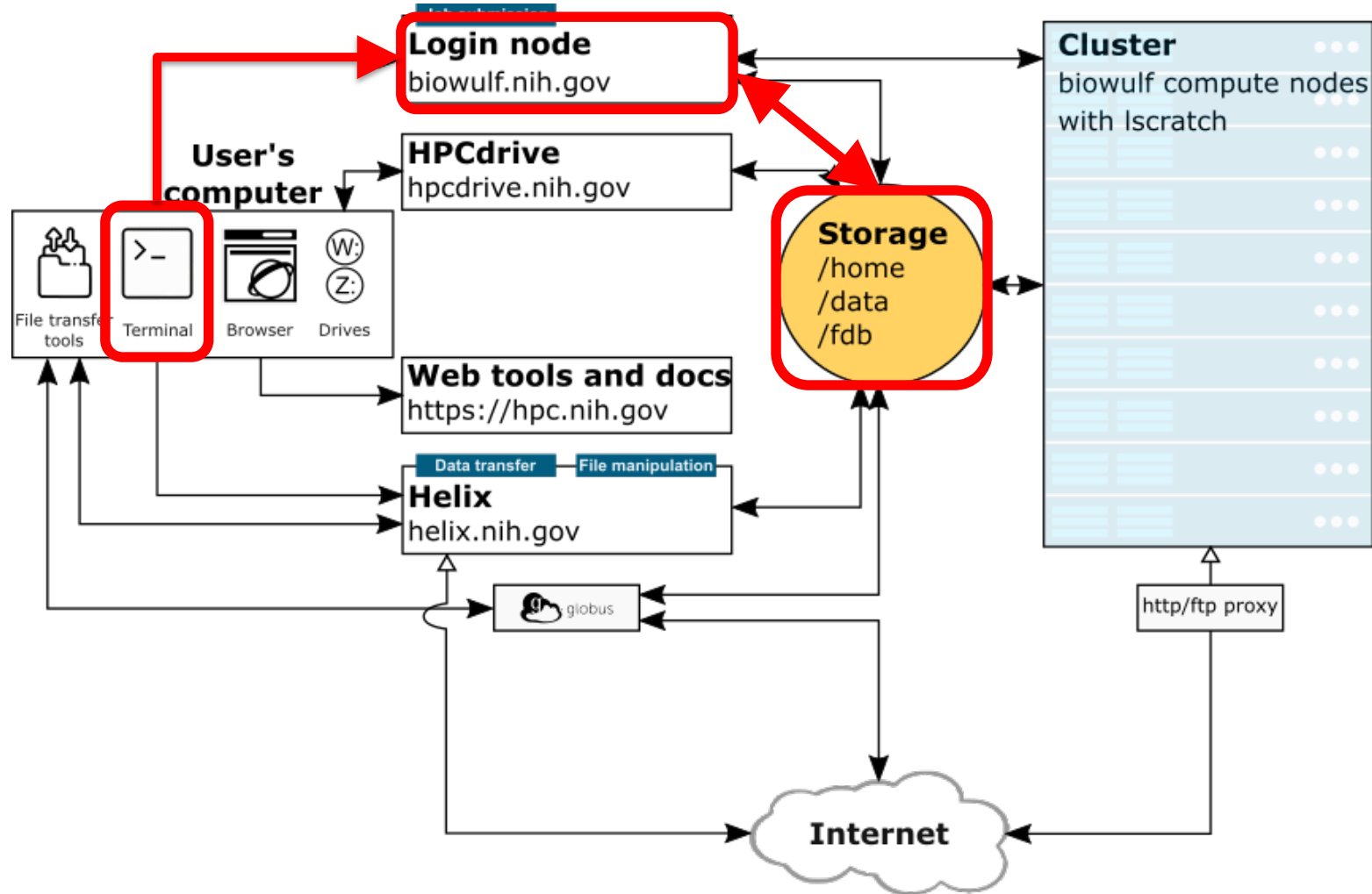
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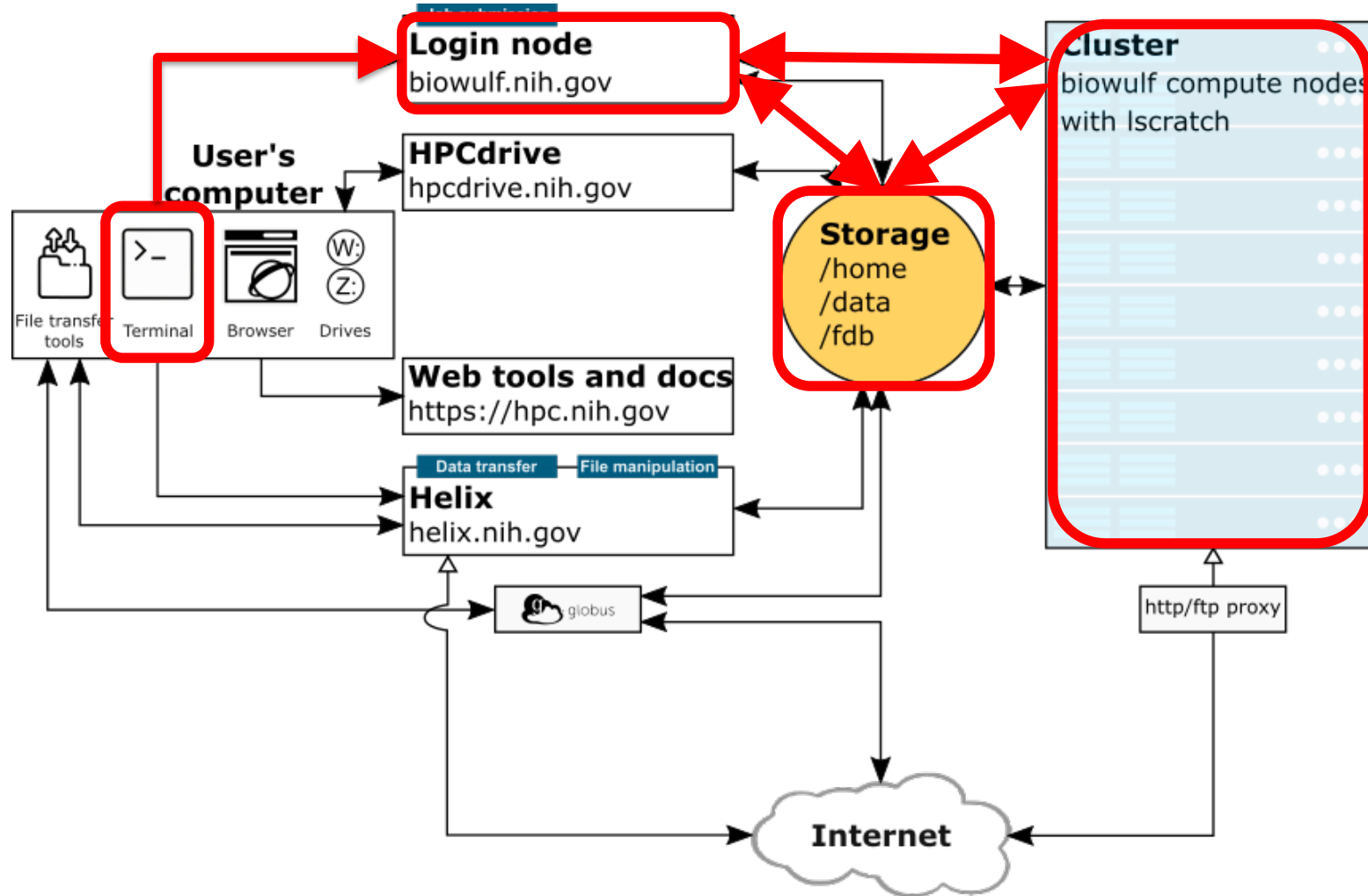
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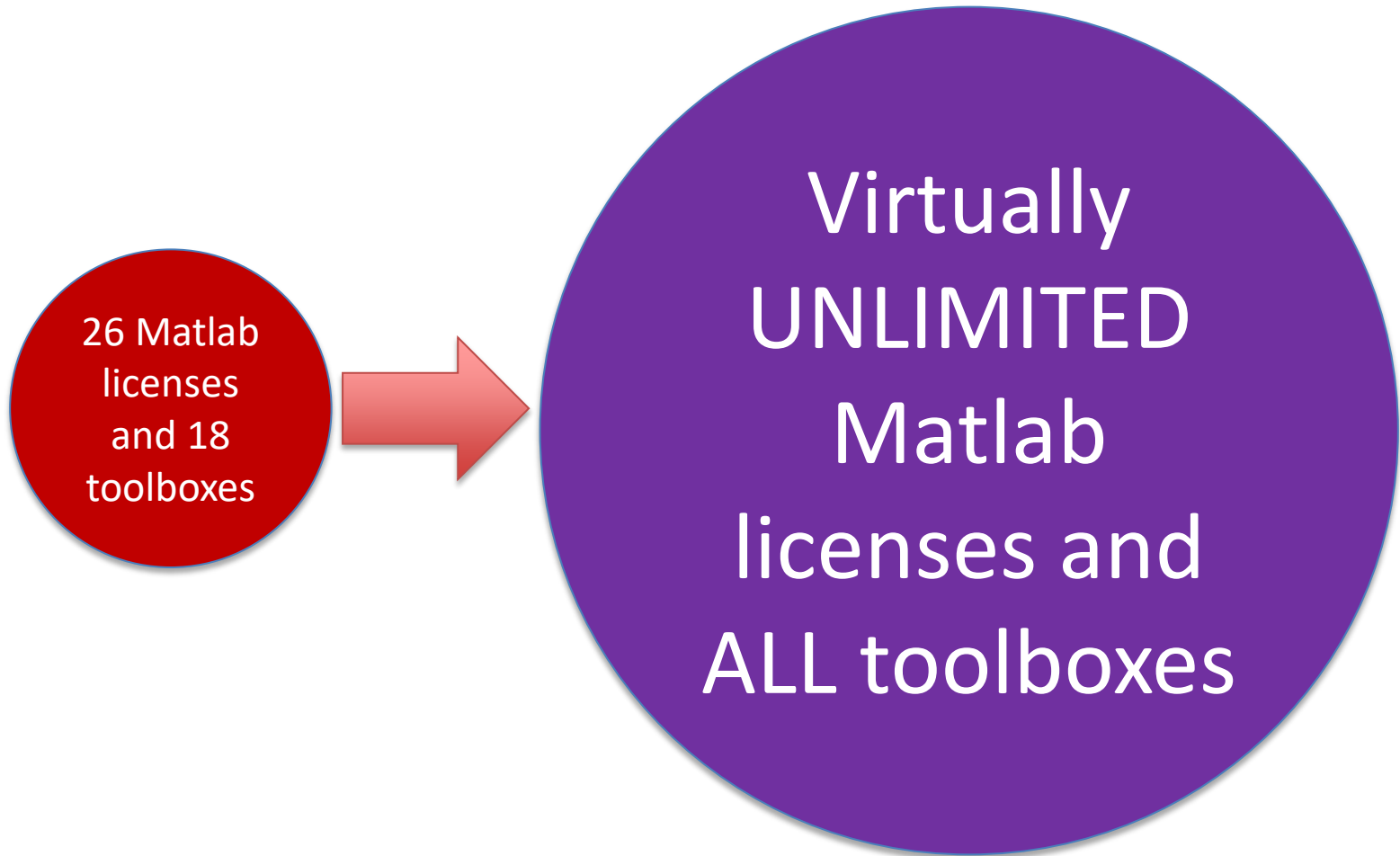


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Matlab Institute Wide License (IWL)

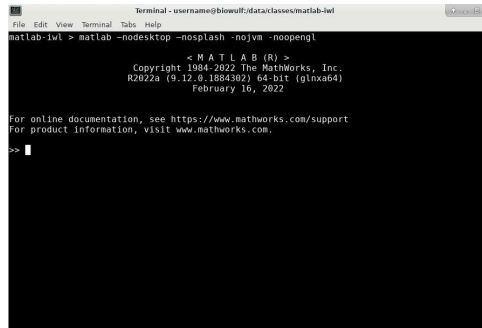


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Running Matlab scripts interactively

Command-line Matlab:



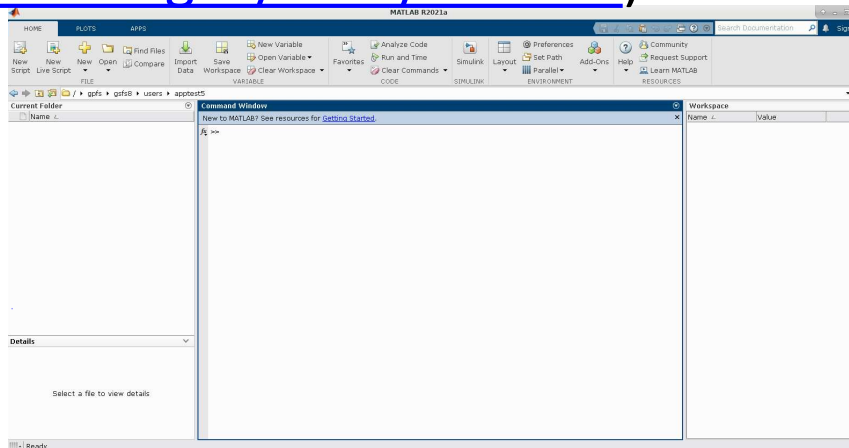
```
Terminal - username@biowulf:/data/classes/matlab-lwl
matlab-lwl > matlab -nodesktop -nosplash -nojvm -noopenGL

< MATLAB (R) >
Copyright 1984-2022 The MathWorks, Inc.
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February 16, 2022

For online documentation, see https://www.mathworks.com/support
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>> |
```

Graphical Matlab using nomachine NX
(see <https://hpc.nih.gov/docs/nx.html>):



Source: <https://hpc.nih.gov/apps/Matlab.html>

Running Matlab scripts interactively

```
local-computer> ssh username@biowulf.nih.gov
biowulf> sinteractive
cn1234> cd /data/$USER
cn1234> cp -r /data/classes/matlab-iwl .
cn1234> cd matlab-iwl
cn1234> module load matlab
[+] Loading Matlab 2022a on cn1234
cn1234> matlab -nodesktop -nosplash -nojvm -noopengl
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< M A T L A B (R) >

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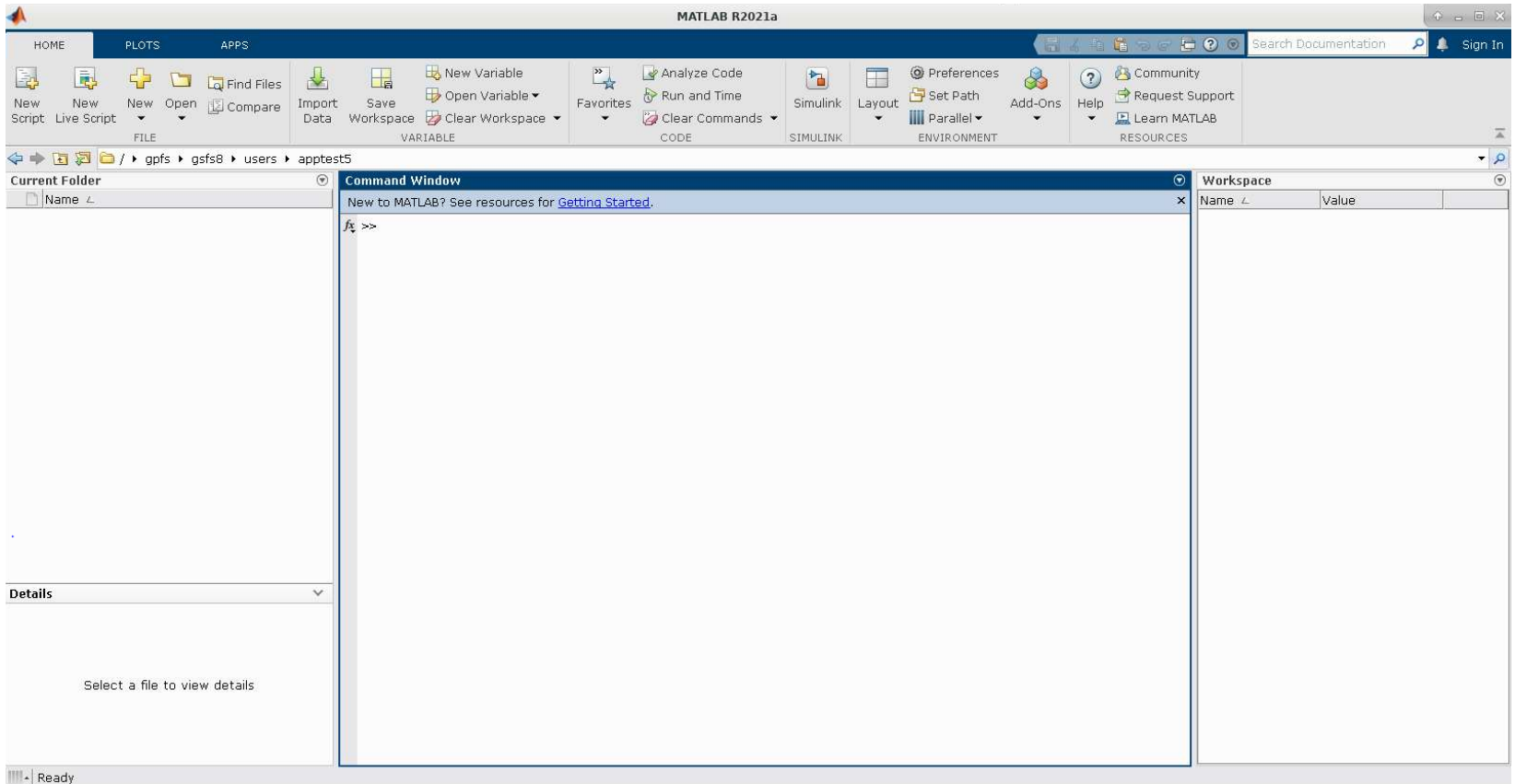
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```
local-computer> ssh username@biowulf.nih.gov
biowulf> sinteractive --mem=4g
cn1234> cd /data/$USER
cn1234> cp -r /data/classes/matlab-iwl .
cn1234> cd matlab-iwl
cn1234> module load matlab
[+] Loading Matlab 2022a on cn1234
cn1234> matlab &
```

Running Matlab scripts interactively

```
local-computer> ssh username@biowulf.nih.gov
biowulf> sinteractive --mem=4g
cn1234> cd /data/$USER
cn1234> cp -r /data/classes/matlab-iwl .
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Running single job with *sbatch*

```
Terminal - teacher@biowulf:/data/teacher/matlab-iwl
File Edit View Terminal Tabs Help
teacher > ls
hyp.m hyp.sh hyp.swarm
teacher > cat hyp.sh
#!/bin/bash
#SBATCH --job-name=hypotenuse
#SBATCH --cpus-per-task=2
#SBATCH --mem=2g
#SBATCH --time=00:30:00

module load matlab

matlab -nodisplay -nodesktop -nojvm -nosplash -r 'hyp(3,4); exit;'
teacher > sbatch hyp.sh
43060138
teacher > ls
hyp.m hyp.sh hyp.swarm slurm-43060138.out
teacher > cat slurm-43060138.out
[+] Loading Matlab 2022a on cn0859

                < M A T L A B (R) >
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H =

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teacher > █
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     5

teacher > █
```

Running single job with *sbatch*

```
Terminal - teacher@biowulf:/data/teacher/matlab-iwl
File Edit View Terminal Tabs Help
teacher > ls
hyp.m hyp.sh hyp.swarm
teacher > cat hyp.sh
#!/bin/bash
#SBATCH --job-name=hypotenuse
#SBATCH --cpus-per-task=2
#SBATCH --mem=2g
#SBATCH --time=00:30:00

module load matlab

matlab -nodisplay -nodesktop -nojvm -nosplash -r 'hyp(3,4); exit;'
teacher > sbatch hyp.sh
43060138
teacher > ls
hyp.m hyp.sh hyp.swarm slurm-43060138.out
teacher > cat slurm-43060138.out
[+] Loading Matlab 2022a on cn0859

                < M A T L A B (R) >
    Copyright 1984-2022 The MathWorks, Inc.
    R2022a (9.12.0.1884302) 64-bit (glnxa64)
    February 16, 2022

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teacher > cat slurm-43060138.out
[+] Loading Matlab 2022a on en0859

                < M A T L A B (R) >
        Copyright 1984-2022 The MathWorks, Inc.
        R2022a (9.12.0.1884302) 64-bit (glnxa64)
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Outline

- Motivation
- Quick review of the Biowulf cluster
- Matlab Institute Wide License
- Running Matlab scripts interactively
- Running Matlab scripts as batch jobs
 - Running single job with *sbatch*
 - Running job array with *swarm*
 - Monitoring jobs
 - Limits, pitfalls and caveats
- Conclusion

Running job array with *swarm*

```
Terminal - teacher@biowulf:/data/teacher/matlab-iwl
File Edit View Terminal Tabs Help
teacher > ls
hyp.m hyp.sh hyp.swarm slurm-43059485.out
teacher > cat hyp.swarm
#SWARM -t 2 -g 2 --time 00:20:00 -m matlab
matlab -nodisplay -nodesktop -nojvm -nosplash -r 'hyp(3,4); exit;'
matlab -nodisplay -nodesktop -nojvm -nosplash -r 'hyp(5,6); exit;'
matlab -nodisplay -nodesktop -nojvm -nosplash -r 'hyp(7,8); exit;'
teacher > swarm hyp.swarm
43059569
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hyp.m hyp.swarm swarm_43059569_0.e swarm_43059569_1.e swarm_43059569_2.e
hyp.sh slurm-43059485.out swarm_43059569_0.o swarm_43059569_1.o swarm_43059569_2.o
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----- COMMAND EXECUTED: -----
( matlab -nodisplay -nodesktop -nojvm -nosplash -r 'hyp(3,4); exit;' )
-----

< M A T L A B (R) >
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< M A T L A B (R) >
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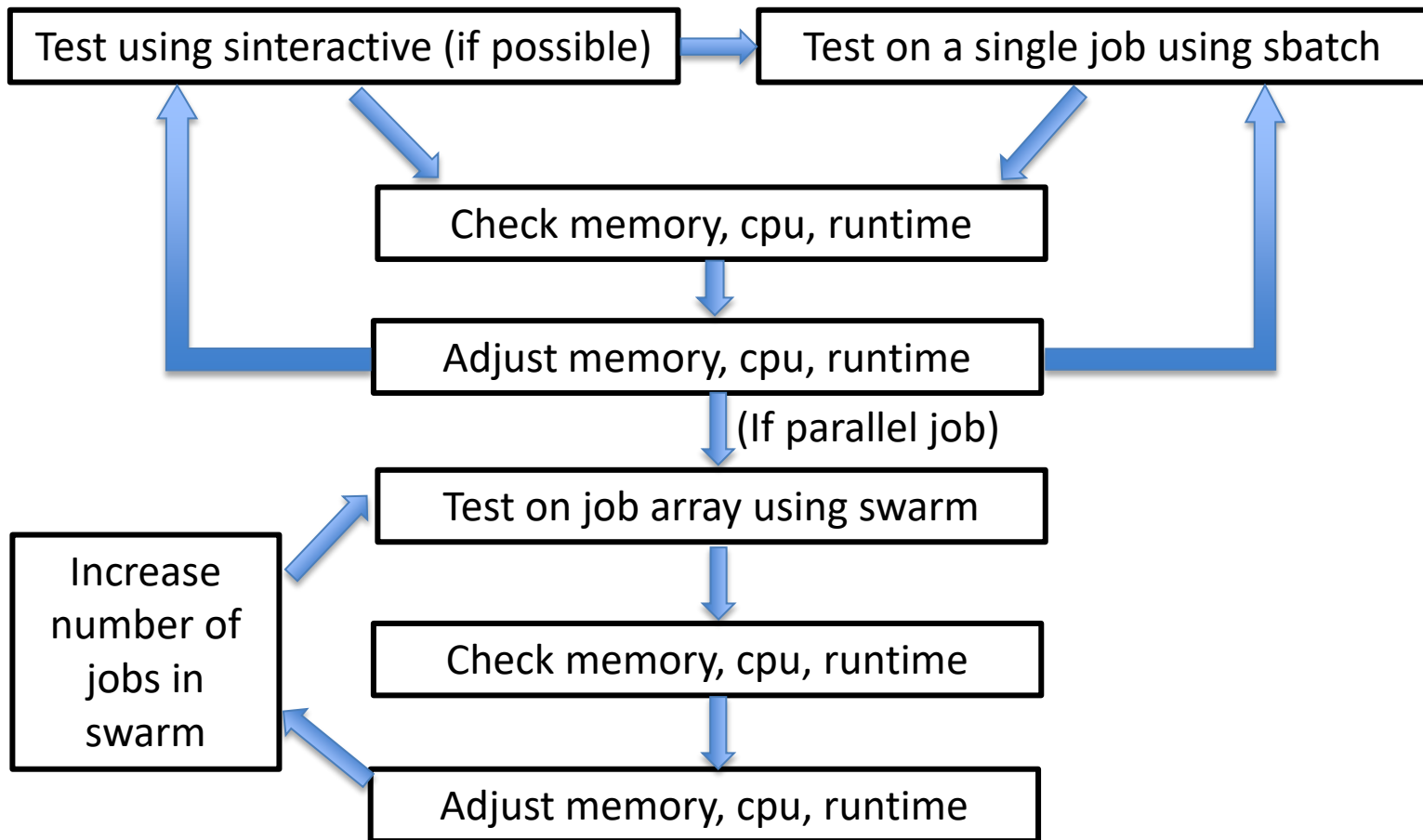
For online documentation, see https://www.mathworks.com/support
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H =

5

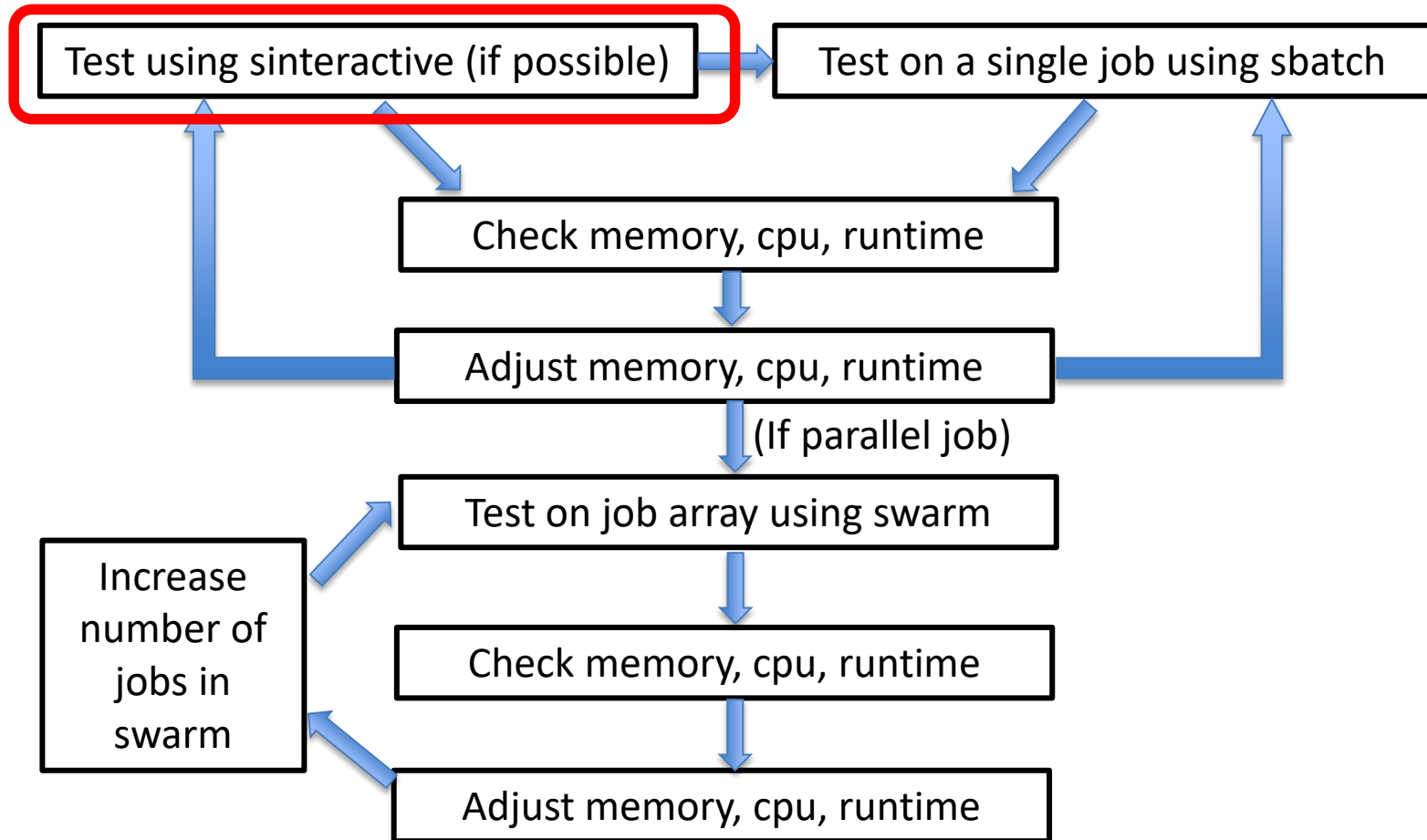
teacher > █
```

How to determine resources for Matlab jobs



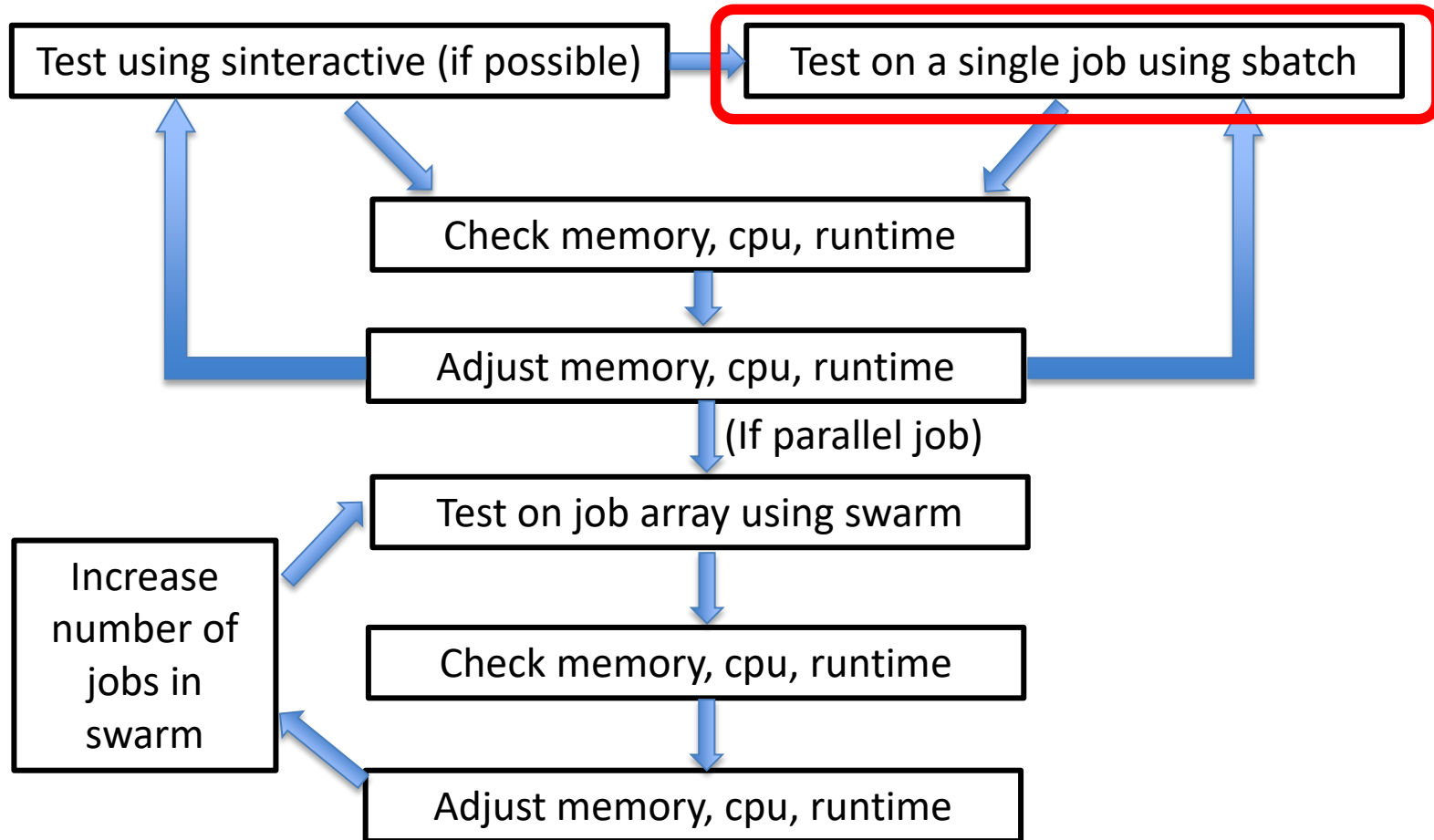
Source: https://hpc.nih.gov/training/intro_biowulf

How to determine resources for Matlab jobs



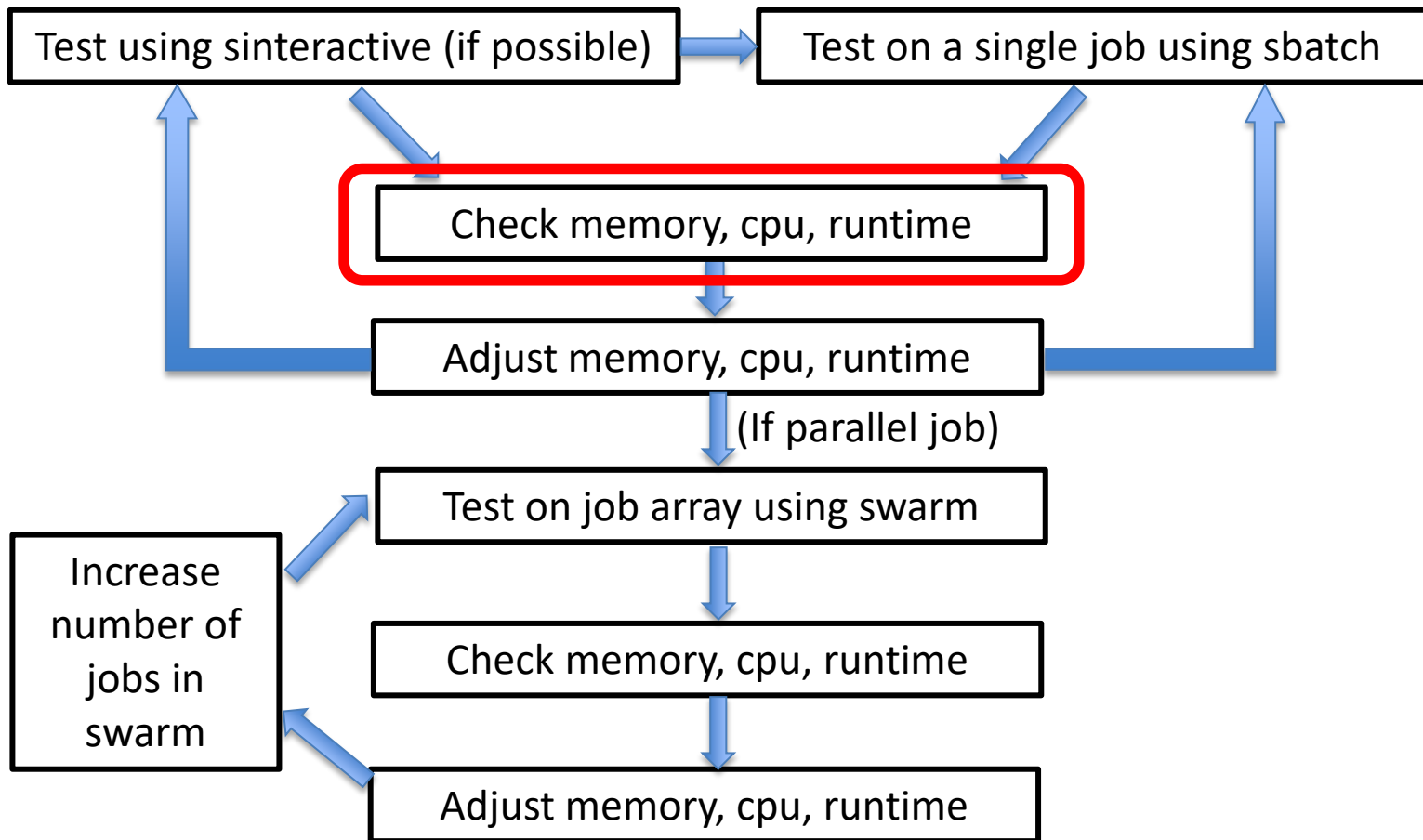
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How to determine resources for Matlab jobs



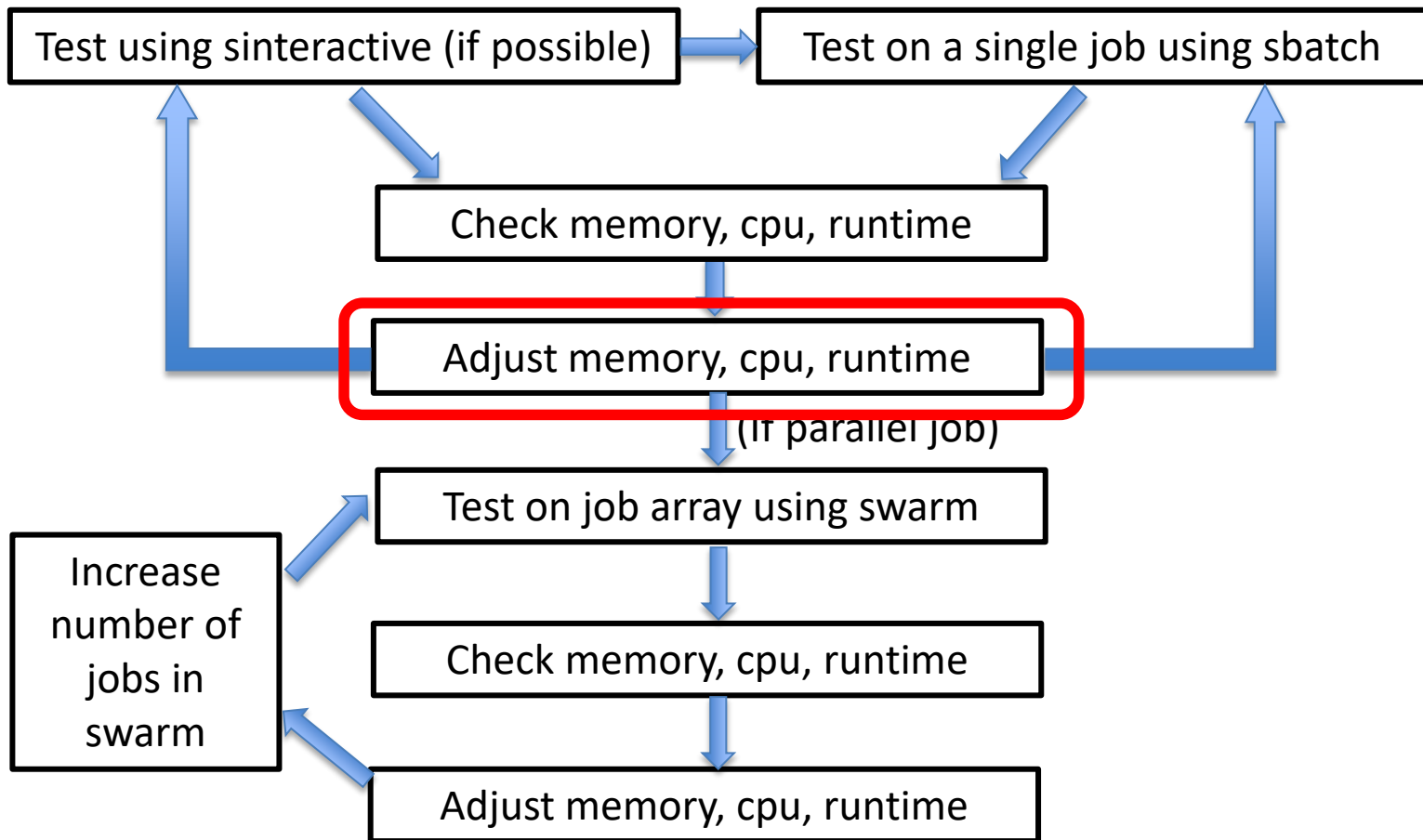
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How to determine resources for Matlab jobs



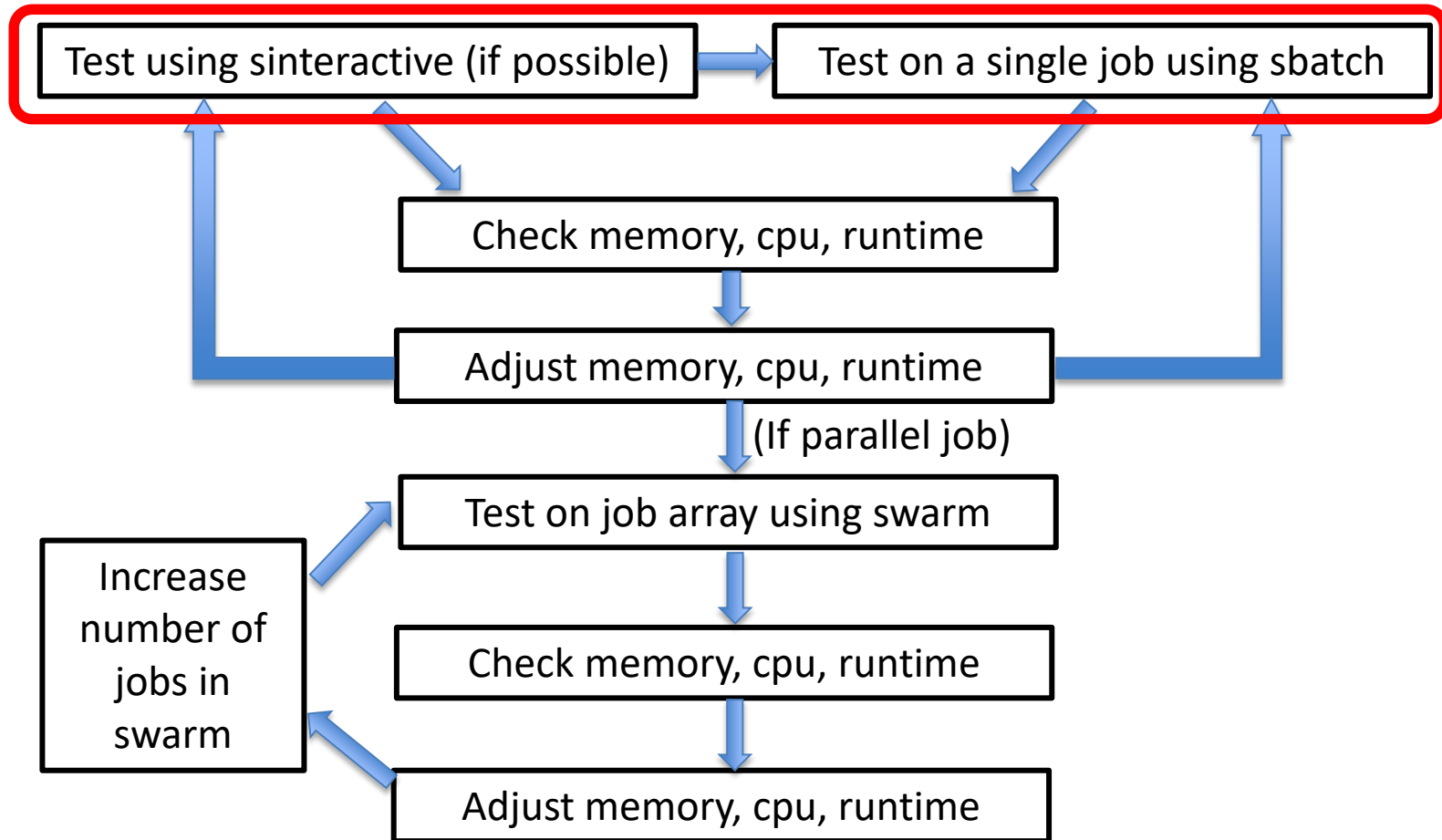
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How to determine resources for Matlab jobs



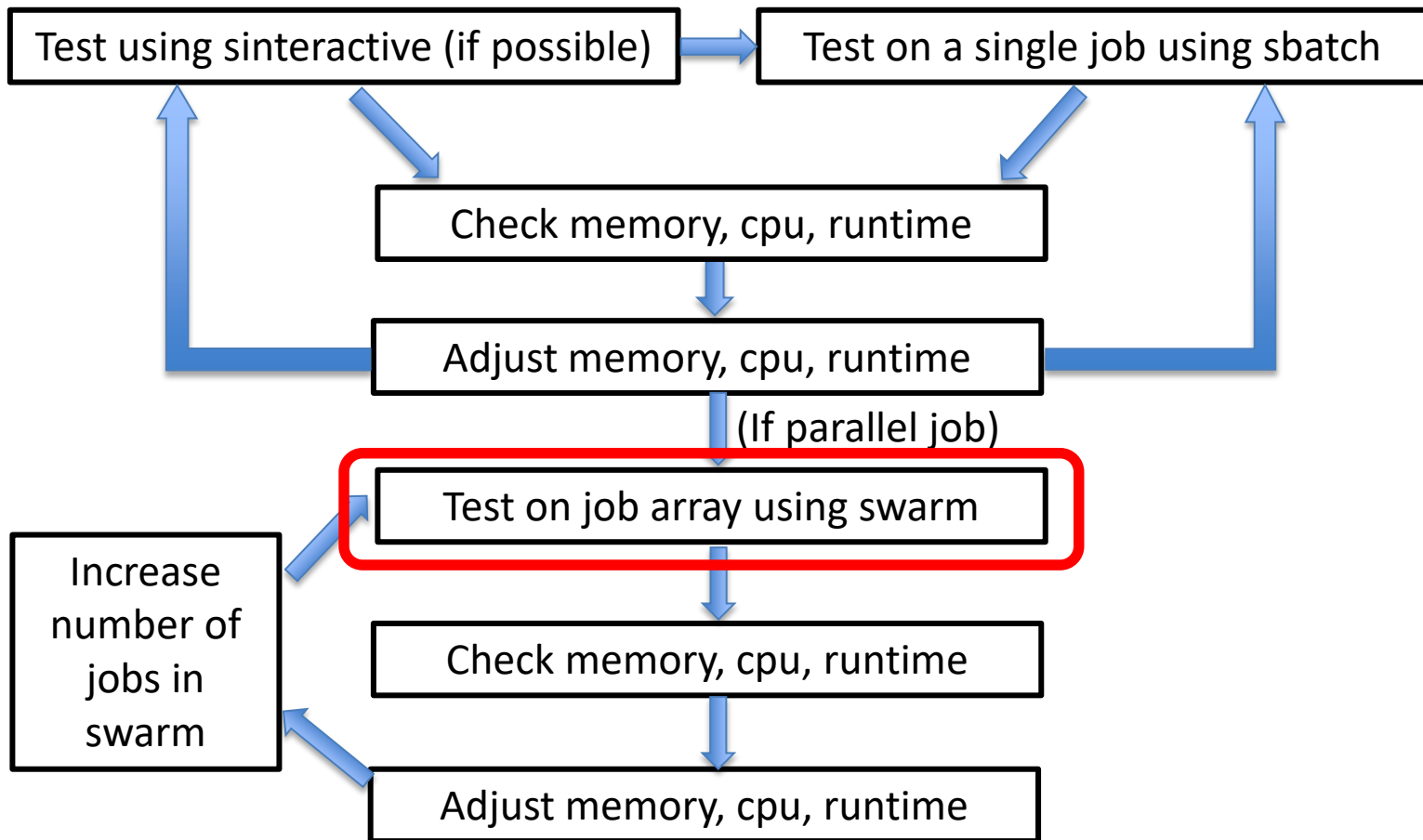
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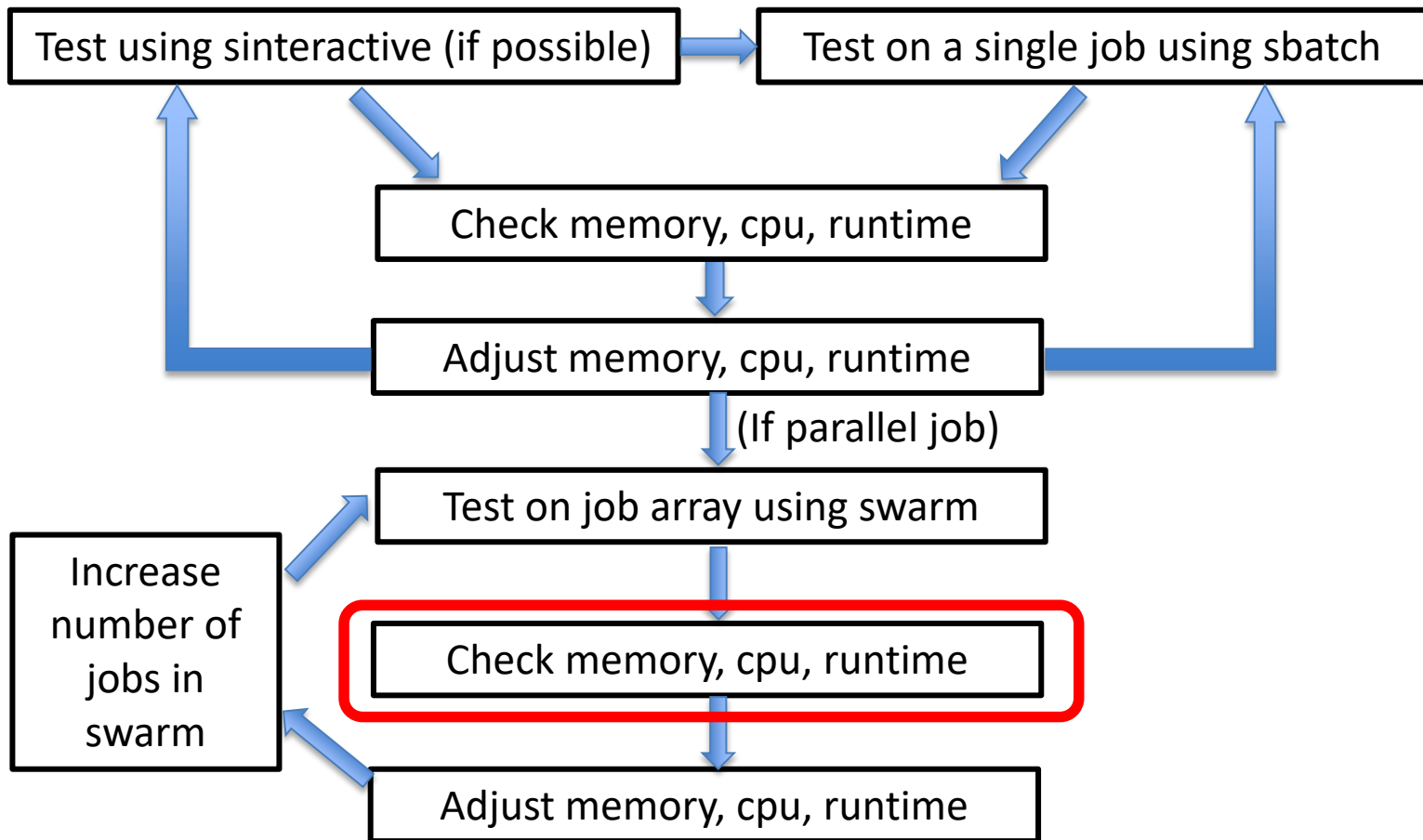
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How to determine resources for Matlab jobs



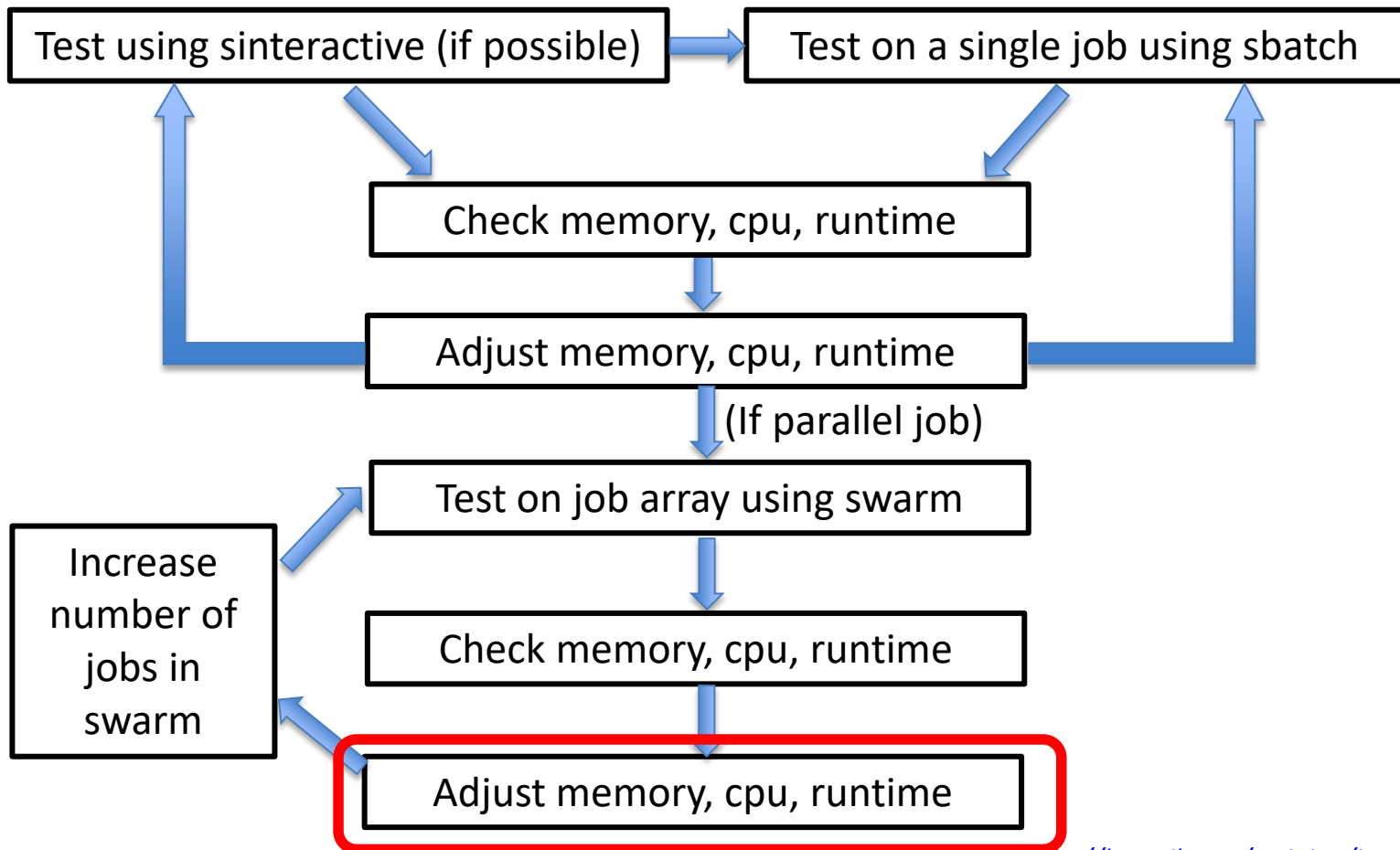
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How to determine resources for Matlab jobs



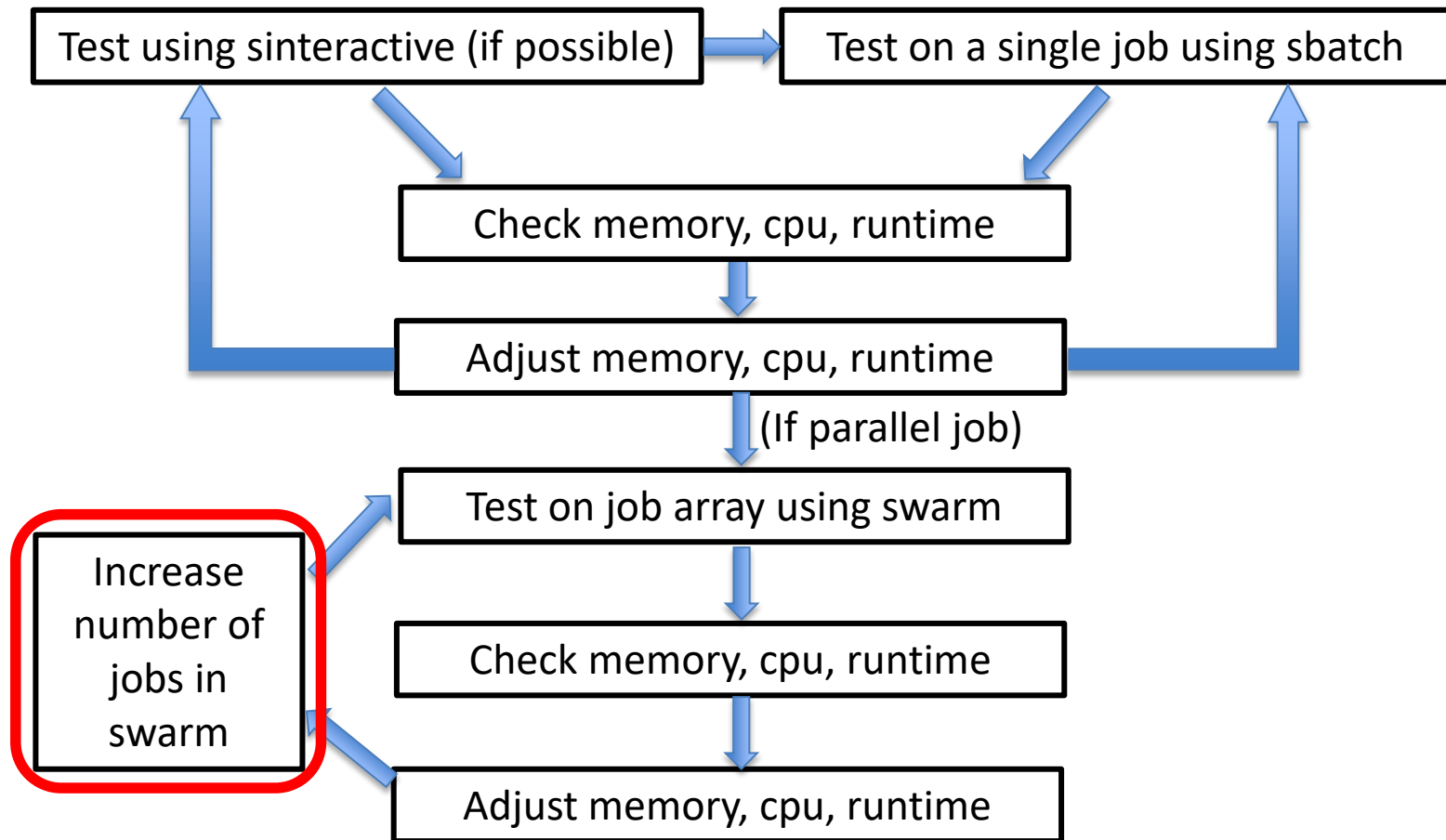
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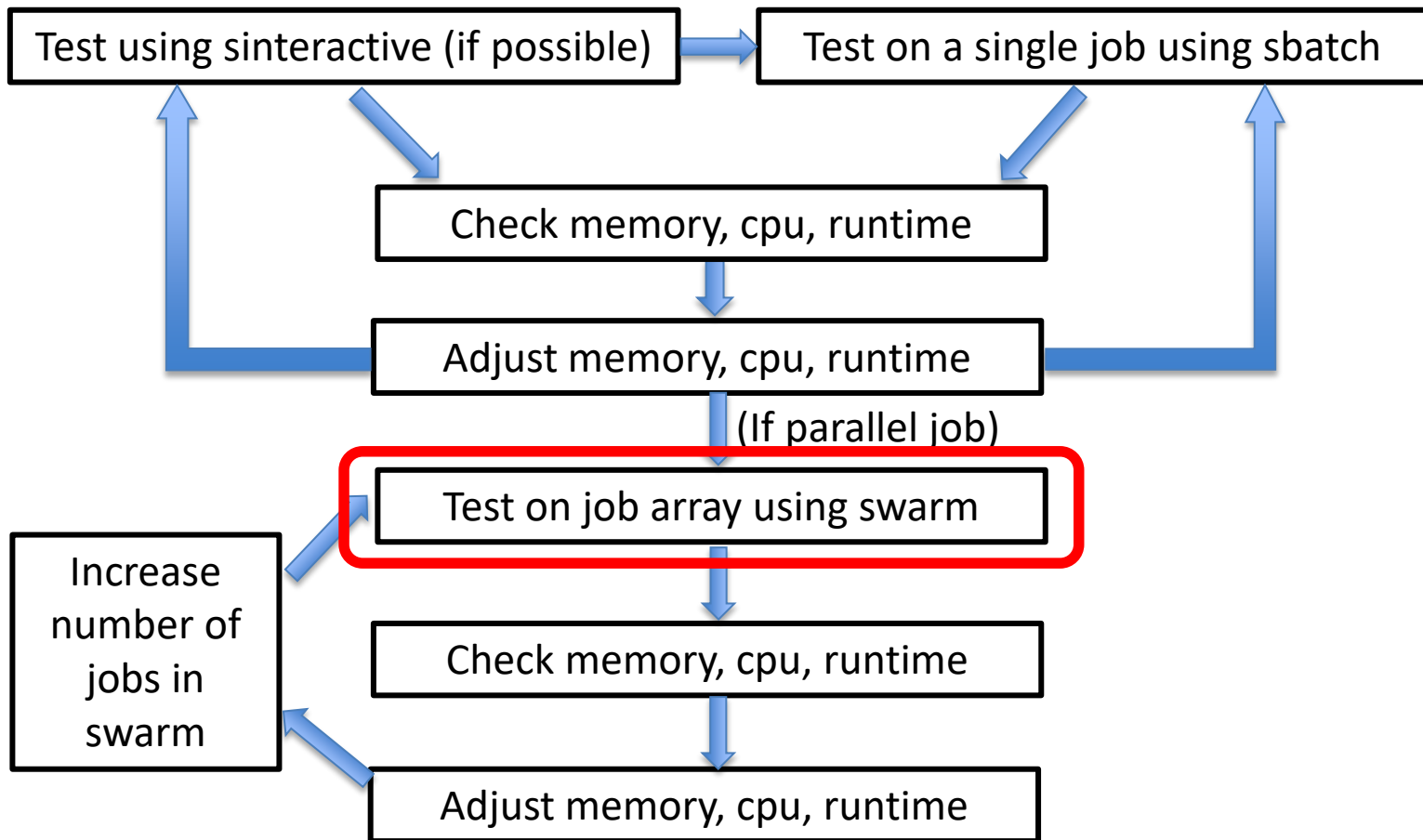
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How to determine resources for Matlab jobs



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Monitoring Matlab jobs

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- Monitoring tells you when a job terminated, whether it completed successfully, and, if the job failed, why it failed.

Monitoring Matlab jobs

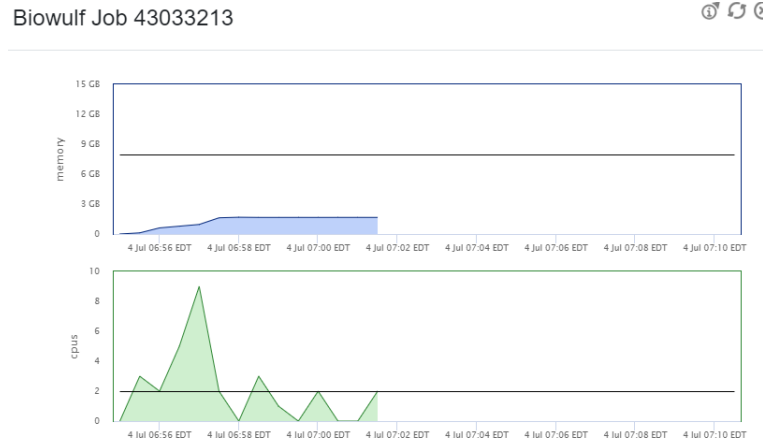
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- Monitoring during testing gives you a sense of what resources (and how much of each resource) you need for future jobs.
- Monitoring tells you when a job terminated, whether it completed successfully, and, if the job failed, why it failed.
- Users are responsible for monitoring their own jobs

Monitoring Matlab jobs

Command-line tools (see hpc.nih.gov/docs/userguide.html)

```
Terminal - username@biowulf.data
File Edit View Terminal Tabs Help
username> dashboard_cli jobs --jobid 43033213 --vertical
jobid: 43033213
state: COMPLETED
submit time: 2022-07-04T06:55:02
partition: interactive
nodes: 1
cpus: 2
mem: 8 GB
timelimit: 8:00:00
gres: -
dependency: -
queued times: -
state reason: -
start time: 2022-07-04T06:55:02
elapsed time: 6:55
end time: 2022-07-04T07:01:57
cpu_max: 9
mem_max: 2 GB
eval: -
username>
```

Graphical dashboard (hpc.nih.gov/dashboard):



Monitoring Matlab jobs

```
Terminal - teacher@biowulf:/data/teacher/matlab-iwl
File Edit View Terminal Tabs Help
teacher > sjobs
=====
User      JobId     JobName    Part      St Reason  Runtime   Walltime   Nodes  CPUs  Memory  Dependency  Nodelist
=====
teacher   43059448 sinteracti interactive R          2:52:02   8:00:00    1     2    4 GB    cn0862
=====
cpus queued = 0
cpus running = 0 / 2
mem queued = 0.0 B
mem running = 2.0 MB / 4.0 GB
jobs queued = 0
jobs running = 1
teacher > jobload
=====
JOBID          TIME          NODES  CPUS  THREADS  LOAD      MEMORY
Elapsed / Wall  Alloc  Active  Used / Alloc
i      43059448  02:52:28 / 08:00:00  cn0862    2      0    0%    0.0 / 4.0 GB
=====
USER SUMMARY
Jobs: 1      Nodes: 1      CPUs: 2      Load Avg: 0%
teacher > jobhist 43059485
JobId       : 43059485
User        : teacher
Submitted   : 20220705 06:22:54
Started     : 20220705 06:22:56
Ended       : 20220705 06:23:17
Submission path : /data/teacher/matlab-iwl
Submission Command : sbatch hyp.sh
=====
JobId      Partition  State  Nodes  CPUs  Walltime  Runtime  MemReq  MemUsed  Nodelist
43059485   norm      COMPLETED  1     2     30:00    0:21    2GB    -    cn0855
teacher >
```

Source: <https://hpc.nih.gov/docs/userguide.html#monitor>

Monitoring Matlab jobs

```
Terminal - teacher@biowulf:/data/teacher/matlab-iwl
File Edit View Terminal Tabs Help
teacher > sjobs
User JobName Part St Reason Runtime Walltime Nodes CPUs Memory Dependency Nodelist
=====
teacher 43059448 sinteracti interactive R 2:52:02 8:00:00 1 2 4 GB cn0862
=====
cpus queued = 0
cpus running = 0 / 2
mem queued = 0.0 B
mem running = 2.0 MB / 4.0 GB
jobs queued = 0
jobs running = 1
teacher > jobload
JOBID TIME NODES CPUS THREADS LOAD MEMORY
Elapsed / Wall Alloc Active Used / Alloc
i 43059448 02:52:28 / 08:00:00 cn0862 2 0 0% 0.0 / 4.0 GB

USER SUMMARY
Jobs: 1 Nodes: 1 CPUs: 2 Load Avg: 0%

teacher > jobhist 43059485
JobId : 43059485
User : teacher
Submitted : 20220705 06:22:54
Started : 20220705 06:22:56
Ended : 20220705 06:23:17
Submission path : /data/teacher/matlab-iwl
Submission Command : sbatch hyp.sh

Jobid Partition State Nodes CPUs Walltime Runtime MemReq MemUsed Nodelist
43059485 norm COMPLETED 1 2 30:00 0:21 2GB - cn0855
teacher >
```

Source: <https://hpc.nih.gov/docs/userguide.html#monitor>

Monitoring Matlab jobs

```
Terminal - teacher@biowulf:/data/teacher/matlab-iwl
File Edit View Terminal Tabs Help
teacher > sjobs
User      JobId    JobName  Part      St Reason Runtime   Walltime  Nodes  CPUs  Memory  Dependency  Nodelist
=====
teacher  43059448 sinteracti interactive R          2:52:02   8:00:00    1     2    4 GB          cn0862
=====
cpus queued = 0
cpus running = 0 / 2
mem queued = 0.0 B
mem running = 2.0 MB / 4.0 GB
jobs queued = 0
jobs running = 1
teacher > jobload
JOBID      TIME          NODES  CPUS  THREADS  LOAD      MEMORY
          Elapsed / Wall  Alloc  Active  %         Used / Alloc
i         43059448  02:52:28 / 08:00:00  cn0862  2      0      0%     0.0 / 4.0 GB

USER SUMMARY
Jobs: 1      Nodes: 1      CPUs: 2      Load Avg: 0%

teacher > jobhist 43059485
JobId      : 43059485
User       : teacher
Submitted  : 20220705 06:22:54
Started    : 20220705 06:22:56
Ended      : 20220705 06:23:17
Submission path : /data/teacher/matlab-iwl
Submission Command : sbatch hyp.sh

JobId      Partition  State  Nodes  CPUs  Walltime  Runtime  MemReq  MemUsed  Nodelist
43059485   norm      COMPLETED  1     2     30:00    0:21    2GB     -     cn0855
teacher > |
```

Source: <https://hpc.nih.gov/docs/userguide.html#monitor>

Monitoring Matlab jobs

```
Terminal - teacher@biowulf:/data/teacher/matlab-iwl
File Edit View Terminal Tabs Help
teacher > sjobs
User      JobId      JobName      Part      St Reason Runtime      Walltime      Nodes CPUs Memory Dependency Nodelist
=====
teacher  43059448  sinteracti  interactive R          2:52:02      8:00:00       1    2   4 GB          cn0862
=====
cpus queued = 0
cpus running = 0 / 2
mem queued = 0.0 B
mem running = 2.0 MB / 4.0 GB
jobs queued = 0
jobs running = 1
teacher > jobload
      JOBID      TIME      NODES CPUS THREADS LOAD MEMORY
      Elapsed / Wall      Alloc Active      Used / Alloc
i      43059448  02:52:28 / 08:00:00 cn0862 2 0 0% 0.0 / 4.0 GB

USER SUMMARY
Jobs: 1 Nodes: 1 CPUs: 2 Load Avg: 0%

teacher > jobhist 43059485
JobId      : 43059485
User       : teacher
Submitted  : 20220705 06:22:54
Started    : 20220705 06:22:56
Ended      : 20220705 06:23:17
Submission path : /data/teacher/matlab-iwl
Submission Command : sbatch hyp.sh

Jobid      Partition State Nodes CPUs Walltime Runtime MemReq MemUsed Nodelist
43059485   norm    COMPLETED 1 2 30:00 0:21 2GB - cn0855
teacher >
```

Source: <https://hpc.nih.gov/docs/userguide.html#monitor>

Monitoring Matlab jobs

```
Terminal - teacher@biowulf:/data/teacher/matlab-iwl
File Edit View Terminal Tabs Help
teacher > dashboard_cli jobs --fields jobid,partition,nodes,cpus,mem,state,elapsed_time,cpu_util,mem_util
jobid      partition  nodes  cpus  mem  state  elapsed_time  cpu_util  mem_util
=====
43041881   interactive  1      2    4 GB  TIMEOUT  8:00:07      50.0%    0.7%
43042454   norm        1      2    2 GB  COMPLETED  0:26      100.0%   40.3%
43042560   norm        1      2    2 GB  COMPLETED  0:22      100.0%   24.1%
43042964   norm        1      2    2 GB  COMPLETED  0:22       50.0%   36.6%
43042975   norm        1      2    2 GB  COMPLETED  0:22       -        -
43043185   norm        1      2    2 GB  COMPLETED  0:23       -        -
43043186   norm        1      2    2 GB  COMPLETED  0:32      50.0%   35.6%
43043187   norm        1      2    2 GB  COMPLETED  0:37      50.0%   26.0%
43043223   norm        1      2    2 GB  COMPLETED  0:17       0.0%    0.0%
43043225   norm        1      2    2 GB  COMPLETED  0:34       0.0%   27.7%
43043226   norm        1      2    2 GB  COMPLETED  0:41      50.0%   16.7%
43059448   interactive  1      2    4 GB  RUNNING   2:54:05     0.0%    0.0%
43059473   norm        1      2    2 GB  COMPLETED  0:16       -        -
43059485   norm        1      2    2 GB  COMPLETED  0:21       -        -
43059569   norm        1      2    2 GB  COMPLETED  0:18       -        -
43059596   norm        1      2    2 GB  COMPLETED  0:16       -        -
43059597   norm        1      2    2 GB  COMPLETED  0:17       -        -
43060138   norm        1      2    2 GB  COMPLETED  0:15       0.0%    2.3%
teacher > █
```

Source: https://hpc.nih.gov/docs/biowulf_tools.html#dashboard_cli

Monitoring Matlab jobs

```
Terminal - teacher@biowulf:/data/teacher/matlab-iwl
File Edit View Terminal Tabs Help
teacher > dashboard_cli jobs --fields jobid,partition,nodes,cpus,mem,state,elapsed_time,cpu_util,mem_util
jobid partition nodes cpus mem state elapsed_time cpu_util mem_util
=====
43041881 interactive 1 2 4 GB TIMEOUT 8:00:07 50.0% 0.7%
43042454 norm 1 2 2 GB COMPLETED 0:26 100.0% 40.3%
43042560 norm 1 2 2 GB COMPLETED 0:22 100.0% 24.1%
43042964 norm 1 2 2 GB COMPLETED 0:22 50.0% 36.6%
43042975 norm 1 2 2 GB COMPLETED 0:22 - -
43043185 norm 1 2 2 GB COMPLETED 0:23 - -
43043186 norm 1 2 2 GB COMPLETED 0:32 50.0% 35.6%
43043187 norm 1 2 2 GB COMPLETED 0:37 50.0% 26.0%
43043223 norm 1 2 2 GB COMPLETED 0:17 0.0% 0.0%
43043225 norm 1 2 2 GB COMPLETED 0:34 0.0% 27.7%
43043226 norm 1 2 2 GB COMPLETED 0:41 50.0% 16.7%
43059448 interactive 1 2 4 GB RUNNING 2:54:05 0.0% 0.0%
43059473 norm 1 2 2 GB COMPLETED 0:16 - -
43059485 norm 1 2 2 GB COMPLETED 0:21 - -
43059569 norm 1 2 2 GB COMPLETED 0:18 - -
43059596 norm 1 2 2 GB COMPLETED 0:16 - -
43059597 norm 1 2 2 GB COMPLETED 0:17 - -
43060138 norm 1 2 2 GB COMPLETED 0:15 0.0% 2.3%
teacher > █
```

Source: https://hpc.nih.gov/docs/biowulf_tools.html#dashboard_cli

Monitoring Matlab jobs

```
Terminal - teacher@biowulf:/data/teacher/matlab-iwl
File Edit View Terminal Tabs Help
teacher > dashboard_cli jobs --fields jobid,partition,nodes,cpus,mem,state,elapsed_time,cpu_util,mem_util
jobid
=====
43041881 interactive 1 2 4 GB TIMEOUT 8:00:07 50.0% 0.7%
43042454 norm 1 2 2 GB COMPLETED 0:26 100.0% 40.3%
43042560 norm 1 2 2 GB COMPLETED 0:22 100.0% 24.1%
43042964 norm 1 2 2 GB COMPLETED 0:22 50.0% 36.6%
43042975 norm 1 2 2 GB COMPLETED 0:22 - -
43043185 norm 1 2 2 GB COMPLETED 0:23 - -
43043186 norm 1 2 2 GB COMPLETED 0:32 50.0% 35.6%
43043187 norm 1 2 2 GB COMPLETED 0:37 50.0% 26.0%
43043223 norm 1 2 2 GB COMPLETED 0:17 0.0% 0.0%
43043225 norm 1 2 2 GB COMPLETED 0:34 0.0% 27.7%
43043226 norm 1 2 2 GB COMPLETED 0:41 50.0% 16.7%
43059448 interactive 1 2 4 GB RUNNING 2:54:05 0.0% 0.0%
43059473 norm 1 2 2 GB COMPLETED 0:16 - -
43059485 norm 1 2 2 GB COMPLETED 0:21 - -
43059569 norm 1 2 2 GB COMPLETED 0:18 - -
43059596 norm 1 2 2 GB COMPLETED 0:16 - -
43059597 norm 1 2 2 GB COMPLETED 0:17 - -
43060138 norm 1 2 2 GB COMPLETED 0:15 0.0% 2.3%
teacher > █
```

Source: https://hpc.nih.gov/docs/biowulf_tools.html#dashboard_cli

Monitoring Matlab jobs

User Dashboard

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Accounts Disk Usage **Job Info** Usage Report Speedtest

Job Info

last updated: 2022-07-04 15:38:43 EDT

Configuration

jobid	jobname	state	statetime	nodelist
43043223_1	swarm	COMPLETED	2022-07-04 15:21:53 EDT	cn0941
43043223_0	swarm	COMPLETED	2022-07-04 15:21:46 EDT	cn0887
43043223_2	swarm	COMPLETED	2022-07-04 15:21:29 EDT	cn0953
43043185_1	swarm	COMPLETED	2022-07-04 15:12:21 EDT	cn0941
43043185_0	swarm	COMPLETED	2022-07-04 15:12:16 EDT	cn0887
43043185_2	swarm	COMPLETED	2022-07-04 15:12:07 EDT	cn0953
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43042964	hypotenuse	COMPLETED	2022-07-04 14:54:36 EDT	cn0862
43042560	hypotenuse	COMPLETED	2022-07-04 14:33:40 EDT	cn0868
43042454	hypotenuse	COMPLETED	2022-07-04 14:30:06 EDT	cn0868

jobid state statetime

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jobid state statetime

Download as CSV

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Monitoring Matlab jobs

Biowulf Job 43041881

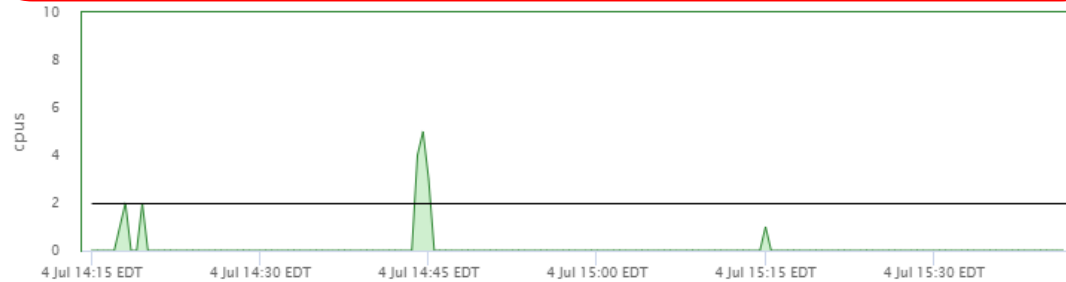
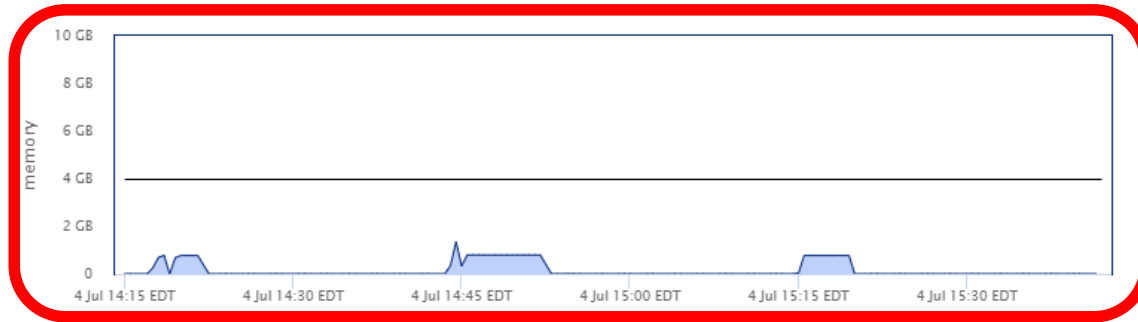


Export to PNG

Source: <https://hpc.nih.gov/dashboard>

Monitoring Matlab jobs

Biowulf Job 43041881

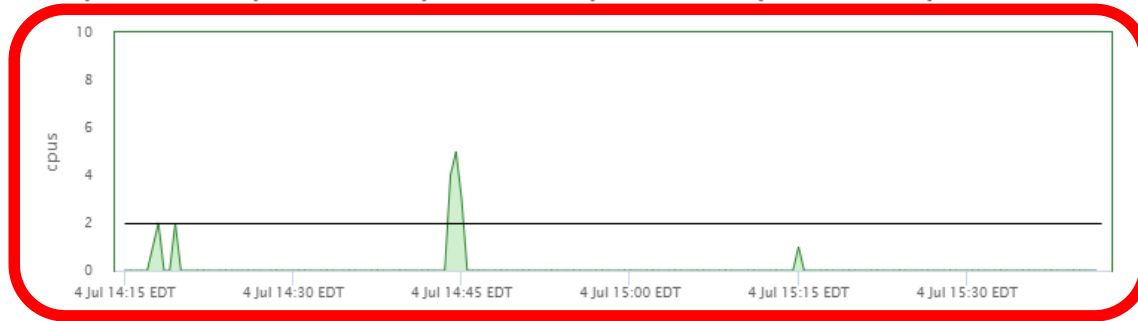
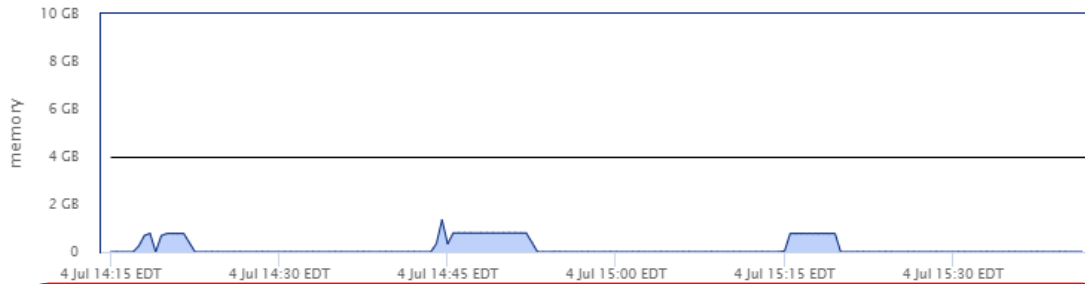


Export to PNG

Source: <https://hpc.nih.gov/dashboard>

Monitoring Matlab jobs

Biowulf Job 43041881



Export to PNG

Source: <https://hpc.nih.gov/dashboard>

Limits, pitfalls, and caveats

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Limits, pitfalls, and caveats

- Test before running large jobs: Make sure you know what resources (memory, CPU, GPU, disk space) your job needs and for how long (walltime).
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- Starting matlab is computationally expensive so try to limit (to 1 preferably) the times you start matlab within a job.
- Make sure you have enough space in your data directory for your jobs
- Try to run jobs with walltime > 15 minutes
- Read your NIH email in case Biowulf staff needs to contact you regarding your running jobs

Conclusion

Hopefully you:

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- Are aware of the benefits of the IWL Matlab license on Biowulf

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Hopefully you:

- Are aware of the benefits of the IWL Matlab license on Biowulf
- Know how to run Matlab both in an interactive session and as a batch job
- Know how to avoid common pitfalls while running Matlab batch jobs

Biowulf staff



Steve Bailey



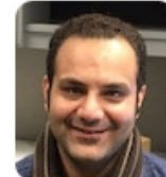
Susan Chacko,
Ph.D.



Gennady Denisov,
Ph.D.

Picture
unavailable

Afif Elghraoui



Ali Erfani



Andrew Fant, Ph.D.



Jonathan Goodson,
Ph.D.



David Hoover, Ph.D.



Patsy Jones

Picture
unavailable

Charles Lehr



Jean Mao, Ph.D.



Tim Miller



Nitish Narula, M.S.



Charlene Osborn



David O'Brien



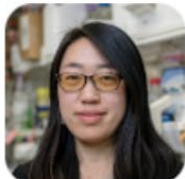
Mark Patkus



Wolfgang Resch,
Ph.D.



Antonio Ulloa, Ph.D.



Qi Yu, Ph.D.

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staff@hpc.nih.gov