Week 1 – Introduction

02613 Python and High-Performance Computing

Today

1. Practical information

2. Python and High-Performance Computing

3. DTU's HPC system

Instructor:

Matthias Bo Stuart

Behind the scenes:

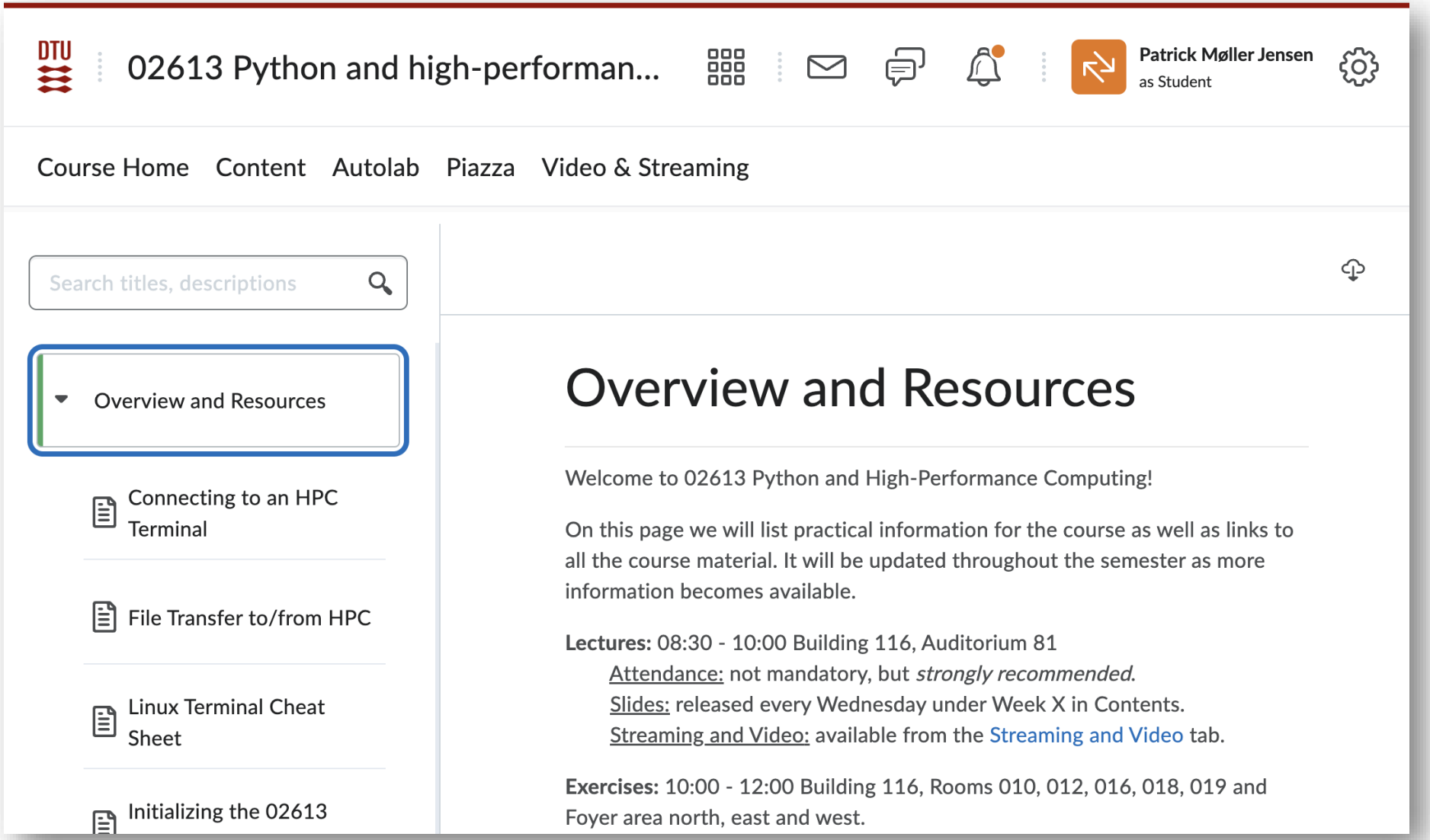
Sven Karlsson

Bernd Damman

Teaching Assistants (TAs):

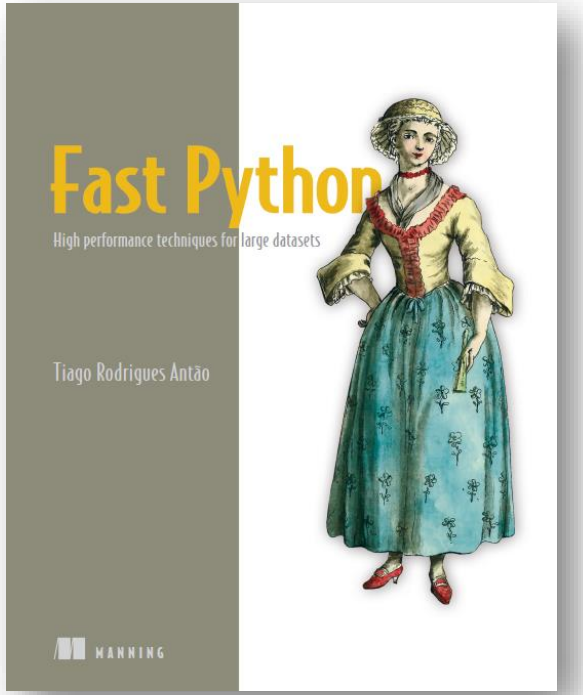
Christian K. Rasmussen
Juliane B. Budde
Jeppe Klitgaard
Jacob A. Wæver
Magnus G. Pedersen
Rasmus J. Pedersen
Abdulrahman Ramadan
Michail Dikaiopoulos
Erik B. Christensen
Lucas Pedersen
Alba G. Primo

learn.inside.dtu.dk

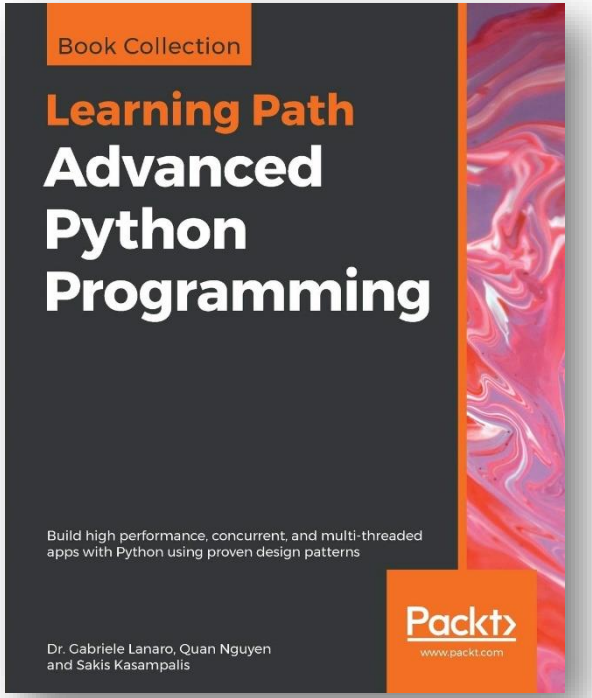


Lectures: Wednesdays 8:30 – 10:00, Building 116, Auditorium 81
Streamed online using Panopto

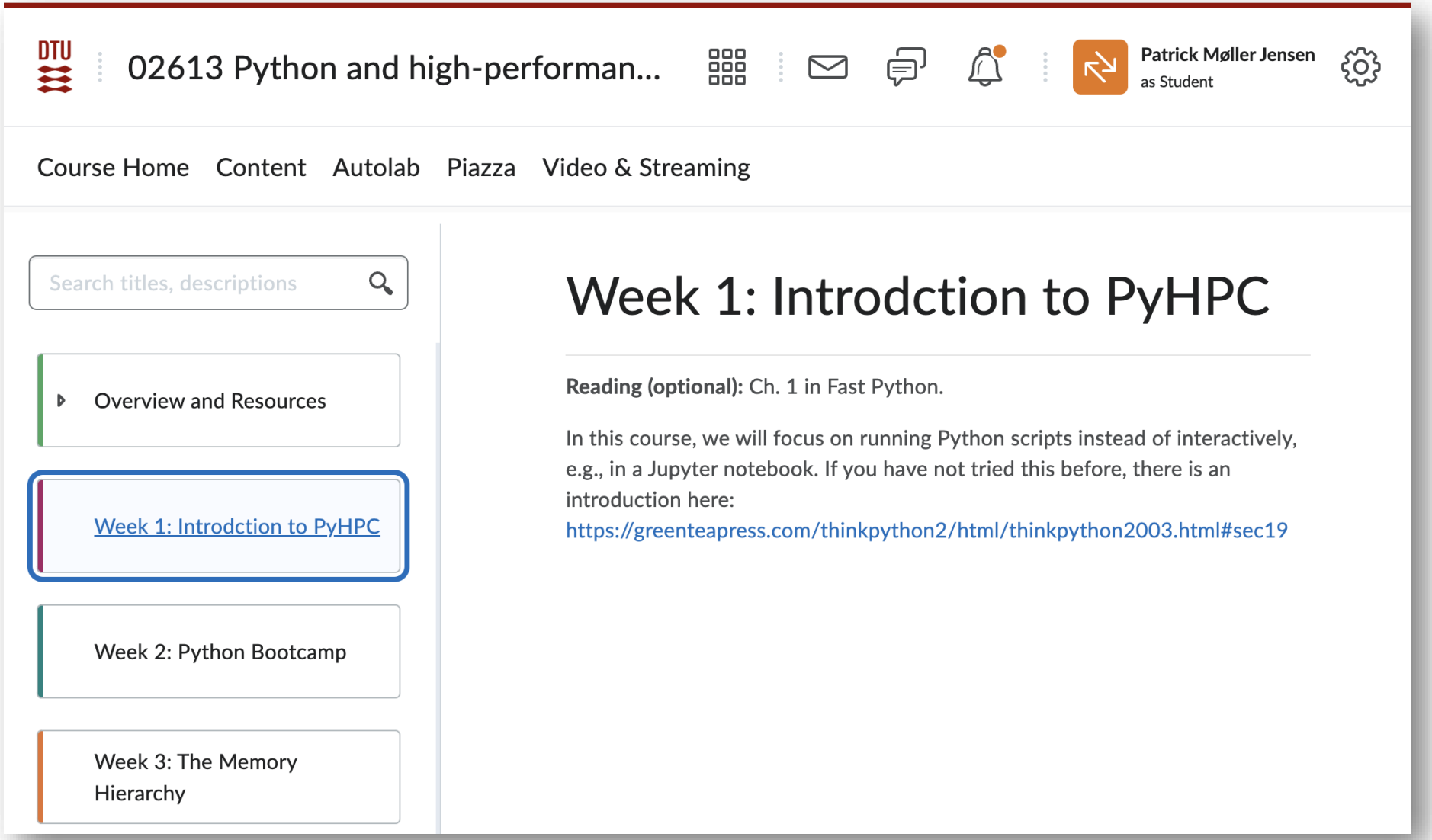
Books: Fast Python



Advanced Python Programming (free online)



learn.inside.dtu.dk



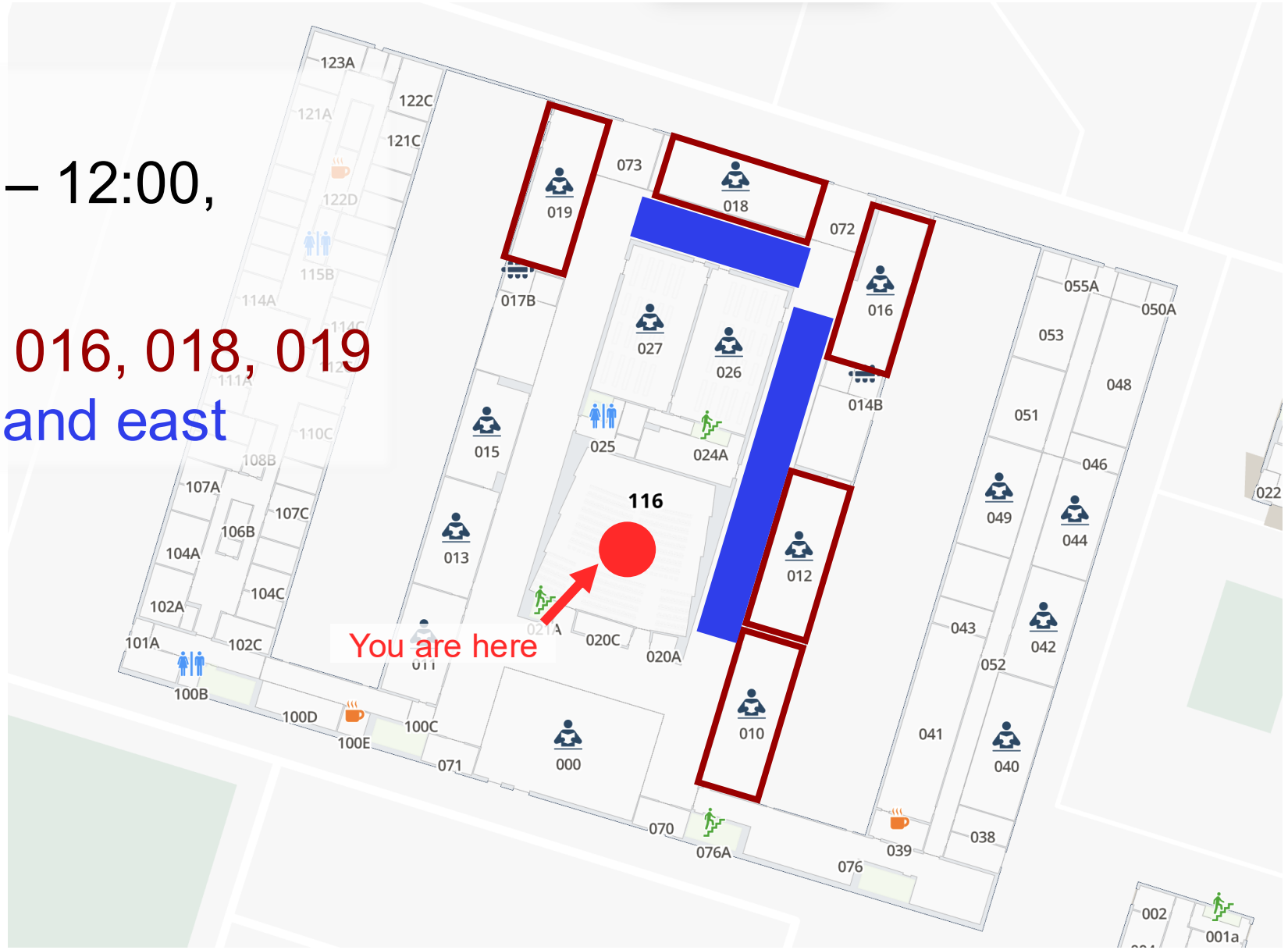
Exercises:

Wednesdays 10:00 – 12:00,

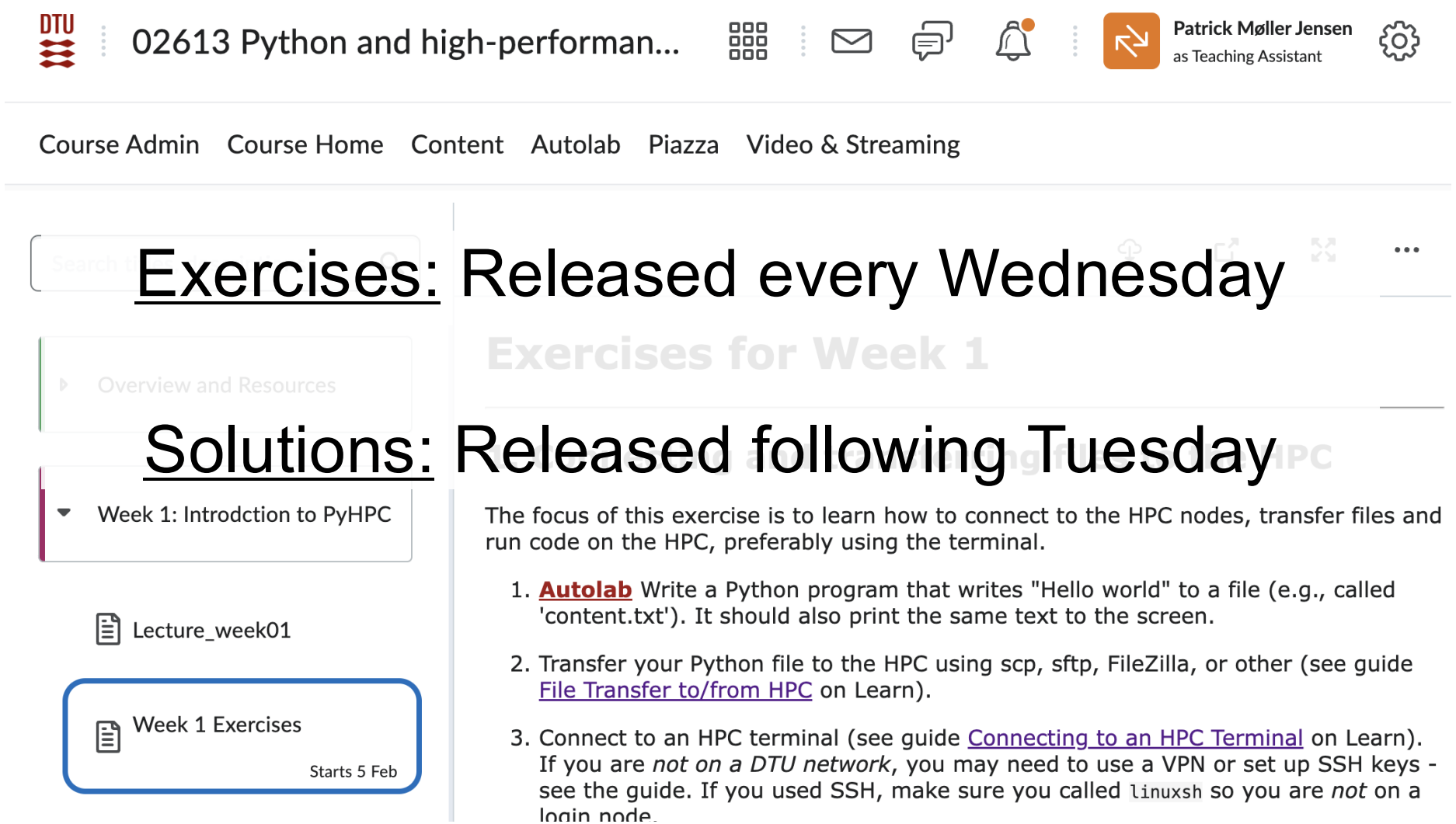
Building 116

Rooms 010, 012, 016, 018, 019

Foyer area north and east



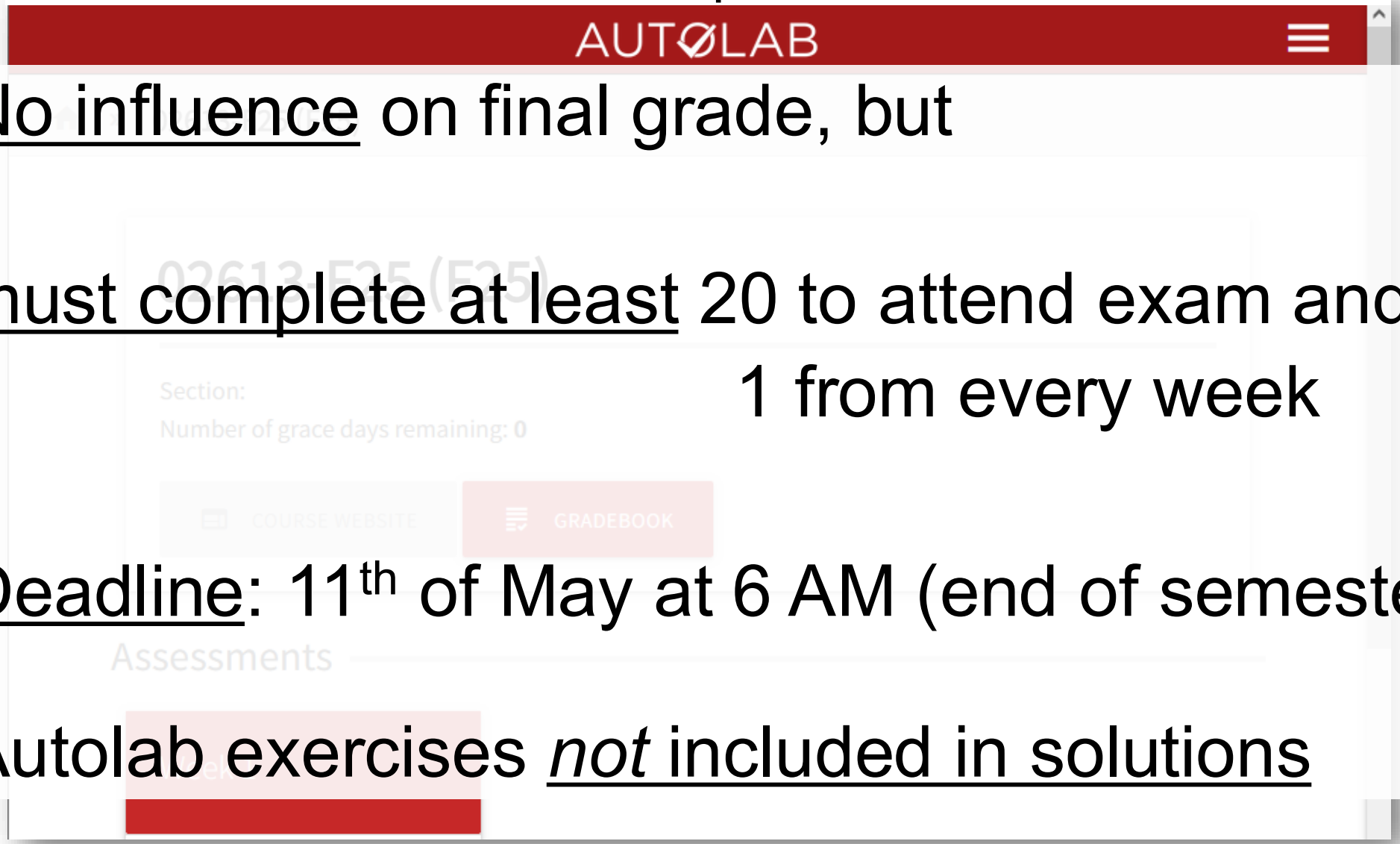
learn.inside.dtu.dk



Exercises: Released every Wednesday

Solutions: Released following Tuesday

autolab.compute.dtu.dk



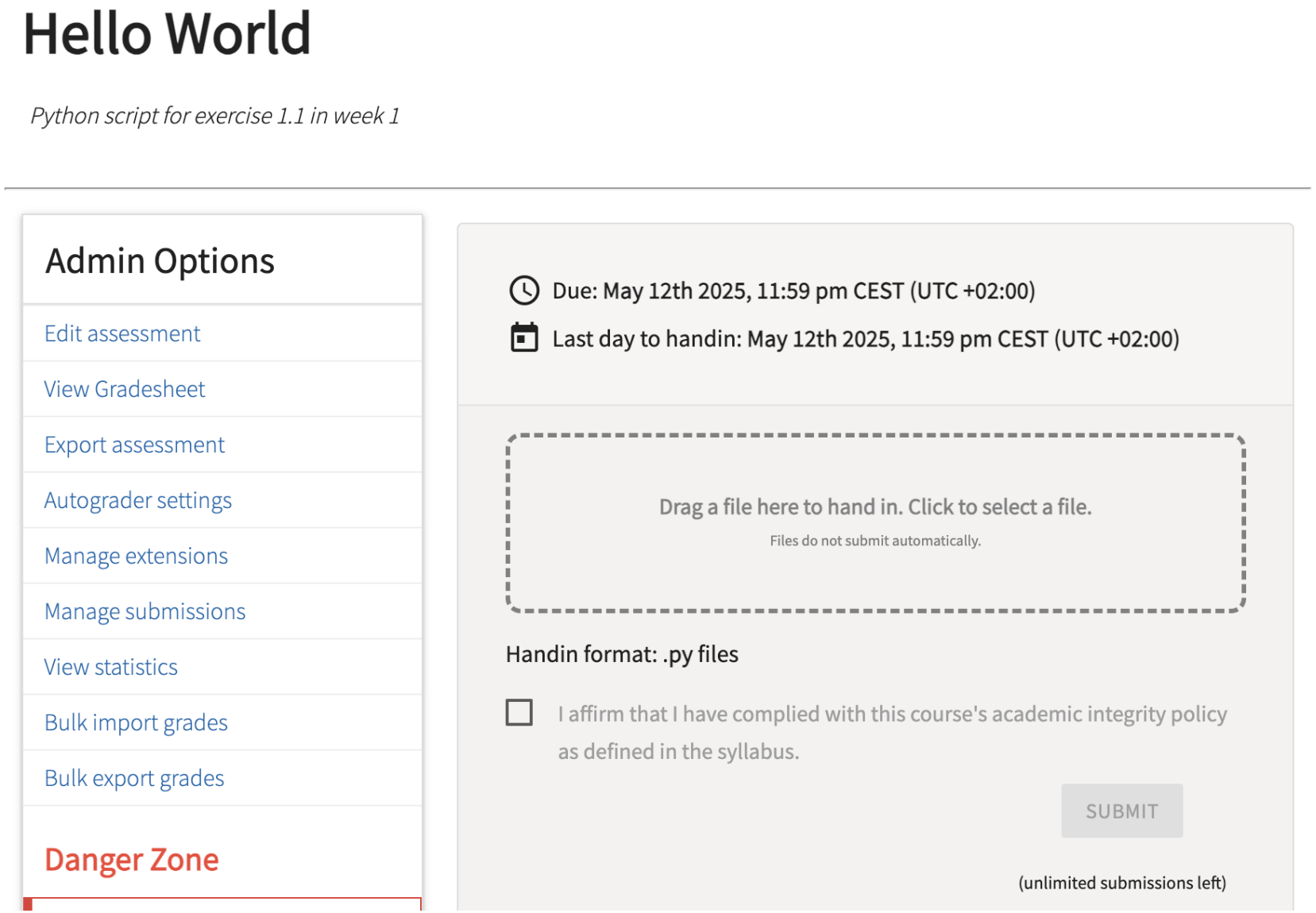
No influence on final grade, but

must complete at least 20 to attend exam and 1 from every week

Deadline: 11th of May at 6 AM (end of semester)

Autolab exercises *not* included in solutions

autolab.compute.dtu.dk



autolab.compute.dtu.dk

Submission Summary

Ver	File	Submission Date	Correctness (100.0)	Days Late (Grace Days Used)	Total Score (100.0)	Tweak	Instructor Actions
1	View Source Download Submission	2025-01-07 16:35:03 +0100	100.0	0 days (0 days)	100.0	–	(Regrade) (Destroy) (Edit)

autolab.compute.dtu.dk

Autograding Result for Hello World - Correctness (patmjen@dtu.dk)

Feedback

Completed

```
Autograder [Tue Jan 14 12:10:13 2025]: Received job 02613-F25_Hello-World_1_patmjen@dtu.dk:1
Autograder [Tue Jan 14 12:10:15 2025]: Success: Autodriver returned normally
Autograder [Tue Jan 14 12:10:15 2025]: Here is the output from the autograder:
---
Autodriver: Job exited with status 0

Running submission file...
Checking result...
 * Ran succesfully: True
 * Printed 'Hello world': True
 * Printed nothing on stderr: True
 * Made new file: True
 * File content is same as printed: True

{"scores": {"Correctness": 100.0}}
```

Results

Autograder Scores

Correctness:	100.0
Autograding Total:	100.0

Paste in code

Paste your function (and only your function) here:

```
def listsum(arr):
    # Your code
```

☐ I affirm that I have complied with this course's academic integrity policy as defined in the syllabus.

SUBMIT QUERY

Quizzes

What does HPC stand for?

- ○ Holistic Program Computations
- ○ High Performance Compute
- ○ Half Price Cost

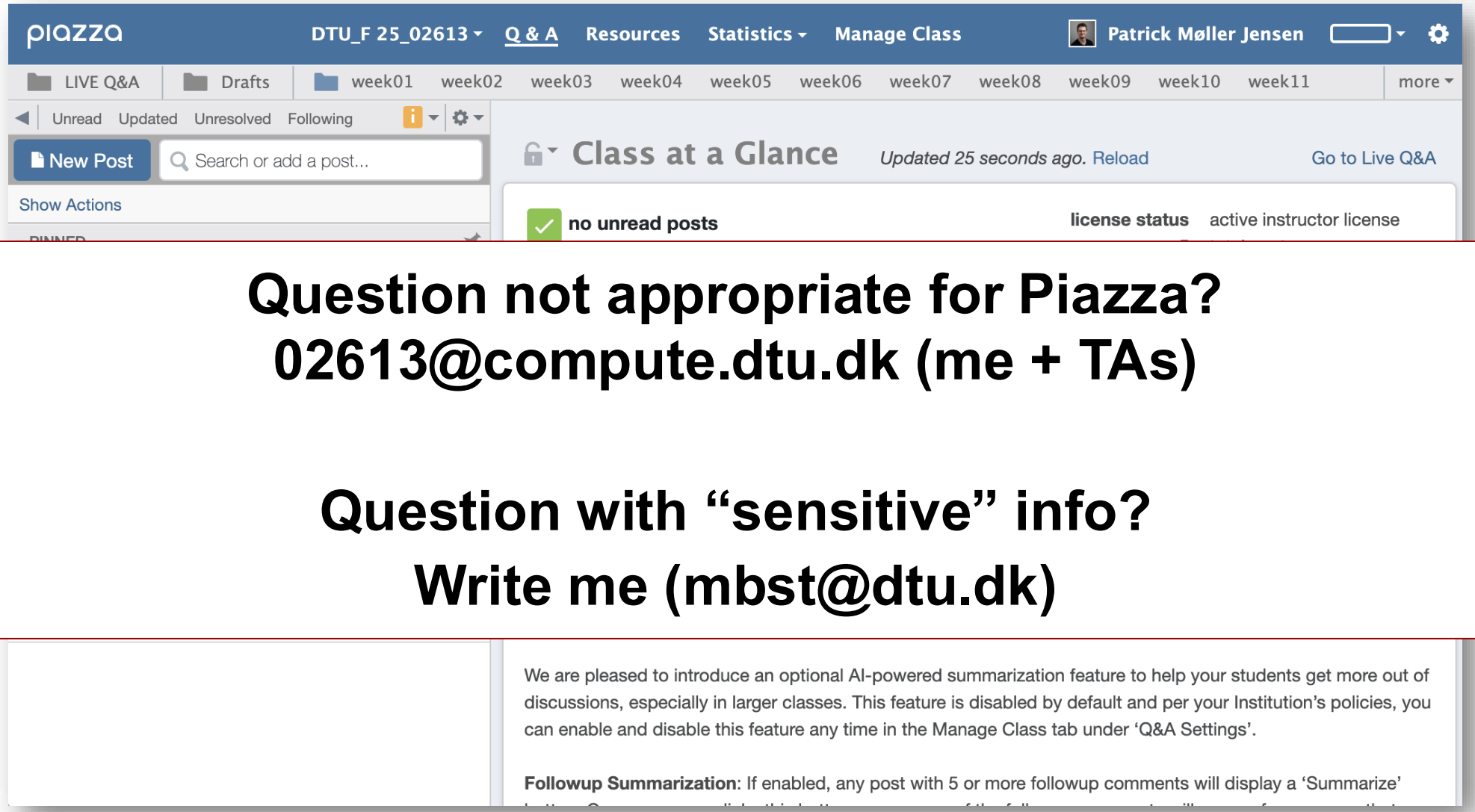
What is the Python language named after?

- ○ The snake!
- ○ Monty Python's Flying Circus
- ○ Nobody knows...

☐ I affirm that I have complied with this course's academic integrity policy as defined in the syllabus.

SUBMIT QUERY

piazza.com (link on Learn)



Mini-Project

Goal: work with course topics in a more “real” way

Work in groups of 3 or 4

Will be released in week 4

Hand-in: Small report on

Sunday 3rd of May, 2026 at 23:59 (week 12)

Must be **completed and approved** to attend exam

Exam:

4 hours written (digital) exam

All aids and materials permitted - without internet access.

Laptop, tablet, and similar devices allowed.

Generative AI is not allowed.

Previous exams + solutions available on Learn.

Full details on learn

Questions?

Join the Vevox session

Go to **vevox.app**

Enter the session ID: **113-073-658**

Or scan the QR code

Join at: **vevox.app** ID: **XXX-XXX-XXX**

Question slide

What do you work with?

Machine Learning and Deep Learning

##.##%

Statistics

##.##%

Modelling and Simulation

##.##%

Optimization

##.##%

Robotics

##.##%

Other

##.##%

Join at: **vevox.app** ID: **XXX-XXX-XXX**

Results slide

What do you work with?

Machine Learning and Deep Learning ##.##%

Statistics ##.##%

Modelling and Simulation ##.##%

Optimization ##.##%

Robotics ##.##%

Other ##.##%

RESULTS SLIDE

Join at: **vevox.app** ID: **XXX-XXX-XXX**

Question slide

What is your experience with Python

Never used it

##.##%

Used it once

##.##%

Used it a little, e.g., for one course

##.##%

Used it a lot

##.##%

"I'm literally a snake!"

##.##%

Join at: **vevox.app** ID: **XXX-XXX-XXX**

Results slide

What is your experience with Python

Never used it

##.##%

Used it once

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Used it a little, e.g., for one course

##.##%

Used it a lot

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"I'm literally a snake!"

##.##%

RESULTS SLIDE

Join at: **vevox.app** ID: **XXX-XXX-XXX**

Question slide

What is your experience with the Linux terminal?

Never used it

##.##%

Used it once

##.##%

Used it a little, e.g., for one course

##.##%

Used it a lot

##.##%

“I stream Netflix as ASCII art!"

##.##%

Join at: **vevox.app** ID: **XXX-XXX-XXX**

Results slide

What is your experience with the Linux terminal?

Never used it

##.##%

Used it once

##.##%

Used it a little, e.g., for one course

##.##%

Used it a lot

##.##%

“I stream Netflix as ASCII art!"

##.##%

RESULTS SLIDE

Join at: **vevox.app** ID: **XXX-XXX-XXX**

Question slide

What is your experience with DTU's HPC systems?

Never used it

##.##%

Used ThinLinc once or twice

##.##%

Used it in interactive mode

##.##%

Used the batch job system

##.##%

"I bsub my breakfast!"

##.##%

Join at: **vevox.app** ID: **XXX-XXX-XXX**

What is your experience with DTU's HPC systems?

Never used it

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Used it in interactive mode

##.##%

Used the batch job system

##.##%

"I bsub my breakfast!"

##.##%

RESULTS SLIDE

Who we expect:

Experience:
Expected

Experience:
Nice but not needed

Today's lecture

1. Practical information

2. Python and High-Performance Computing

3. DTU's HPC system

What is high-performance computing?

Join at: **vevox.app** ID: **XXX-XXX-XXX**

Question slide

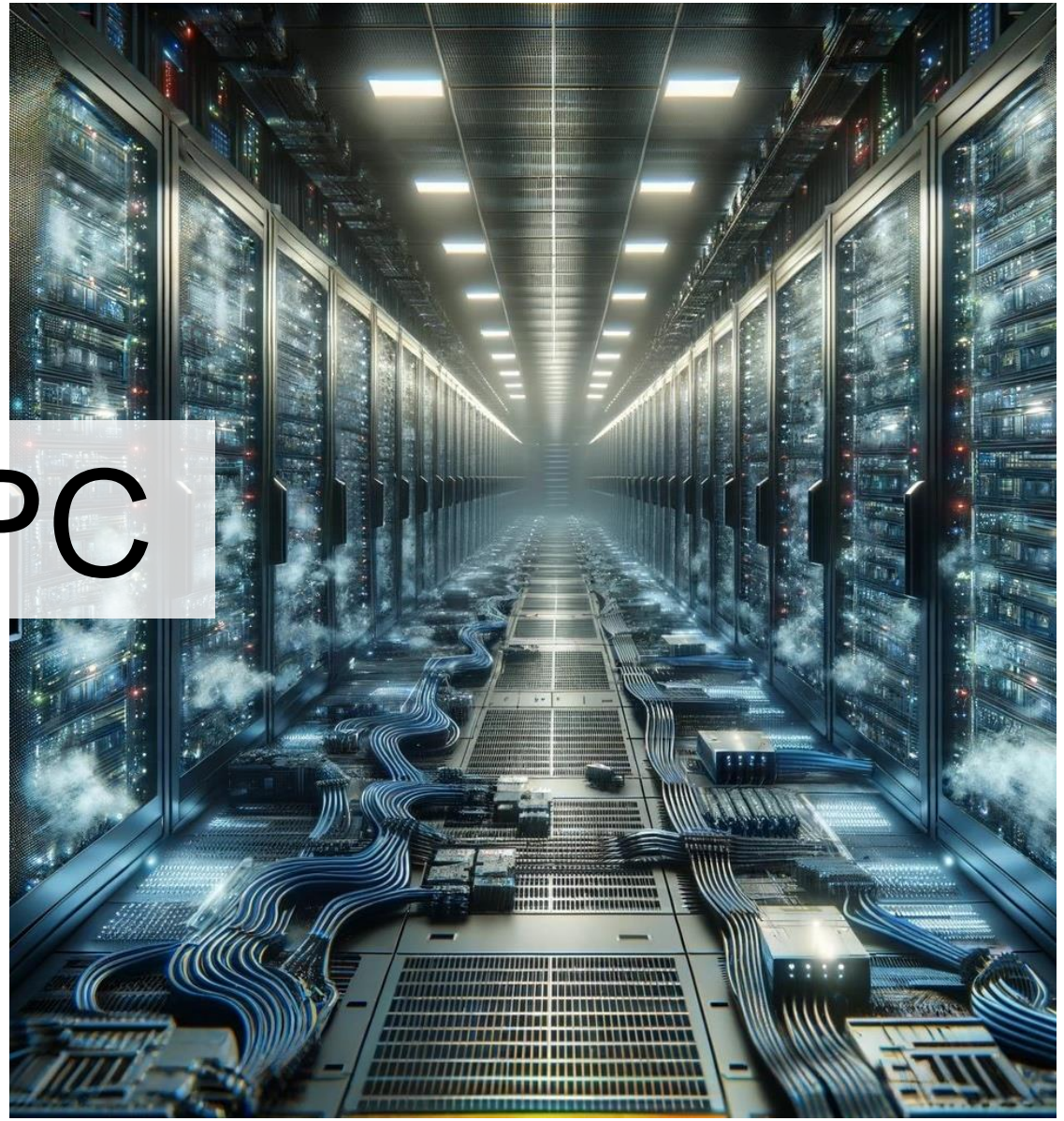
What does High Performance Computing mean to you?

Join at: **vevox.app** ID: **XXX-XXX-XXX**

What does High Performance Computing mean to you?

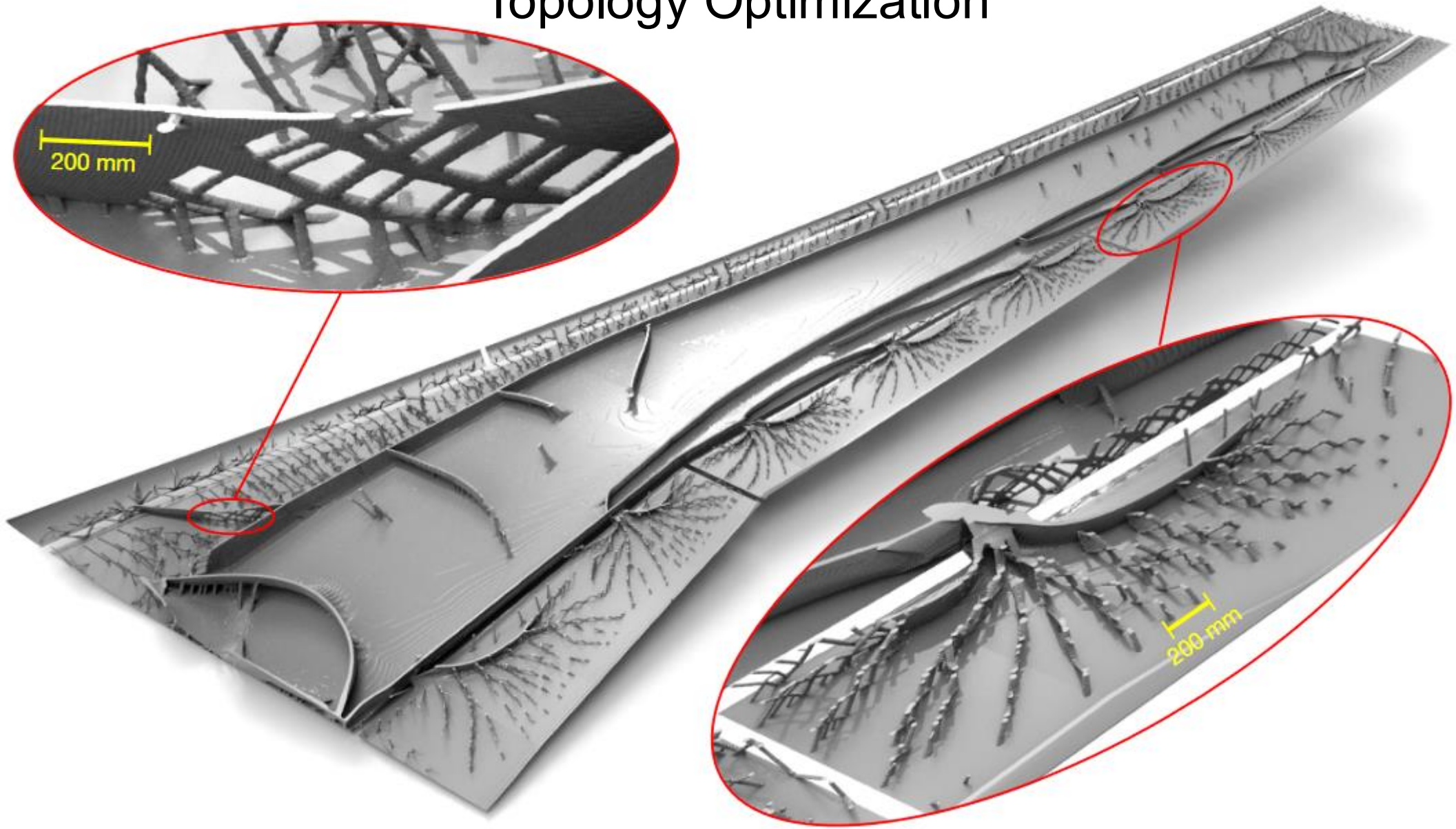
RESULTS SLIDE

HPC



Why high-performance computing?

Topology Optimization

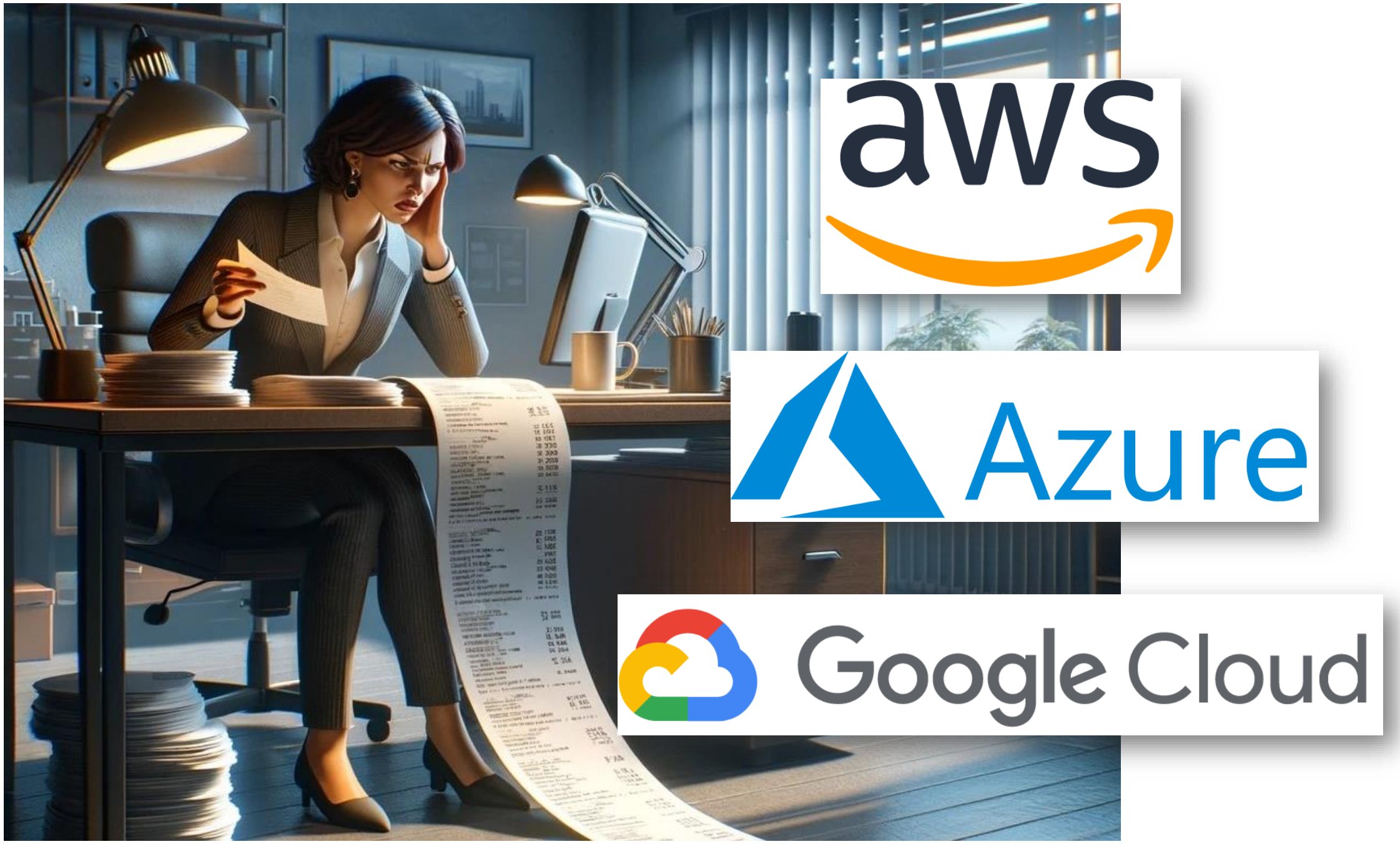


Wind Turbine Design

ChatGPT

GitHub Copilot

Why me?


aws
Azure
Google Cloud

Course goals

- Identify slow code and improve its performance
- Understand how hardware affects performance
- Efficiently utilize single core, multi core and GPU resources
- Use a modern HPC system (not just your own laptop/PC)

Official list on course base page

Week by week

Week 1	Intro meeting, diagnostic test, HPC intro	CPU
Week 2	Python primer and running Python on HPC	
Week 3	Memory hierarchy: caches, disks, etc.	
Week 4	Profiling and High-Performance NumPy	(mini-project released)
Week 5 + 6	Parallelism: Scalability and Amdahl's law	
Week 7	High-Performance Pandas and Apache Arrow	
Week 8	Storing Big Data	
Week 9	Numba and GPU Computing	GPU
Week 10	CuPy and GPU profiling	
Week 11	HPC Workflows	HPC Workflows
Week 12	Project Work (hand-in Sunday)	
Week 13	Common HPC Pitfalls and Q&A	

Today's lecture

1. Practical information

2. Python and High-Performance Computing

3. DTU's HPC system


HPC SERVER
CAMPUS COMPUTER SYSTEM
TECHNICAL UNIVERSITY OF DENMARK

What is an HPC cluster?

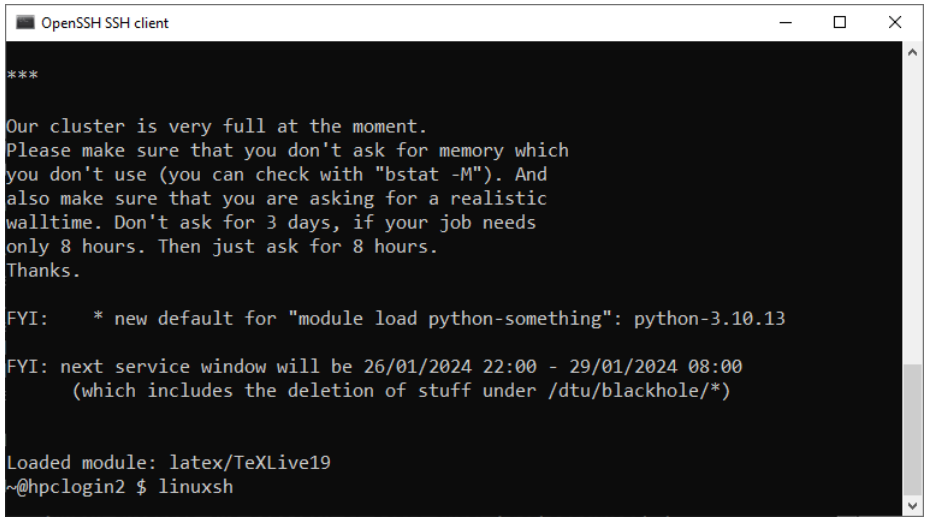
How do I access it!?

Your computer

Your computer

SSH or ThinLinc

Login node



node = a computer

Your computer

SSH or ThinLinc

Login node

```
OpenSSH SSH client

***

Our cluster is very full at the moment.
Please make sure that you don't ask for memory which
you don't use (you can check with "bstat -M"). And
also make sure that you are asking for a realistic
walltime. Don't ask for 3 days, if your job needs
only 8 hours. Then just ask for 8 hours.
Thanks.

FYI:    * new default for "module load python-something": python-3.10.13

FYI: next service window will be 26/01/2024 22:00 - 29/01/2024 08:00
     (which includes the deletion of stuff under /dtu/blackhole/*)


Loaded module: latex/TeXLive19
~@hpclogin2 $ linuxsh
```

Jump

Interactive nodes

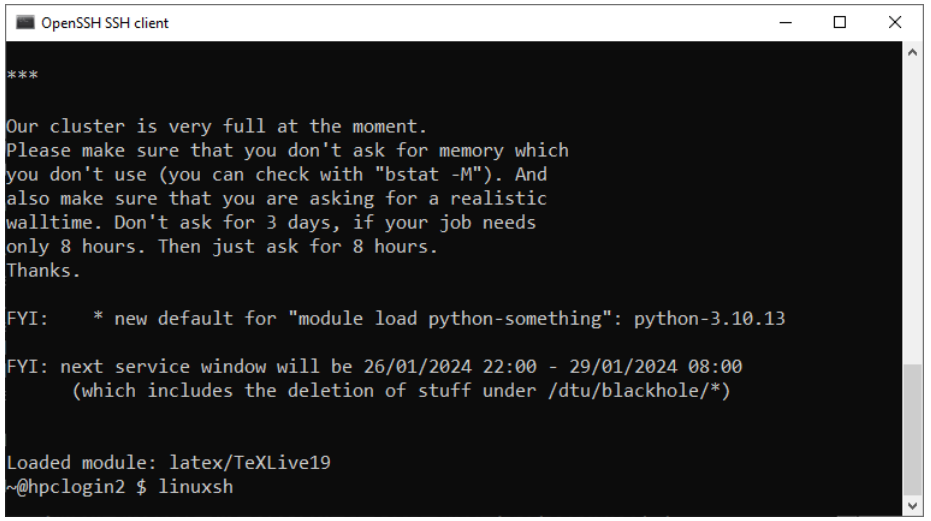
```
OpenSSH SSH client

~@n-62-11-19 $
```

Your computer

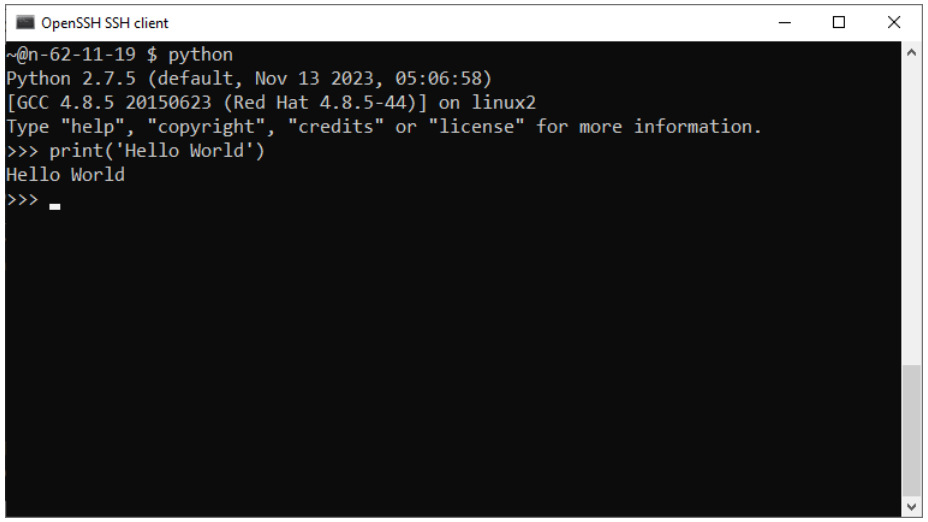
SSH or ThinLinc

Login node



Jump

Interactive nodes



Your computer

SSH or ThinLinc

Login node

Jump

Interactive nodes

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OpenSSH SSH client

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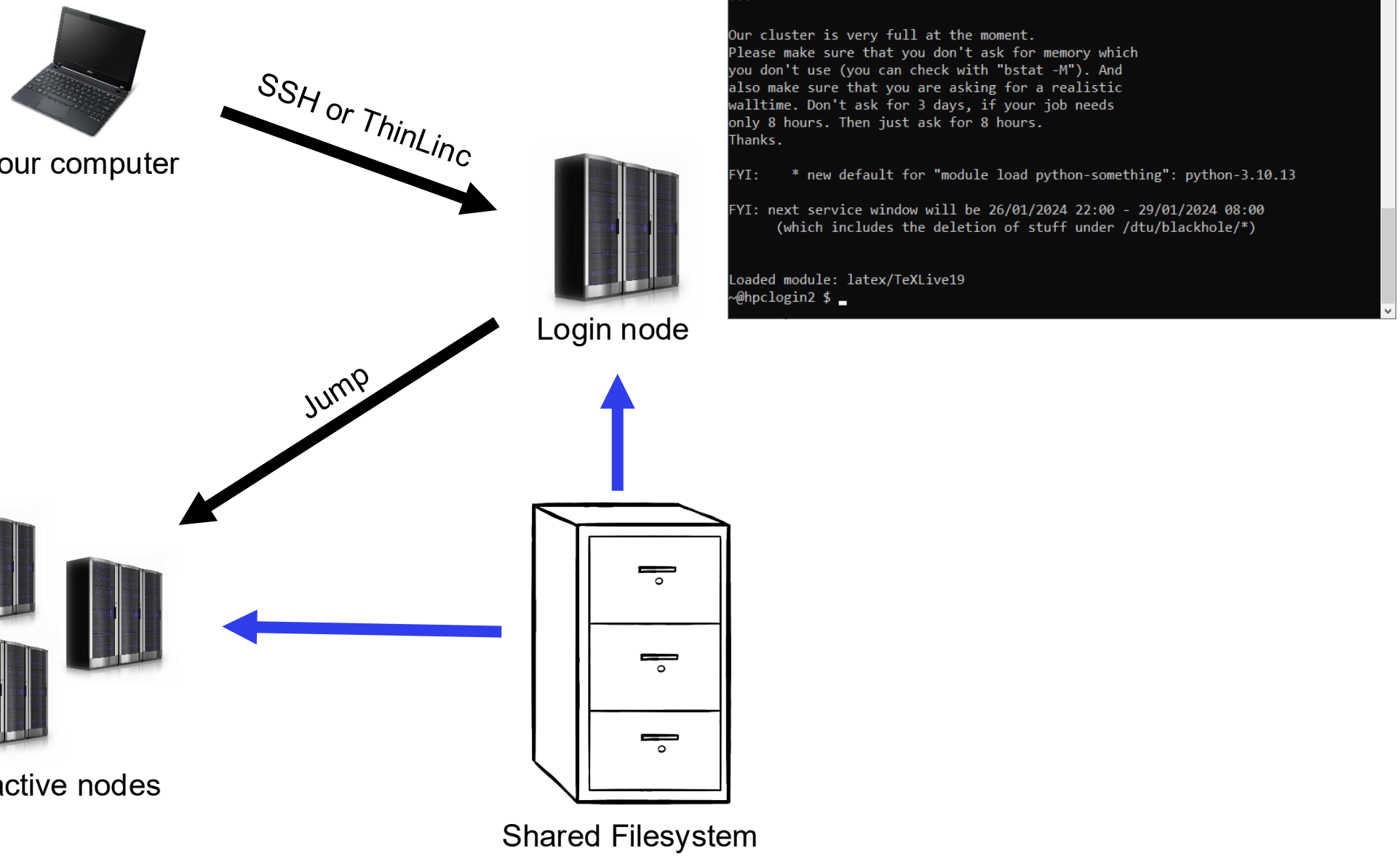
Your computer
SSH or ThinLinc
Login node
Jump
Interactive nodes
Shared Filesystem
OpenSSH SSH client
***
Our cluster is very full at the moment.
Please make sure that you don't ask for memory which
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Loaded module: latex/TeXLive19
~@hpclogin2 $

Your computer

SSH or ThinLinc

Login node

OpenSSH SSH client

```
***

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Loaded module: latex/TeXLive19
~@hpclogin2 $
```
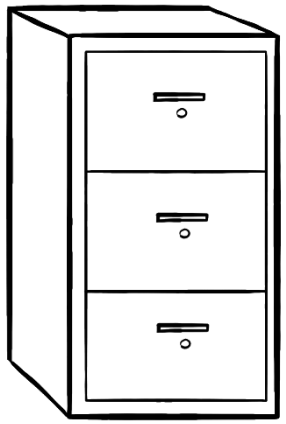

Jump

Batch jobs

Interactive nodes



Shared Filesystem

Non-Interactive nodes

Batch jobs: the simplest script

```
#!/bin/bash
sleep 60
```

submit.sh

Batch jobs: the simplest script

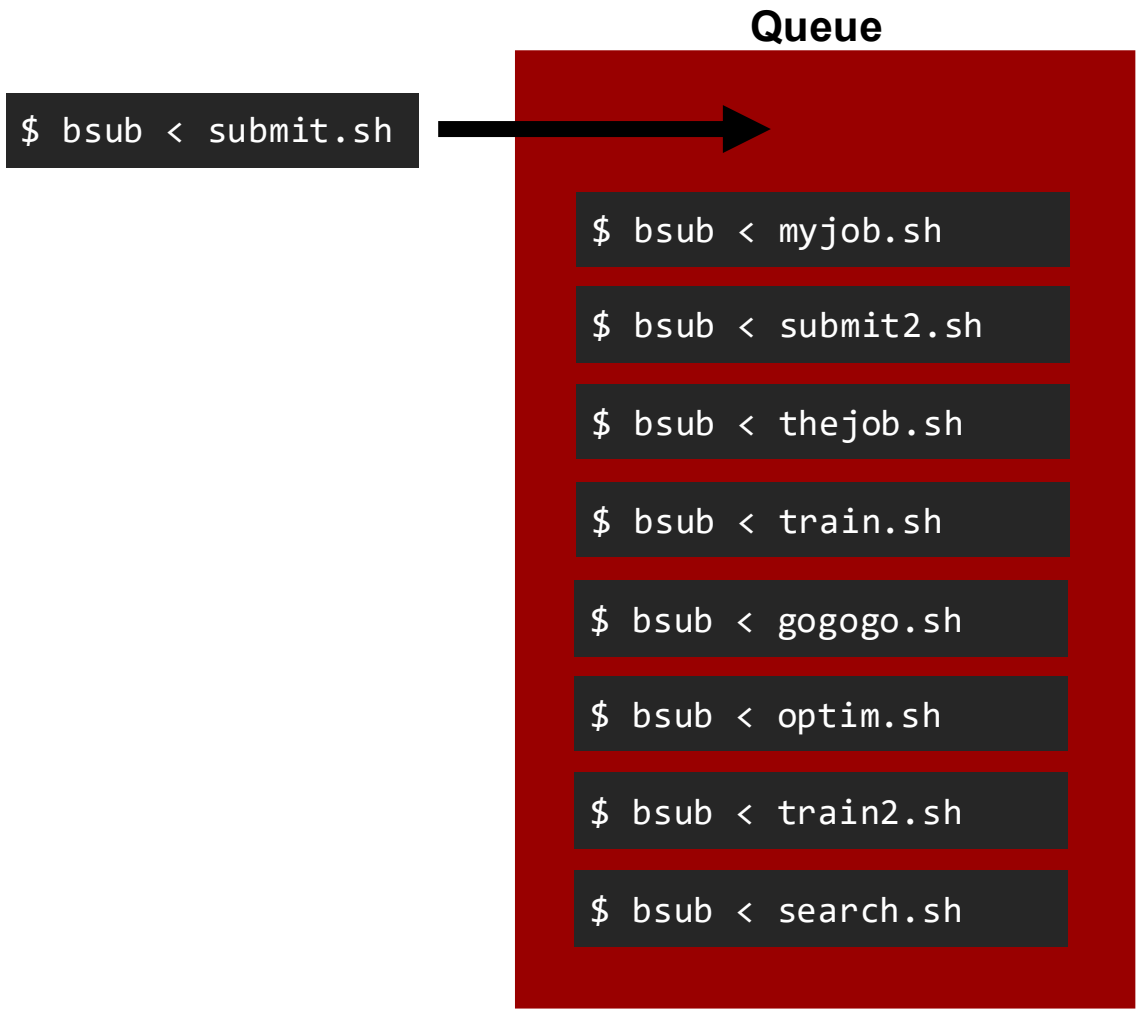
```
#!/bin/bash
sleep 60
```

submit.sh

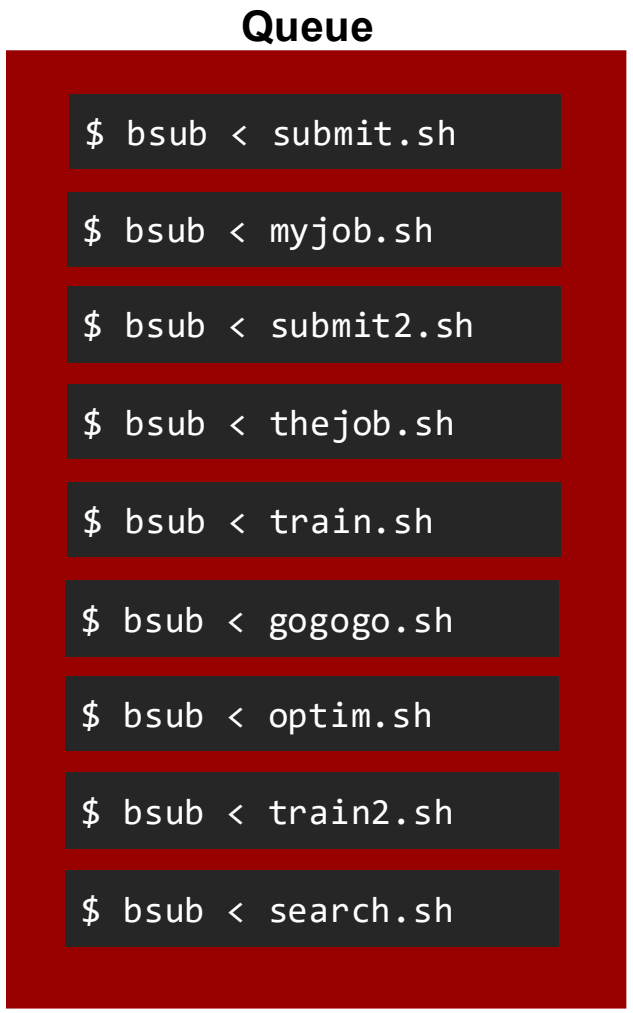
```
$ bsub < submit.sh
Job <702572> is submitted to default queue <hpc>.
$
```

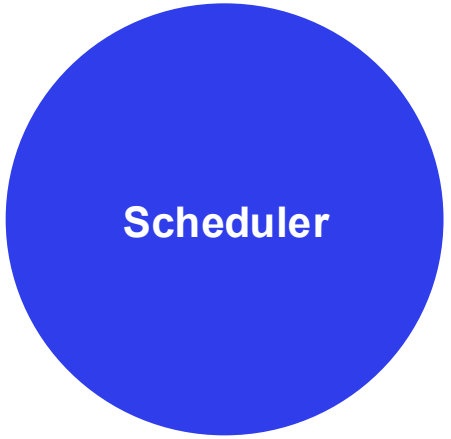
What happens now?

Interlude: queues and resource managers

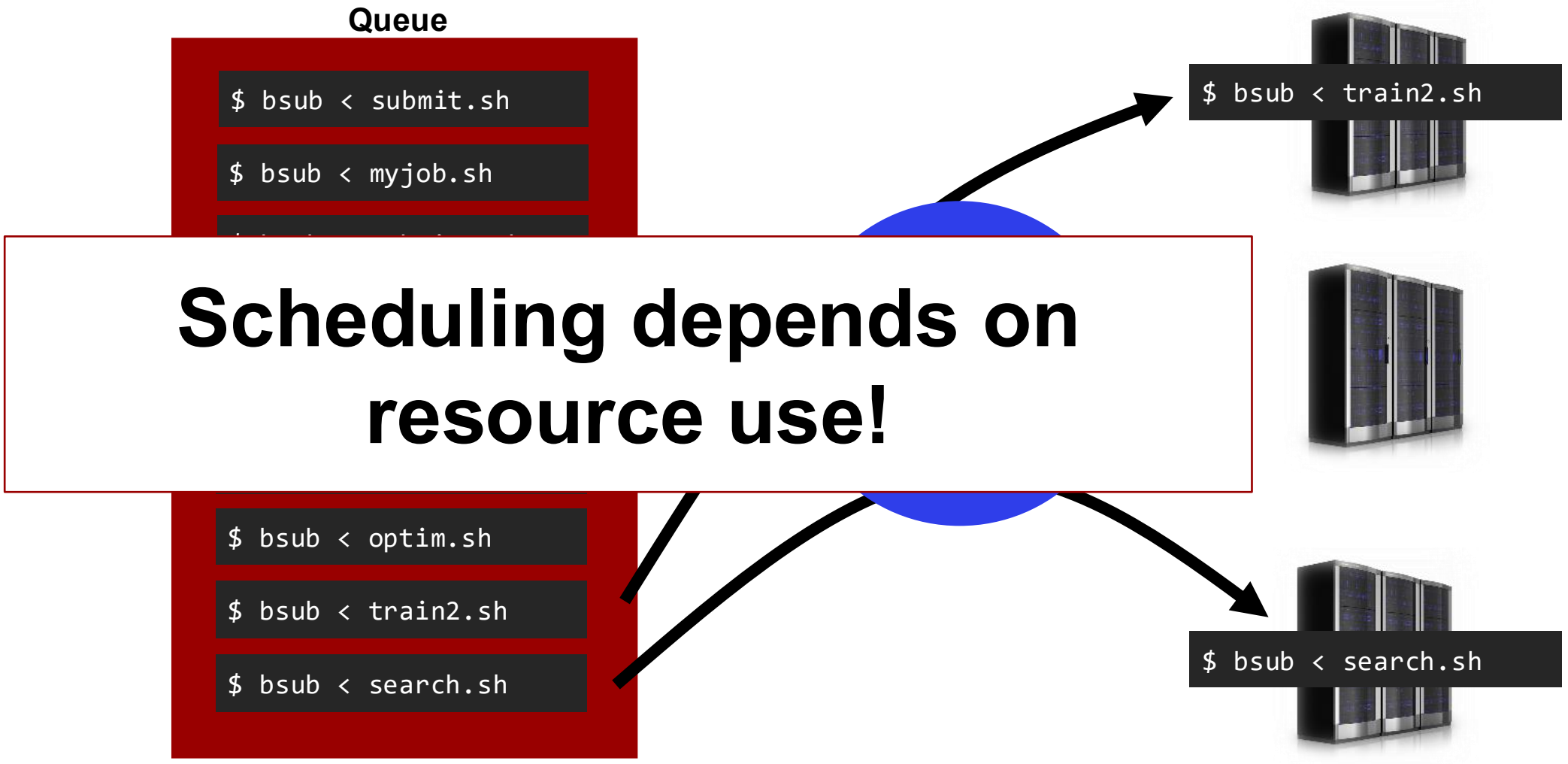


Interlude: queues and resource managers





Interlude: queues and resource managers



Scheduling depends on resource use!

Interlude: queues and resource managers

#	CPU	RAM	GPU	
31 x	2x Xeon E5 2650 v4	252 – 504 GB		hpc
46 x	2x Xeon E5 2660 v3	126 GB		
24 x	2x Xeon Gold 6126	189 – 756 GB		
4 x	2x Xeon Gold 6142	378 GB		
26 x	2x Xeon Gold 6226R	378 – 756 GB		
4 x	2x Xeon Gold 6342	504 GB		
8x	2x Xeon Gold 6126	189 – 378 GB	2x NVIDIA V100 16-32GB	gpuv100
3x	2x Xeon Gold 6142	378 GB	4x NVIDIA V100 32GB	
4x	2x Xeon Gold 6242	378 GB	2x NVIDIA V100 32GB	
5x	2x Xeon Gold 6226R	756 GB	2x NVIDIA A100 40GB	gpua100
6x	2x Xeon Gold 6326	1008 GB	2x NVIDIA A100 80GB	

… and more

Batch jobs: the simplest script

```
#!/bin/bash
sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702572> is submitted to default queue <hpc>.
$
```

Batch jobs: the simplest script

```
#!/bin/bash
sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702572> is submitted to default queue <hpc>.
$ bstat
JOBID  USER    QUEUE JOB_NAME SLOTS STAT START_TIME    ELAPSED
702572 patmjen hpc   NONAME   1     PEND      -         0:00:00
$
```

Batch jobs: the simplest script

```
#!/bin/bash
sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702572> is submitted to default queue <hpc>.
$ bstat
JOBID  USER    QUEUE JOB_NAME SLOTS STAT START_TIME    ELAPSED
702572 patmjen hpc   NONAME   1     RUN  Dec 13 12:17  0:00:00
$
```

Batch jobs: the simplest script

```
#!/bin/bash
sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702572> is submitted to default queue <hpc>.
$ bstat
JOBID  USER    QUEUE JOB_NAME SLOTS STAT START_TIME    ELAPSED
702572 patmjen hpc   NONAME   1     RUN  Dec 13 12:17  0:00:00
$ bjobs
JOBID  USER    QUEUE JOB_NAME SLOTS STAT START_TIME   TIME_LEFT
702572 patmjen hpc   NONAME   1     RUN  Dec 13 12:17 00:02:00 L
$
```

Batch jobs: the simplest script

```
#!/bin/bash
sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702572> is submitted to default queue <hpc>.
$ bstat
JOBID  USER    QUEUE JOB_NAME SLOTS STAT START_TIME    ELAPSED
702572 patmjen hpc   NONAME   1     RUN  Dec 13 12:17  0:00:00
$ bjobs
JOBID  USER    QUEUE JOB_NAME SLOTS STAT START_TIME   TIME_LEFT
702572 patmjen hpc   NONAME   1     RUN  Dec 13 12:17 00:02:00 L
$ ls -1
NONAME_702572.out
submit.sh
$
```

Batch jobs: the simplest script

```
#!/bin/bash
sleep 60
```

submit.sh

```
$ bsub < submit.sh
```

Batch jobs: the simplest script

```
#!/bin/bash
sleep 60
```

submit.sh

```
$ bsub < submit.sh
bsub info: Job has no name! Setting it to NONAME!
bsub info: Job has no wall-clock time! Setting it to 15 minutes!
bsub info: Job has no output file! Setting it to NONAME_%J.out!
bsub info: Job has no memory requirements! Setting it to 1024 MB!
bsub info:   You need to specify at least -R "rusage[mem=...]"!
Job <702572> is submitted to default queue <hpc>.
$
```

Need to specify resources!

Batch jobs: the simple script

Job name
Queue name
Wall-clock time
Resources (mem)
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702573> is submitted to queue <hpc>.
$
```

Batch jobs: the simple script

Job name
Queue name
Wall-clock time
Resources (mem)
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702573> is submitted to queue <hpc>.
$ ls -1
sleeper_702573.out
sleeper_702573.err
submit.sh
$
```

Batch jobs: output files

Job name
Queue name
Wall-clock time
Resources (mem)
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
<printed output if any>
------------------------------------------------------------
Sender: LSF System <lsfadmin@hpc.dtu.dk>
Subject: Job 19953623: <sleeper> in cluster <dcc> Done

Job <sleeper> was submitted from host <n-62-11-19> by user
<patmjen> in cluster <dcc> at Mon Jan 22 11:11:23 2024
Job was executed on host(s) <n-62-31-4>, in queue <hpc>, as user
<patmjen> in cluster <dcc> at Mon Jan 22 11:11:25 2024
</zhome/9d/d/98006> was used as the home directory.
</zhome/9d/d/98006/Documents/02613> was used as the working
directory.
Started at Mon Jan 22 11:11:25 2024
Terminated at Mon Jan 22 11:12:27 2024
Results reported at Mon Jan 22 11:12:27 2024

… more
```

sleeper_702573.out

Batch jobs: output files

Job name
Queue name
Wall-clock time
Resources (mem)
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
…
Your job looked like:

------------------------------------------------------------
# LSBATCH: User input
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R "rusage[mem=512MB]"
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60

… more
```

sleeper_702573.out

Batch jobs: output files

Job name
Queue name
Wall-clock time
Resources (mem)
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
…
------------------------------------------------------------

Successfully completed.

Resource usage summary:

    CPU time :                                   0.82 sec.
    Max Memory :                                 4 MB
    Average Memory :                             4.00 MB
    Total Requested Memory :                     512.00 MB
    Delta Memory :                               508.00 MB
    Max Swap :                                   -
    Max Processes :                              4
    Max Threads :                                5
    Run time :                                   62 sec.
    Turnaround time :                            64 sec.
```

sleeper_702573.out

Batch jobs: multiple cores

Job name
Queue name
Wall-clock time
Resources (mem)
Number of cores
Number of hosts
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -n 4
#BSUB -R ”span[hosts=1]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702574> is submitted to queue <hpc>.
$
```

Note: memory usage is *multiplied* by number of requested cores!

Actual requested memory: 2048 MB = 2GB

Interlude: what is my actual hardware?

```
$ lscpu
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                48
On-line CPU(s) list:   0-47
Thread(s) per core:    2
Core(s) per socket:    12
Socket(s):             2
NUMA node(s):          2
Vendor ID
CPU famil
Model:
Model nar
Stepping
CPU MHz:
BogoMIPS
Virtuali
L1d cach
L1i cache:             32K
L2 cache:              1024K
L3 cache:              19712K
NUMA node0 CPU(s):     0-11,24-35
NUMA node1 CPU(s):     12-23,36-47
Flags:                 <omitted…>
```

Number of threads

Number of cores / socket

Number of sockets

Note: shows hardware cores.
***Not* what you requested!**

Interlude: what is my actual hardware?

```
$ cpucount
48
$ echo $CPUTYPEV
XeonGold6226
```

Batch jobs: selecting hardware

Job name
Queue name
Wall-clock time
Resources (mem)
CPU model
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -R "select[model==XeonGold6226R]"
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

lscpu
sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702575> is submitted to queue <hpc>.
$
```

Batch jobs: selecting hardware

Job name
Queue name
Wall-clock time
Resources (mem)
CPU model
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -R "select[model==XeonGold6226R]"
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

lscpu
sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702575> is submitted to queue <hpc>.
$ cat sleeper_702575.out
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                48
On-line CPU(s) list:   0-47
Thread(s) per core:    2
Core(s) per socket:    12
Socket(s):             2
NUMA node(s):          2
Vendor ID:             GenuineIntel
CPU family:            6
Model:                 85
Model name:            Intel(R) Xeon(R) Gold 6226
…
------------------------------------------------

Sender: LSF System <lsfadmin@hpc.dtu.dk>
…
```

Batch jobs: checking the output

Job name
Queue name
Wall-clock time
Resources (mem)
CPU model
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -R "select[model==XeonGold6226R]"
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

lscpu
sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702575> is submitted to queue <hpc>.
$ bpeek
<< output from stdout >>
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                48
On-line CPU(s) list:   0-47
Thread(s) per core:    2
Core(s) per socket:    12
Socket(s):             2
NUMA node(s):          2
…
<< output from stderr >>
$
```

Batch jobs: checking the output

Job name
Queue name
Wall-clock time
Resources (mem)
CPU model
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -R "select[model==XeonGold6226R]"
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

lscpu
sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702575> is submitted to queue <hpc>.
$ bpeek 702575
<< output from stdout >>
Architecture:          x86_64
CPU op-mode(s):        32-bit, 64-bit
Byte Order:            Little Endian
CPU(s):                48
On-line CPU(s) list:   0-47
Thread(s) per core:    2
Core(s) per socket:    12
Socket(s):             2
NUMA node(s):          2
…
<< output from stderr >>
$
```

What if I make a mistake?

Batch jobs: invalid jobs

Job name
Queue name
Wall-clock time
Resources (mem)
Number of cores
Number of hosts
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -n 99
#BSUB -R ”span[hosts=1]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
$ bsub < submit.sh
```

Batch jobs: invalid jobs

Job name
Queue name
Wall-clock time
Resources (mem)
Number of cores
Number of hosts
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -n 99
#BSUB -R ”span[hosts=1]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702576> is submitted to queue <hpc>.
$
```

Batch jobs: invalid jobs

Job name
Queue name
Wall-clock time
Resources (mem)
Number of cores
Number of hosts
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -n 99
#BSUB -R ”span[hosts=1]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702576> is submitted to queue <hpc>.
$ bstat
JOBID   USER     QUEUE JOB_NAME NALLOC STAT START_TIME  ELAPSED
702576  patmjen  hpc   sleeper       0 PEND      -      0:00:00
$
```

Job will never start!

Batch jobs: invalid jobs

Job name
Queue name
Wall-clock time
Resources (mem)
Number of cores
Number of hosts
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=512MB]”
#BSUB -n 99
#BSUB -R ”span[hosts=1]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702576> is submitted to queue <hpc>.
$ bstat
JOBID   USER     QUEUE JOB_NAME NALLOC STAT START_TIME  ELAPSED
702576  patmjen  hpc   sleeper       0 PEND      -      0:00:00
$ bjobs -p
JOBID   USER     STAT  QUEUE  FROM_HOST  EXEC_HOST JOB_NAME …
702576  patmjen  PEND  hpc    hpclogin2            sleeper  …
 Not enough job slot(s): 10 hosts;
$
```

Batch jobs: invalid jobs

Job name
Queue name
Wall-clock time
Resources (mem)
Number of cores
Number of hosts
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=250GB]”
#BSUB -n 8
#BSUB -R ”span[hosts=1]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702577> is submitted to queue <hpc>.
$ bstat
JOBID   USER     QUEUE JOB_NAME NALLOC STAT START_TIME  ELAPSED
702577  patmjen  hpc   sleeper       0 PEND      -      0:00:00
$
```

Batch jobs: invalid jobs

Job name
Queue name
Wall-clock time
Resources (mem)
Number of cores
Number of hosts
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=250GB]”
#BSUB -n 8
#BSUB -R ”span[hosts=1]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702577> is submitted to queue <hpc>.
$ bstat
JOBID   USER     QUEUE JOB_NAME NALLOC STAT START_TIME  ELAPSED
702577  patmjen  hpc   sleeper       0 PEND      -      0:00:00
$ bjobs -p
JOBID   USER     STAT  QUEUE  FROM_HOST  EXEC_HOST JOB_NAME …
702577  patmjen  PEND  hpc    hpclogin2            sleeper  …
 Job's requirements for resource reservation not satisfied: 10
hosts;
$
```

Note: sometimes you just have to wait! Help out by giving good resource requirements.

Batch jobs: invalid jobs

Job name
Queue name
Wall-clock time
Resources (mem)
Number of cores
Number of hosts
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=250GB]”
#BSUB -n 8
#BSUB -R ”span[hosts=1]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702577> is submitted to queue <hpc>.
$ bstat
JOBID   USER     QUEUE JOB_NAME NALLOC STAT START_TIME  ELAPSED
702577  patmjen  hpc   sleeper       0 PEND      -      0:00:00
$ bjobs -p
JOBID   USER     STAT  QUEUE  FROM_HOST  EXEC_HOST JOB_NAME …
702577  patmjen  PEND  hpc    hpclogin2            sleeper  …
 Job's requirements for resource reservation not satisfied: 10
hosts;
$
```

Batch jobs: invalid jobs

Job name
Queue name
Wall-clock time
Resources (mem)
Number of cores
Number of hosts
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=250GB]”
#BSUB -n 8
#BSUB -R ”span[hosts=1]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702577> is submitted to queue <hpc>.
$ bstat
JOBID   USER     QUEUE JOB_NAME NALLOC STAT START_TIME  ELAPSED
702577  patmjen  hpc   sleeper       0 PEND      -      0:00:00
$ bjobs -p
JOBID   USER     STAT  QUEUE  FROM_HOST  EXEC_HOST JOB_NAME …
702577  patmjen  PEND  hpc    hpclogin2            sleeper  …
 Job's requirements for resource reservation not satisfied: 10
hosts;
$ bkill 702577
Job <702577> is being terminated
$
```

Batch jobs: invalid jobs

Job name
Queue name
Wall-clock time
Resources (mem)
Number of cores
Number of hosts
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -W 2
#BSUB -R ”rusage[mem=250GB]”
#BSUB -n 8
#BSUB -R ”span[hosts=1]”
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702577> is submitted to queue <hpc>.
$ bstat
JOBID   USER     QUEUE JOB_NAME NALLOC STAT START_TIME  ELAPSED
702577  patmjen  hpc   sleeper       0 PEND      -      0:00:00
$ bjobs -p
JOBID   USER     STAT  QUEUE  FROM_HOST  EXEC_HOST JOB_NAME …
702577  patmjen  PEND  hpc    hpclogin2            sleeper  …
 Job's requirements for resource reservation not satisfied: 10
hosts;
$ bkill 702577
Job <702577> is being terminated
$
```

Please clean after yourselves with bkill

Batch jobs: invalid jobs

Job name
Queue name
Wall-clock ti
Resources (m
Number of co
Number of hosts
Output file (stdout)
Output file (stderr)

```
#!/bin/bash
#BSUB -J sleeper
#BSUB -q hpc
#BSUB -R ”span[h
#BSUB -o sleeper_%J.out
#BSUB -e sleeper_%J.err

sleep 60
```

submit.sh

```
$ bsub < submit.sh
Job <702577> is submitted to queue <hpc>.
$ bstat
JOBID   USER     QUEUE JOB_NAME NALLOC STAT START_TIME  ELAPSED
        patmjen  hpc   sleeper       0 PEND      -       0:00:00

                                                EXEC_HOST JOB_NAME …
 Job's requirements
hosts;
$ bkill 702577
Job <702577> is being terminated
$
```

More available – Links to guides on Learn

Today’s exercise

Get set up and get familiar:

1. File upload and download
2. Python scripts on interactive nodes
3. Simple batch jobs

Python on HPC: shared Anaconda env

```
$
```

Python on HPC: shared Anaconda env

```
$ source /dtu/projects/02613_2025/conda/conda_init.sh
$ conda activate 02613
```

Python on HPC: shared Anaconda env

```
$ source /dtu/projects/02613_2024/conda/conda_init.sh
$ conda activate 02613
(02613) $
```

Python on HPC: shared Anaconda env

```
$ source /dtu/projects/02613_2024/conda/conda_init.sh
$ conda activate 02613
(02613) $ python -c "import sys; print(sys.executable)”
/dtu/projects/02613_2025/conda/miniconda3/envs/02613/bin/python
(02613) $
```

Python on HPC: shared Anaconda env

```
$ source /dtu/projects/02613_2024/conda/conda_init.sh
$ conda activate 02613
(02613) $ python -c "import sys; print(sys.executable)”
/dtu/projects/02613_2024/conda/miniconda3/envs/02613/bin/python
(02613) $
```

Must do this everytime you change node!

Python on HPC: shared Anaconda env

```
$ source /dtu/projects/02613_2024/conda/conda_init.sh
$ conda activate 02613
(02613) $ python -c "import sys; print(sys.executable)”
/dtu/projects/02613_2024/conda/miniconda3/envs/02613/bin/python
(02613) $
```

Check ”Initializing the 02613 Conda Environment” in Learn for known issues

Useful commands

Log on to HPC
ssh <username>@login.hpc.dtu.dk
ssh <username>@login2.hpc.dtu.dk

Initialize course Anaconda environment
source /dtu/projects/02613_2024/conda/conda_init.sh
conda activate 02613

Change to work node
linuxsh

Terminal commands (directory == folder)

```
pwd                 # print working directory
ls                  # list contents of working directory
ls <path>           # list contents of path
cd <path>           # change directory to path
mkdir -p <path>     # make new directory
```

Check CPU
lscpu

Submit job script
bsub < submit.sh

Job status
bstat
bjobs
bjobs –p # pending reason

Check job output
bpeek
bpeek <JOBID>

Kill job
bkill <JOBID>