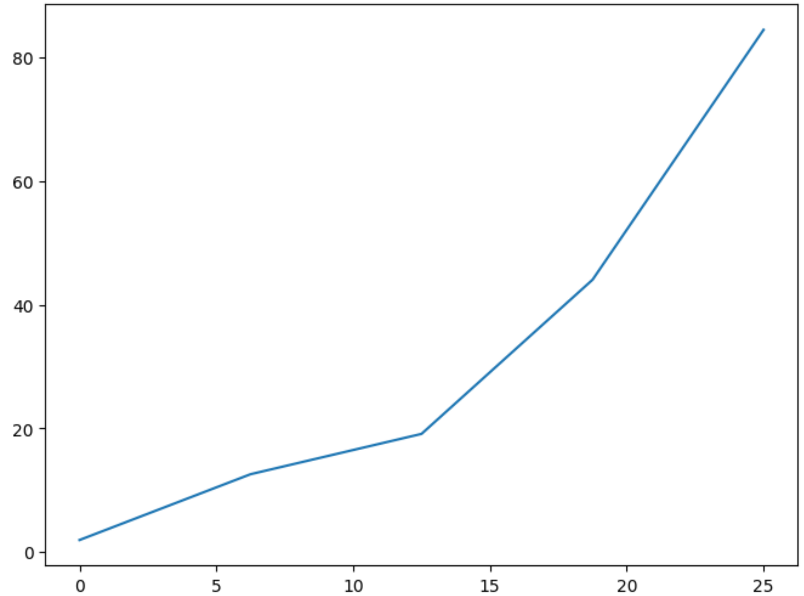
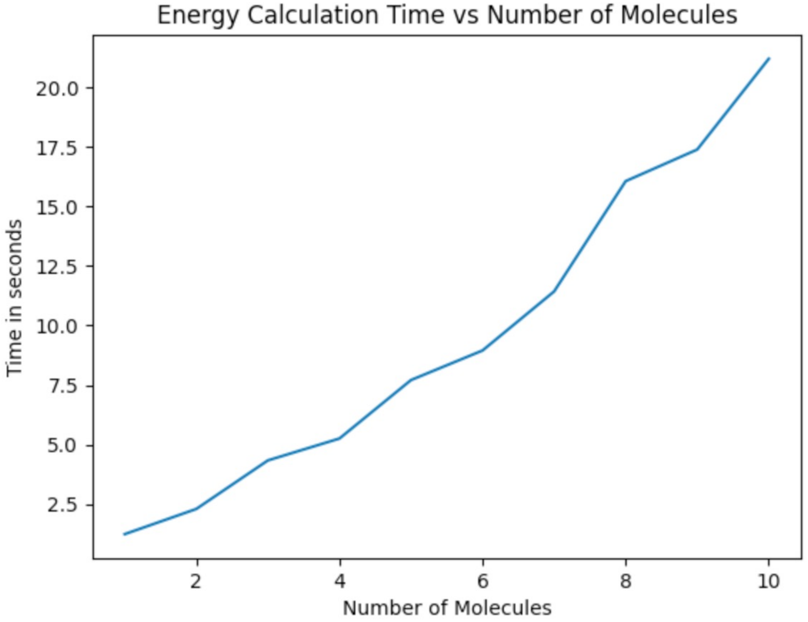
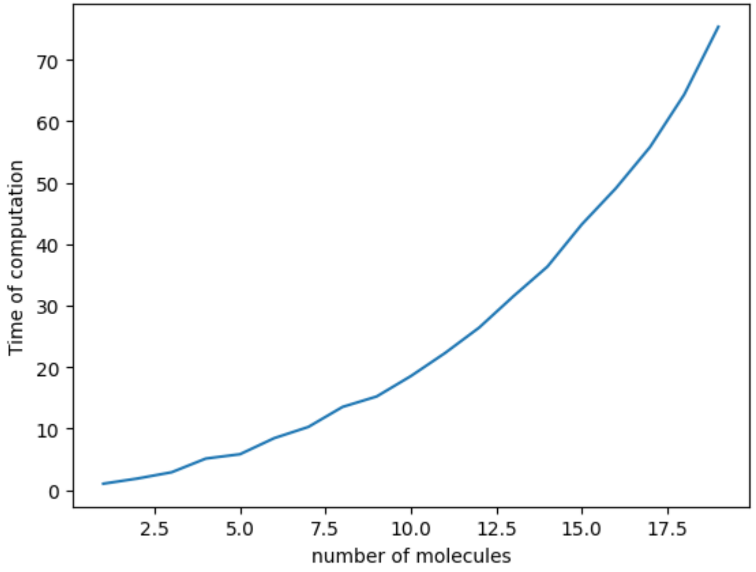
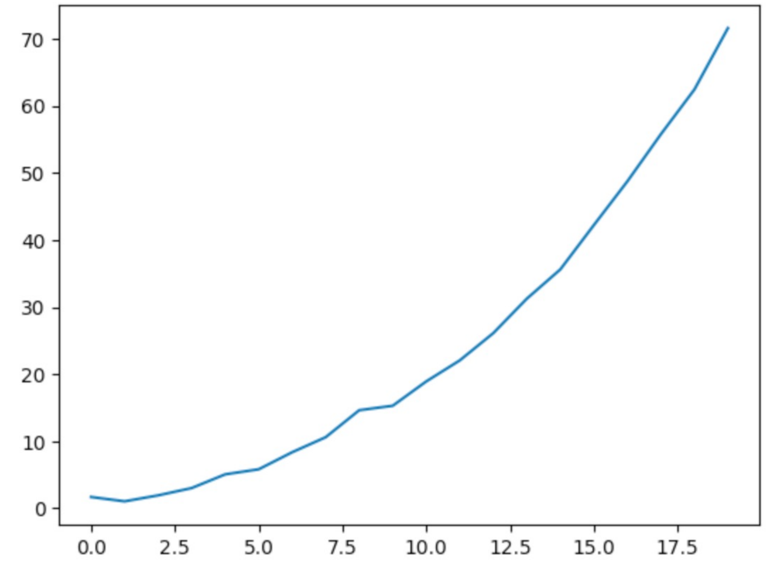
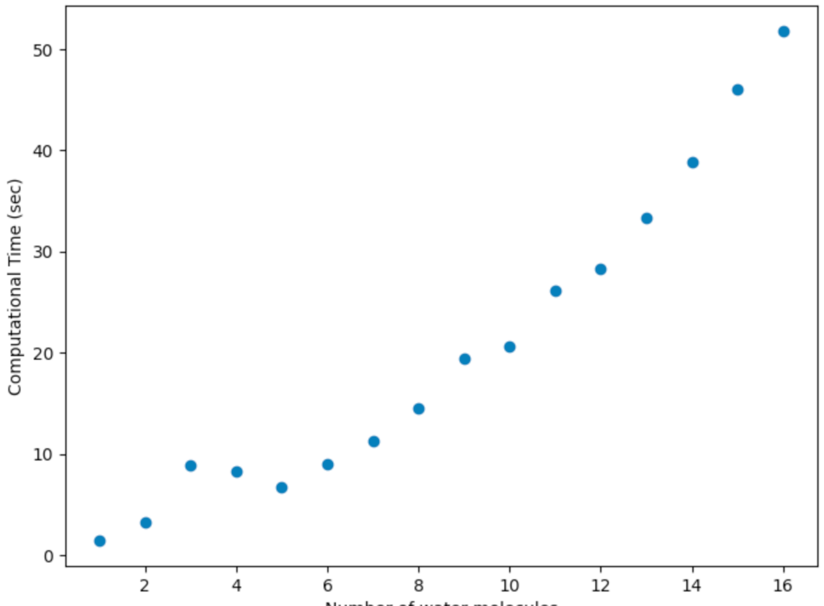
HW15 Runtime Calculation: # of Molecules vs Time

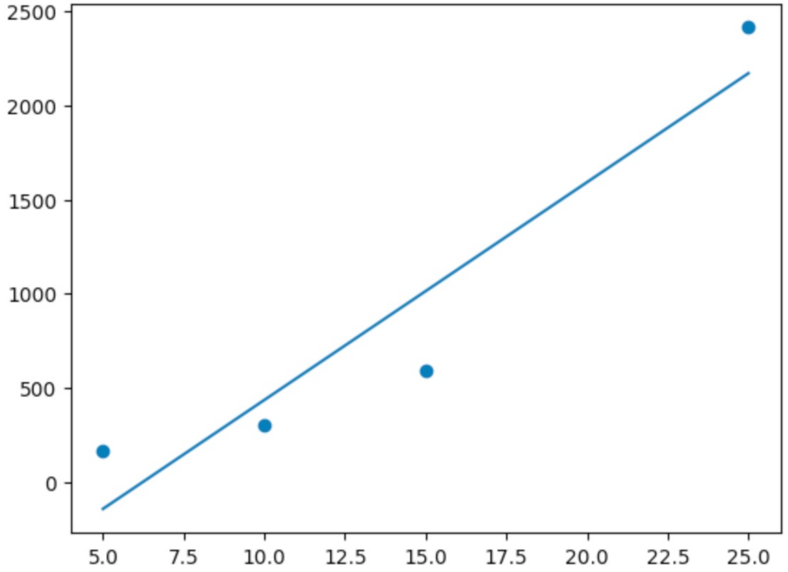


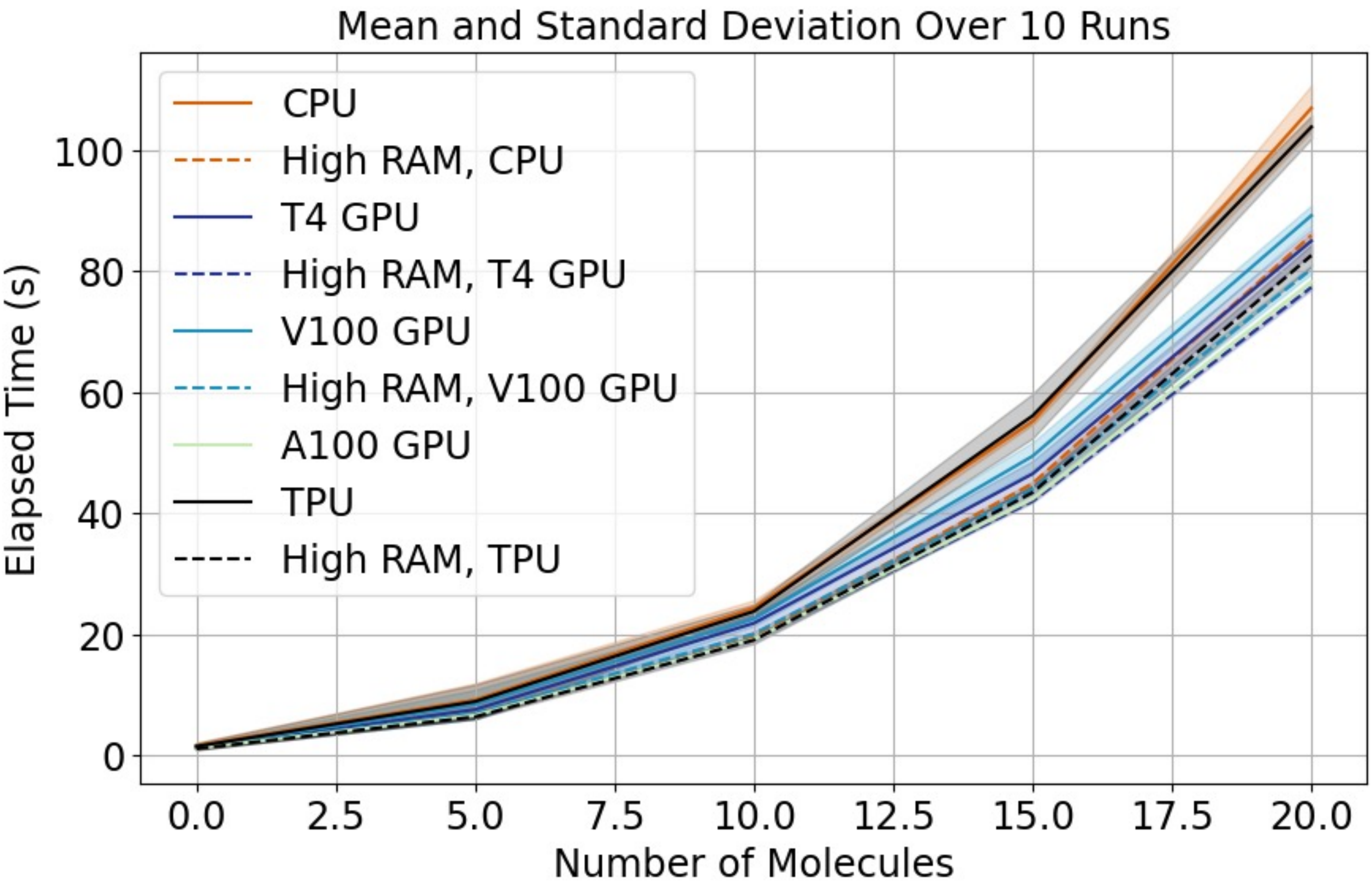






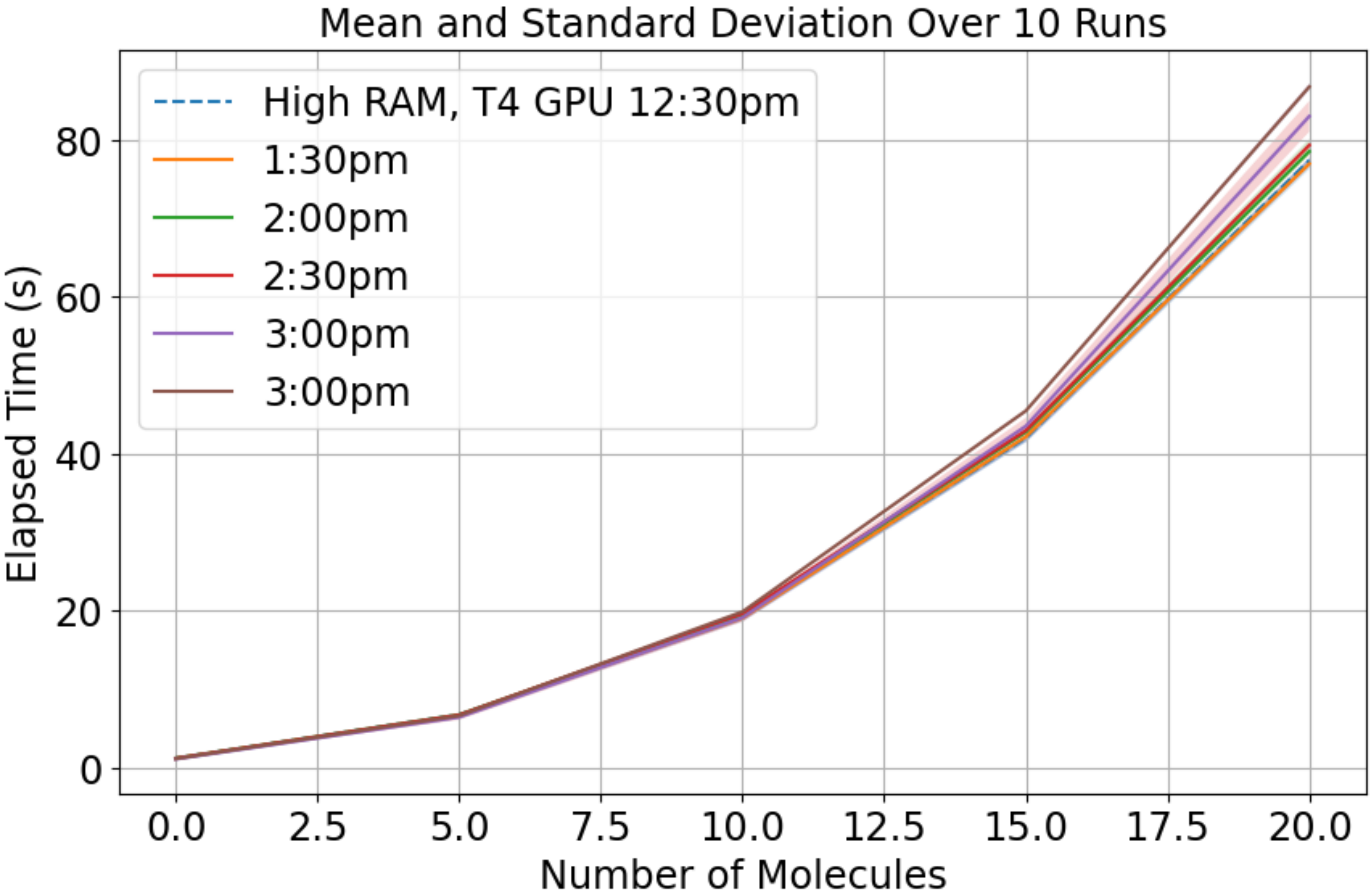






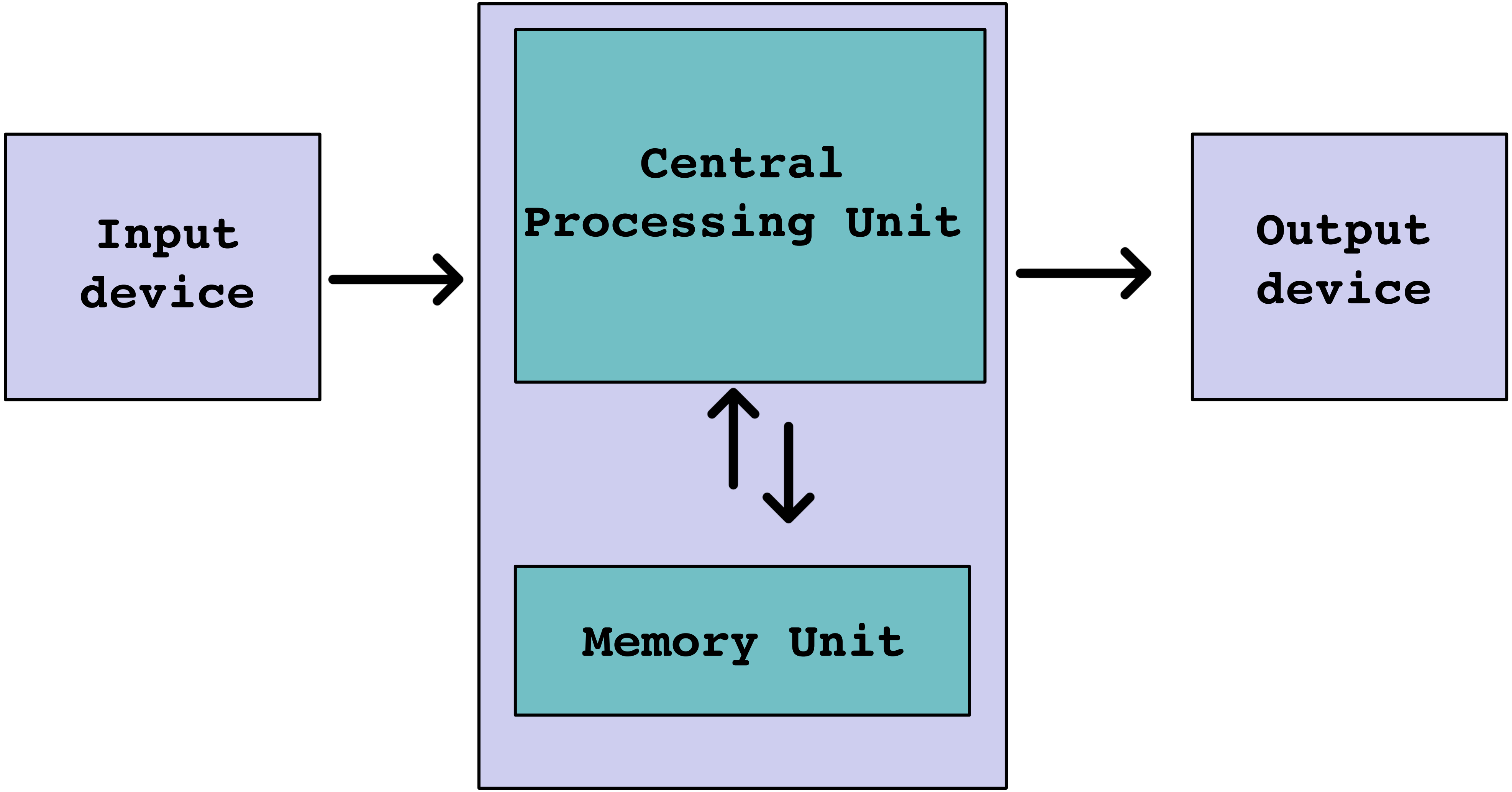
“Benchmarking” done on Google Colab

March 25th, 2024 ~12:00pm Claremont, CA

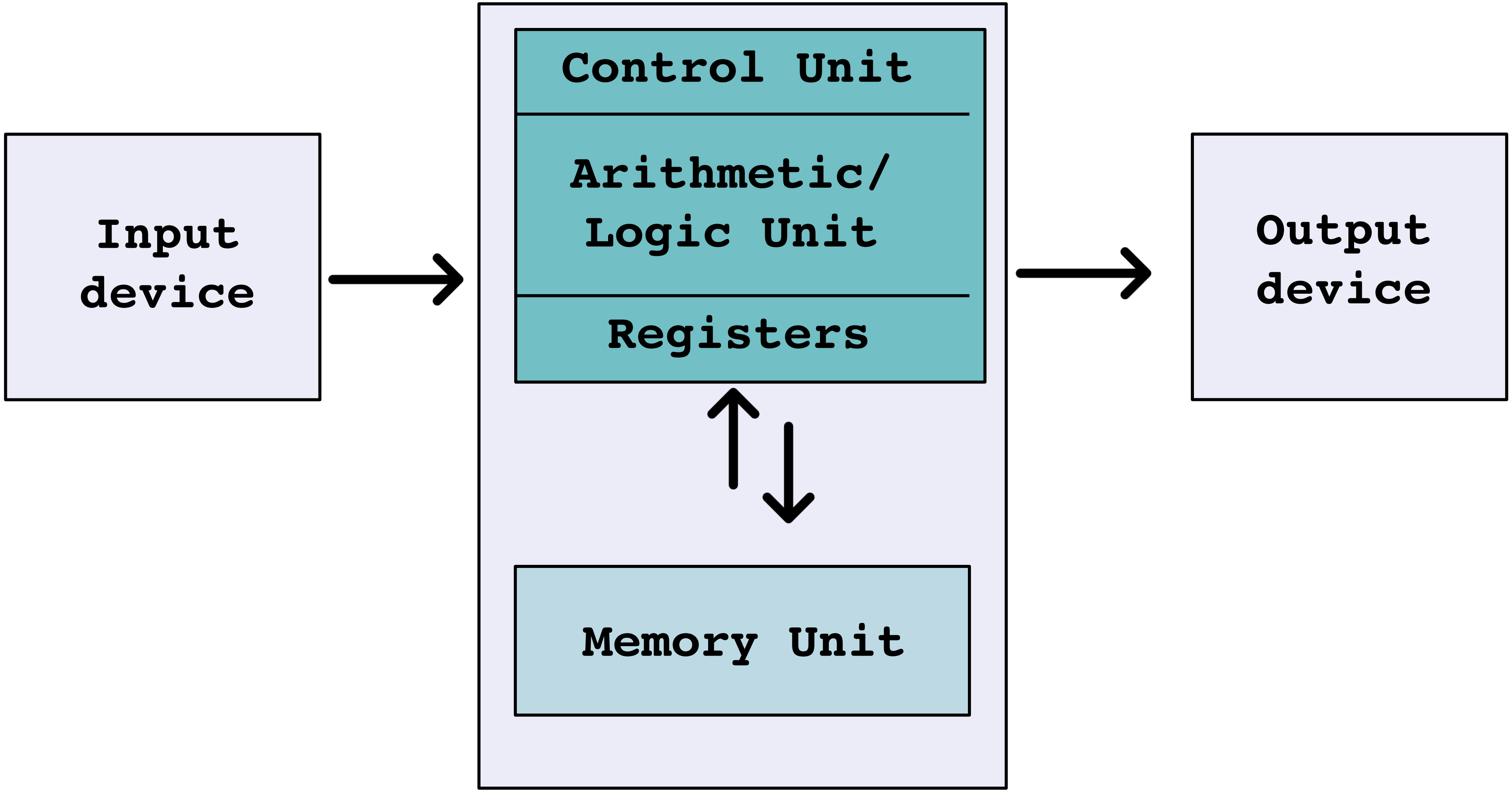


Why does runtime look like it is increasing overtime?

A computer
(von Neumann architecture)

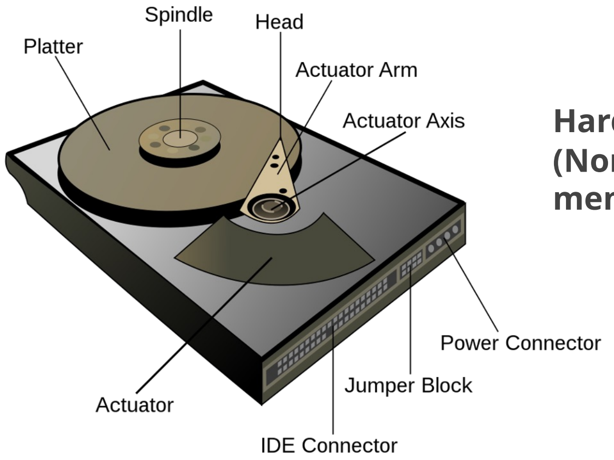


A computer
(von Neumann architecture)



Memory

- Different kinds of memory have different properties.
- Typically some trade-off between power requirements, cost, and speed.
- Memory *usually* refers to *volatile memory* in the form of RAM.



Hard Drive (Non-volatile memory)

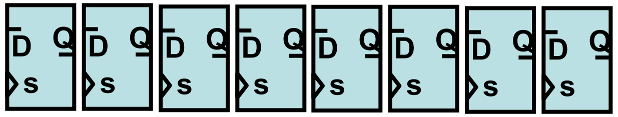
RAM (Volatile memory)

Memory can mean difference things

Registers

on the Central Processing Unit

8 flip-flops are an 8-bit **register**



100 Registers of 8-64 bits each

~ 10,000 bits

Main Memory

(volatile memory)

~ 10 billion bits +

1 GB memory

Disk Drive

(non-volatile memory)

~10 trillion bits (or more)

1 TB drive

	Registers	Main Memory	Disk Drive
Time	1 clock cycle 10^{-9} sec	100 cycles 10^{-7} sec	10^{7} cycles 10^{-2} sec
If a cycle == 1 minute	**1 min**	**1.5 hours**	**19 YEARS**

What is HPC?

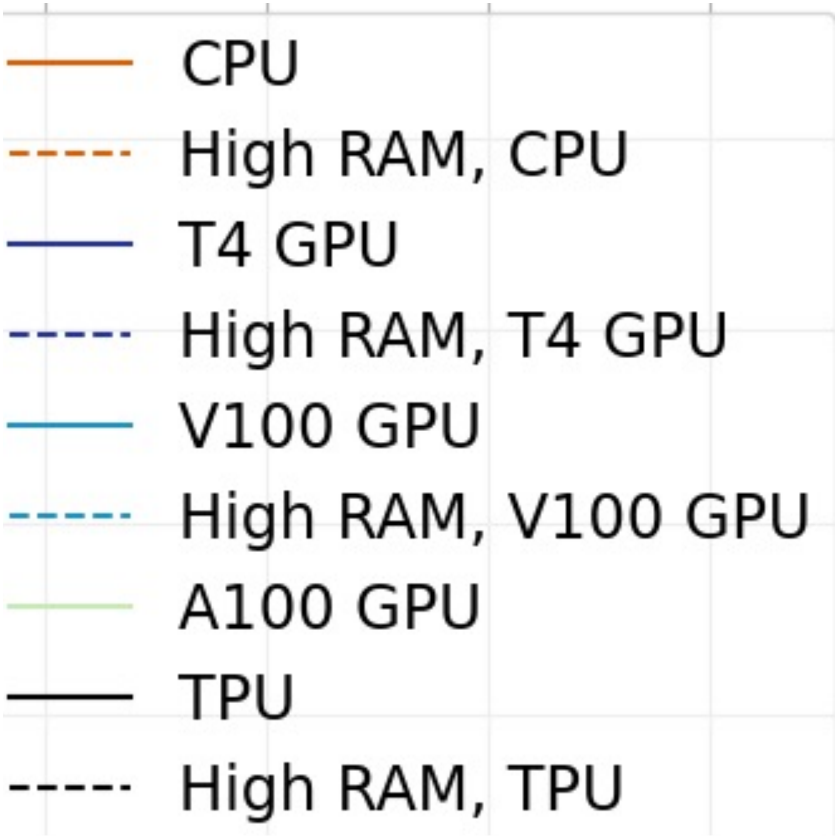
HPC stands for:
High Performance Computing

It essentially means computing that cannot be (tractably) performed on a personal computer.

Note: Orb of glowing lines not strictly necessary for HPC.

High Performance Memory

- You need high memory whenever you have a large dataset, model, or other structure that needs to be held *all in memory at once*, or at least frequently accessed during calculations, e.g.
  - Climate models!



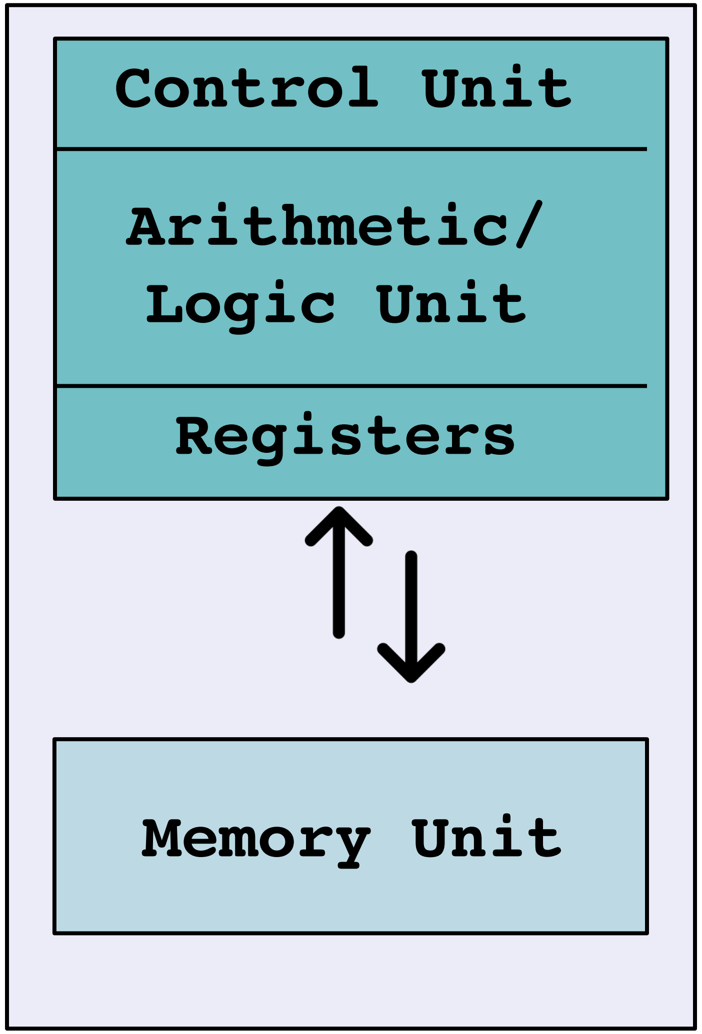
12.7 GB RAM
51 GB RAM
12.7 GB RAM
51 GB RAM
12.7 GB RAM
51 GB RAM
83.5 GB RAM
12.7 GB RAM
35.2 GB RAM

Processing Power

The *processor* is the element of the computer that performs operations.

Processing speed is affected by a number of factors, including:

- The number of cores
- The clock speed/processor speed
- Cache size



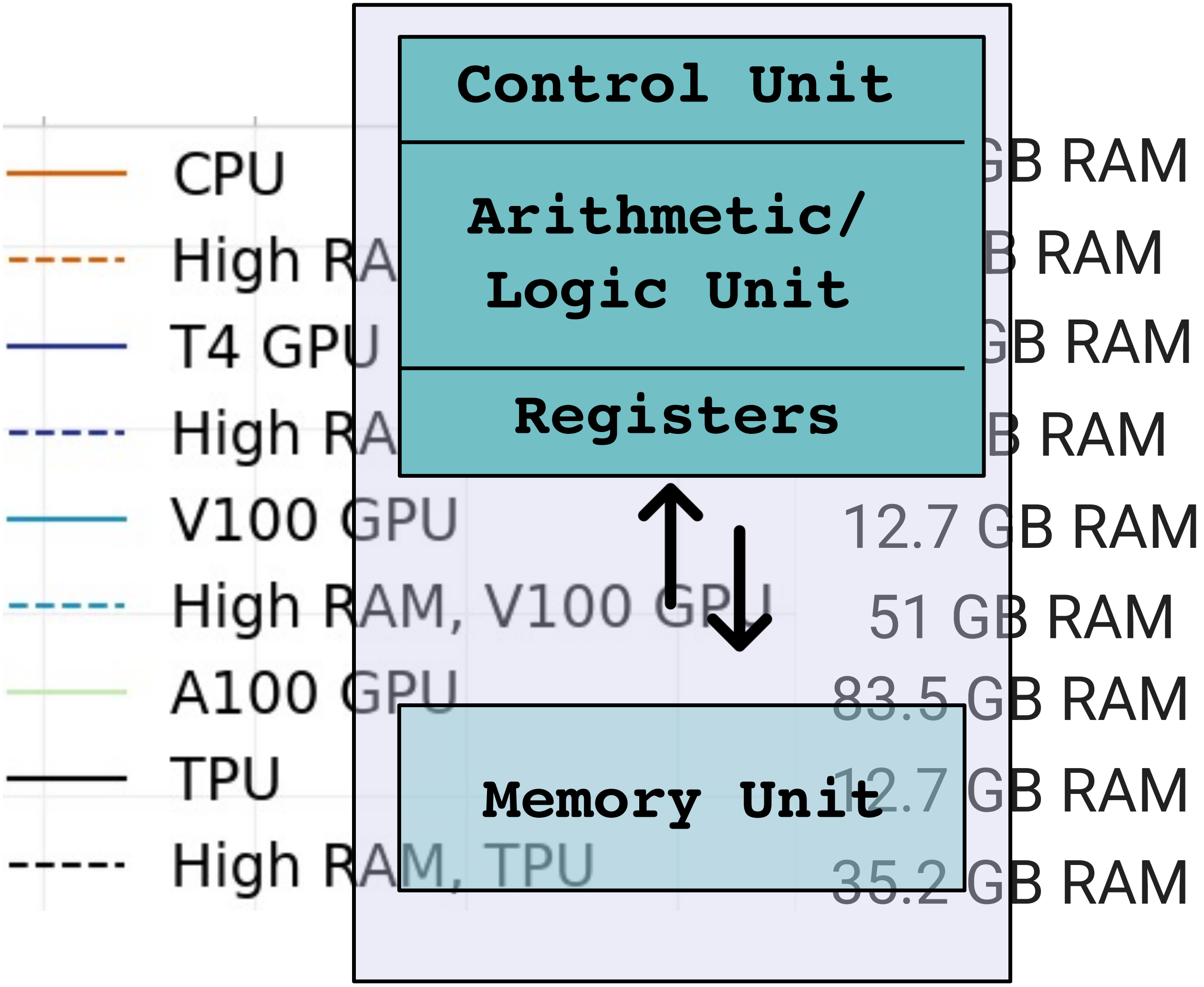
Processing Power - GPUs

There is another type of processor hardware: GPUs.

GPU = **G**raphics **P**rocessing **U**nit

GPUs are special purpose hardware originally designed for video processing and computer graphics - they have *many* processing cores, but the cores are less independent (they do the same operation over a block of data).

GPU memory is also typically a *separate** pool from the memory available to your CPU.



* Modern Apple hardware has implemented a hybrid memory model, with memory shared between CPU and GPU cores.

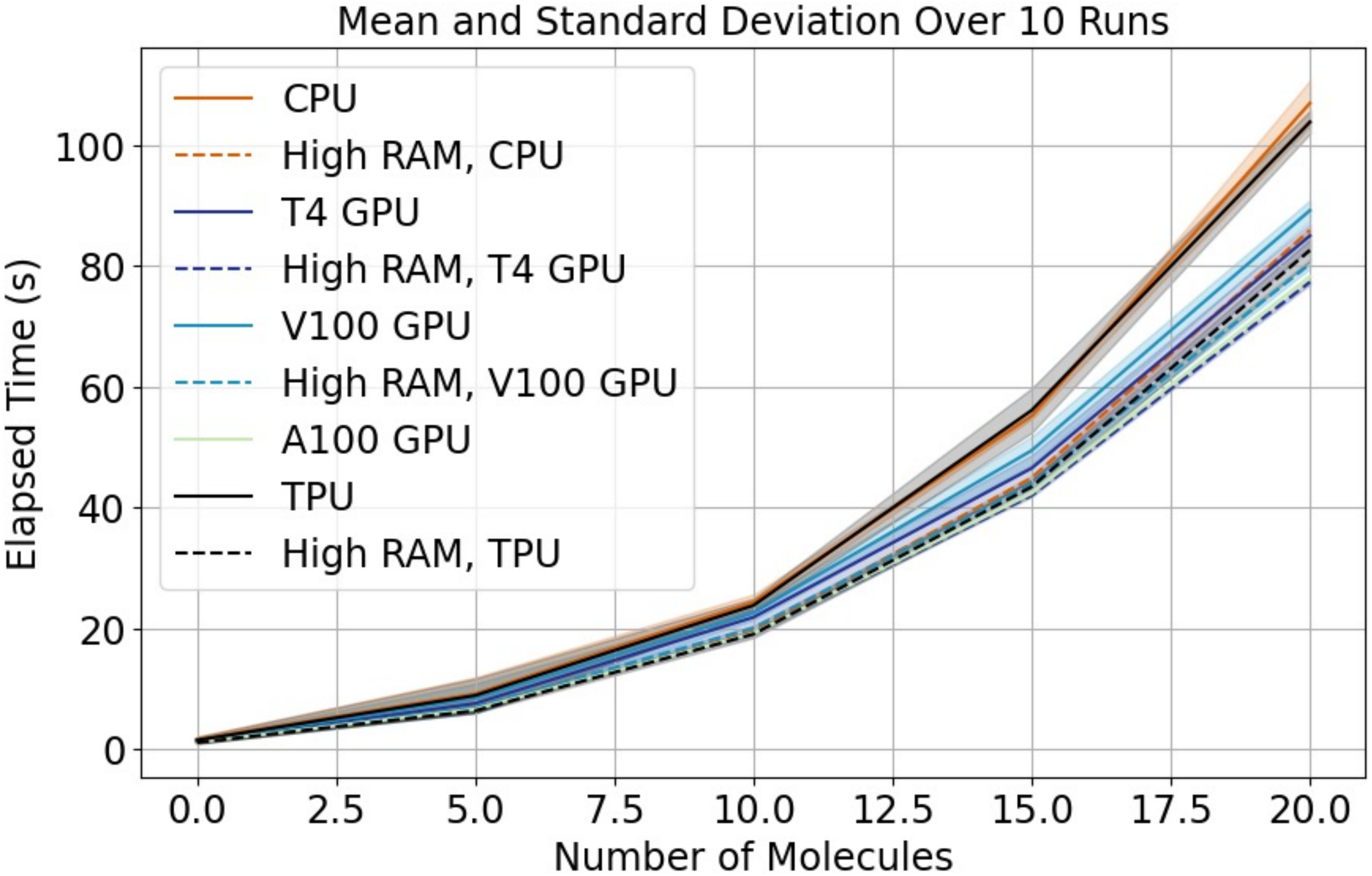
GPU or CPU?

To take advantage of a GPU, you must have a computational problem that is well-suited to GPU architecture. Common examples include:

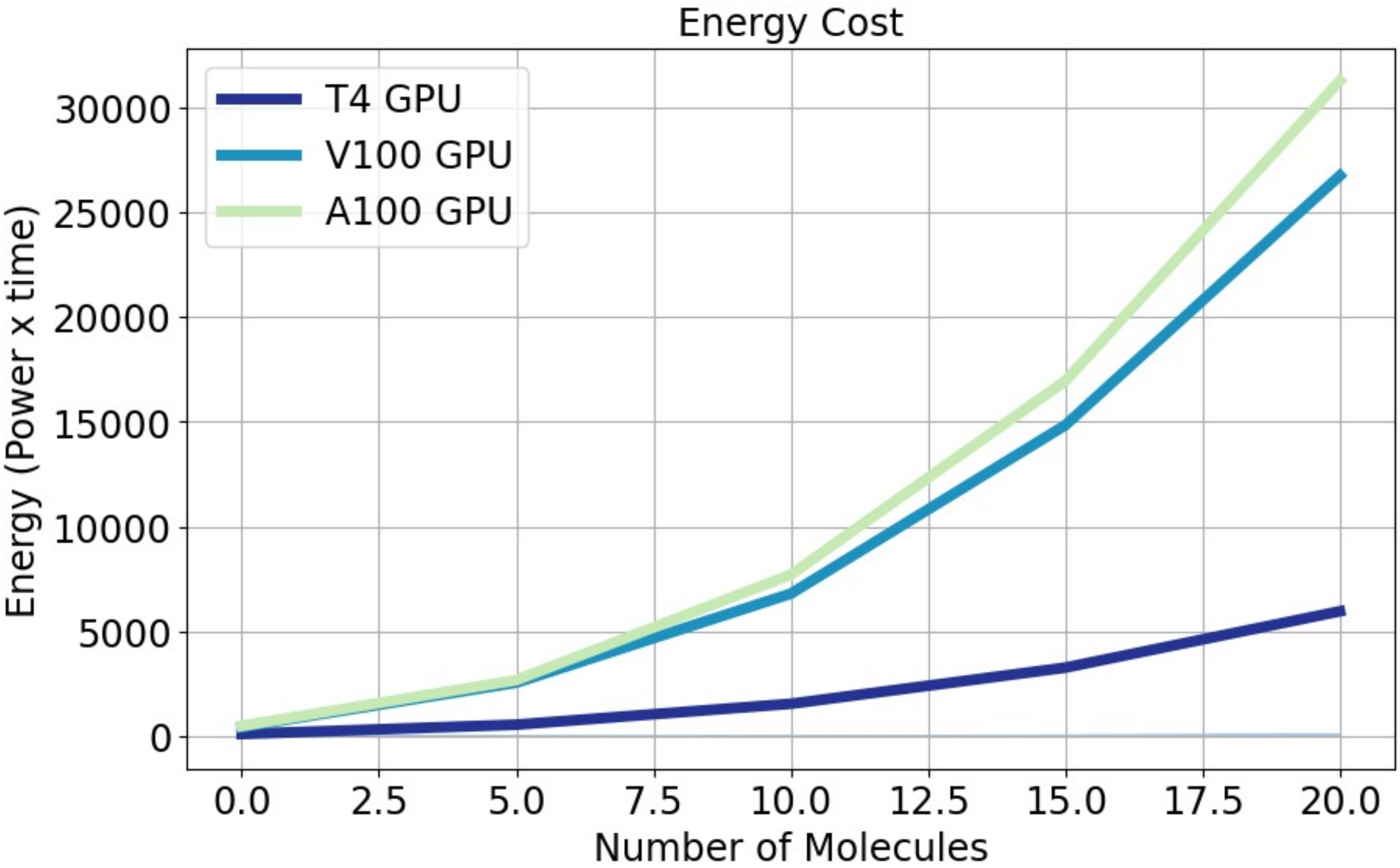
- Graphics and video processing
- Neural networks

But, there is a cost to using a GPU! Some problems that don't benefit from a GPU are typically better done on a CPU, like:

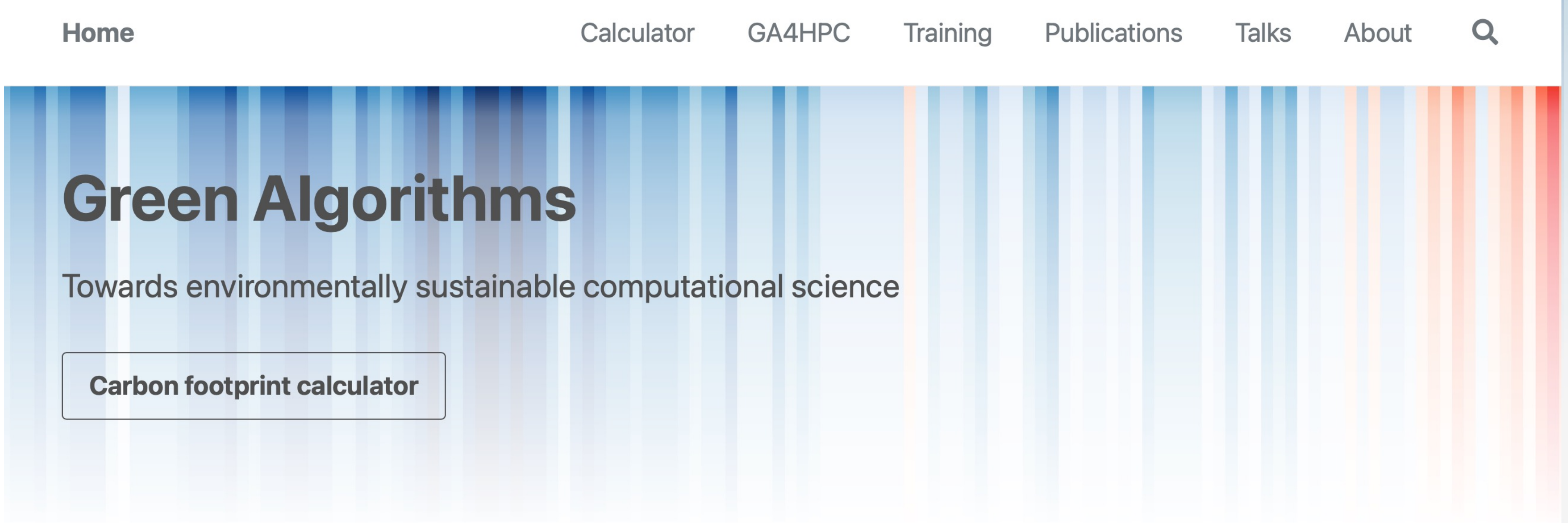
- Problems with a sequence of independent calculations (e.g. solving ODEs!)



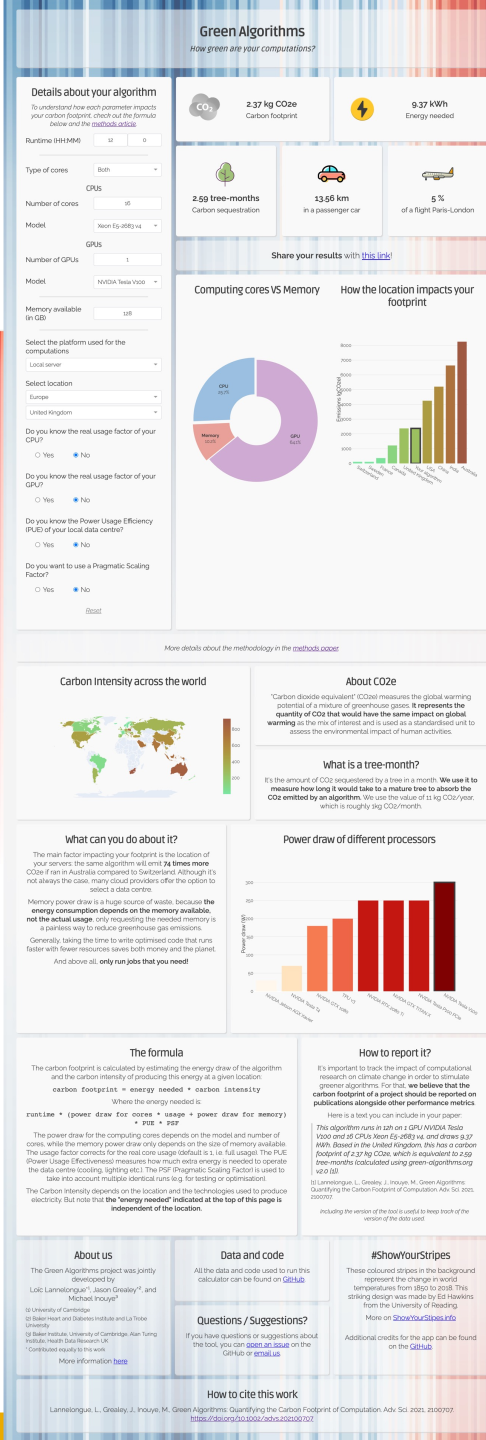
Mean and Standard Deviation Over 10 Runs
CPU
High RAM, CPU
T4 GPU
High RAM, T4 GPU
V100 GPU
High RAM, V100 GPU
A100 GPU
TPU
High RAM, TPU
Elapsed Time (s)
0
20
40
60
80
100
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
Number of Molecules

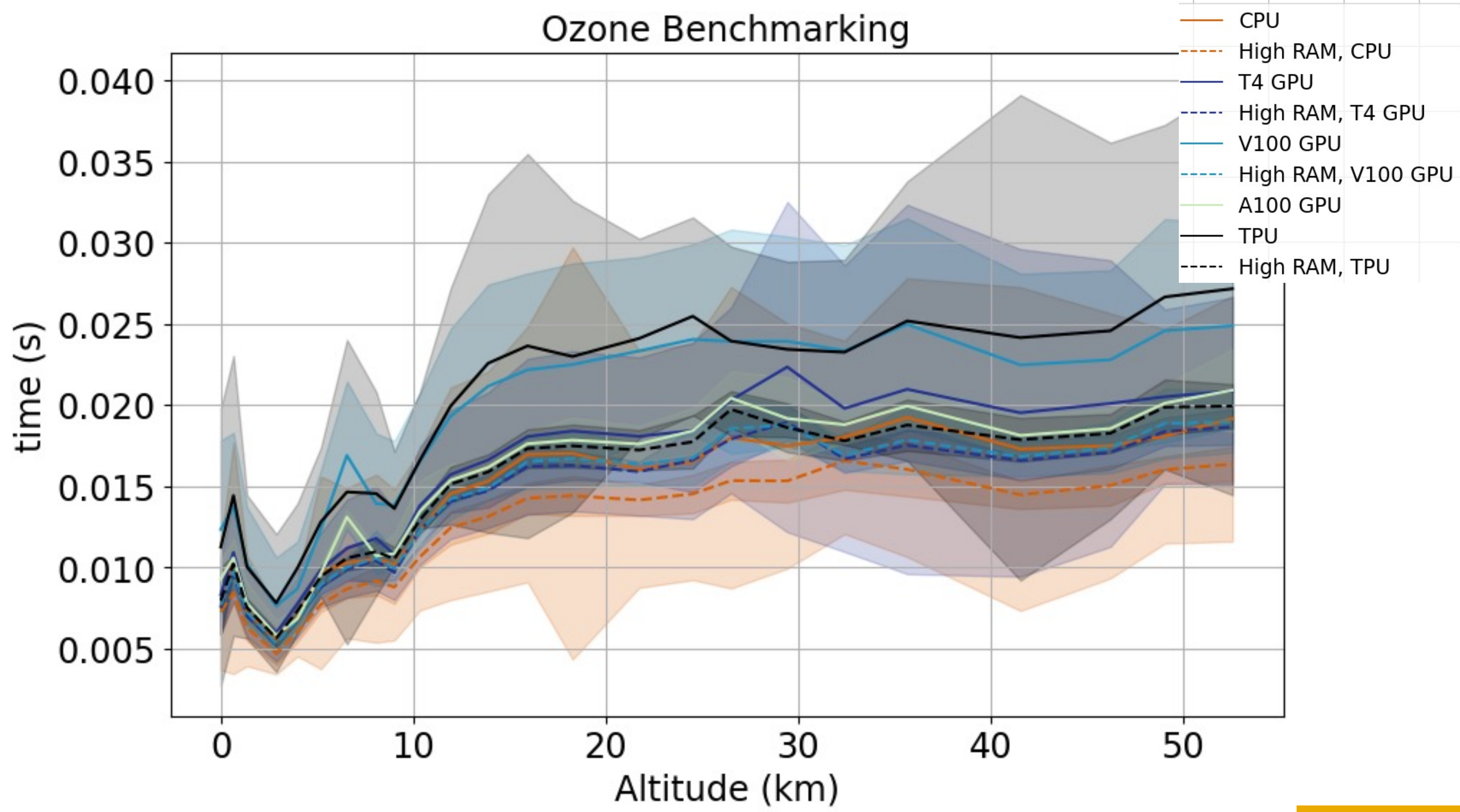

Energy Cost
T4 GPU
V100 GPU
A100 GPU
30000
25000
20000
15000
10000
5000
0
Energy (Power x time)
0.0
2.5
5.0
7.5
10.0
12.5
15.0
17.5
20.0
Number of Molecules

This is Green Chemistry!



https://www.green-algorithms.org




Ozone Benchmarking
time (s)
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0
10
20
30
40
50
Altitude (km)
CPU
High RAM, CPU
T4 GPU
High RAM, T4 GPU
V100 GPU
High RAM, V100 GPU
A100 GPU
TPU
High RAM, TPU

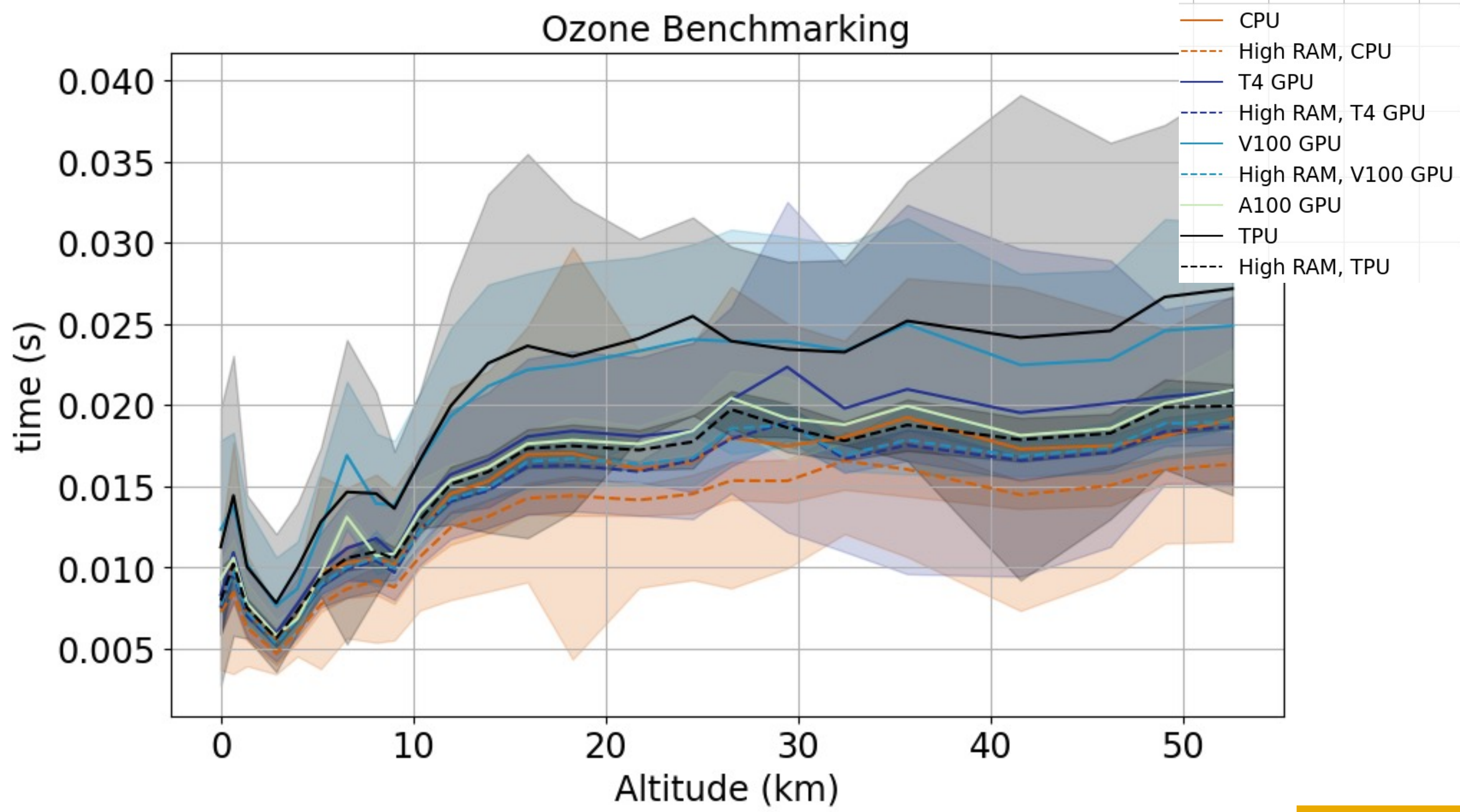
Hardware Control

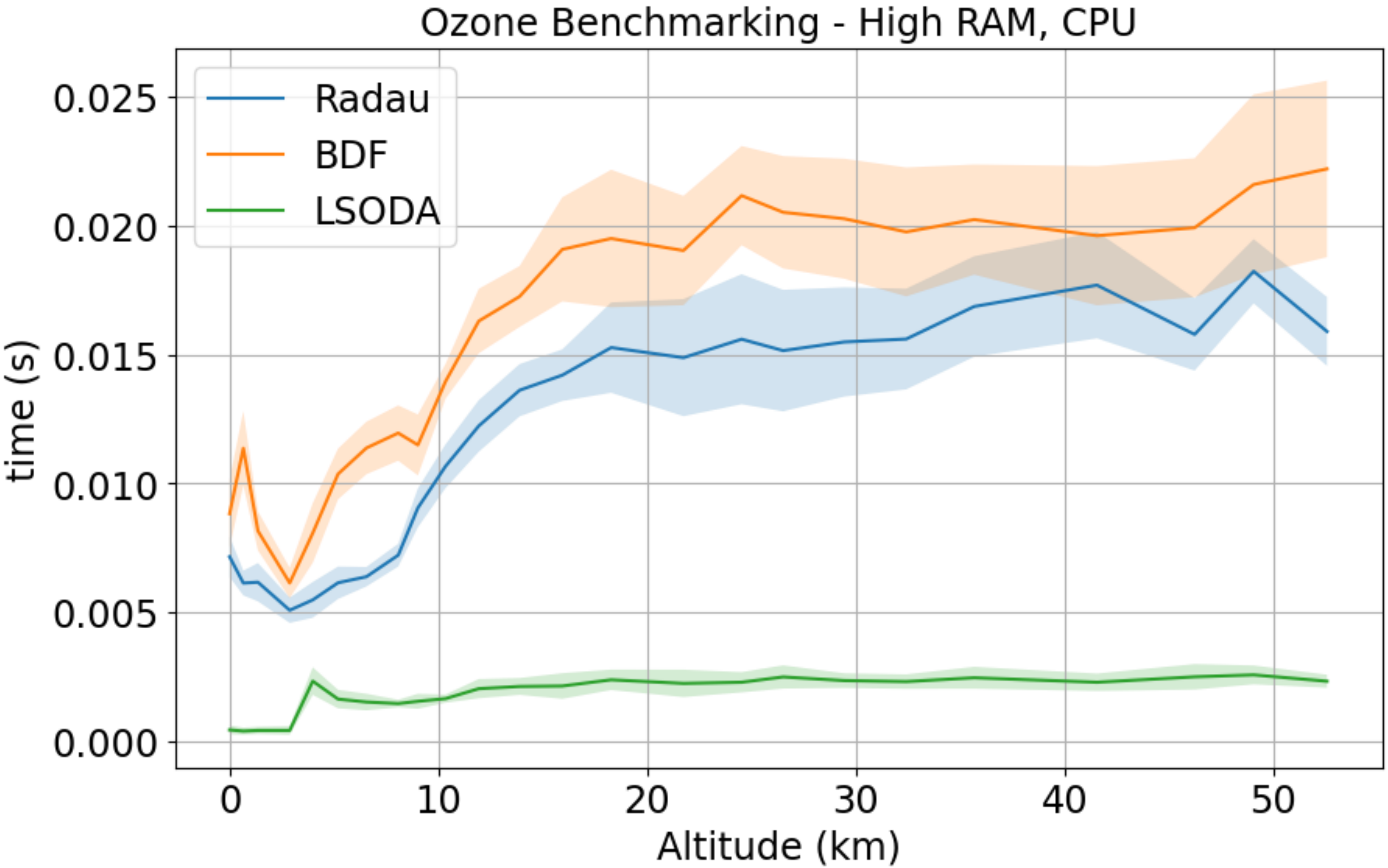
Sometimes your research might involve *how* an answer gets computed, and you need precise knowledge or control over what hardware is involved.

Many standard HPC solutions abstract this away (e.g. cloud services might not tell you what machine is processing your information, or might assign a different architecture each time).

Examples of research where this would be a concern include:

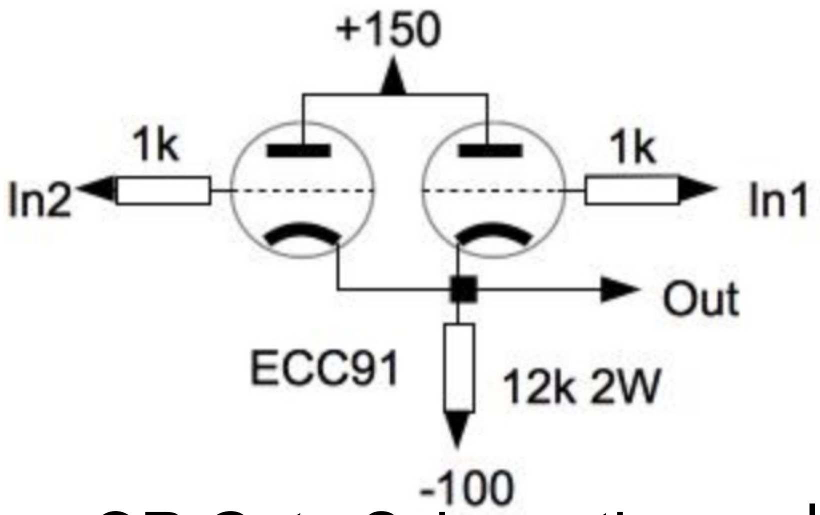
- Power consumption experiments
- Software or hardware benchmarking


Ozone Benchmarking
time (s)
Altitude (km)
0.040
0.035
0.030
0.025
0.020
0.015
0.010
0.005
0
10
20
30
40
50
CPU
High RAM, CPU
T4 GPU
High RAM, T4 GPU
V100 GPU
High RAM, V100 GPU
A100 GPU
TPU
High RAM, TPU


Ozone Benchmarking - High RAM, CPU
Radau
BDF
LSODA
0.025
0.020
0.015
0.010
0.005
0.000
time (s)
0
10
20
30
40
50
Altitude (km)

What are computers *actually* made of?

Early 1950s: vacuum tubes
Late 1950s: transistors
Late 1960s: printed/integrated circuits
1970s: Microprocessors



OR Gate Schematic

I borrowed these slides from the year I co-taught CS5:
https://www.cs.hmc.edu/twiki/bin/view/CS5Spring2022

What are computers *actually* made of?

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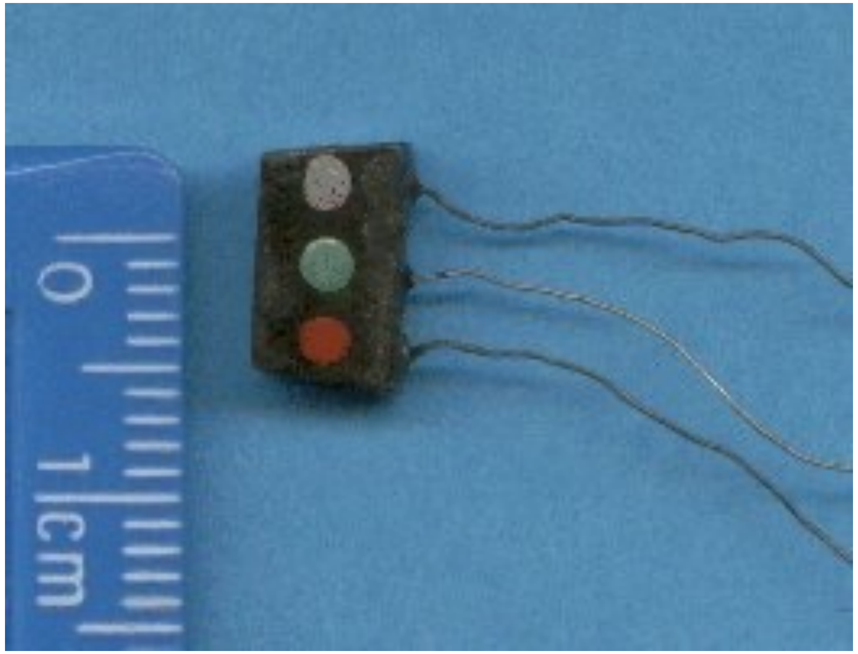

"The most important invention of the 20th century…"

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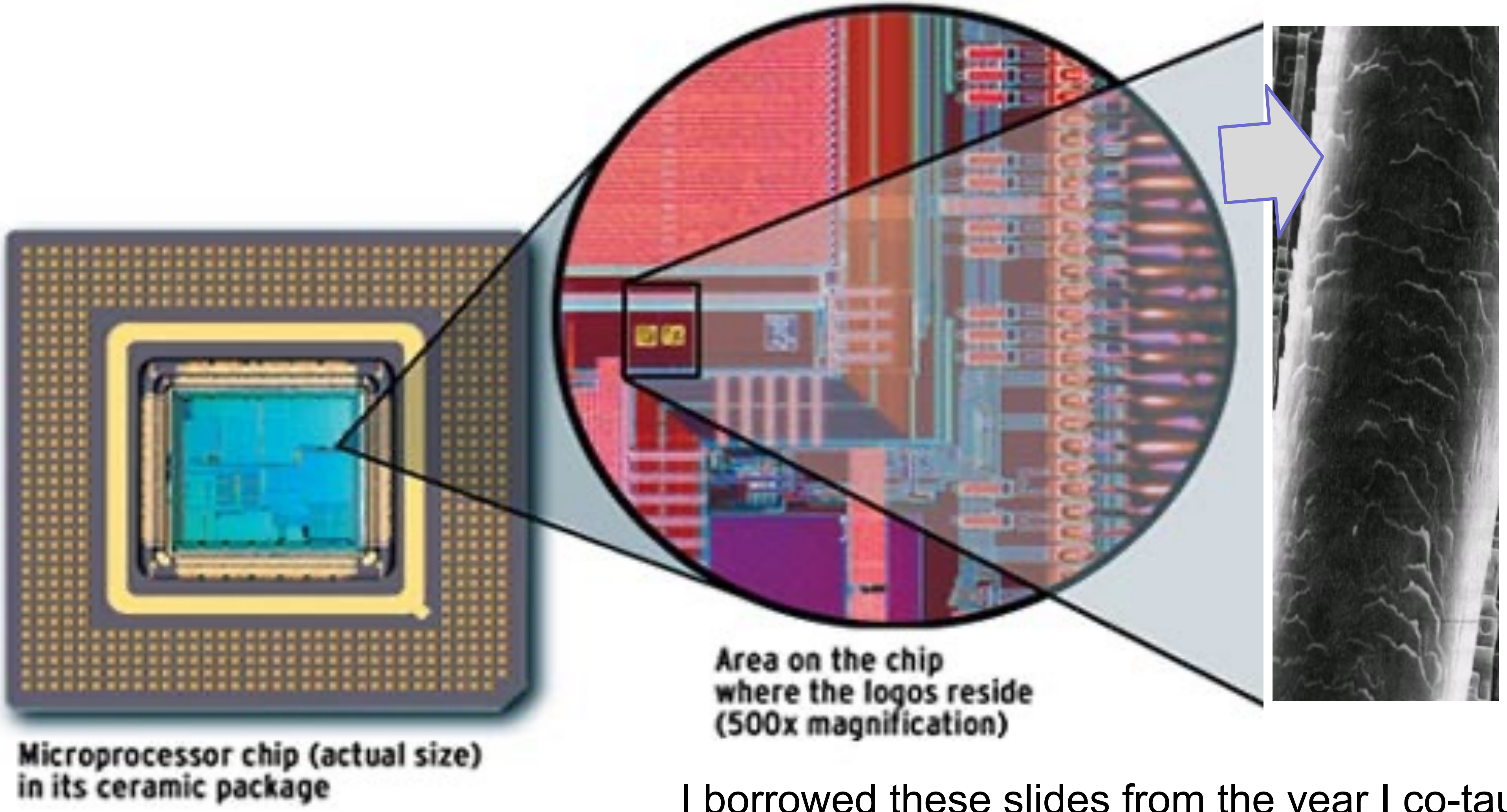
https://www.cs.hmc.edu/twiki/bin/view/CS5Spring2022

Today's gates?



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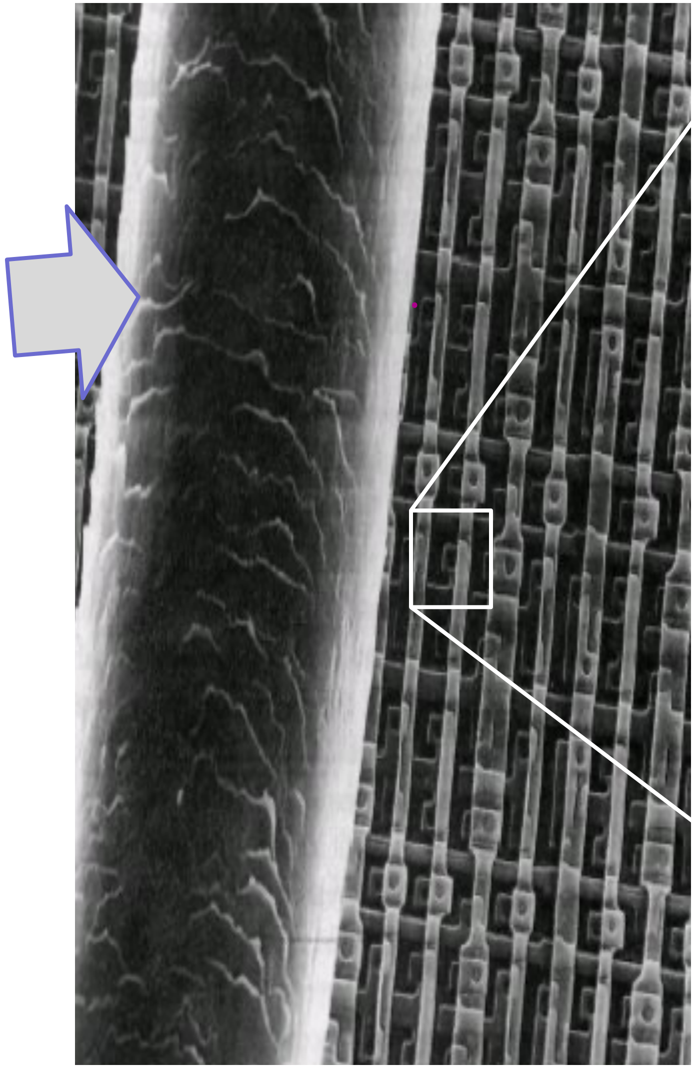
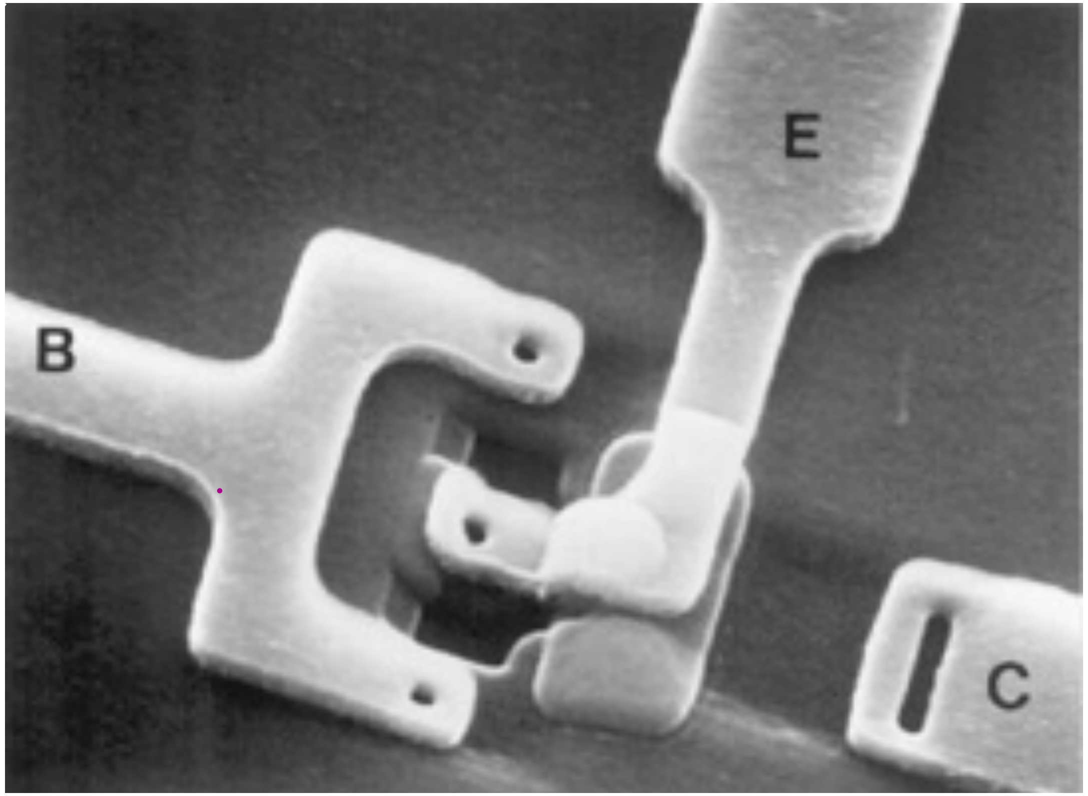
are from silicon-based switches ~ ***transistors***

switches?





a single etched transistor labeled with
base (b), emitter (e), and collector (c)

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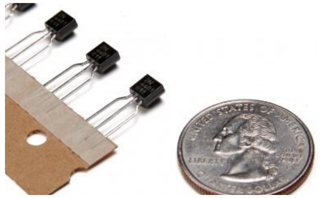
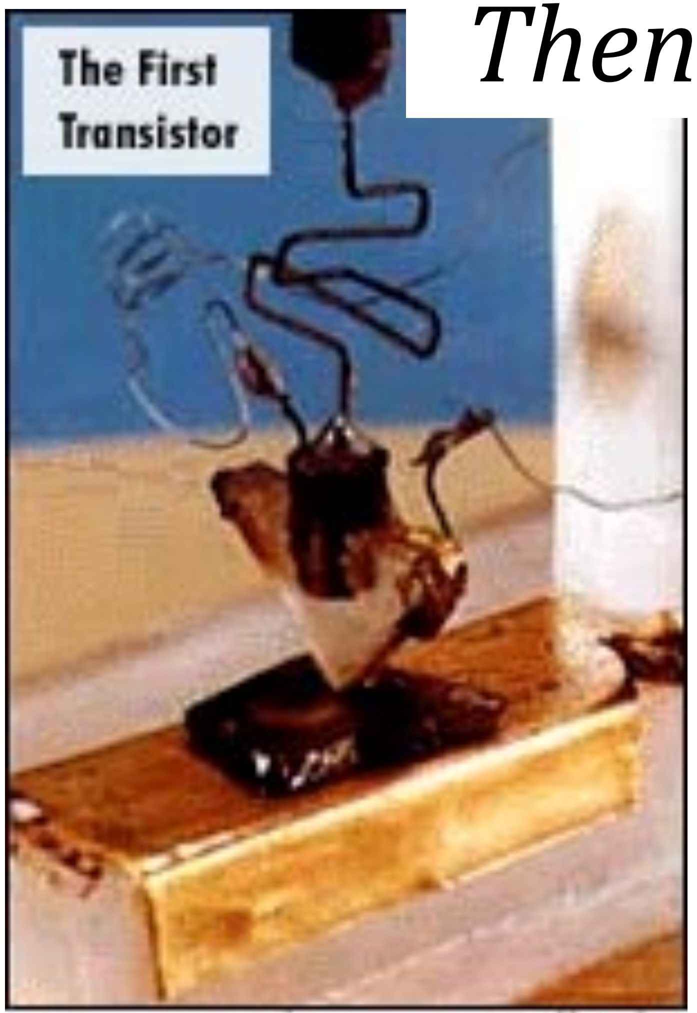
Single electron tunnelling



Fry's transistors

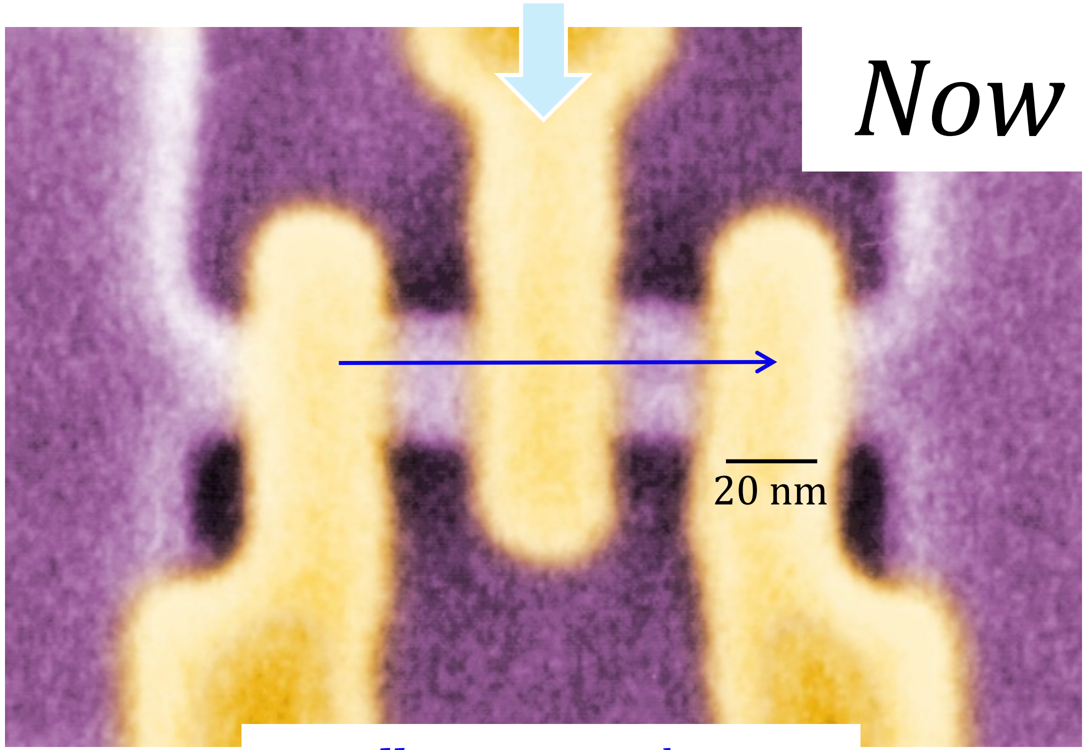


Then

Bell Labs

"high"

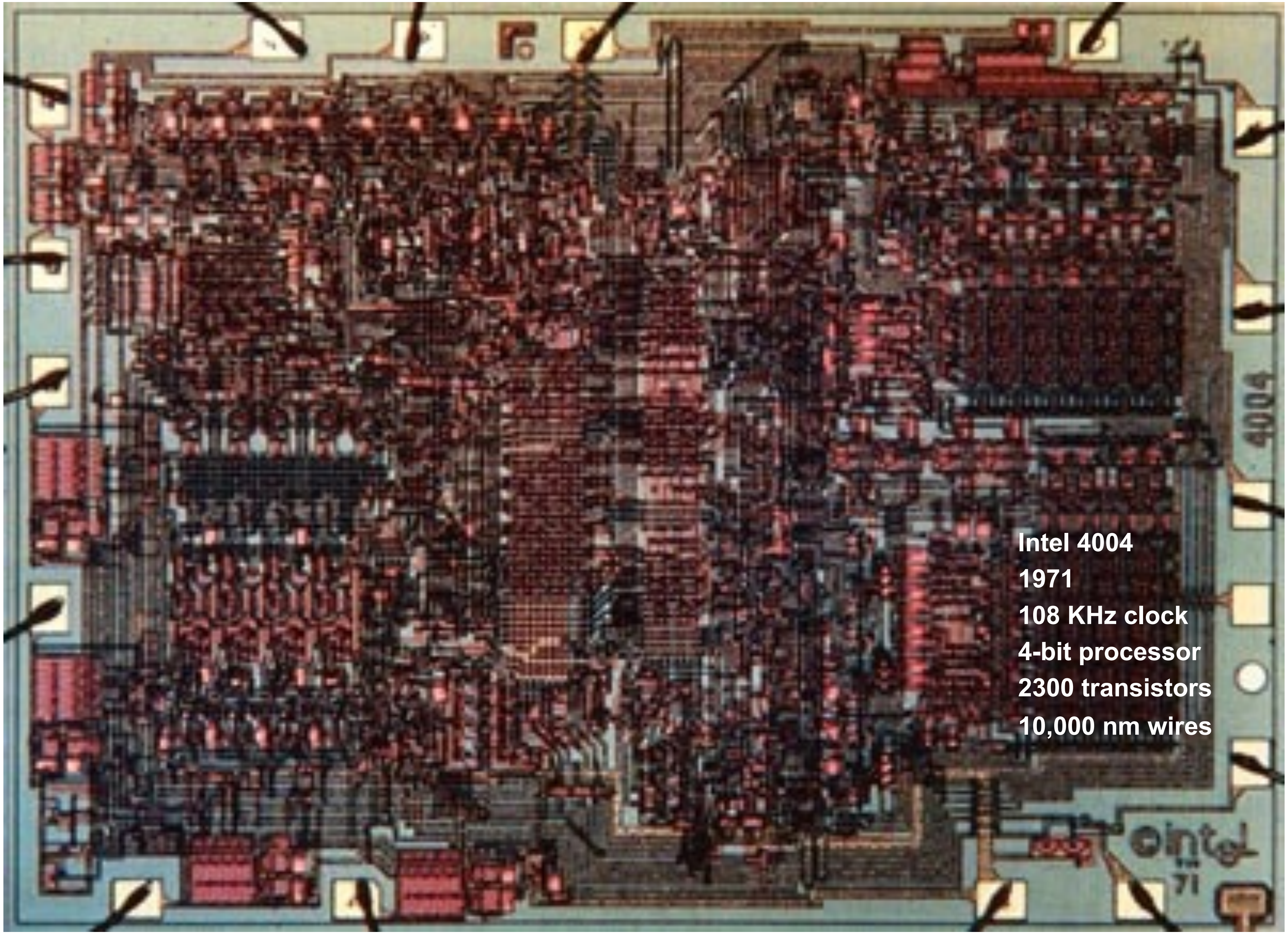
a +5v voltage here



Now

allows current here

I borrowed these slides from the year I co-taught CS5: https://www.cs.hmc.edu/twiki/bin/view/CS5Spring2022


Intel 4004
1971
108 KHz clock
4-bit processor
2300 transistors
10,000 nm wires
4004
intel

2006

Intel Core 2 Duo

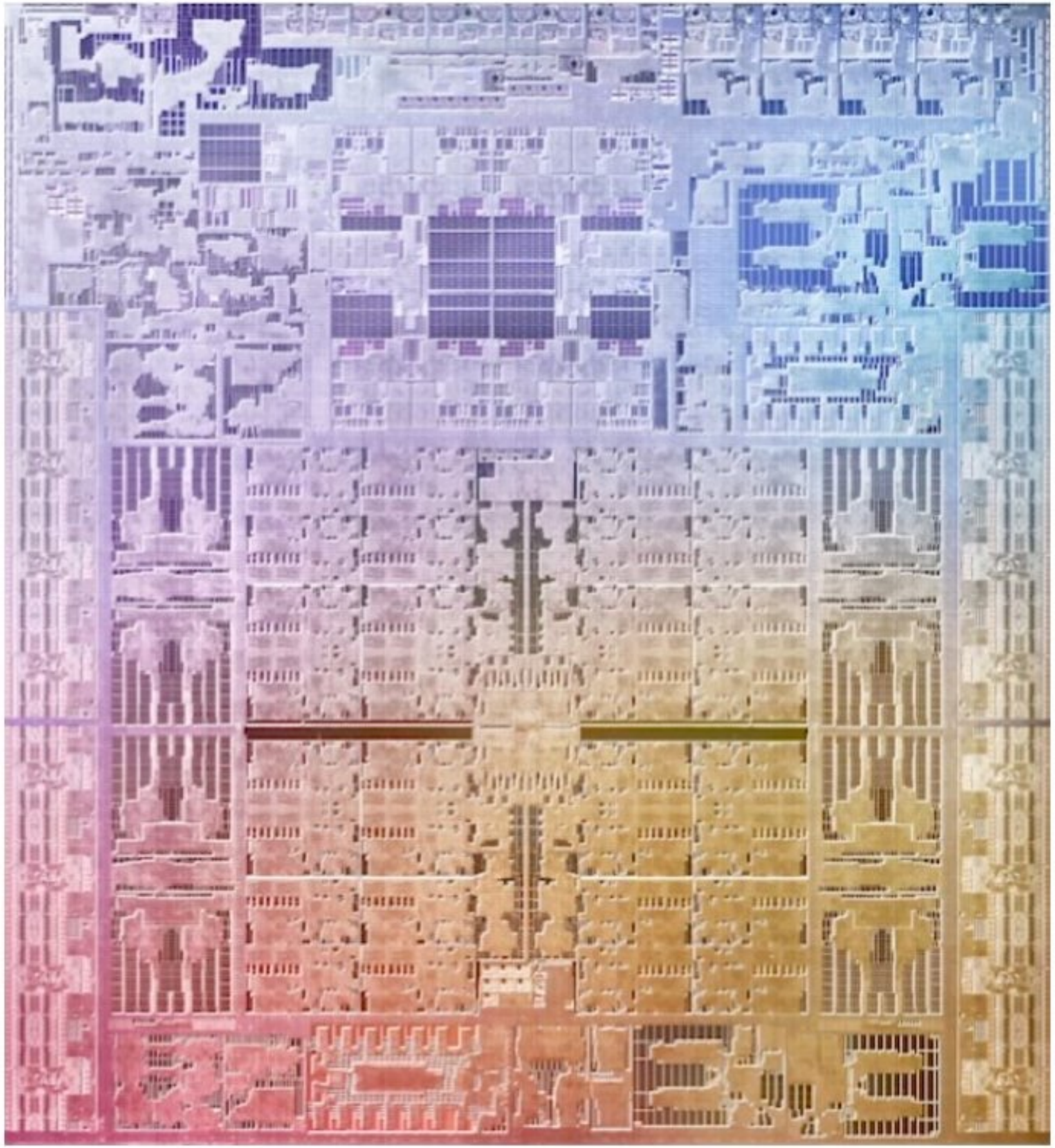
3 GHz clock

64-bit processor

291 million transistors

65 nm wires

I see these designers had excellent taste!



Apple M1 Max (2021)

In-Class Submission

Find an application – a paper, preferably – that shows how *chemistry* has changed *computing*