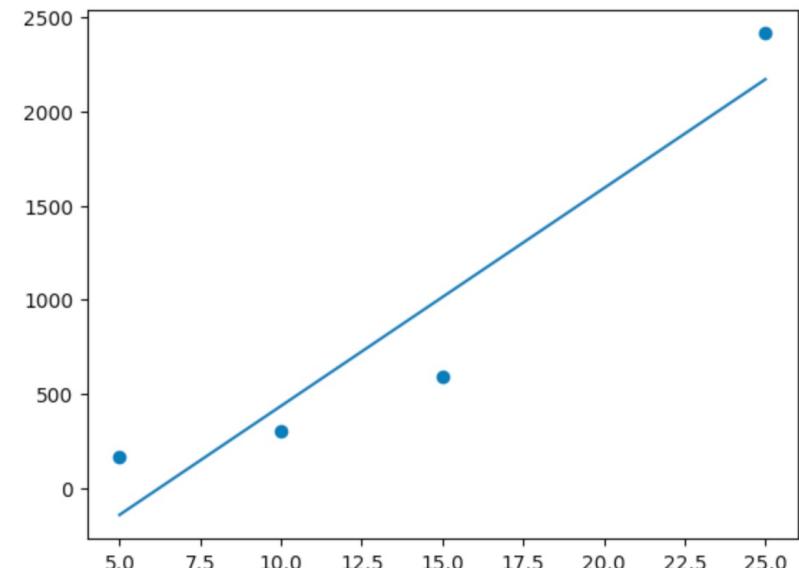
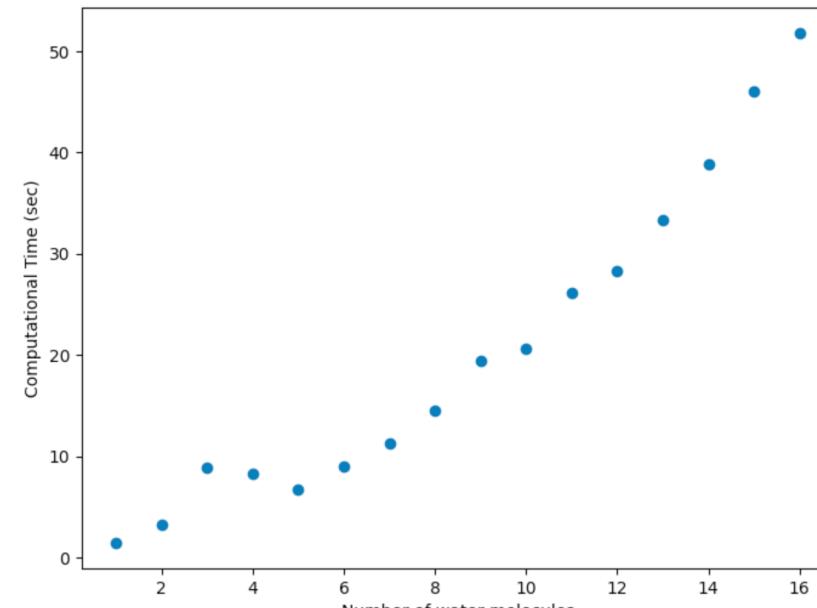
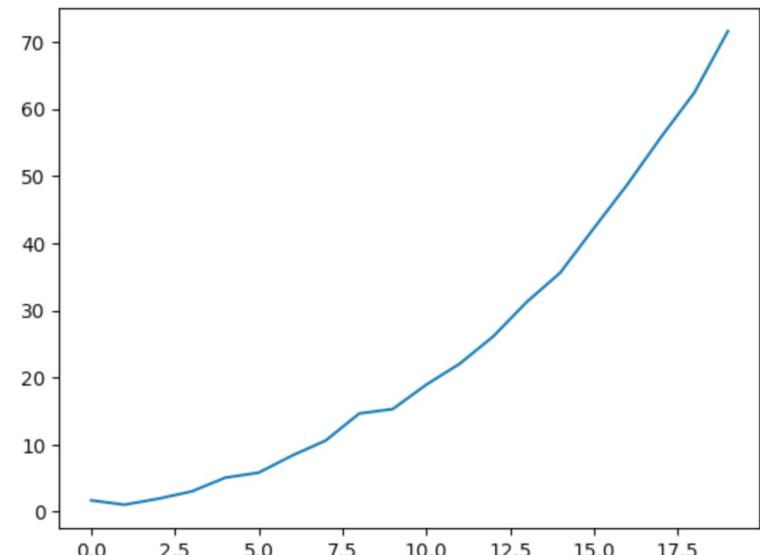
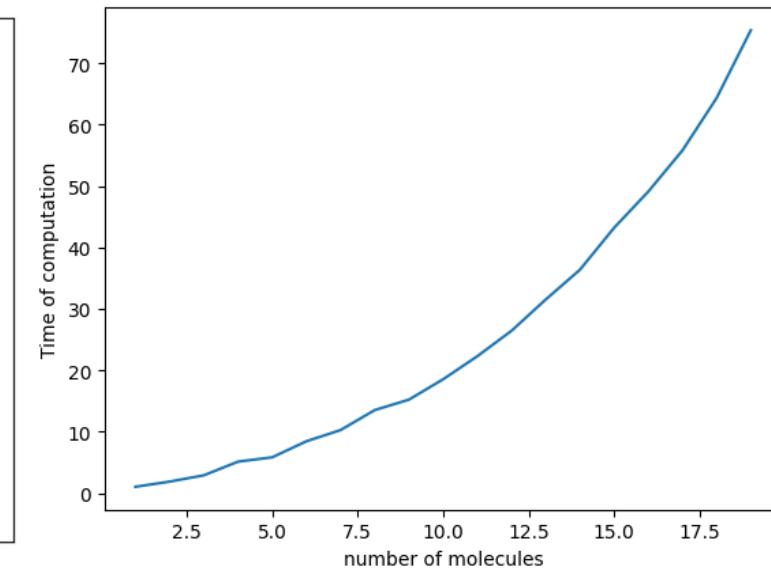
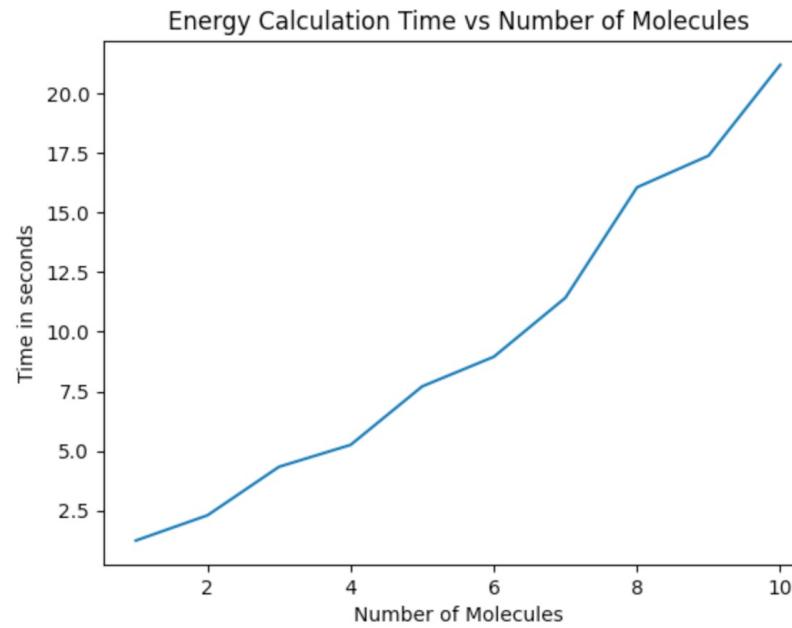
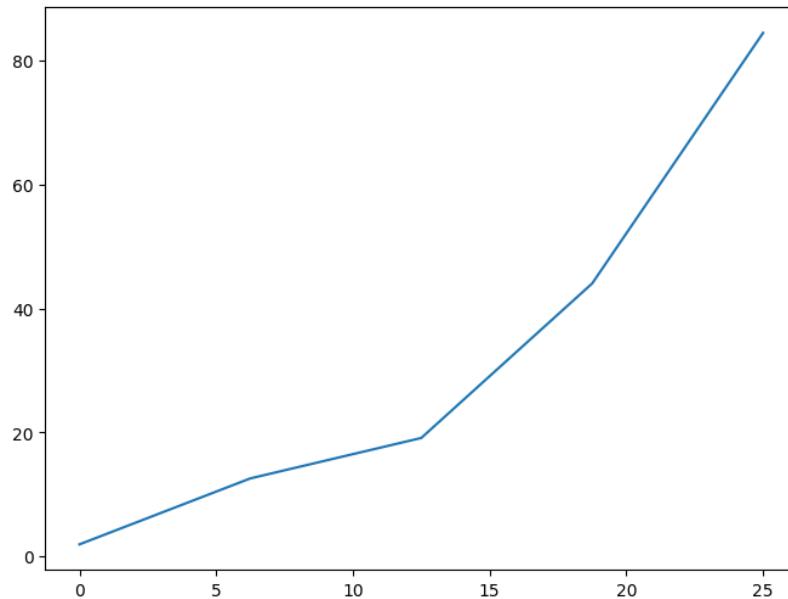
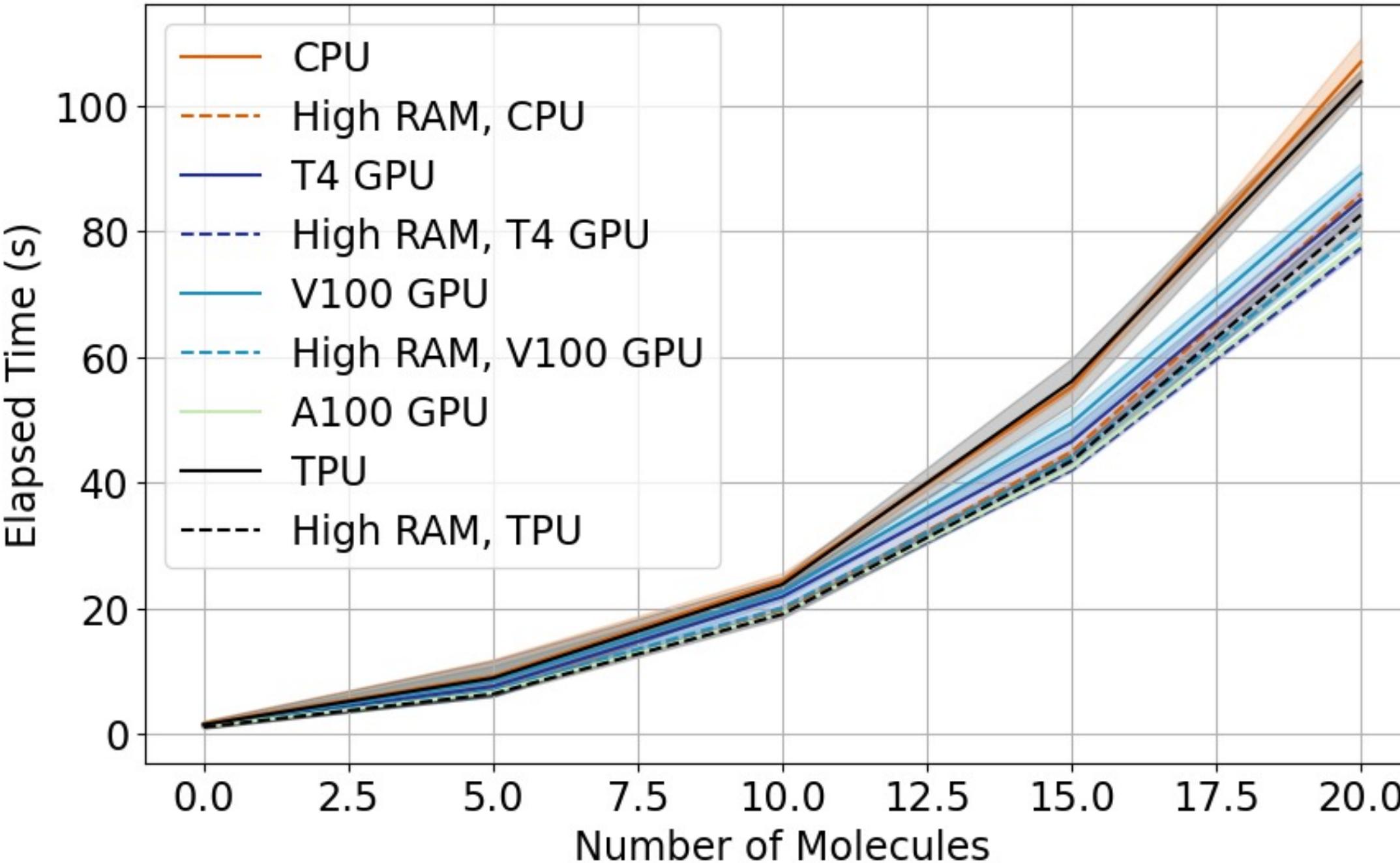


# HW15 Runtime Calculation: # of Molecules vs Time



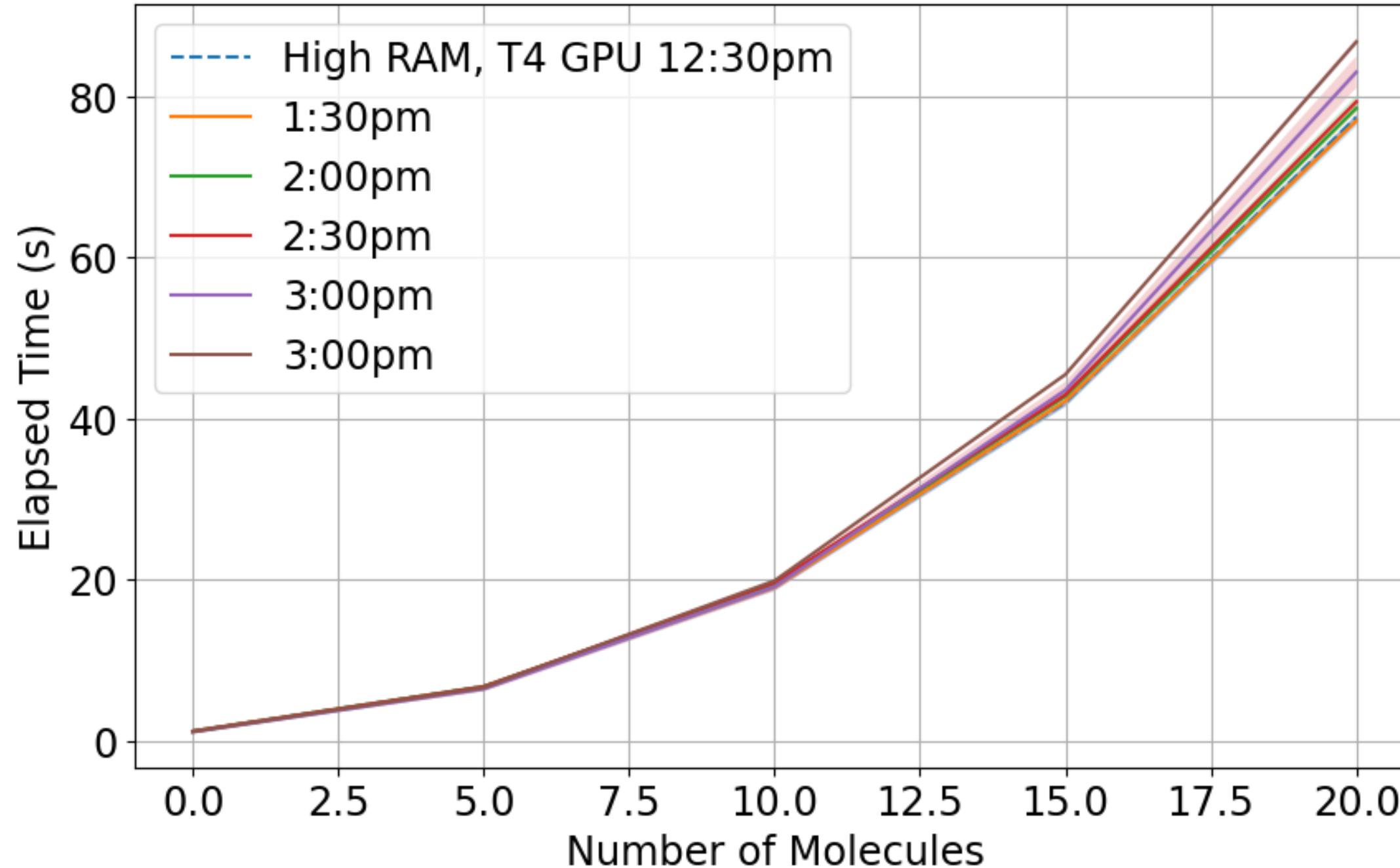
# Mean and Standard Deviation Over 10 Runs



“Benchmarking”  
done on Google  
Colab

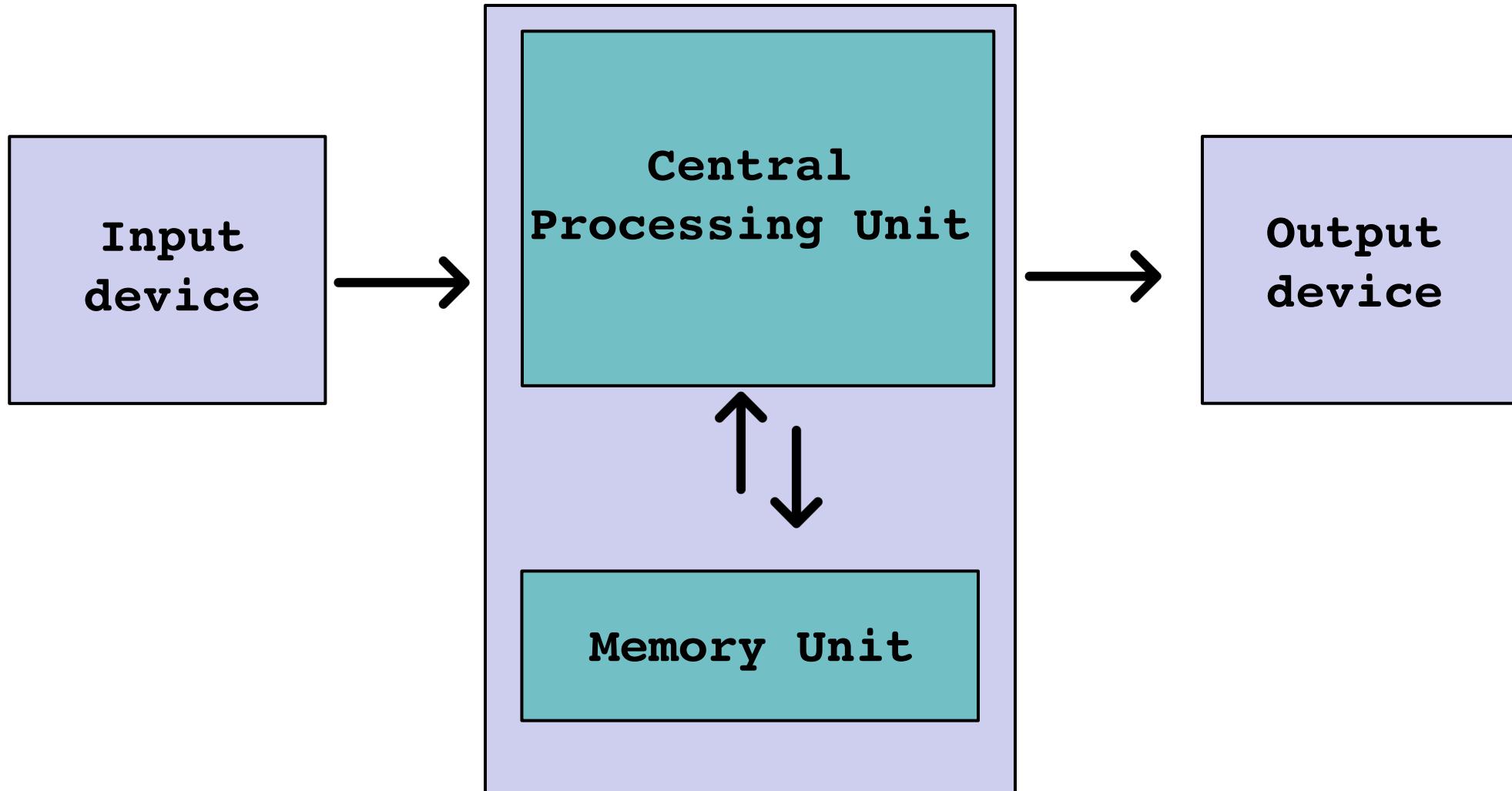
March 25<sup>th</sup>,  
2024 ~12:00pm  
Claremont, CA

# Mean and Standard Deviation Over 10 Runs

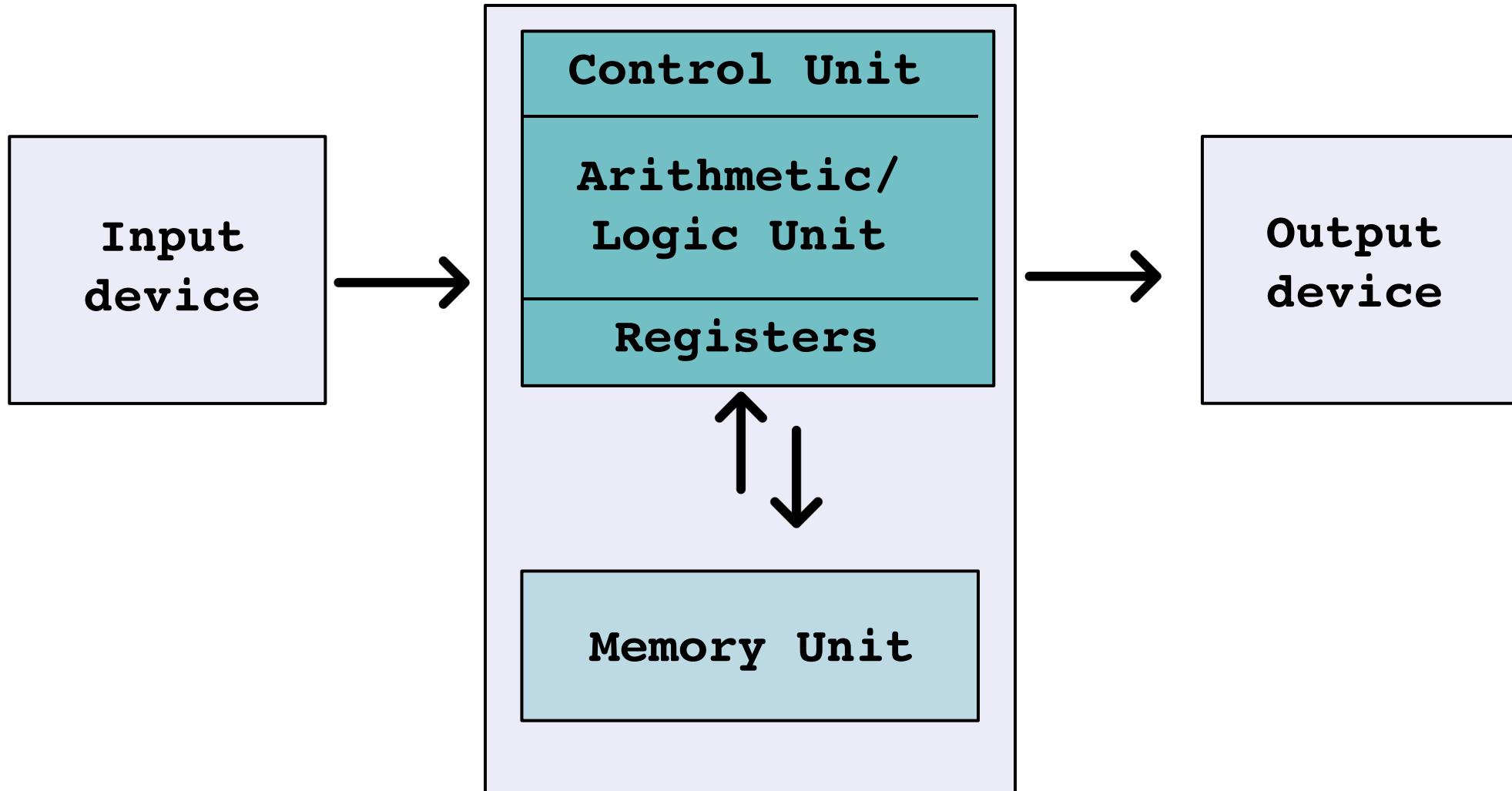


Why does runtime look like it is increasing overtime?

# A computer (von Neumann architecture)

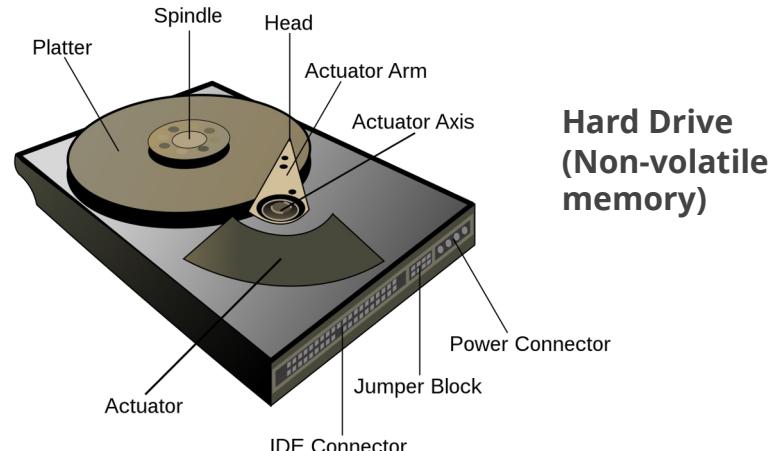


# A computer (von Neumann architecture)

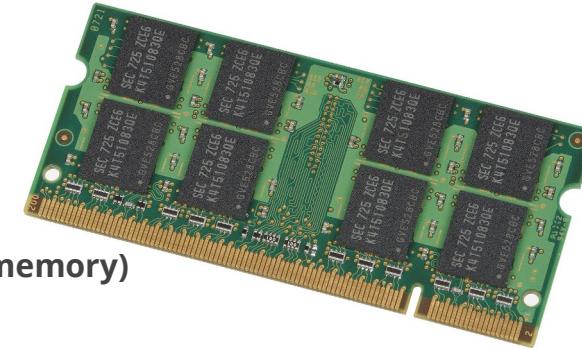


# Memory

- 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)



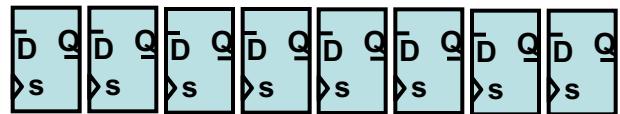
**RAM**  
(Volatile memory)

# 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

Time

1 clock cycle  
 $10^{-9}$  sec

If a cycle ==  
1 minute

**1 min**

## Main Memory

(volatile memory )



~ 10 billion bits +  
1 GB memory

100 cycles  
 $10^{-7}$  sec

**1.5 hours**

## Disk Drive

(non-volatile memory)



~10 trillion bits (or more)  
1 TB drive

$10^7$  cycles  
 $10^{-2}$  sec

**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!

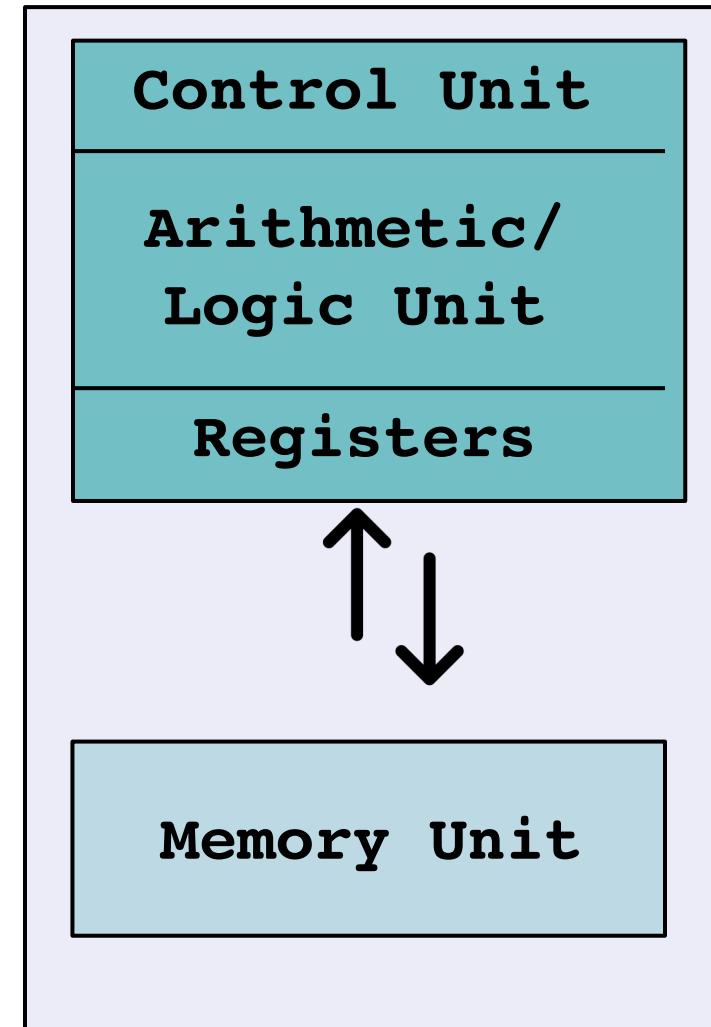
 CPU	12.7 GB RAM
 High RAM, CPU	51 GB RAM
 T4 GPU	12.7 GB RAM
 High RAM, T4 GPU	51 GB RAM
 V100 GPU	12.7 GB RAM
 High RAM, V100 GPU	51 GB RAM
 A100 GPU	83.5 GB RAM
 TPU	12.7 GB RAM
 High RAM, TPU	35.2 GB RAM

# 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



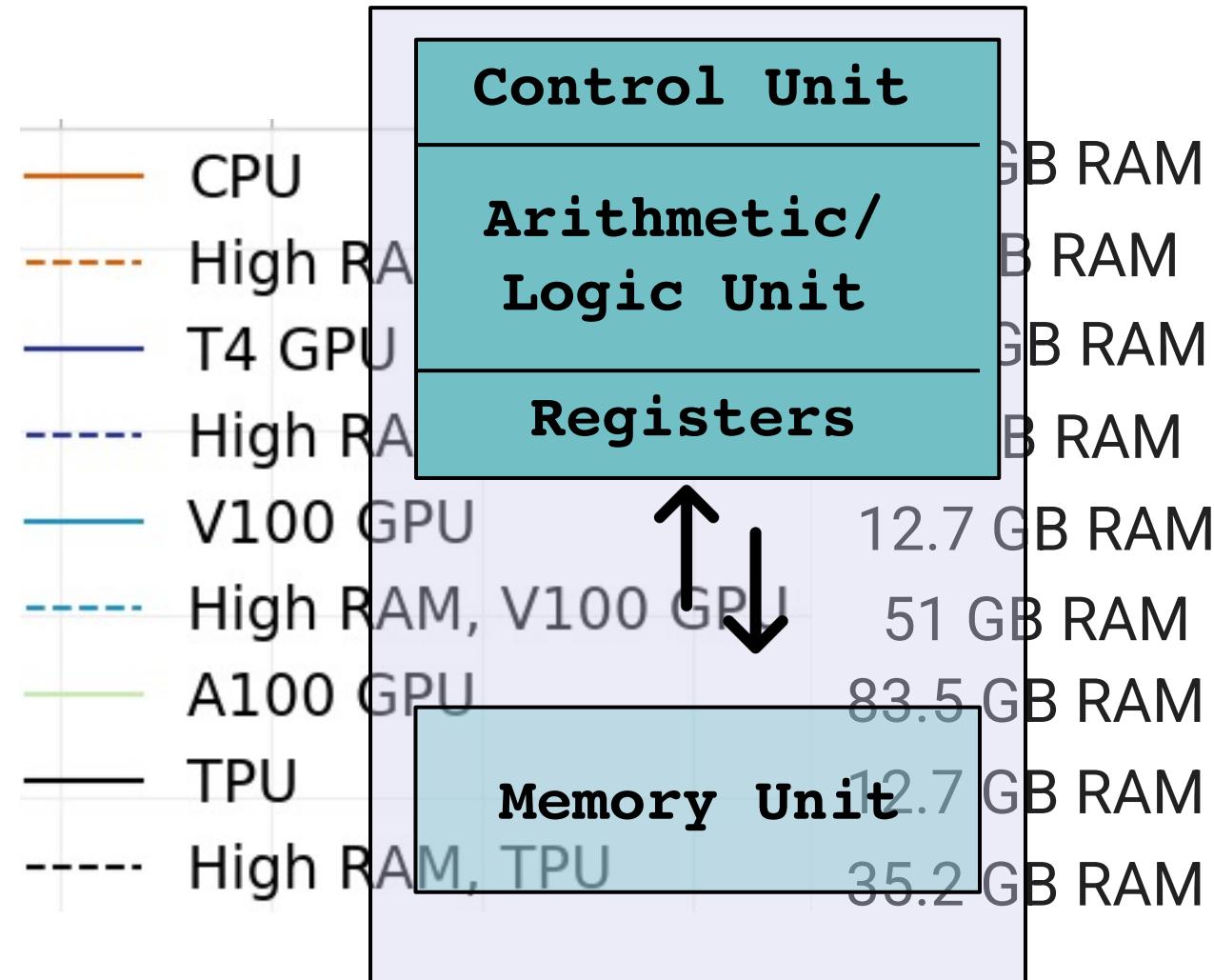
# Processing Power - GPUs

There is another type of processor hardware: GPUs.

**GPU = Graphics Processing Unit**

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?

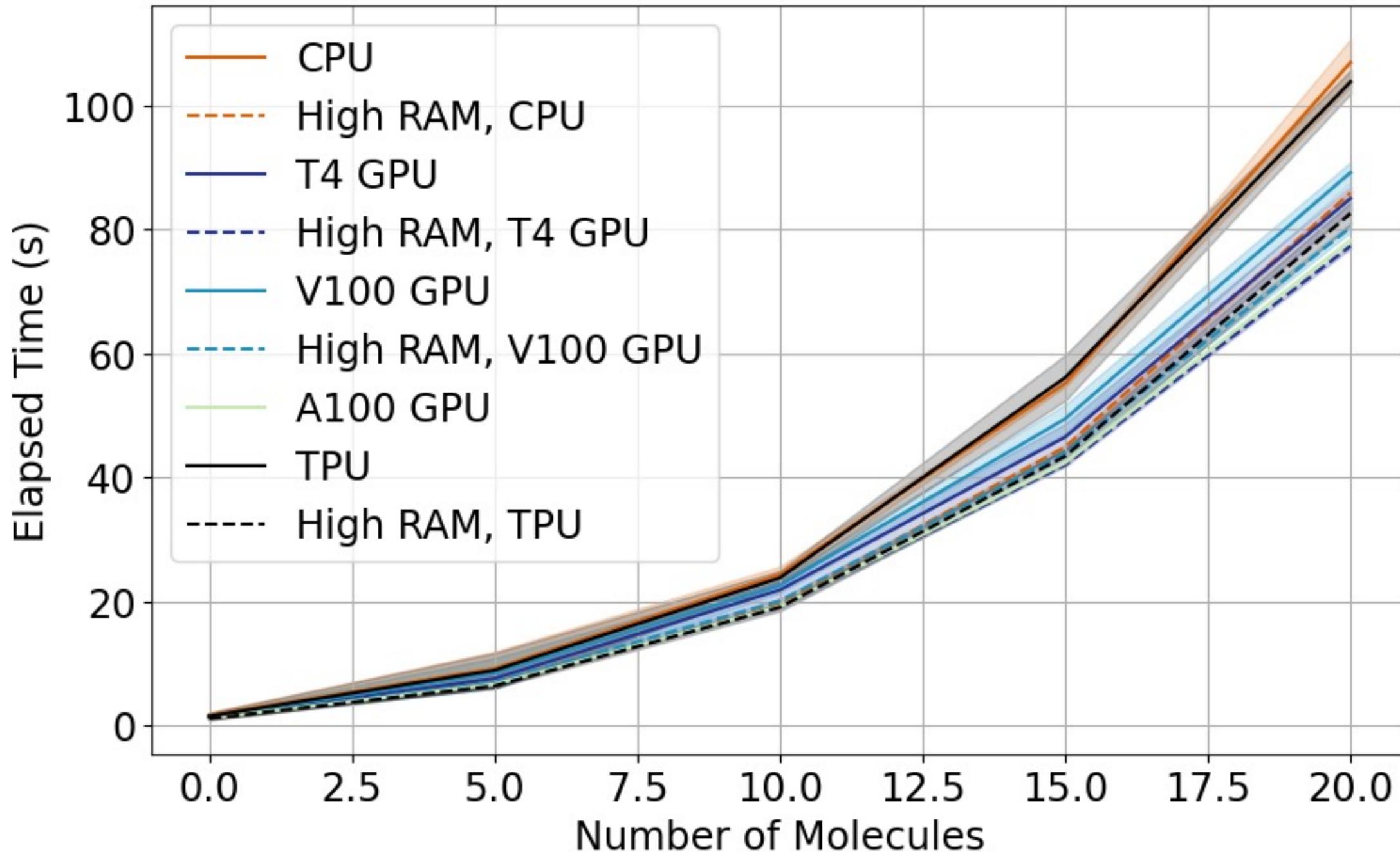
To take advantage of a GPU, you must have a computational problem that is well-suited to GPU architecture. Common examples include:

- Graphics and video processing
- Neural networks

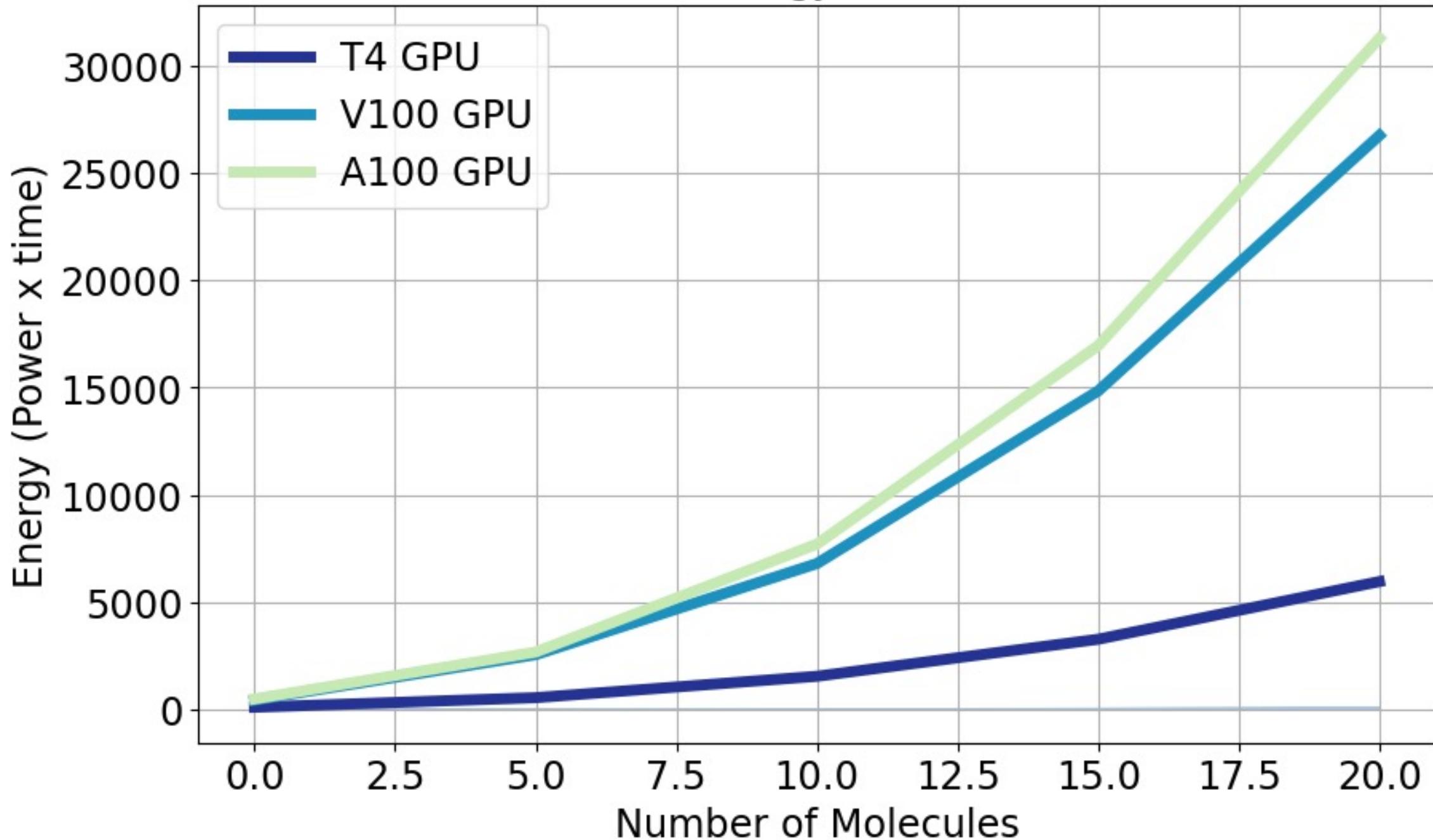
But, there is a cost to using a GPU! Some problems that don't benefit from a GPU are typically better done on a CPU, like:

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

## Mean and Standard Deviation Over 10 Runs



# Energy Cost



# This is Green Chemistry!

## Home

## Calculator

GA4HPC

## Training

## Publications

# Talks

## About

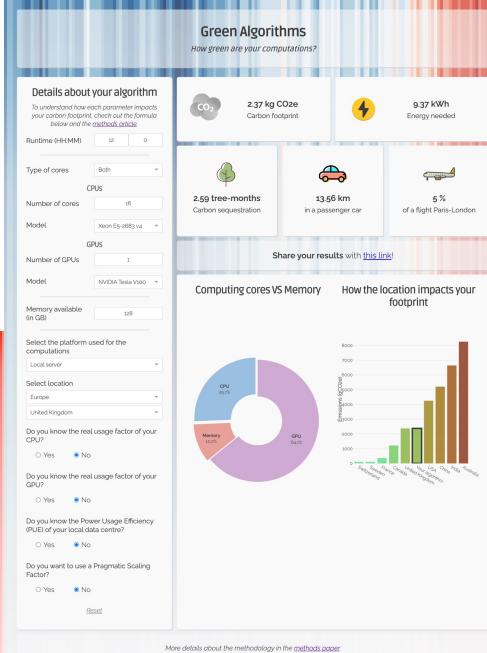


# Green Algorithms

# Towards environmentally sustainable computational science

## Carbon footprint calculator

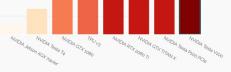
<https://www.green-algorithms.org>



What can you do about it?

The main factor impacting your footprint is the location of your servers; the same algorithm will emit **74 times more CO<sub>2</sub>** if ran in Australia compared to Switzerland. Although it's not always the case, many cloud providers offer the option to

Memory Size	Power usage (W)
1GB	~100
2GB	~110
4GB	~120
8GB	~180
16GB	~185
32GB	~185



The formula

The carbon footprint is calculated by estimating the energy draw of the algorithm and the carbon intensity of producing this energy at a given location:

$$\text{carbon footprint} = \text{energy needed} \times \text{carbon intensity}$$

When the energy needed is runtime \* (power draw for cores \* usage + power draw for memory) PUE = PSF The power draw for the compute depends on the model and number of cores, while the memory power draw only depends on the size of memory available. The usage factor corrects for the real core usage (default is 1, i.e. full usage). The PUE (Power Usage Effectiveness) measures how much extra energy is needed to operate publications alongside other performance metrics.

The data centre (cooling, lighting etc). The PSF (Pragmatic Scaling Factor) is used to take into account multiple identical runs (e.g. testing or optimisation).

The Carbon Intensity depends on the location and the technologies used to produce electricity. But note that the "energy needed" indicated at the top of this page is independent of the location.

PERIODIC TABLE OF THE GLOSS WORDS

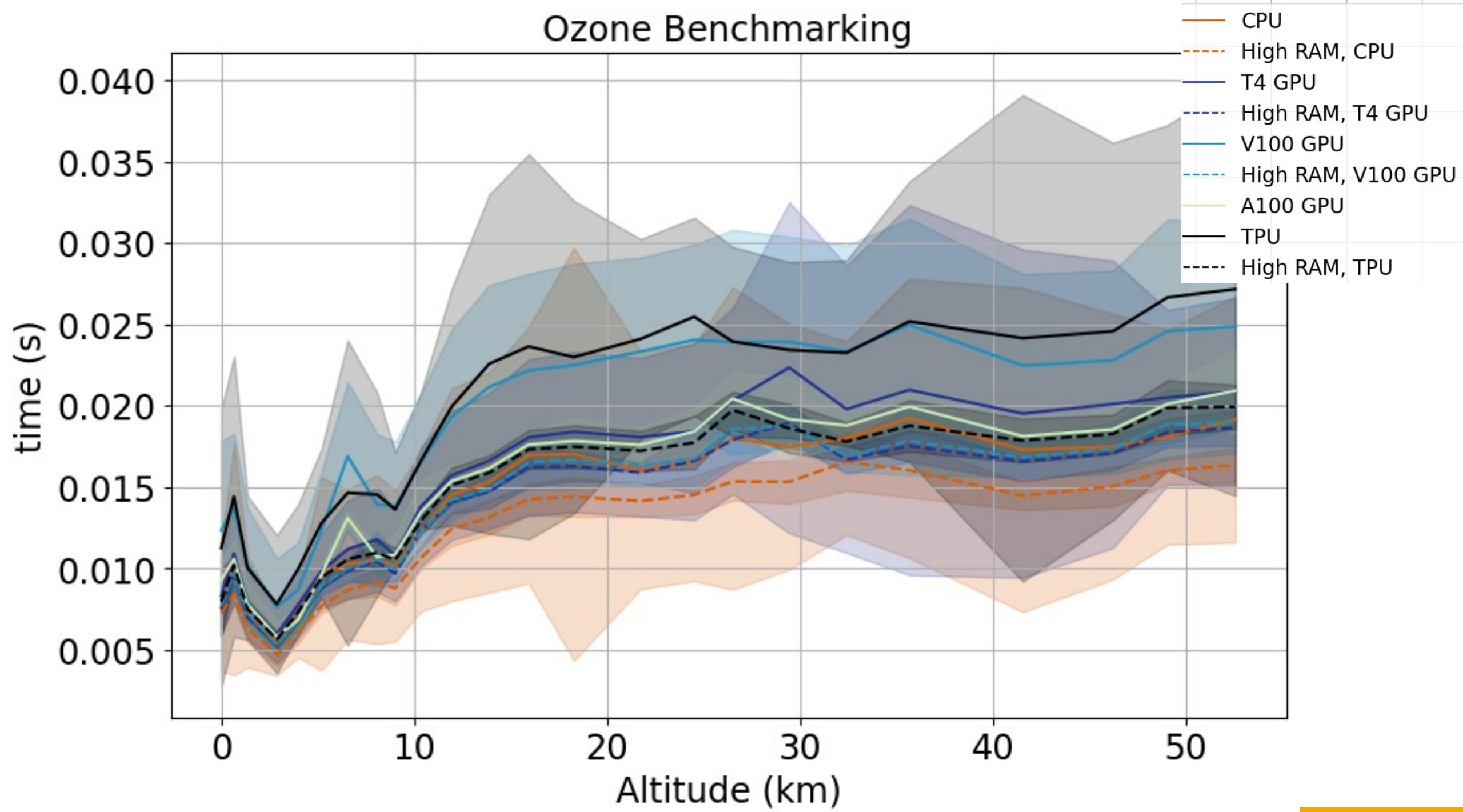
The Green Algorithms project was jointly developed by Loïc Lannelongue<sup>1</sup>, Jason Greyley<sup>2</sup>, and [all the data and code used to run this calculator can be found on GitHub](#). These coloured stripes in the background represent the change in world temperatures from 1860 to 2018. This “temperature stripe” visualization was created by [Michael Mann](#).

Michael Inouye  
University of Cambridge  
(2) Baker Heart and Diabetes Institute and La Trobe University  
University of Cambridge, Michael Inouye, Michael Inouye  
Questions / Suggestions? [ShowYourStress.info](#)

If you have questions or suggestions about the tool, you can [open an issue](#) on the GitHub page.

#### How to cite this work

## Ozone Benchmarking



# Hardware Control

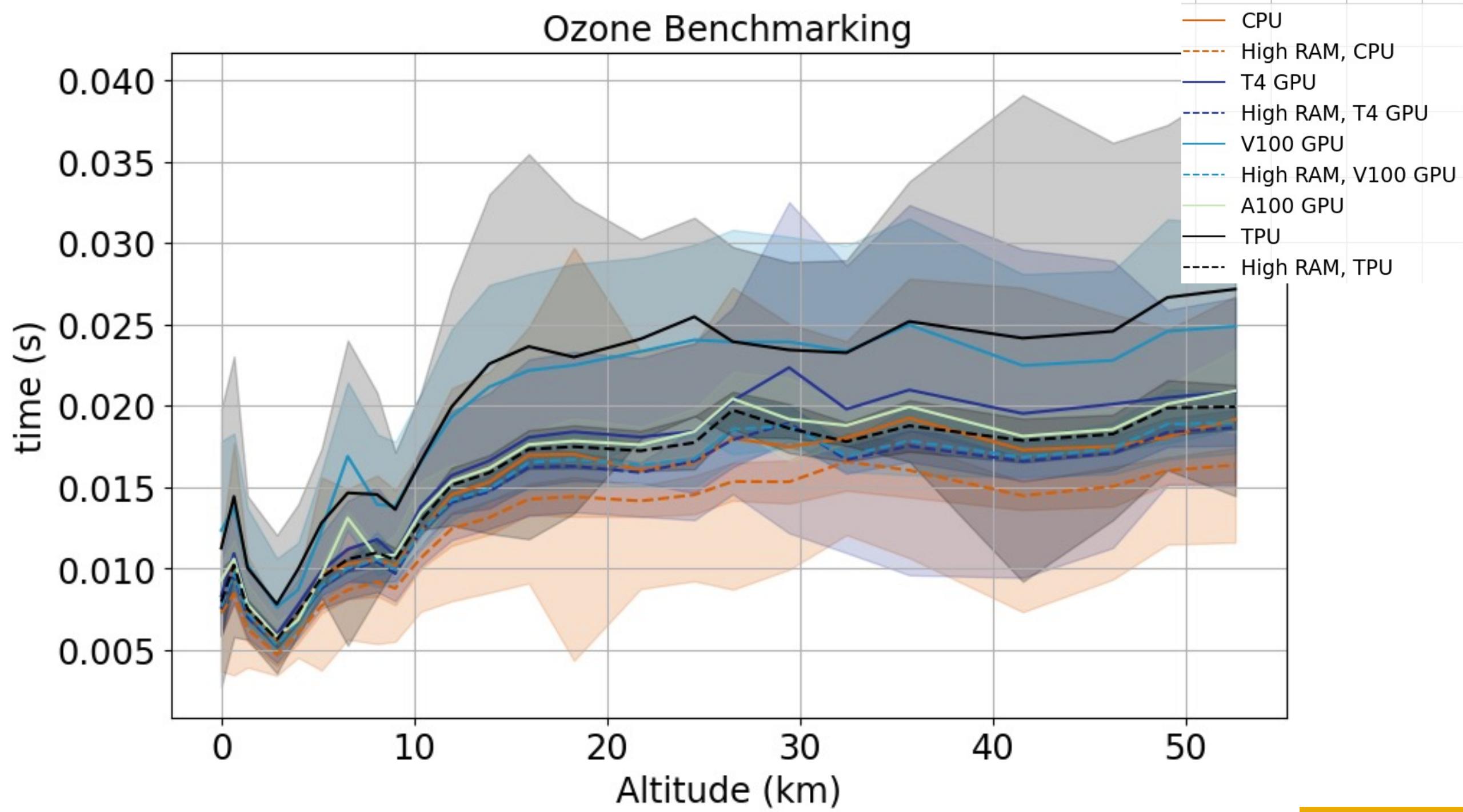
Sometimes your research might involve *how* an answer gets computed, and you need precise knowledge or control over what hardware is involved.

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).

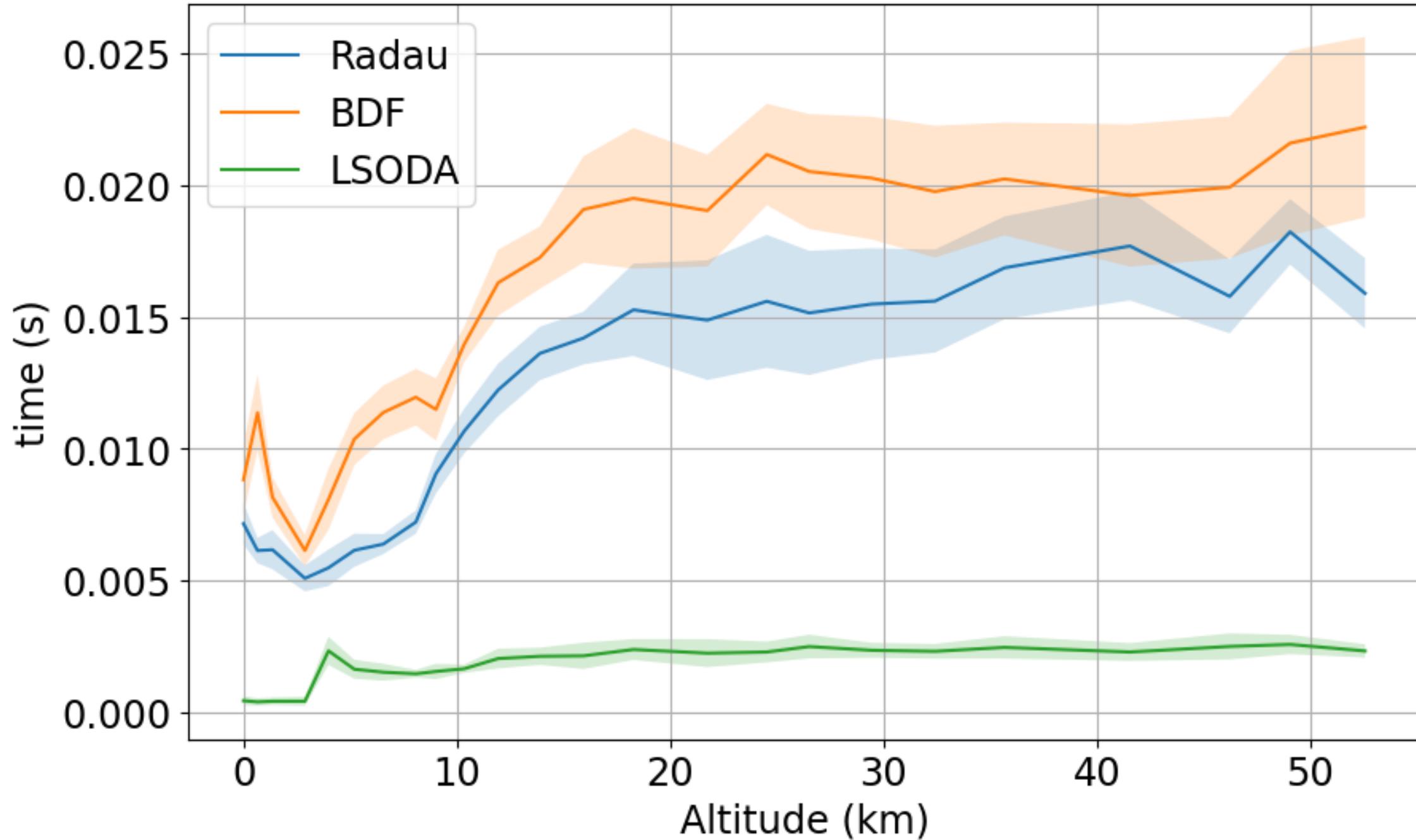
Examples of research where this would be a concern include:

- Power consumption experiments
- Software or hardware benchmarking

## Ozone Benchmarking



# Ozone Benchmarking - High RAM, CPU



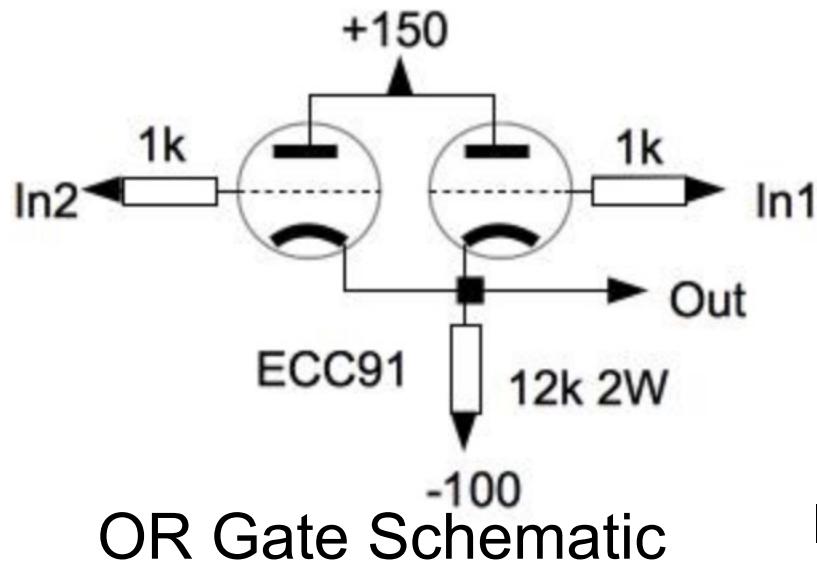
# What are computers *actually* made of?

Early 1950s: vacuum tubes

Late 1950s: transistors

Late 1960s: printed/integrated circuits

1970s: Microprocessors



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

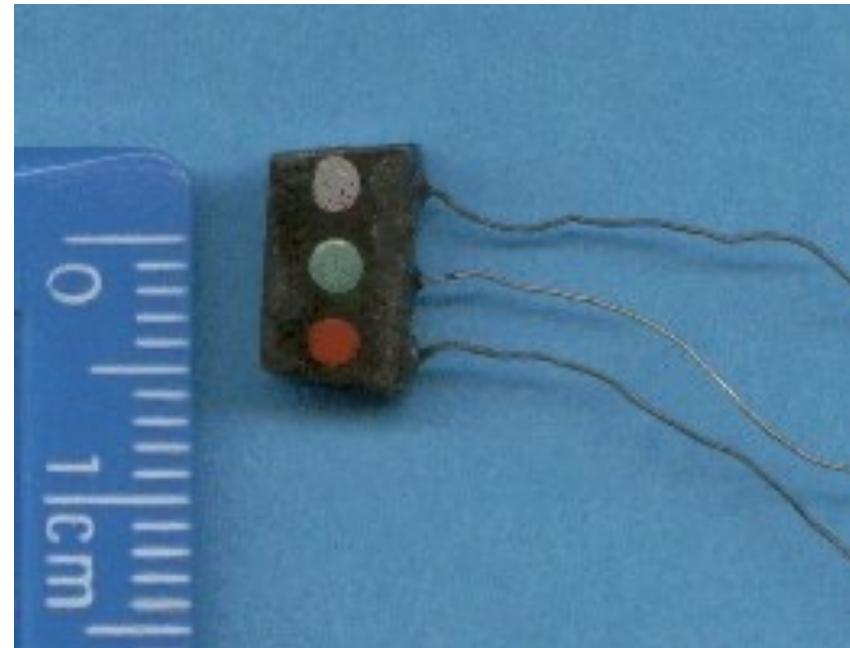
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**Late 1950s: transistors**

Late 1960s: printed/integrated circuits

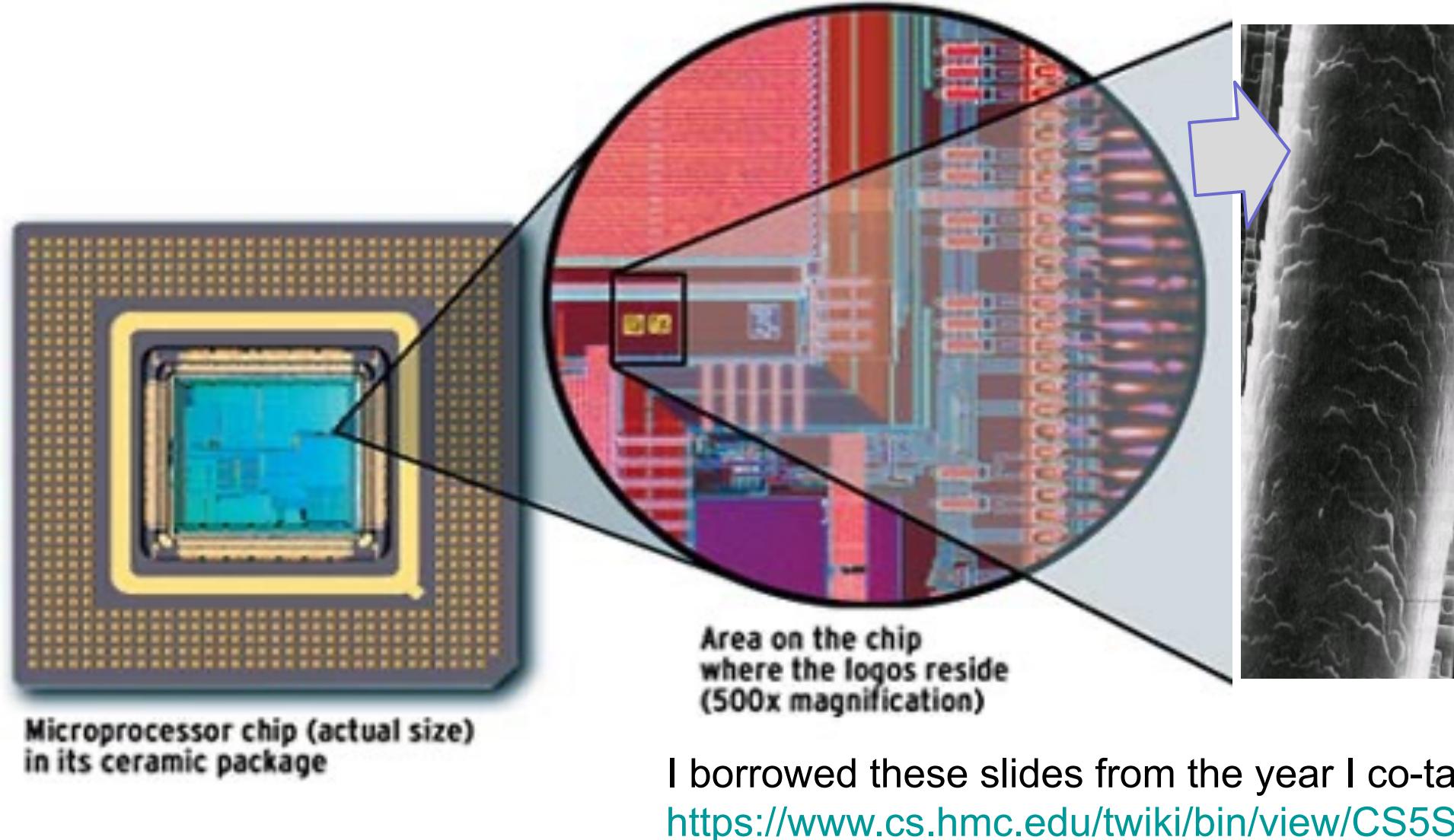
1970s: Microprocessors



***“The most important invention of the 20<sup>th</sup> century...”***

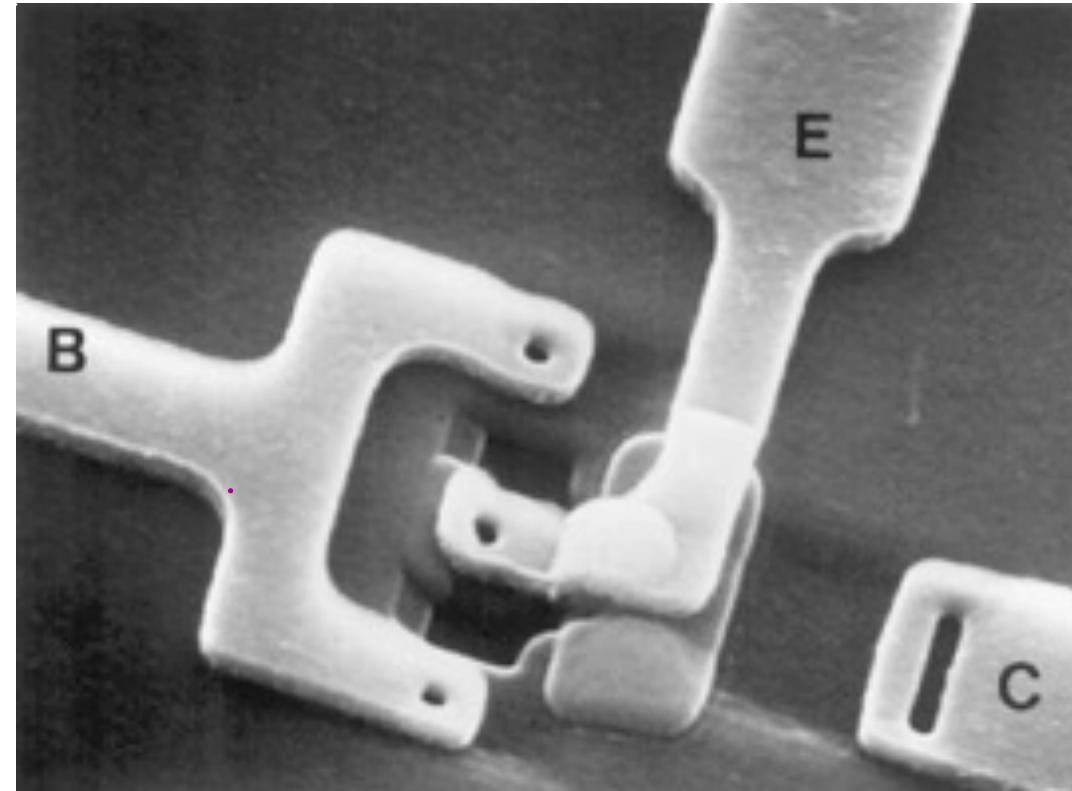
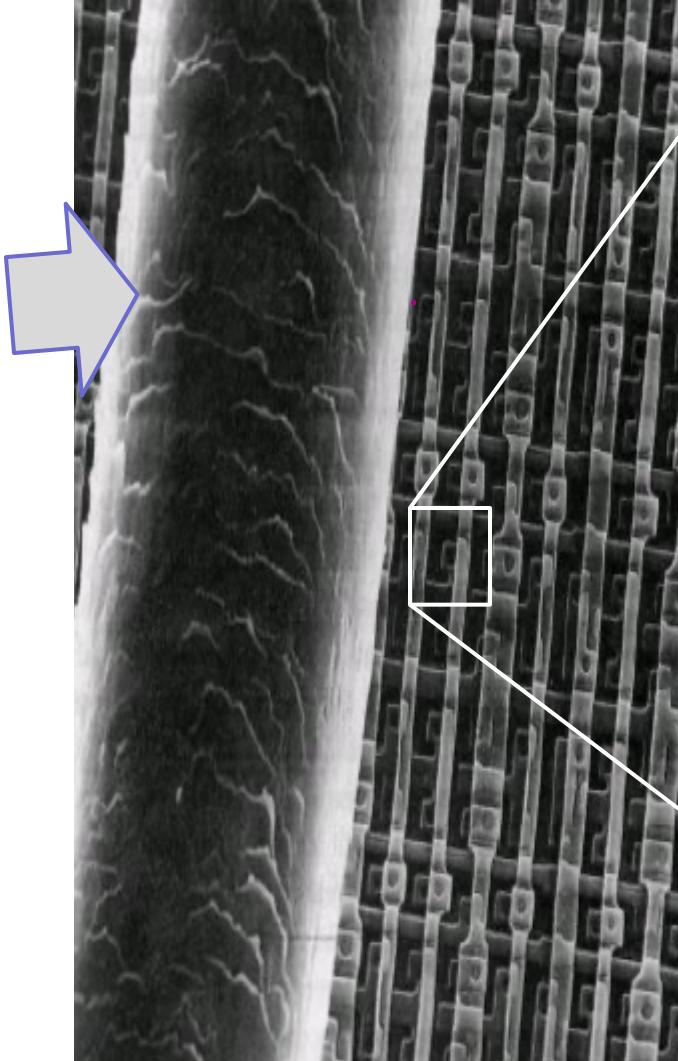
I borrowed these slides from the year I co-taught CS5:  
<https://www.cs.hmc.edu/twiki/bin/view/CS5Spring2022>

# Today's gates?



are from silicon-based switches ~ *transistors*

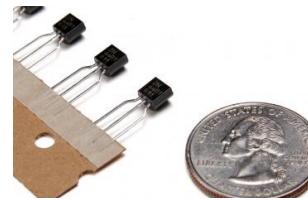
switches?



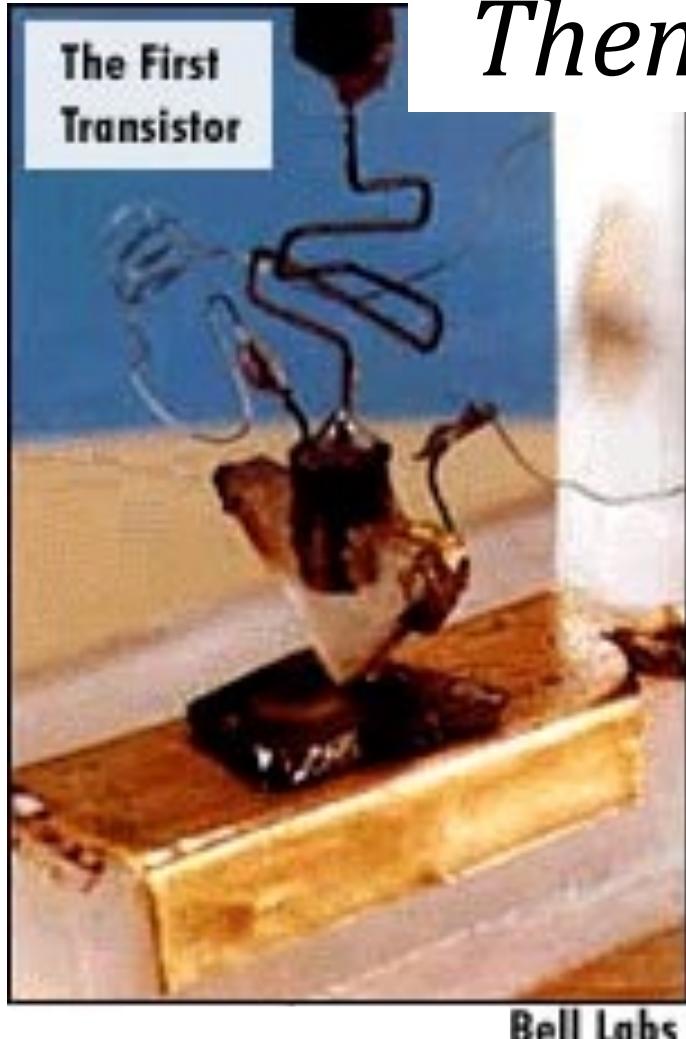
a single etched transistor labeled with  
base (b), emitter (e), and collector (c)

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

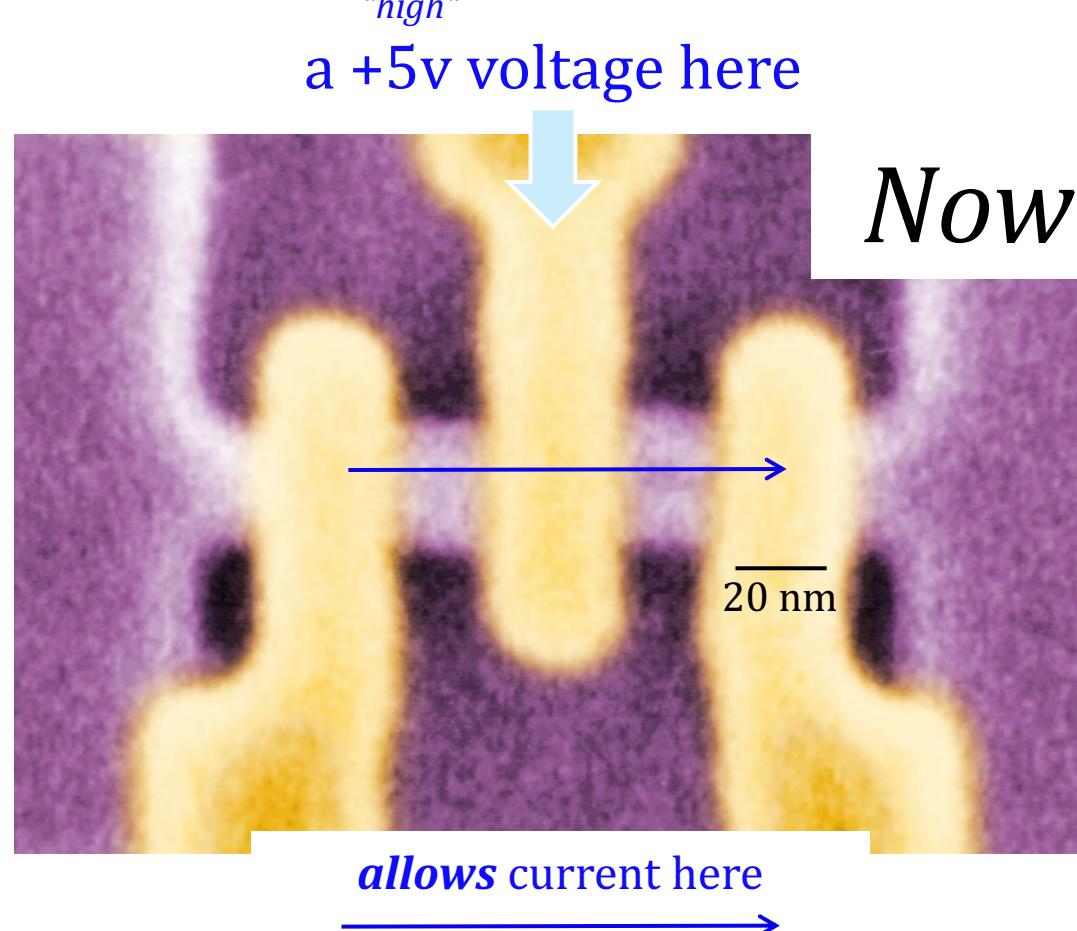
# *Single electron tunnelling*



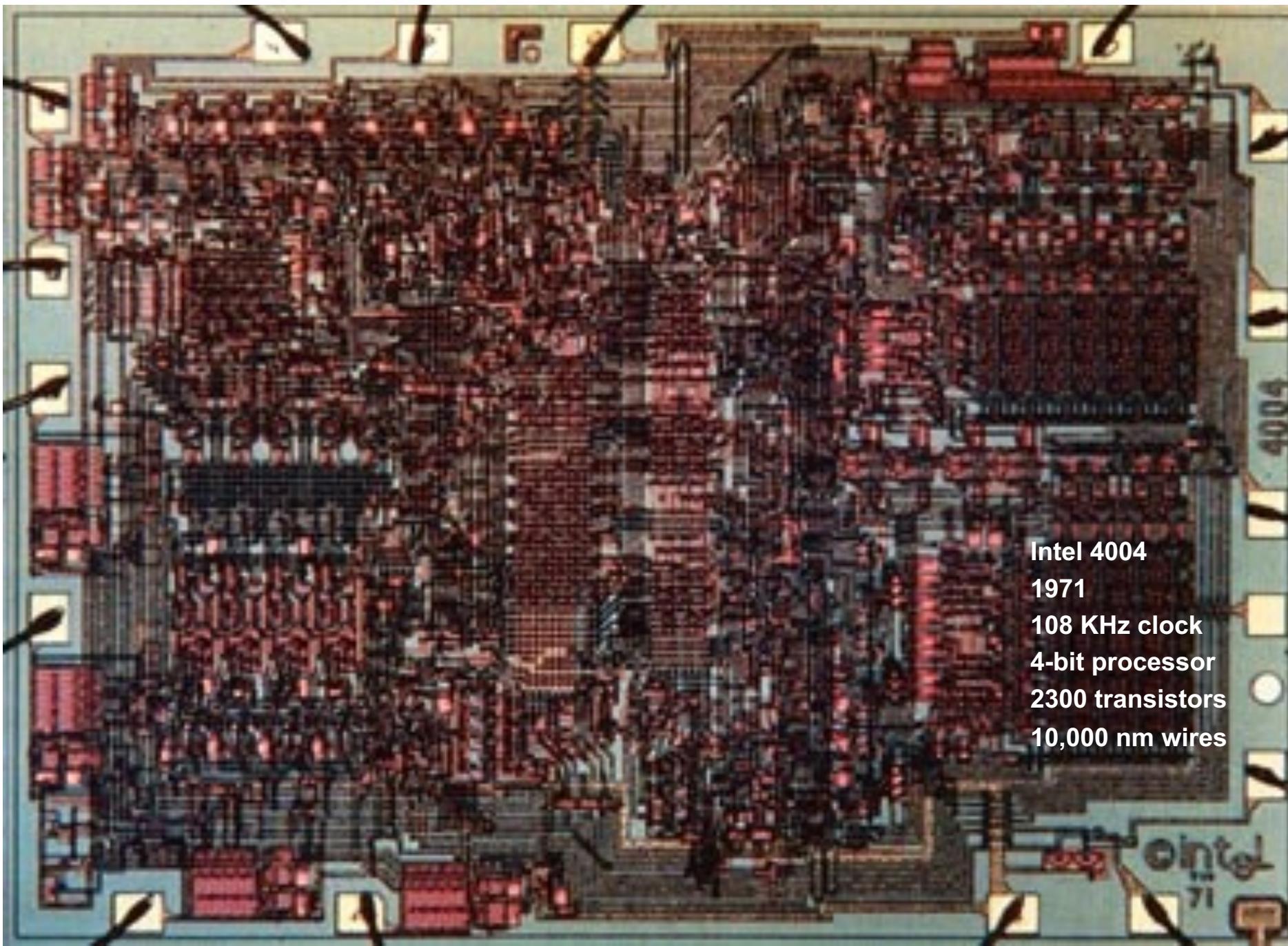
Fry's transistors



*Then*



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**



2006

Intel Core 2 Duo

3 GHz clock

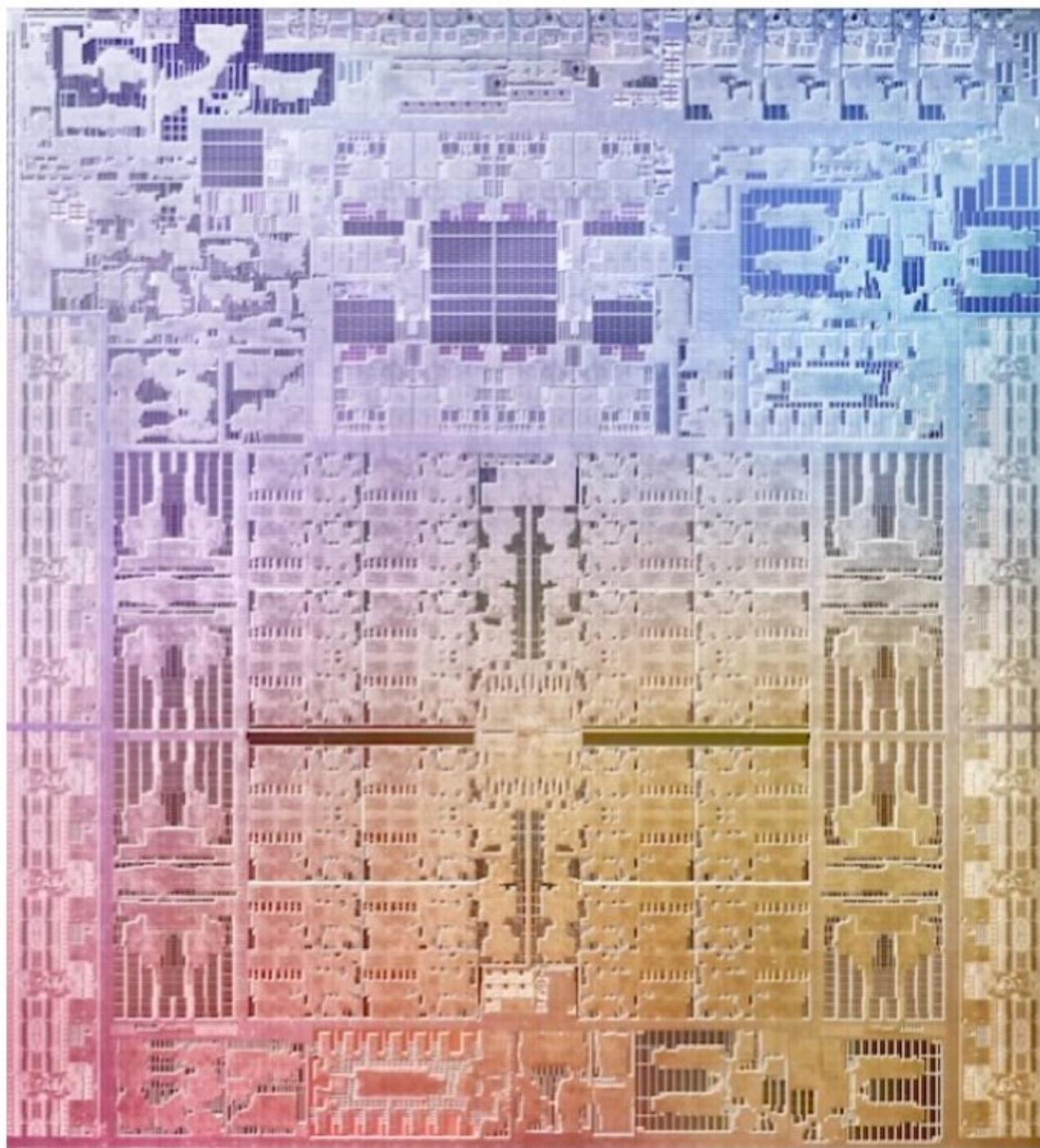
64-bit processor

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*