

Memory Bound Computing

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Advanced Scientific Programming in Python

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“No sensible decision can be made any longer without taking into account not only the world as it is, but the world as it will be.”

— *Isaac Asimov*

“No sensible decision can be made any longer without taking into account not only the **computer** as it is, but the **computer** as it will be.”

— My own rephrasing

Overview

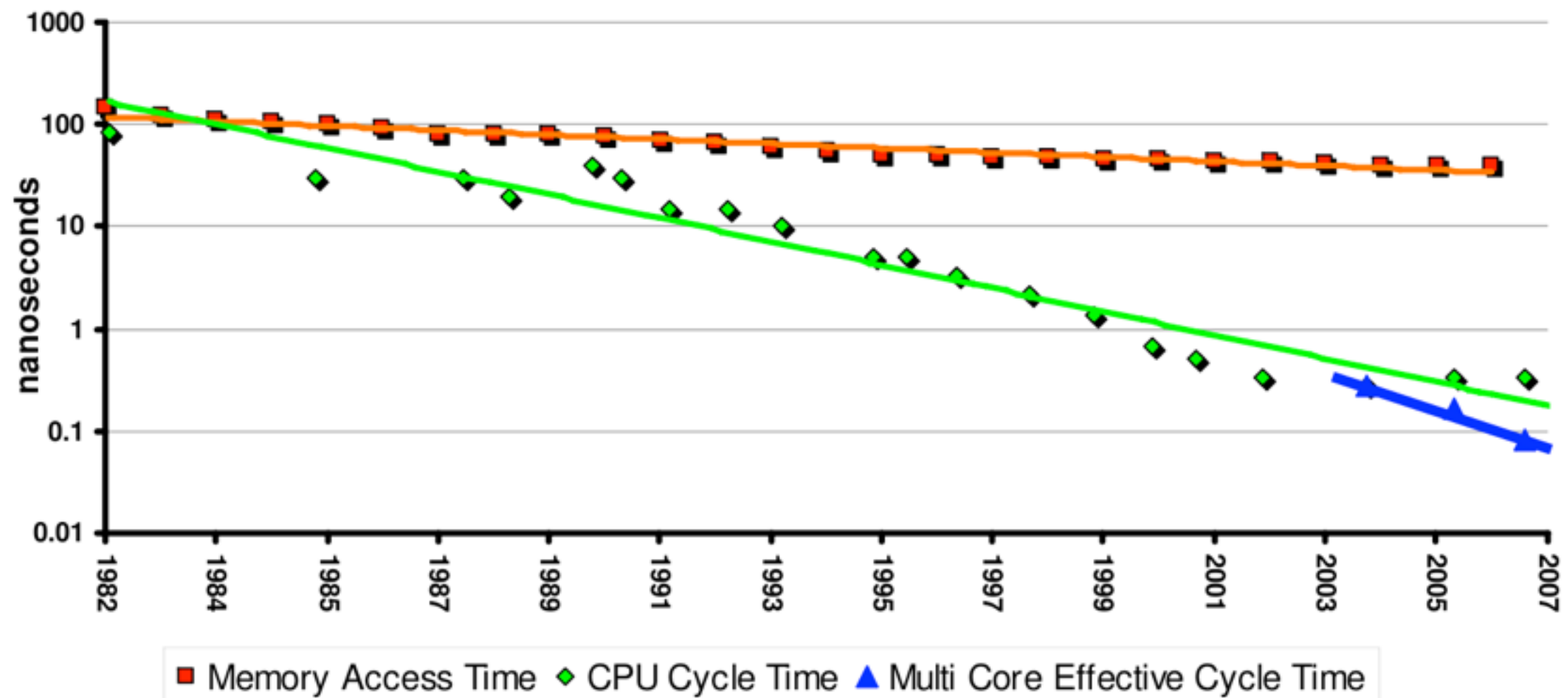
- The Starving CPU problem
- Recent trends in computer architecture
- Handling Big Data: storing and processing as much data as possible with your existing resources

“Across the industry, today’s chips are largely able to execute code faster than we can feed them with instructions and data.”

– Richard Sites, after his article
“It’s The Memory, Stupid!”,
Microprocessor Report, 10(10), 1996

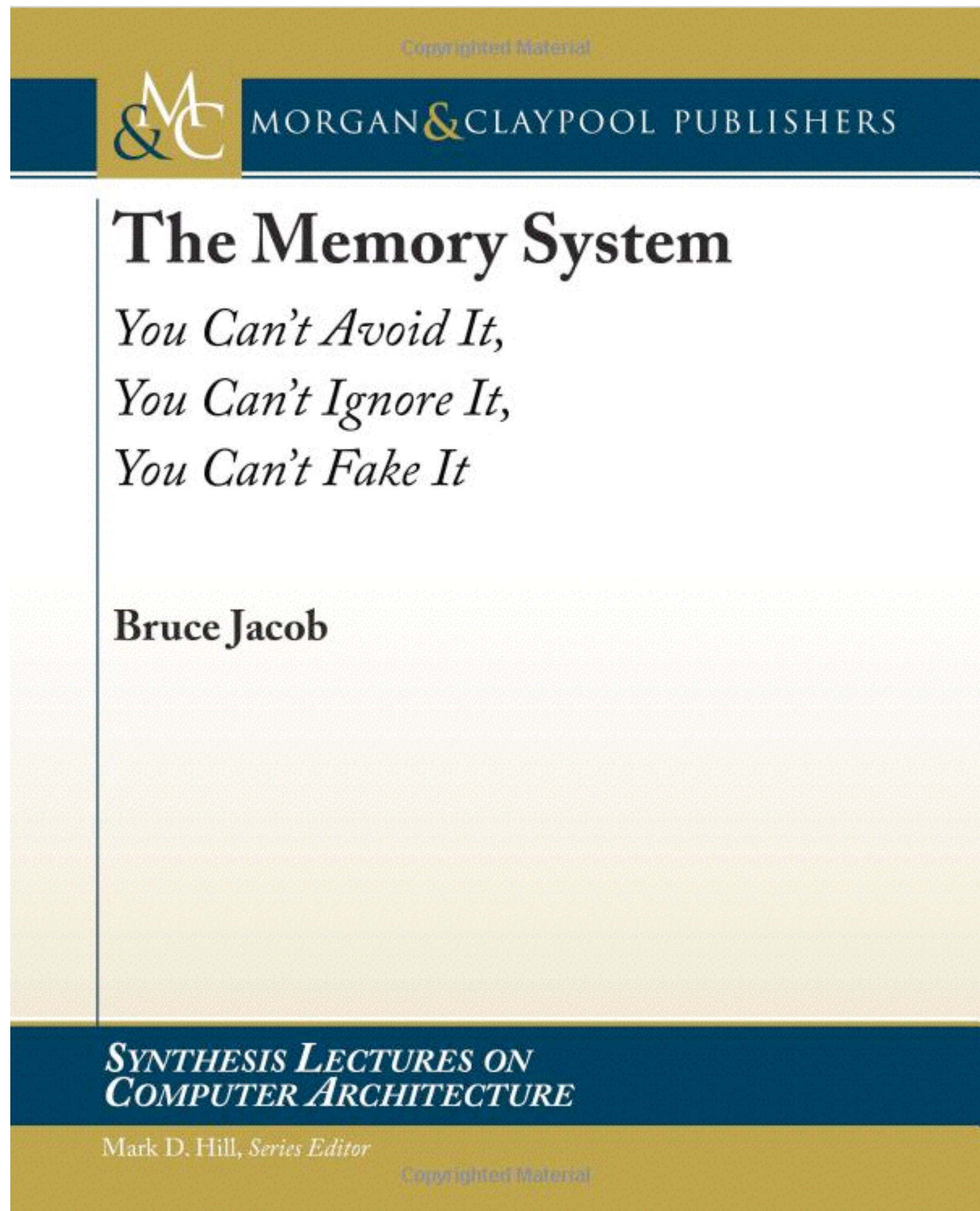
The Starving CPU Problem

Memory Access Time vs CPU Cycle Time



The gap is wide and still opening!

Book in
2009



The Status of CPU Starvation in 2016

- Memory latency is much slower (between 250x and 1000x) than processors.
- Memory bandwidth is improving at a better rate than memory latency, but it is also slower than processors (between 30x and 100x).

CPU Caches to the Rescue

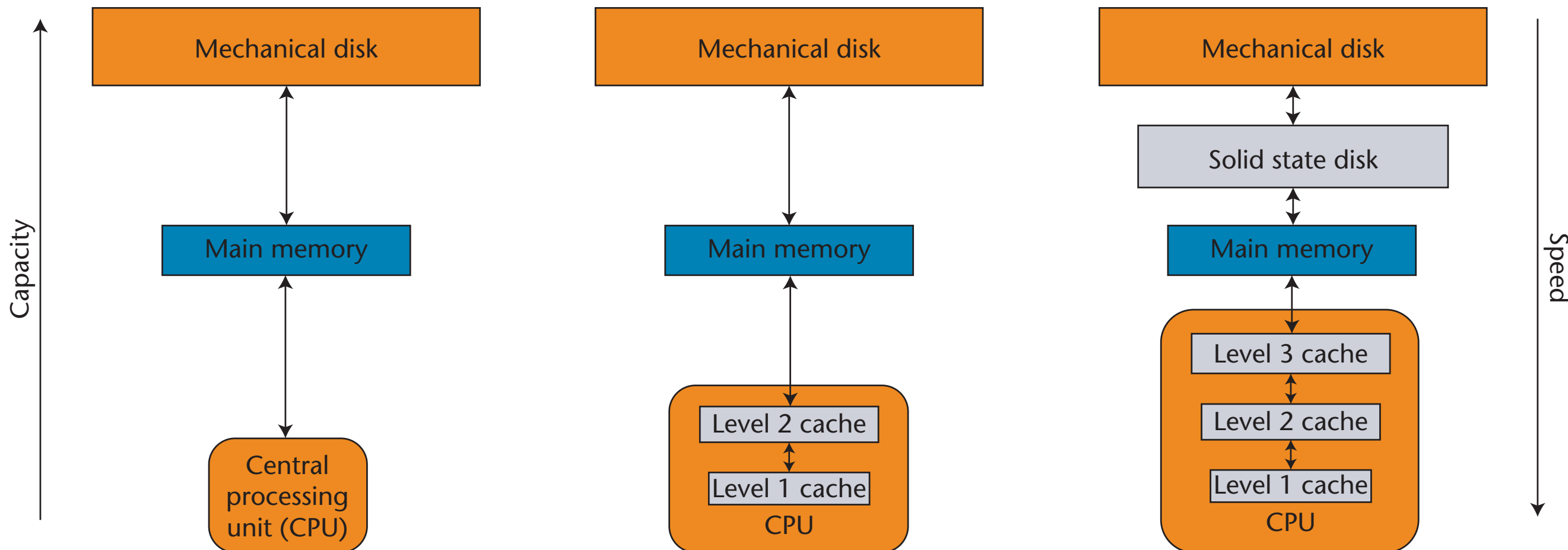
- CPU cache latency and throughput are much better than memory
- However: the faster they run the smaller they must be (because of heat dissipation problems)

Computer Architecture Evolution

Up to end 80's

90's and 2000's

2010's



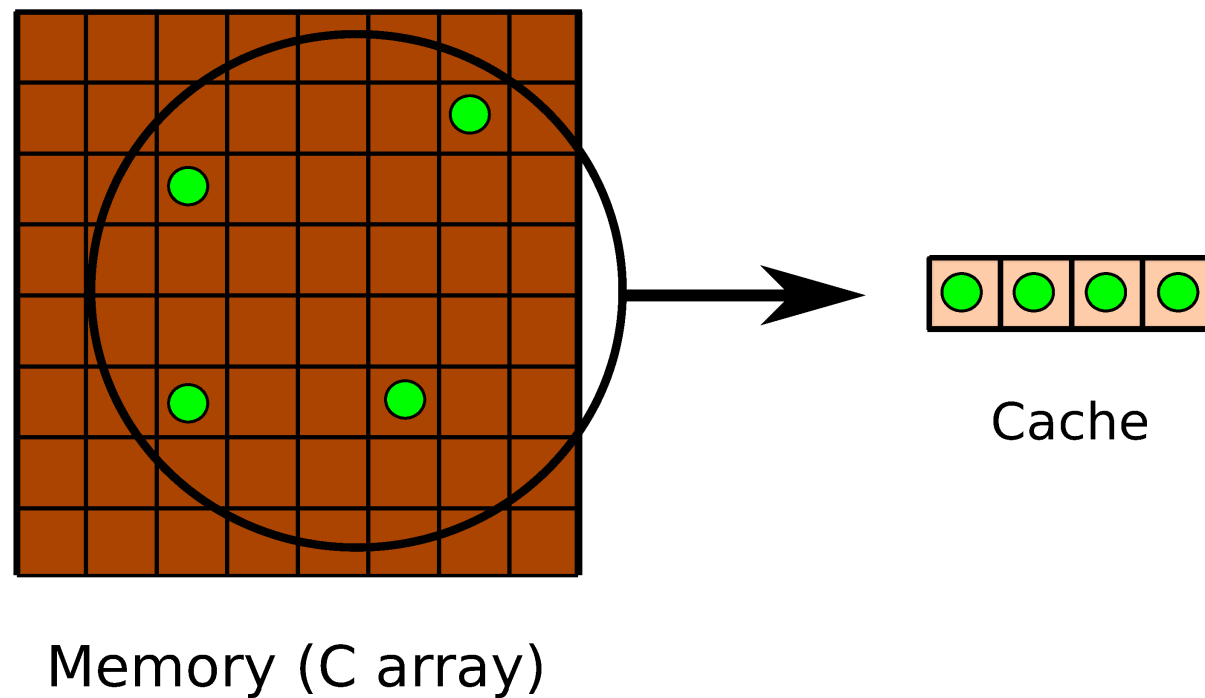
When CPU Caches Are Effective?

Mainly in a couple of scenarios:

- Time locality: when the dataset is reused
- Spatial locality: when the dataset is accessed sequentially

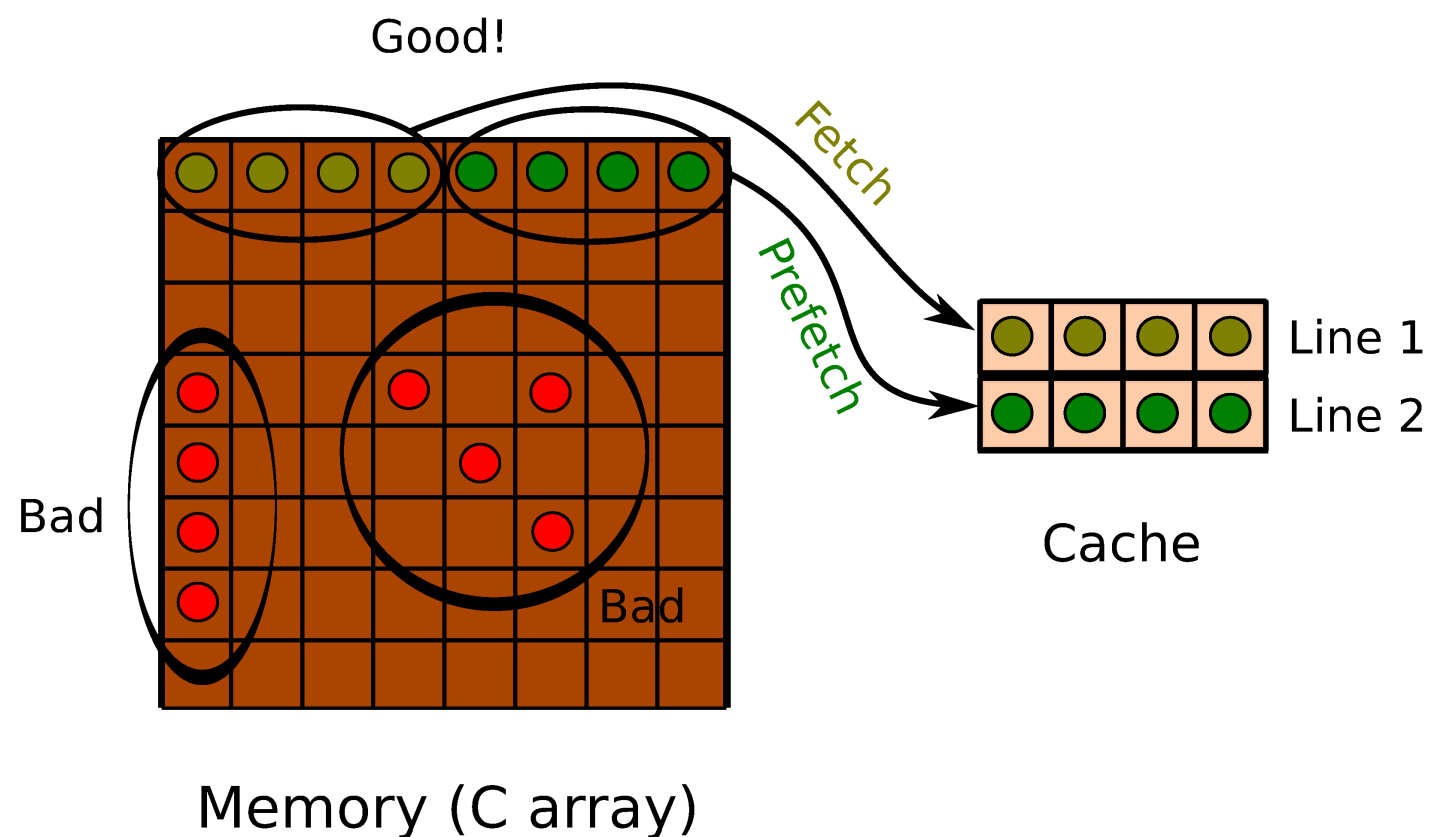
Time Locality

Parts of the dataset are reused



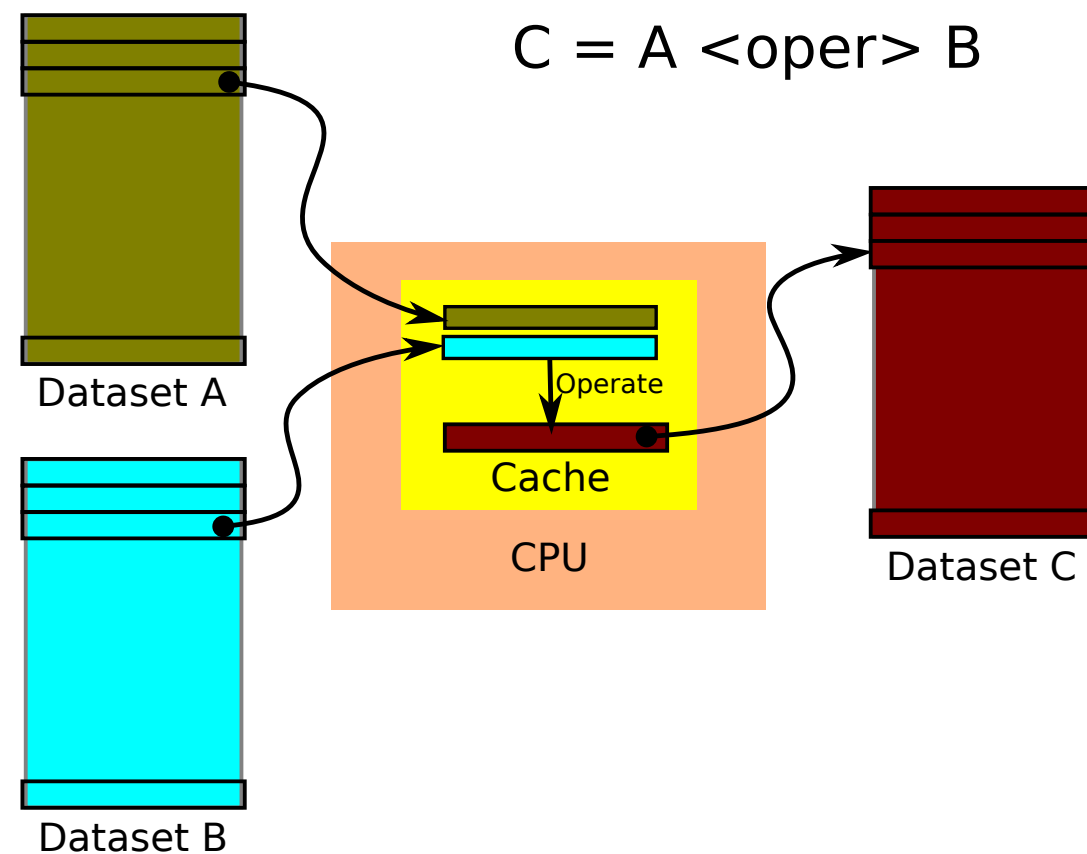
Spatial Locality

Dataset is accessed sequentially



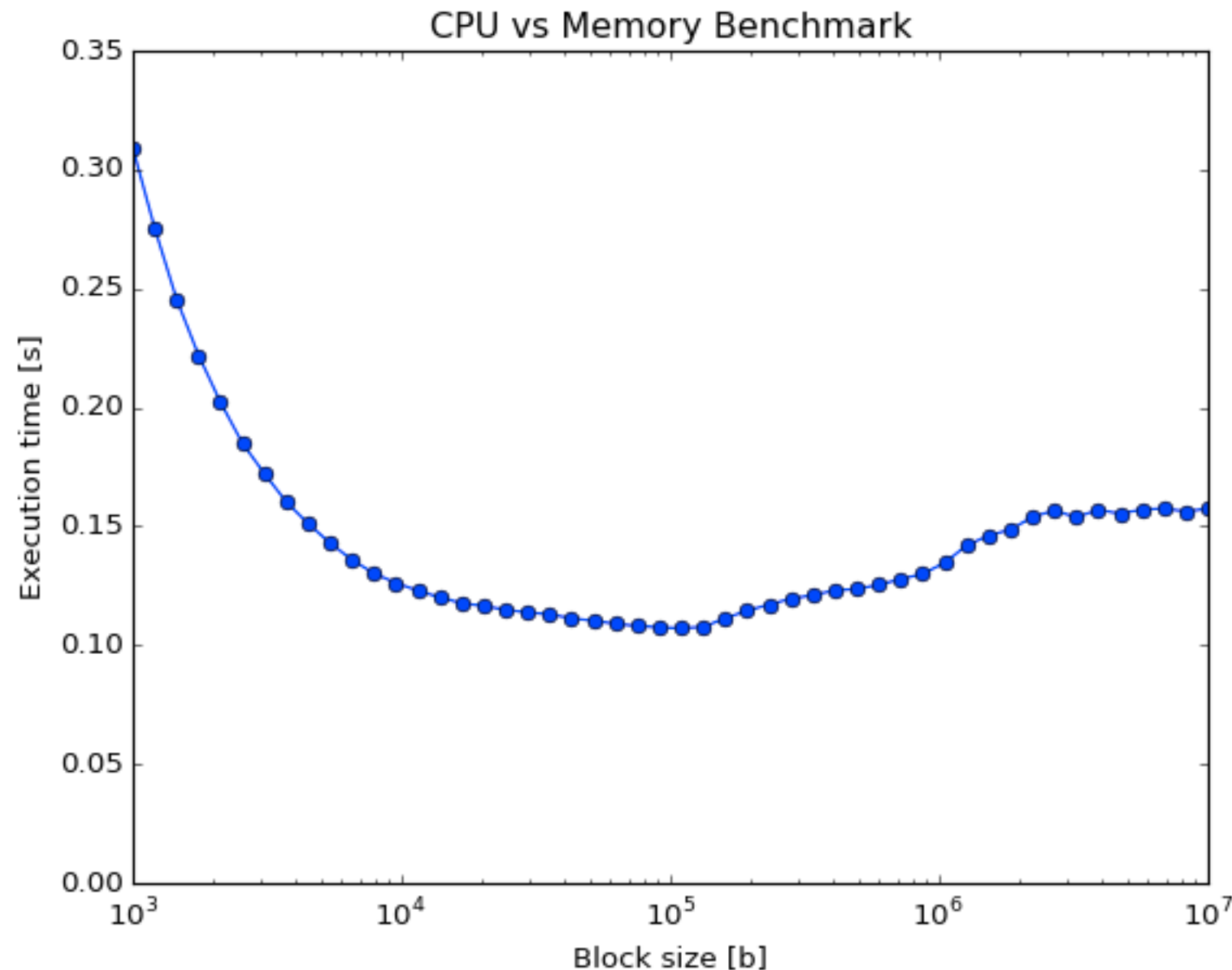
The Blocking Technique

When accessing disk or memory, get a **contiguous** block that fits in CPU cache, operate upon it and **reuse** it as much as possible.



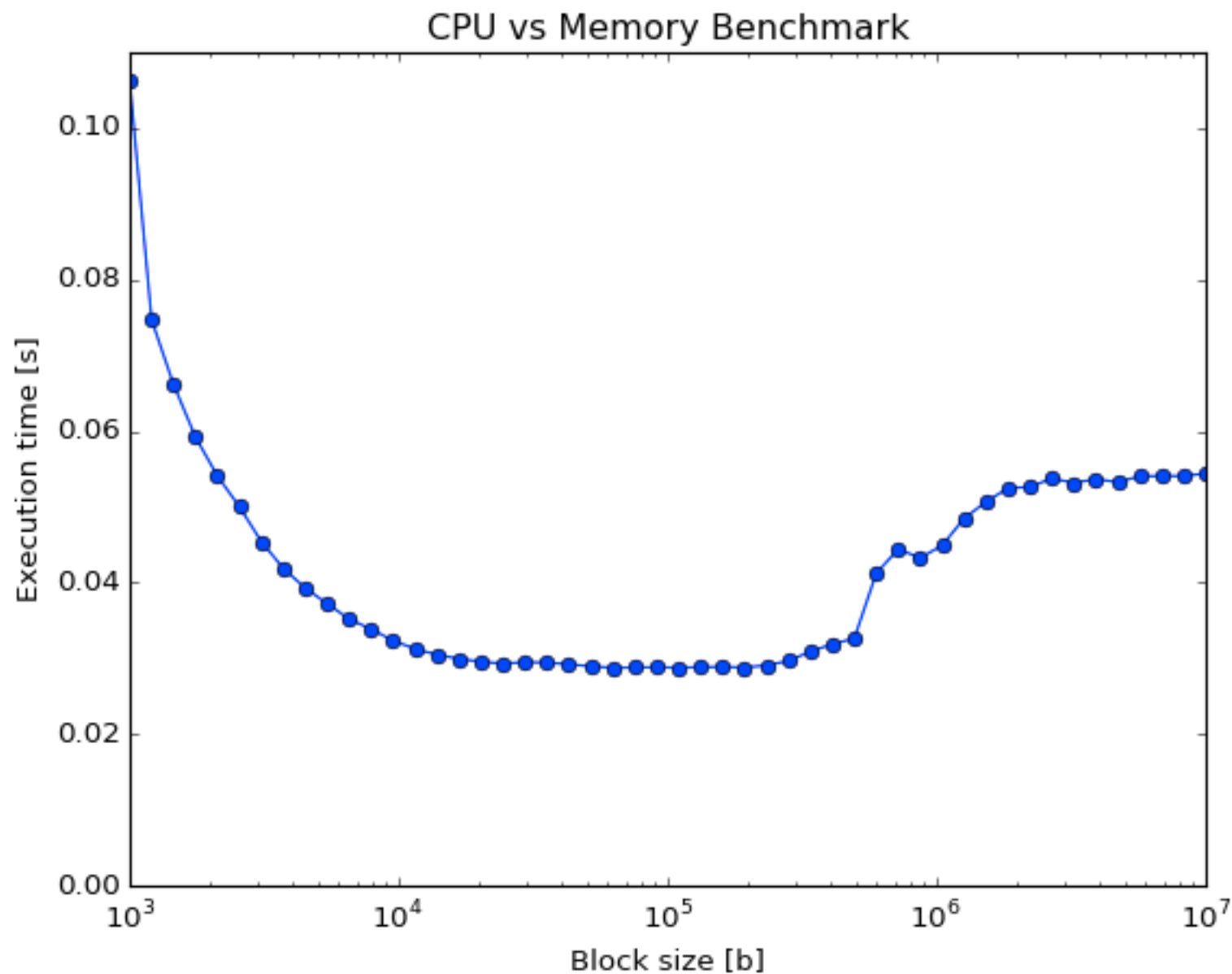
Use this extensively to leverage **spatial** and **temporal** localities

The Blocking Technique in Action (Exercise 0)



CPU: Intel Xeon E312xx @ 2.00GHz (Sandy Bridge)

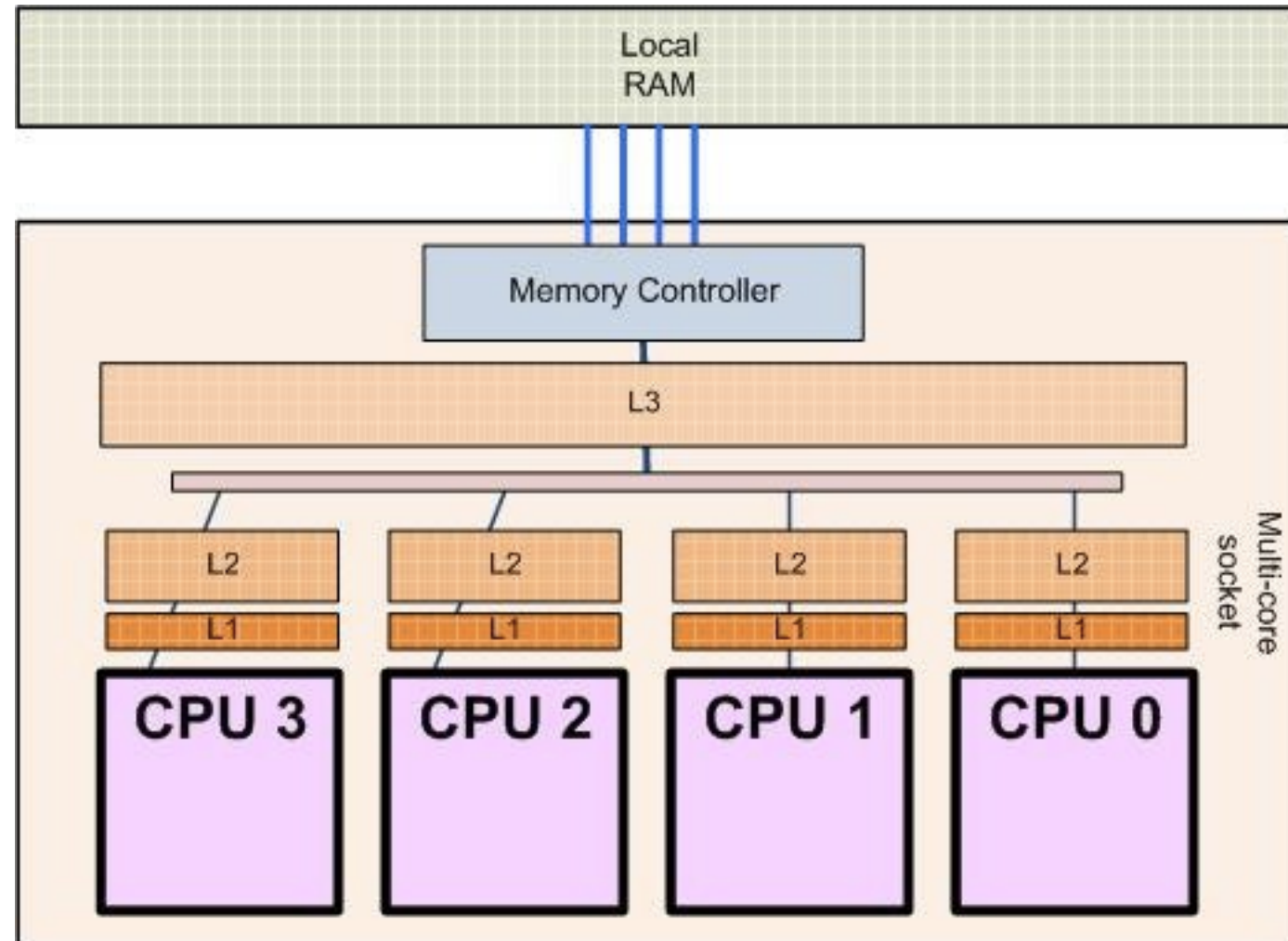
The Blocking Technique in Action (Exercise 0)



CPU: Intel Xeon(R) CPU E3-1245 v5 @ 3.50GHz (Skylake)

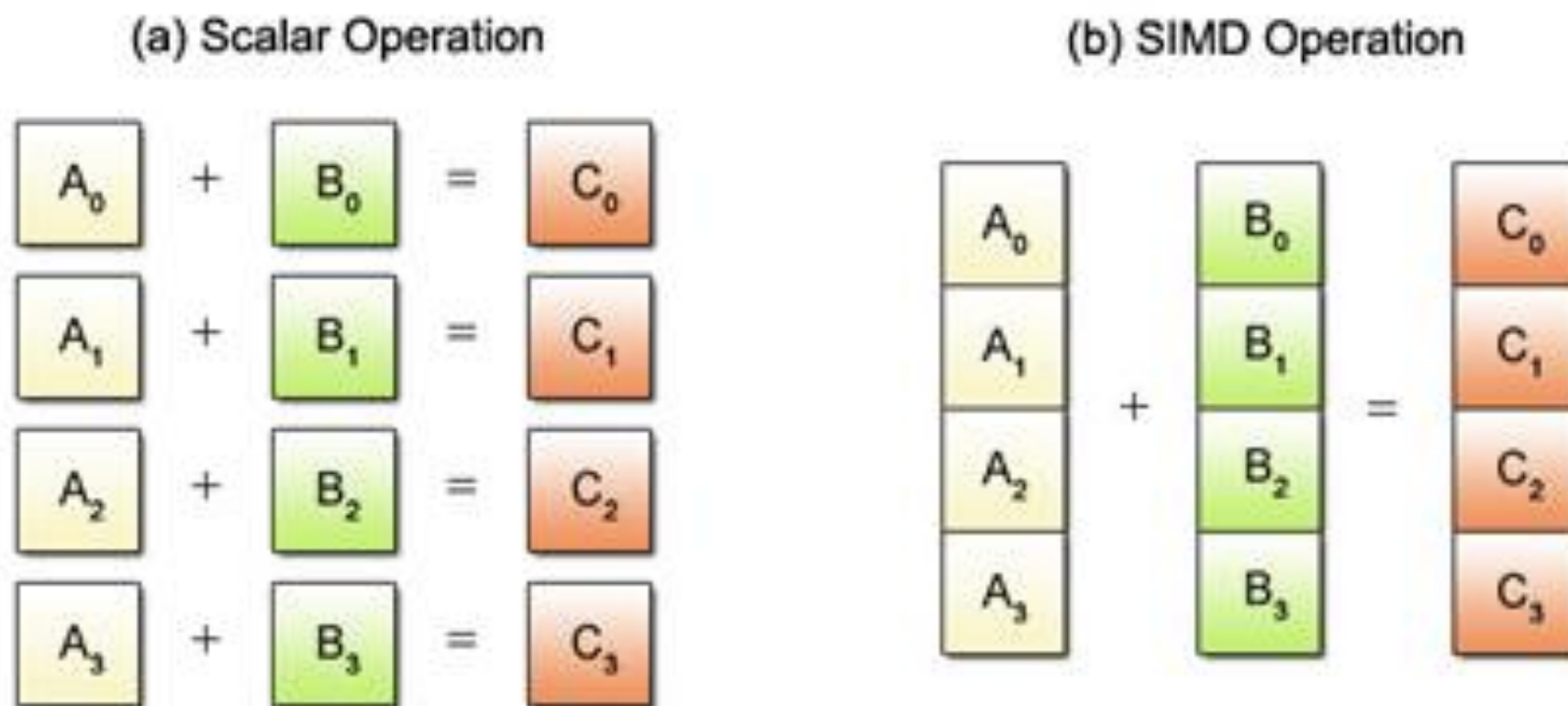
Trends in Computer Architecture

We Are In A Multicore Age



- This requires special programming measures to leverage all its potential: threads, multiprocessing

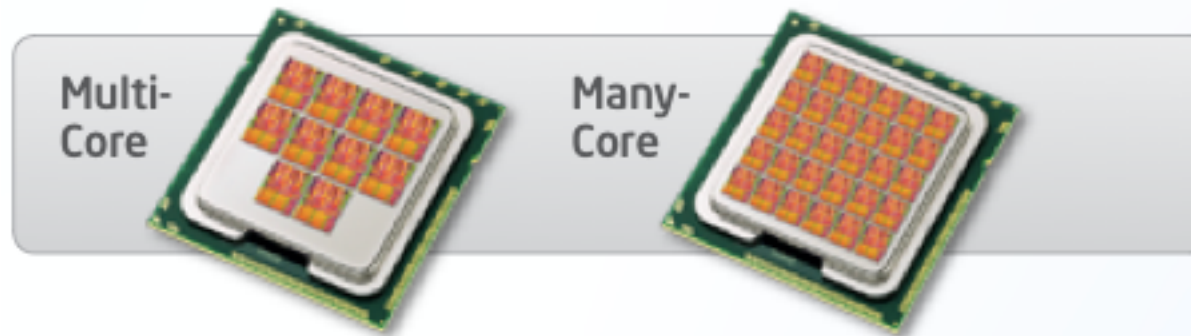
SIMD: Single Instruction, Multiple Data



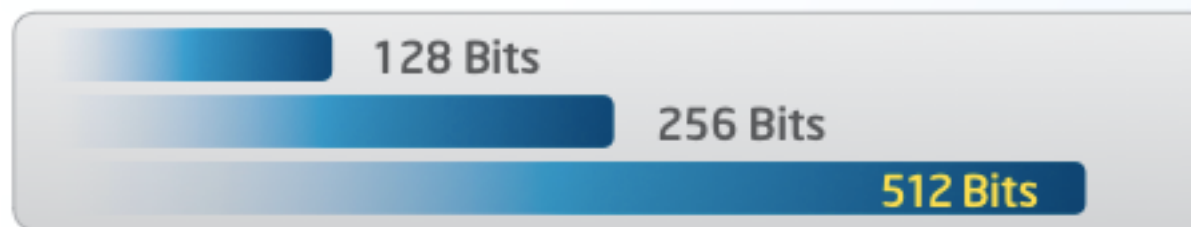
More operations in the same CPU clock

Forthcoming Trends in CPU

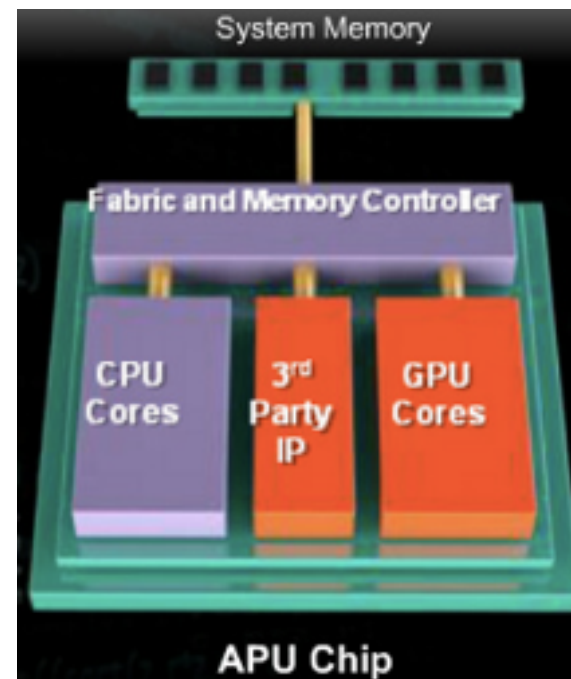
More Cores



Wider Vectors

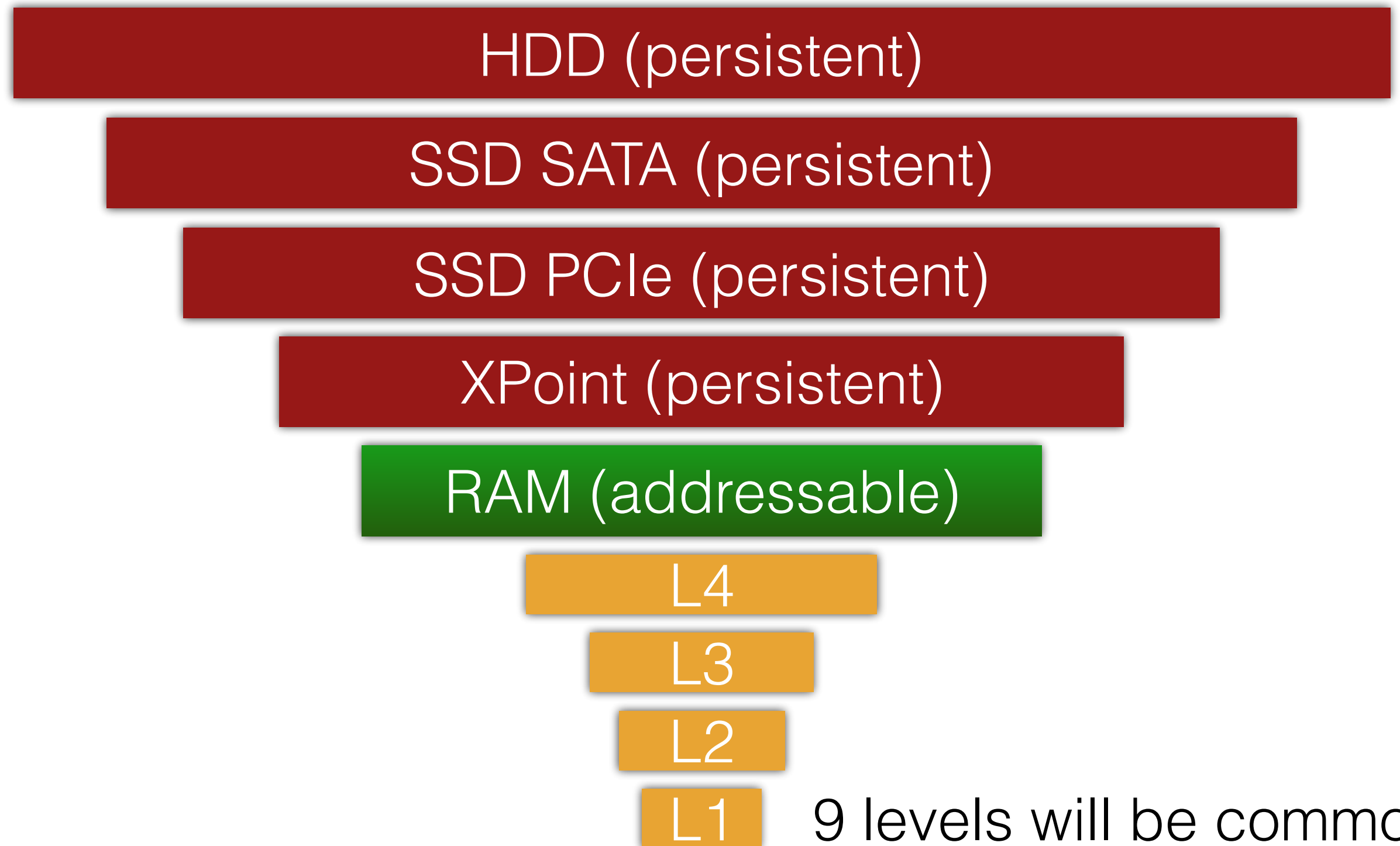


CPU+GPU Integration



Hierarchy of Memory

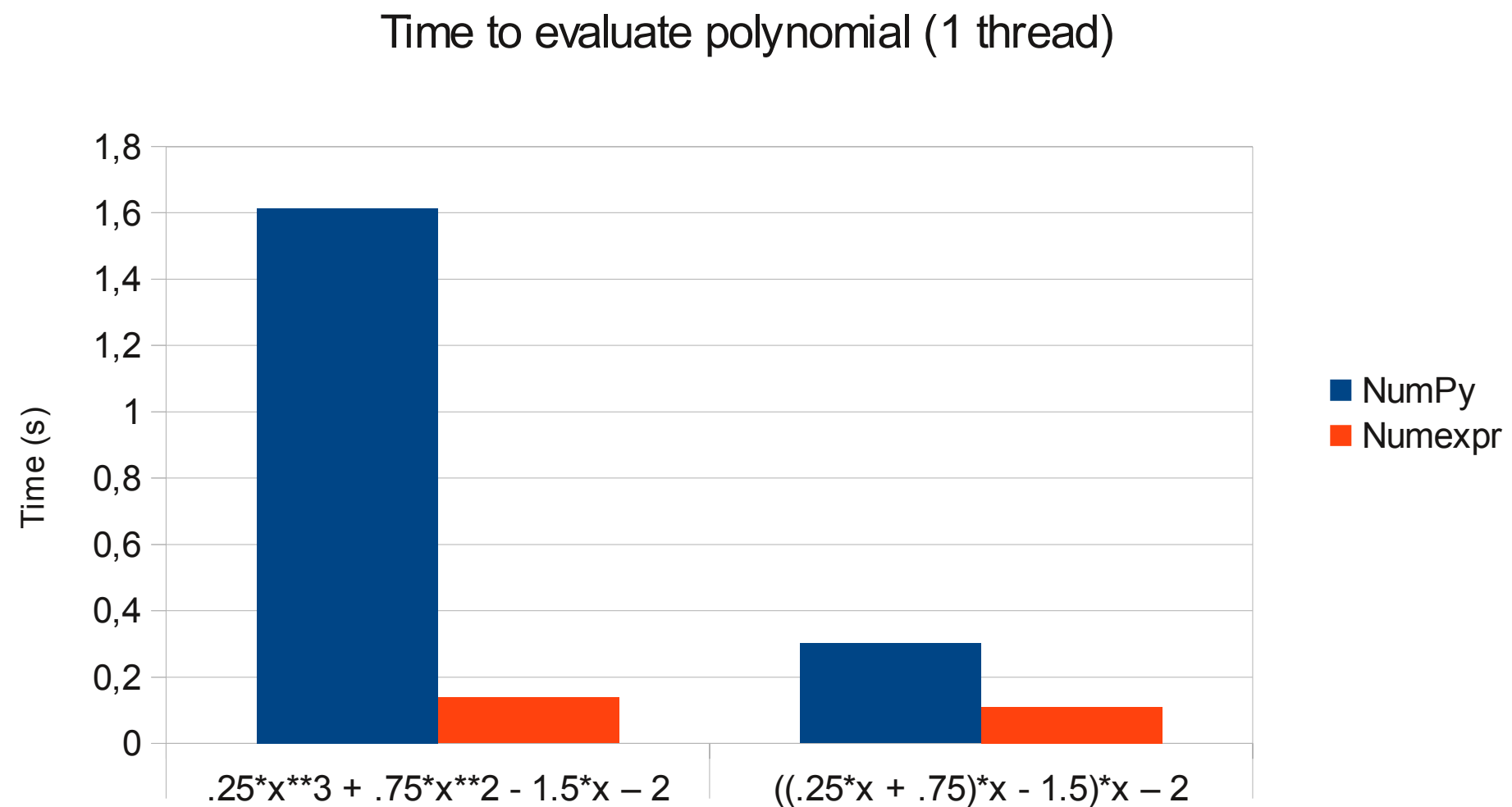
By 2018 (Educated Guess)



numexpr

- It is a computational engine for NumPy that makes a sensible use of the memory hierarchy for better performance
- It can use multi-core (via multi-threading) and SIMD (via Intel's MKL) for better CPU usage.
- PyTables, pandas and bcolz (among others) can all leverage numexpr automatically if installed

Computing with numexpr



Power Expansion

Numexpr expands expression:

$$0.25*x**3 + 0.75*x**2 + 1.5*x - 2$$

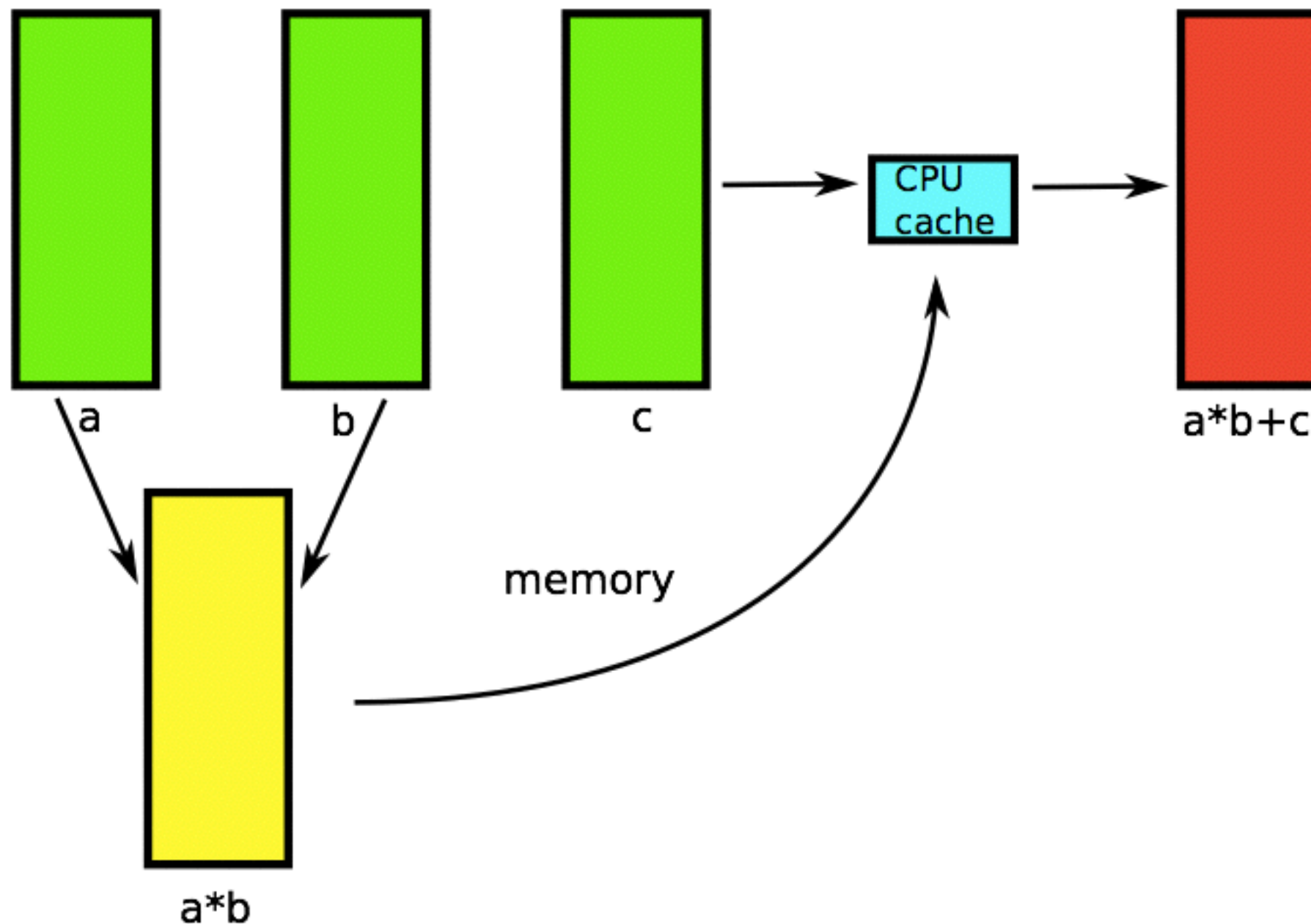
to:

$$0.25*x*x*x + 0.75*x*x + 1.5*x - 2$$

so, no need to use the expensive `pow()`

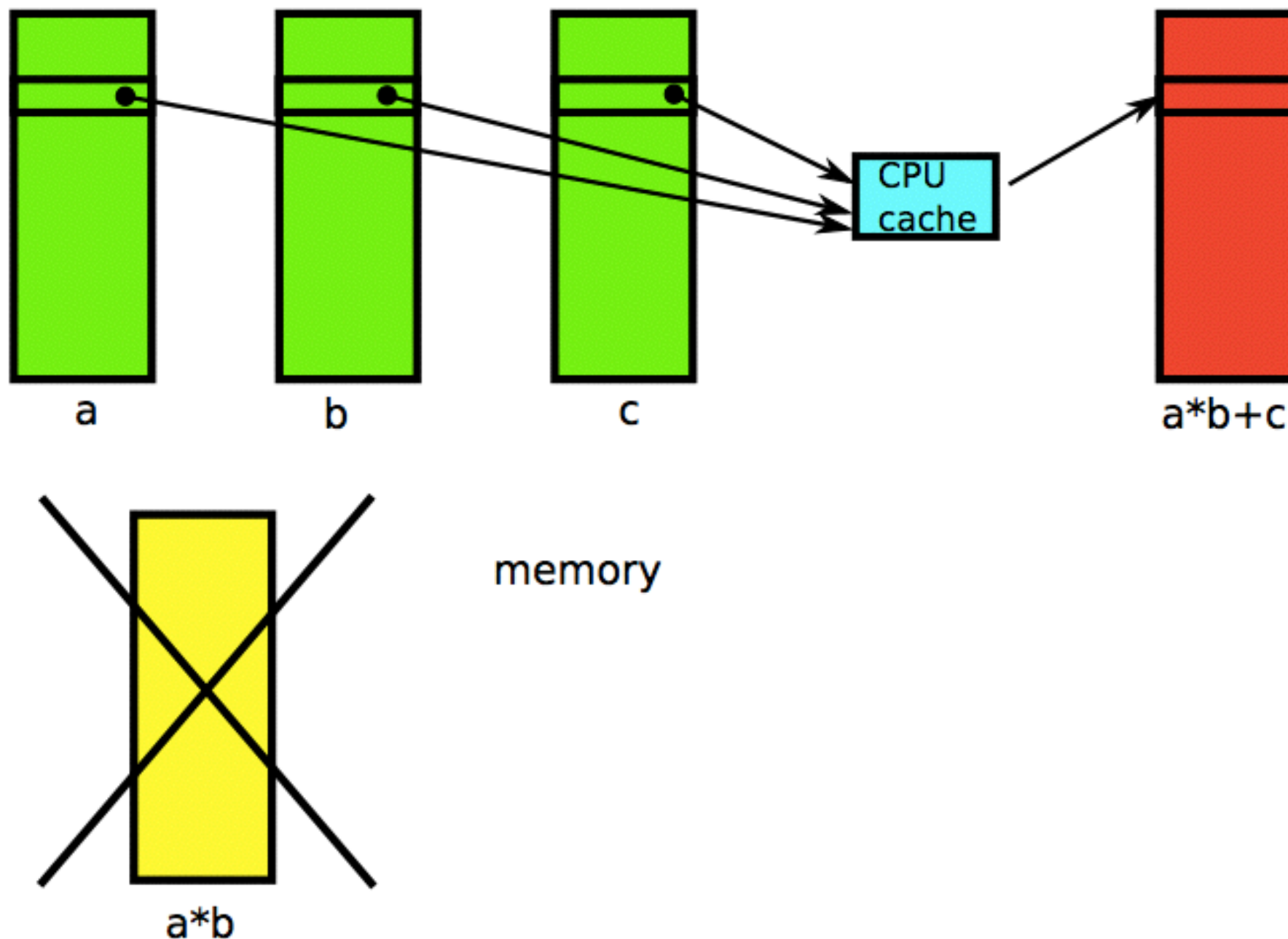
Computing with NumPy

Temporaries go to memory



Computing with numexpr

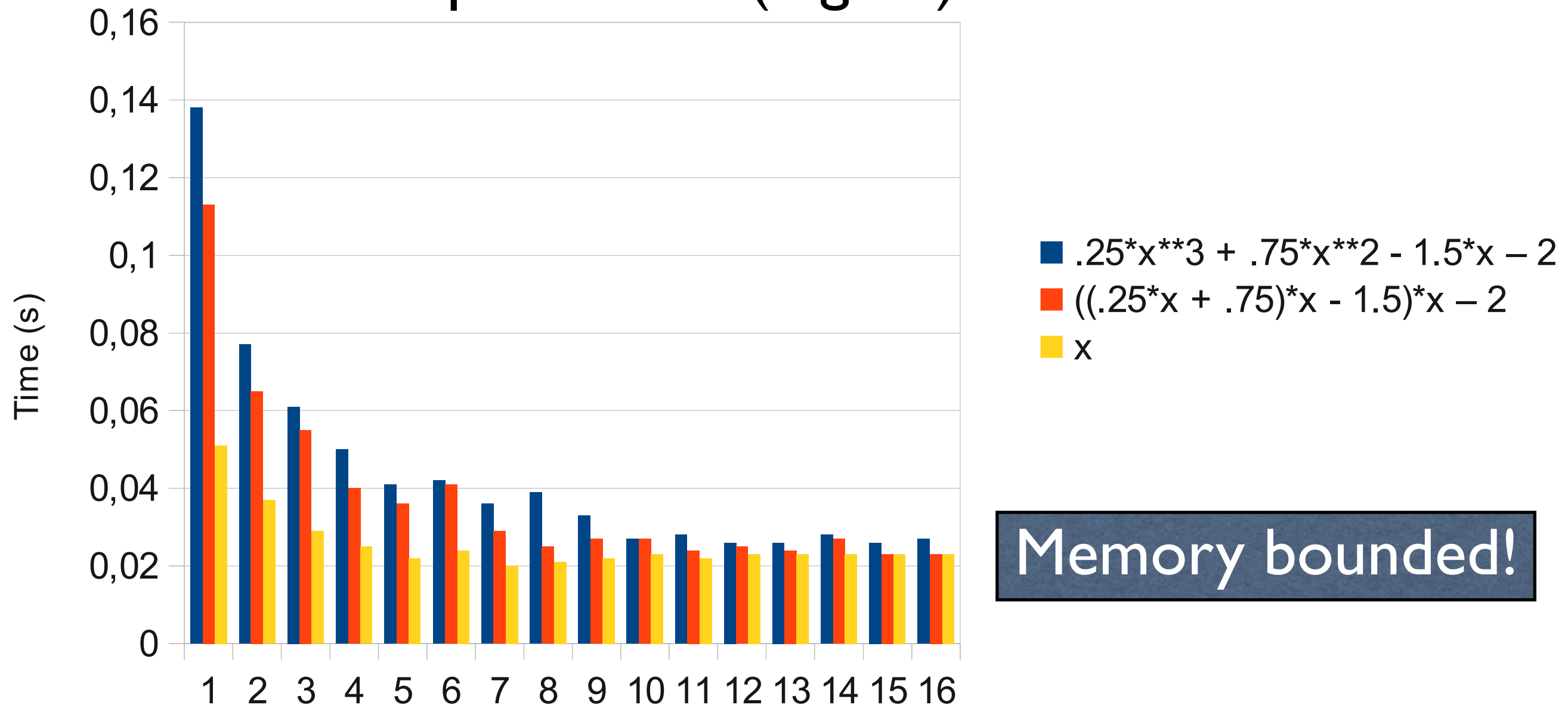
Temporaries stay in cache



Multithreaded numexpr and Beyond: Numba

numexpr Allows Multithreading for Free

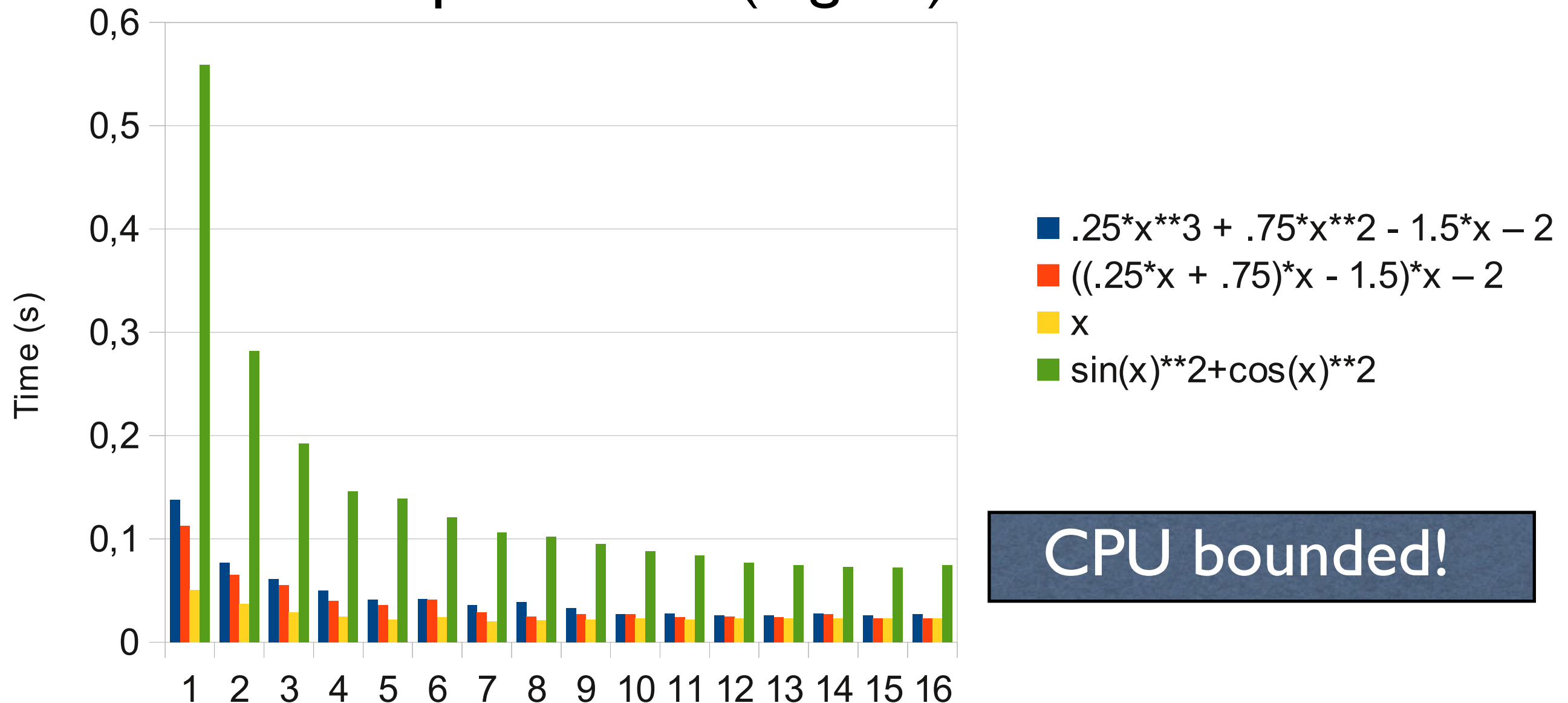
numexpr with 16 (logical) cores



Memory bounded!

Transcendental Functions

numexpr with 16 (logical) cores



CPU bounded!

Numexpr Limitations

- Numexpr only implements element-wise operations, i.e. '**a*b**' is evaluated as:

```
for i in range(N):
```

```
    c[i] = a[i] * b[i]
```

- In particular, it cannot deal with things like:

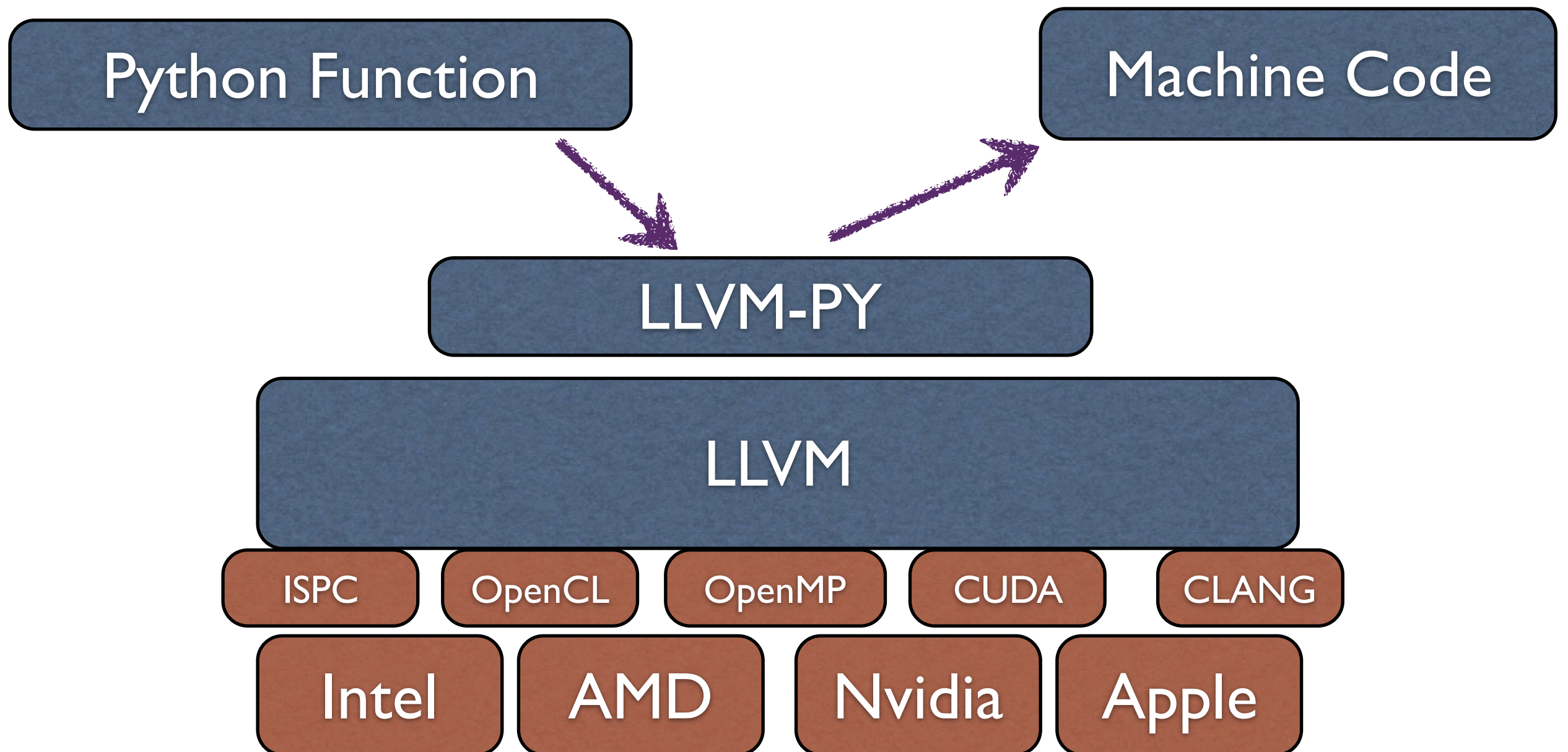
```
for i in range(N):
```

```
    c[i] = a[i-1] + a[i] * b[i]
```

Numba: Overcoming numexpr Limitations

- Numba is a JIT that can translate a subset of the Python language into machine code
- It uses LLVM infrastructure behind the scenes
- Can achieve similar or better performance than numexpr, but with more flexibility

How Numba works



Take-away Messages

- When you have to optimize, have in mind the starving CPU problem.
- Do not always try to parallelize blindly. Give optimization a try first.
- Use proper tools when you need speed. Using one single tool for everything is not going to work well.

What's Next

- Parallel Computing tomorrow (Eilif)
- Efficient Data Containers (in-memory and on-disk)
- Social event this night!