Technische
Universität
Braunschweig

Institut für Betriebssysteme
und Rechnerverbund
Algorithmik

Algorithm Engineering
Lecture 2: CPU Architecture 2

Room for the Tutorial

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Hopefully:

- no more standing in the lecture/tutorial,
- no more sitting on the window sills,
- no more PK 3.3; we have the SN 23.2 (70 official seats) instead.

Optimization Hierarchy

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Correctness comes first! Then:

- choose the right algorithm, then
- choose the right data structures and memory layout, then
- measure performance, help branch prediction, etc.

Today

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Topics today:

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- Finishing caching/memory

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- Compiler optimizations & single instruction, multiple data (SIMD)

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- Finishing caching/memory
- Compiler optimizations & single instruction, multiple data (SIMD)
- Parallelization

Caching: SoA vs AoS

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- Iterating an array of structures skips past unused fields

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Caching: SoA vs AoS

Striding:

- Iterating an array of structures skips past unused fields
- Unless we use most of the parts of the structure
- Fundamental issue in many situations:
  - Array of structures (AoS) is much cleaner from a software engineering perspective
  - Structure of arrays (SoA) can be more performant for several reasons

```cpp
struct Particle {
    float pos[2];
    float speed[2];
    float color[4];
    float shinyness;
    float rotation;
    float age;
    float springiness;
    float density;
    float area;
    float thickness;
    // ...
};
std::vector<Particle> particles;
```

```cpp
struct Particles {
    std::vector<std::array<float,2>> positions;
    std::vector<std::array<float,2>> speeds;
    std::vector<std::array<float,4>> colors;
    std::vector<float> shinyness;
    std::vector<float> rotation;
    std::vector<float> age;
    std::vector<float> springiness;
    std::vector<float> density;
    std::vector<float> area;
    std::vector<float> thickness;
    // ...
};
Particles particles;
```

SoA vs. AoS: Experiment

```cpp
struct Data {
    float touched[2];
    char untouched[N];
};
std::vector<Data> aos;
struct SoA {
    std::vector<std::array<float,2>> touched;
    std::vector<std::array<char,N>> untouched;
};
SoA soa;
```

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Each element:

```cpp
s += (std::abs)(touched[0] - touched[1]);
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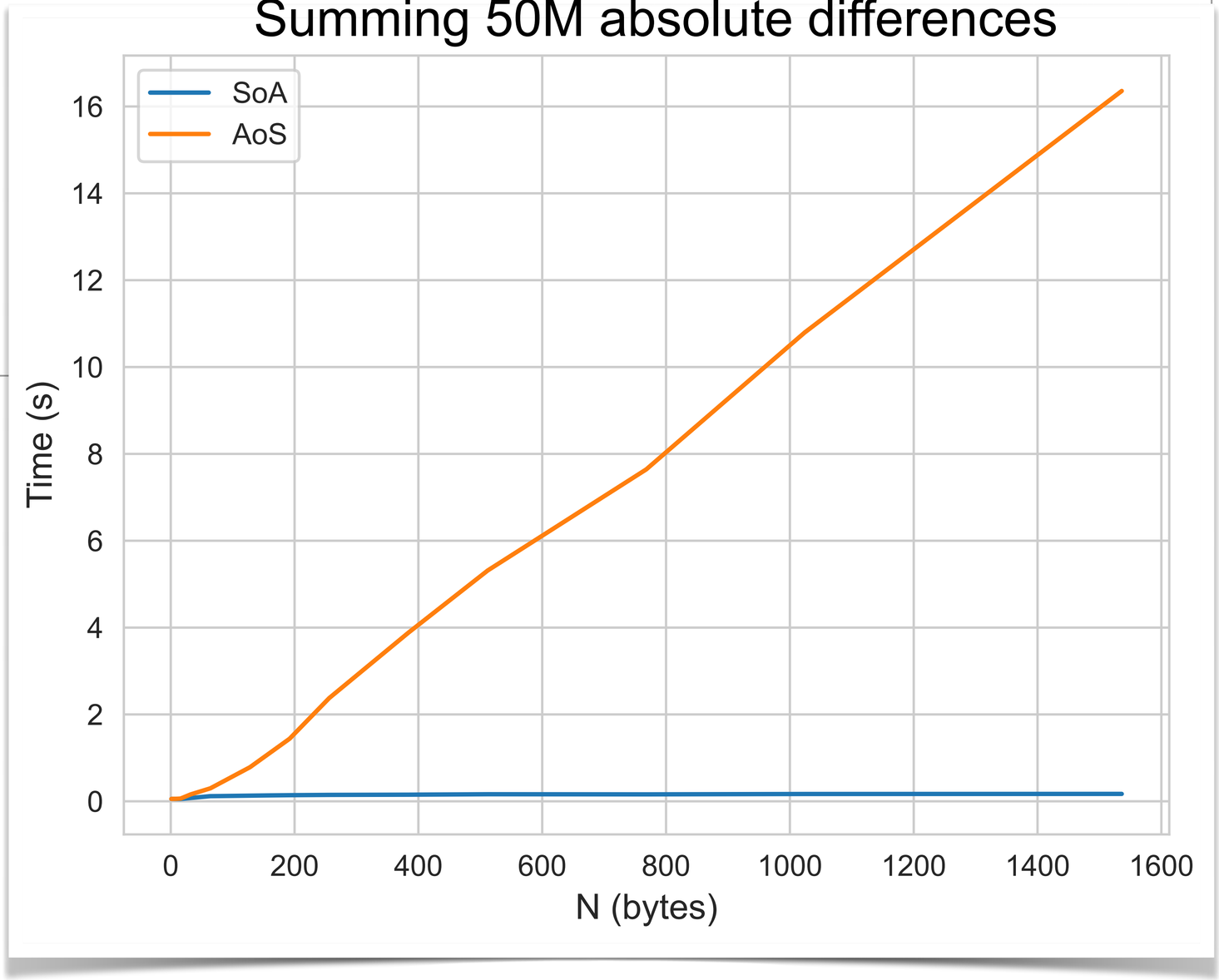

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```
1 // Allocates a new vector EVERY iteration — heap allocation + deallocation each time
2 for (int iter = 0; iter < 1000000; iter++) {
3     std::vector<int> neighbors;            // malloc → heap allocation
4     find_neighbors(node, neighbors);       // fills it
5     best = evaluate(neighbors);            // uses it
6 }   // free → heap deallocation, then repeat
```

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}   // free → heap deallocation, then repeat
```

```cpp
// Allocate once, reuse — no allocation in the hot loop
std::vector<int> neighbors;
for (int iter = 0; iter < 1000000; iter++) {
    neighbors.clear();                     // size → 0, but buffer stays
    find_neighbors(node, neighbors);       // reuses existing capacity
    best = evaluate(neighbors);
}
```

Cost of Memory Allocations

Another

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```
1 // Alloc
2 for (int
3     std:
4     finc
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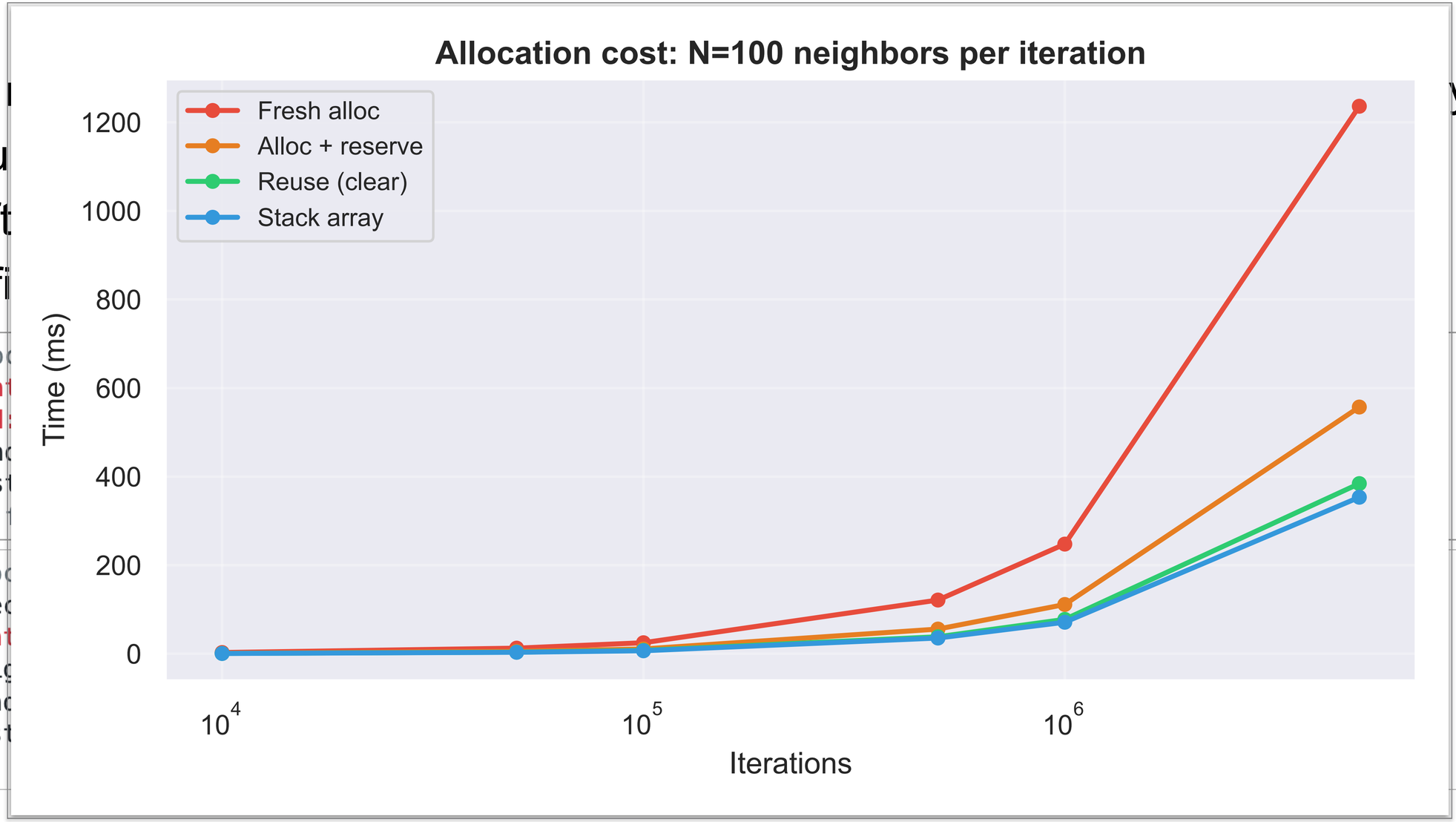

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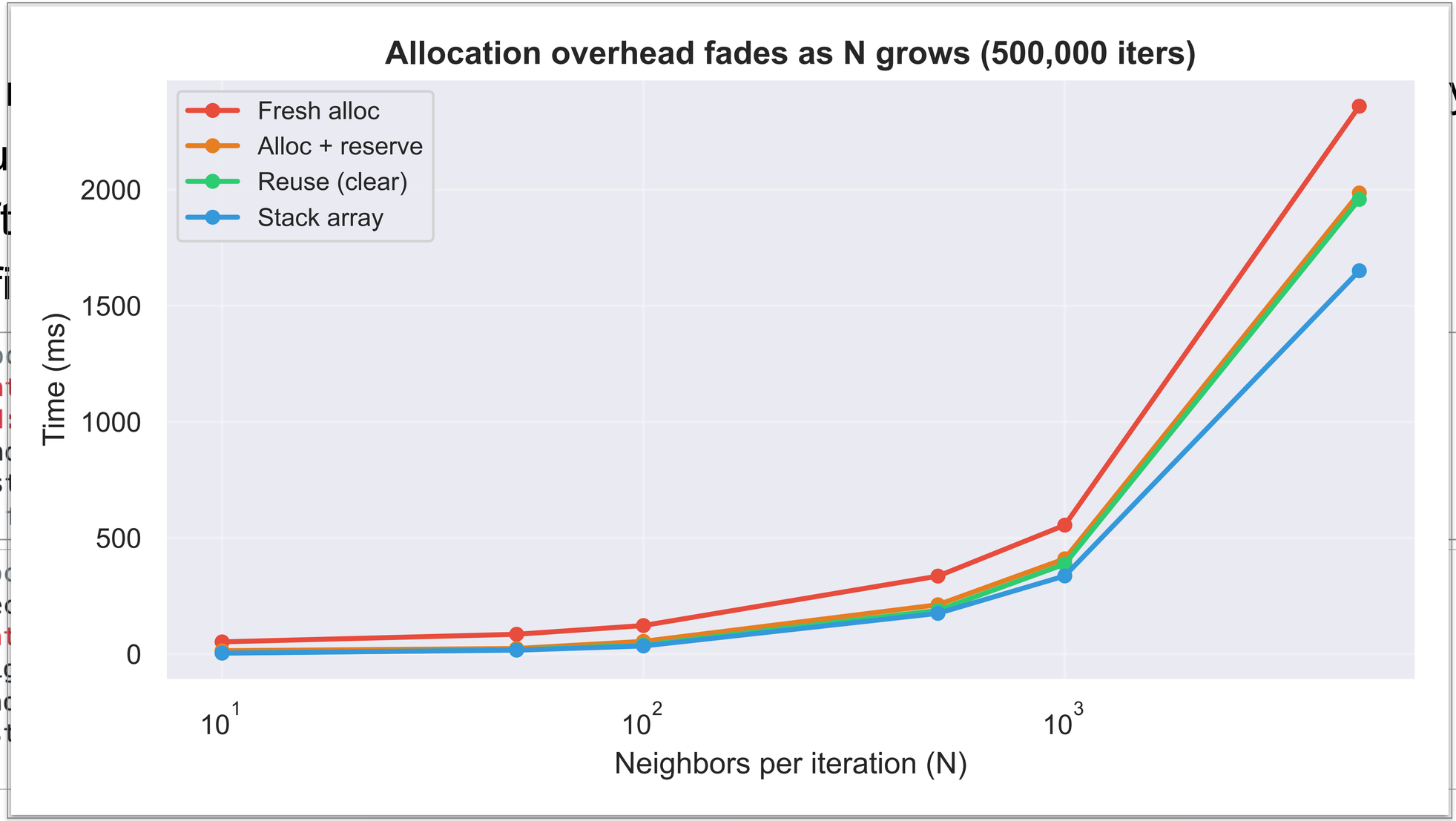

Memory Allocation: More Examples

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Individual allocations (expensive):

```
1  // Branch-and-bound: new node per branch
2  for (auto& child : branches) {
3      auto* node = new BBNode(child);
4      queue.push(node);
5  }
6  // ... later: delete every node
7
8  // String building per iteration
9  for (int i = 0; i < N; i++) {
10     std::string key = build_key(i);
11     map[key] = compute(i);
12 }
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2  std::vector<BBNode> pool(max_nodes);
3  int next = 0;
4  for (auto& child : branches) {
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6      queue.push(&pool[next++]);
7  }
8
9  // Reserve + reuse string buffer
10 std::string key;
11 key.reserve(64);
12 for (int i = 0; i < N; i++) {
13     build_key_into(i, key);  // writes into key
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Hidden allocations: accidental copying/construction of containers, temporaries, …
Misunderstanding of C++: Objects are passed around by value by default
Profile/measure to find such situations!

Why is the stack version cheaper?

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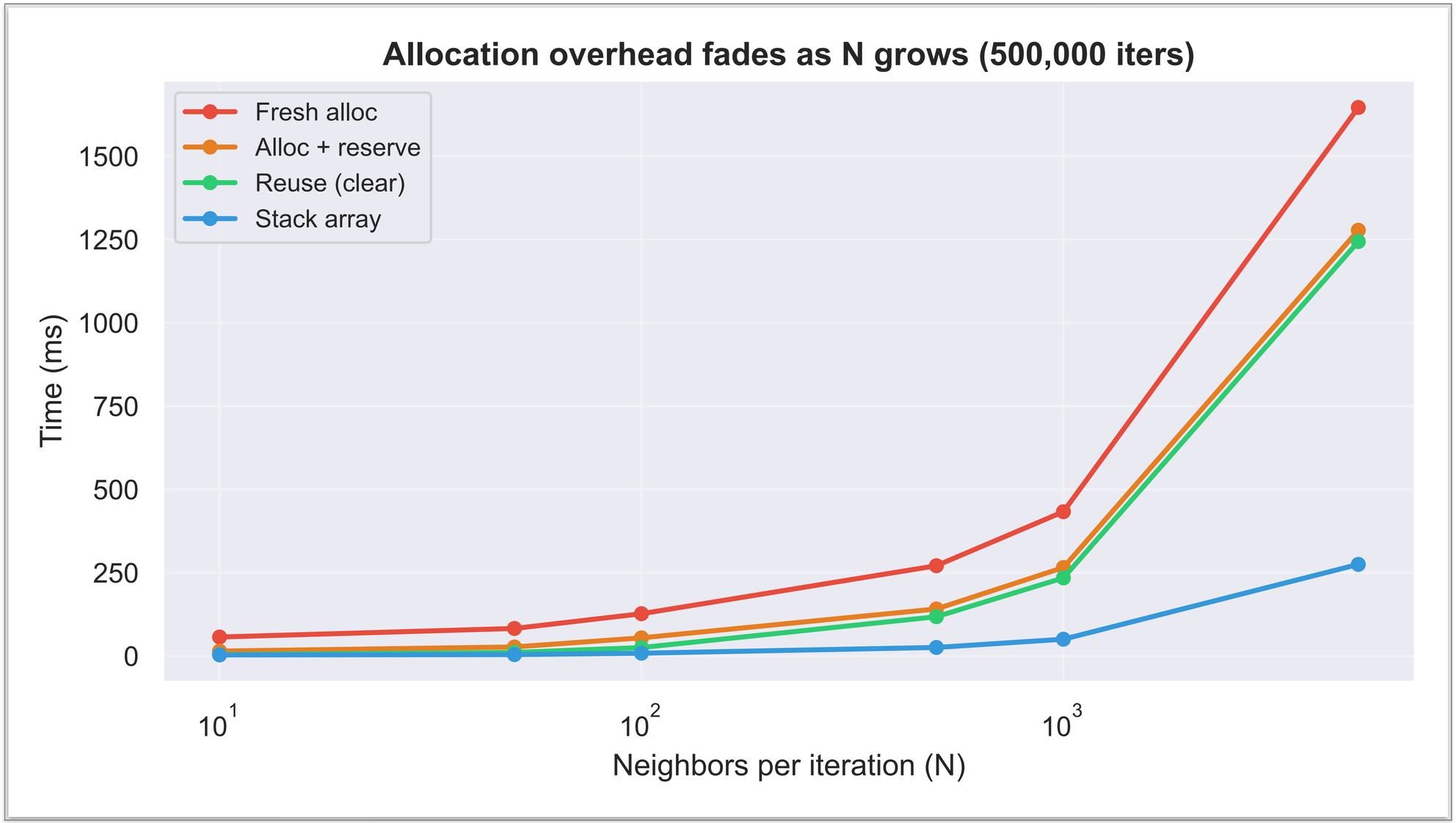

SIMD: Doing more with one instruction

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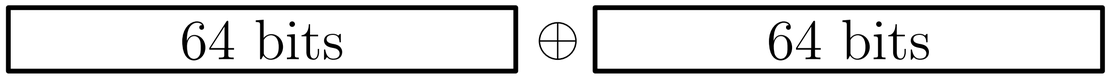
Normal instructions:



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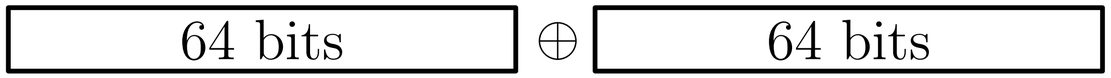
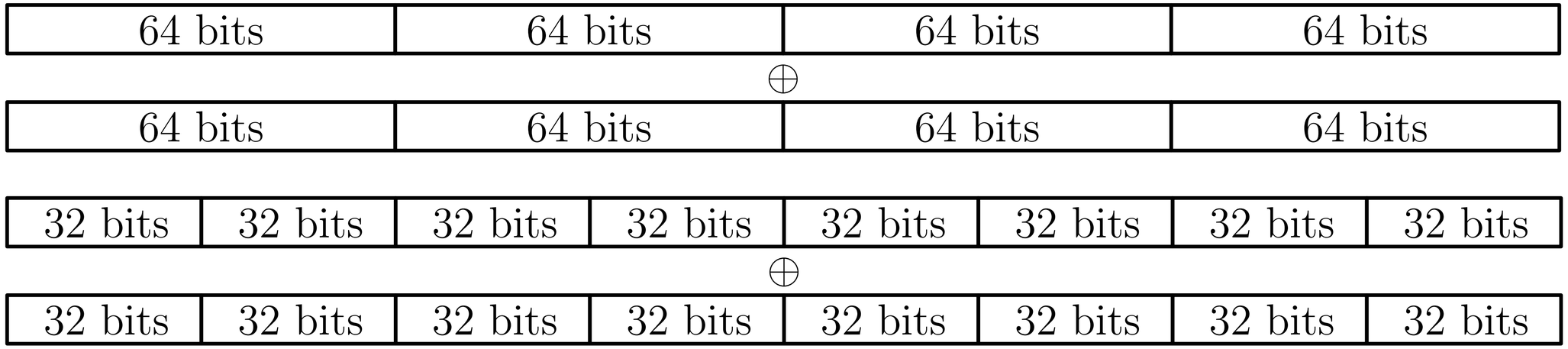


SIMD (single instruction, multiple data) instructions:



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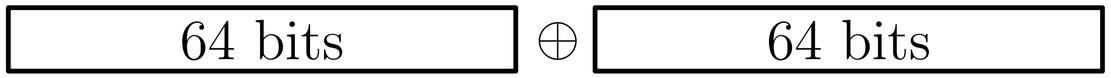

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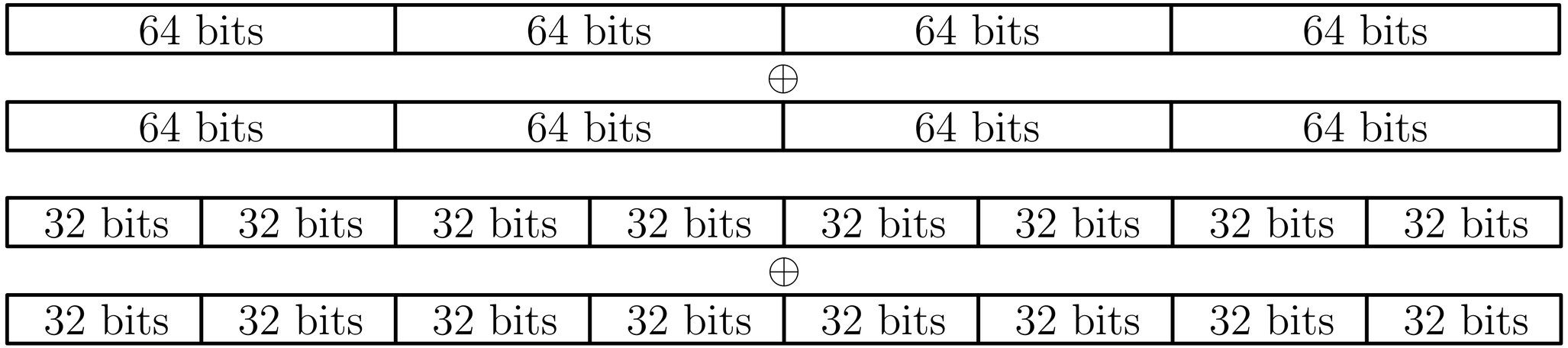

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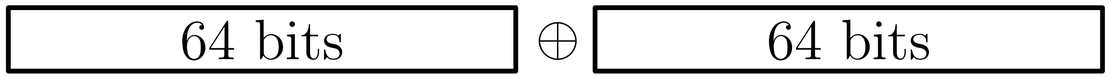

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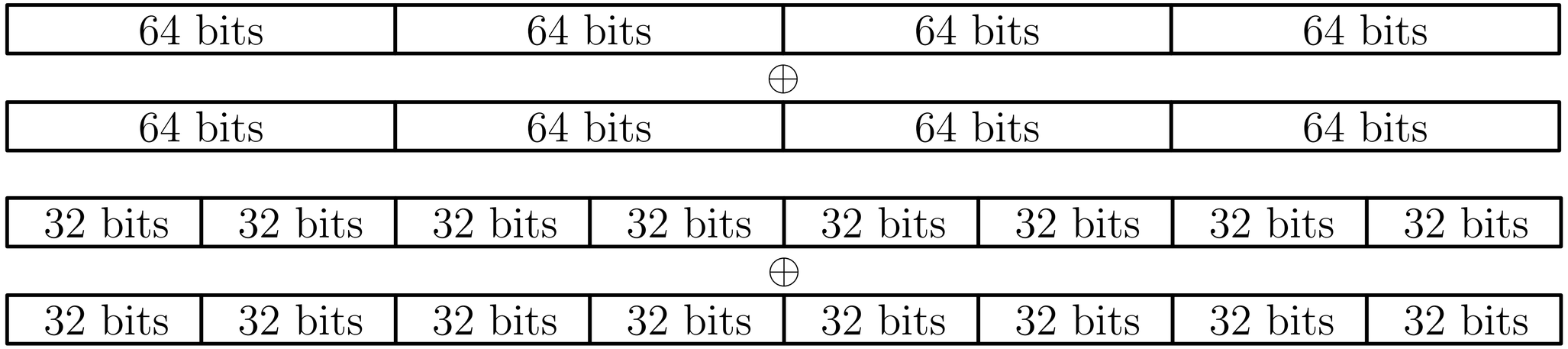

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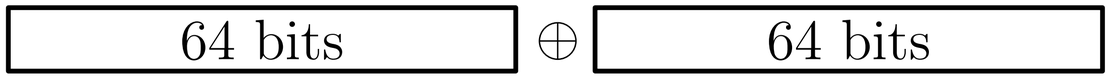

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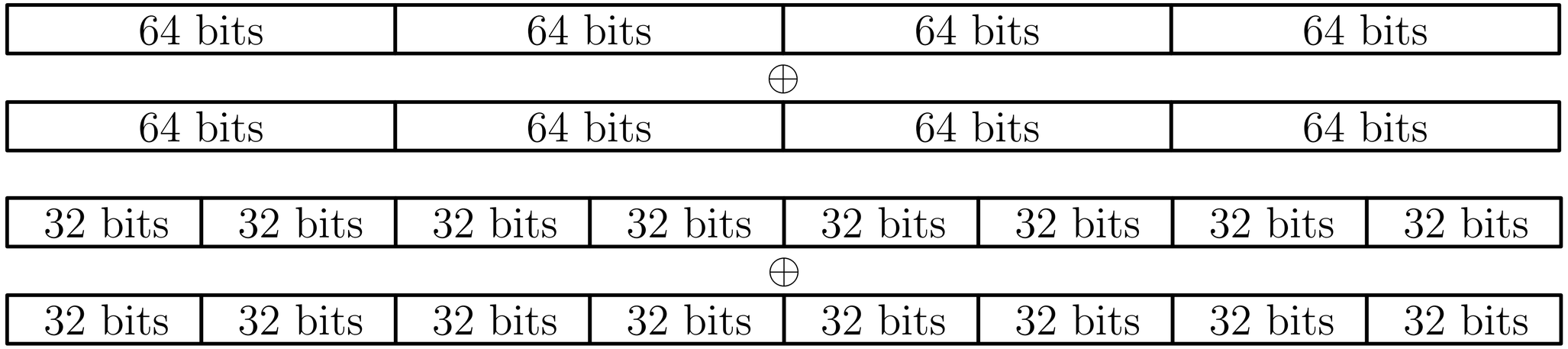

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Comparisons, masking, permuting entries and other horizontal operations, extraction, …

Both integer and floating point, various operand and suboperand sizes (128, 256, 512 bits).

SIMD: Simplest Example

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#include <vector>
#include <numeric>

std::int32_t sum(const std::vector<std::int32_t>& input) {
    return std::reduce(input.begin(), input.end());
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unvectorized (`-O1`)

```
[...]
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vectorized (`-O2 -mavx`)

```asm
[...]
.LBB0_8:
        vpaddd  xmm0, xmm0, xmmword ptr [rdx + 4*rax]
        vpaddd  xmm1, xmm1, xmmword ptr [rdx + 4*rax + 16]
        vpaddd  xmm2, xmm2, xmmword ptr [rdx + 4*rax + 32]
        vpaddd  xmm3, xmm3, xmmword ptr [rdx + 4*rax + 48]
        add     rax, 16
        cmp     r9, rax
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[...]
```

vectorized (`-O2 -mavx2`)

```asm
[...]
.LBB0_8:
        vpaddd  ymm0, ymm0, ymmword ptr [rdx + 4*rax]
        vpaddd  ymm1, ymm1, ymmword ptr [rdx + 4*rax + 32]
        vpaddd  ymm2, ymm2, ymmword ptr [rdx + 4*rax + 64]
        vpaddd  ymm3, ymm3, ymmword ptr [rdx + 4*rax + 96]
        add     rax, 32
        cmp     r9, rax
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[...]
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vectorized (`-O2 -mavx512f`)

```asm
[...]
.LBB0_8:
        vpaddd  zmm0, zmm0, zmmword ptr [rdx + 4*rax]
        vpaddd  zmm1, zmm1, zmmword ptr [rdx + 4*rax + 64]
        vpaddd  zmm2, zmm2, zmmword ptr [rdx + 4*rax + 128]
        vpaddd  zmm3, zmm3, zmmword ptr [rdx + 4*rax + 192]
        add     rax, 64
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- Only then think about potentially doing it yourself

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Simple to medium-complexity cases:

- Usually handled well by the compiler (`-O2` and upwards, depending on extra flags)

Manual intervention:

- Often complex
- Platform- and compiler-dependent
- Needs special compiler/library support (e.g., `<immintrin.h>`)
- Rarely worth it
- Measure first!
- Verify the compiler is not doing it (properly) & try to get the compiler to do it second!
- Only then think about potentially doing it yourself

Auto-vectorization: Why might the compiler not be doing it?

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- Implicit assumptions for, e.g., M1 offer more (newer hardware baseline)

Auto-vectorization: Let’s play a game.

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 2     std::int64_t r = 0;
 3     for(std::size_t i = 0, n = v.size(); i < n; ++i) {
 4         r += v.at(i); // contains a bounds check
 5     }
 6     return r;
 7 }
 8
 9 std::int64_t sum2(const std::vector<std::int64_t>& v) {
10     std::int64_t r = 0;
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MSVC (`/O2 /arch:AVX2`) only vectorizes `sum2` (but eliminates bounds check…)

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2     std::int64_t r = 0;
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4         r += (v[i] - v[i-1]);
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No compiler found the hidden $O(1)$.

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Vectorization: clang (`-O2`): ✅, gcc (`-O3`): ✅, MSVC (`/O2 /Ob3`): ❌

Auto-vectorization: Why might the compiler not be doing it?

```cpp
void sequence2(std::vector<std::int64_t>& v,
               const std::vector<std::int64_t>& w)
{
    if(w.size() != v.size()) {
        return;
    }
    for(std::size_t i = 1, n = v.size(); i < n; ++i) {
        v[i] = v[i-1] * w[i];
    }
}
```

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```

No way to vectorize - dependency chain `v[n-1]` - `v[n-2]` - ... - `v[0]`!

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```
 1 void sequence3(std::vector<std::int64_t>& v,
 2                 const std::vector<std::int64_t>& w)
 3 {
 4     if(w.size() != v.size()) {
 5         return;
 6     }
 7     for(std::size_t i = 0, n = v.size(); i < n - 1; ++i) {
 8         v[i] = v[i+1] * w[i];
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gcc, clang and MSVC: ✅

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```
1 void collatz_update(std::vector<std::int64_t>& v) {
2     for(std::size_t i = 0, n = v.size(); i < n; ++i) {
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clang (`-O2`): ✅, gcc (`-O3`): ✅, MSVC (`/O2 /Ob3`): ❌ (remains branching)

Auto-vectorization: Subtle code issues

```
 1 float floatplus(float y, float z) { return y + z; }
 2
 3 float sum1(const std::vector<float>& x) {
 4     return std::accumulate(x.begin(), x.end());
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 7 float sum2(const std::vector<float>& x) {
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12 float sum3(const std::vector<float>& x) {
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Float addition is commutative, but not strictly speaking associative!

Auto-vectorization: Alternative Version

```cpp
float sum4(const std::vector<float>& x) {
    const std::size_t n = x.size(), i = 0;
    if(n < 32) return std::accumulate(x.begin(), x.end());
    alignas(64) std::array<float, 16> subsums, next;
    std::fill_n(&subsums[0], 16, 0.0f);
    for(; i + 15 < n; i += 16) {
        for(int j = 0; j < 16; ++j) {
            next[j] = x[i + j];
        }
        for(int j = 0; j < 16; ++j) {
            subsums[j] += next[j];
        }
    }
    // handle <= 15 remaining values
    for(std::size_t j = 0; i + j < n; ++j)
        subsums[j] += x[i + j];
    }
    // sum intermediate values
    for(int k = 8; k > 0; k /= 2) {
        for(int j = 0; j < k; ++j) {
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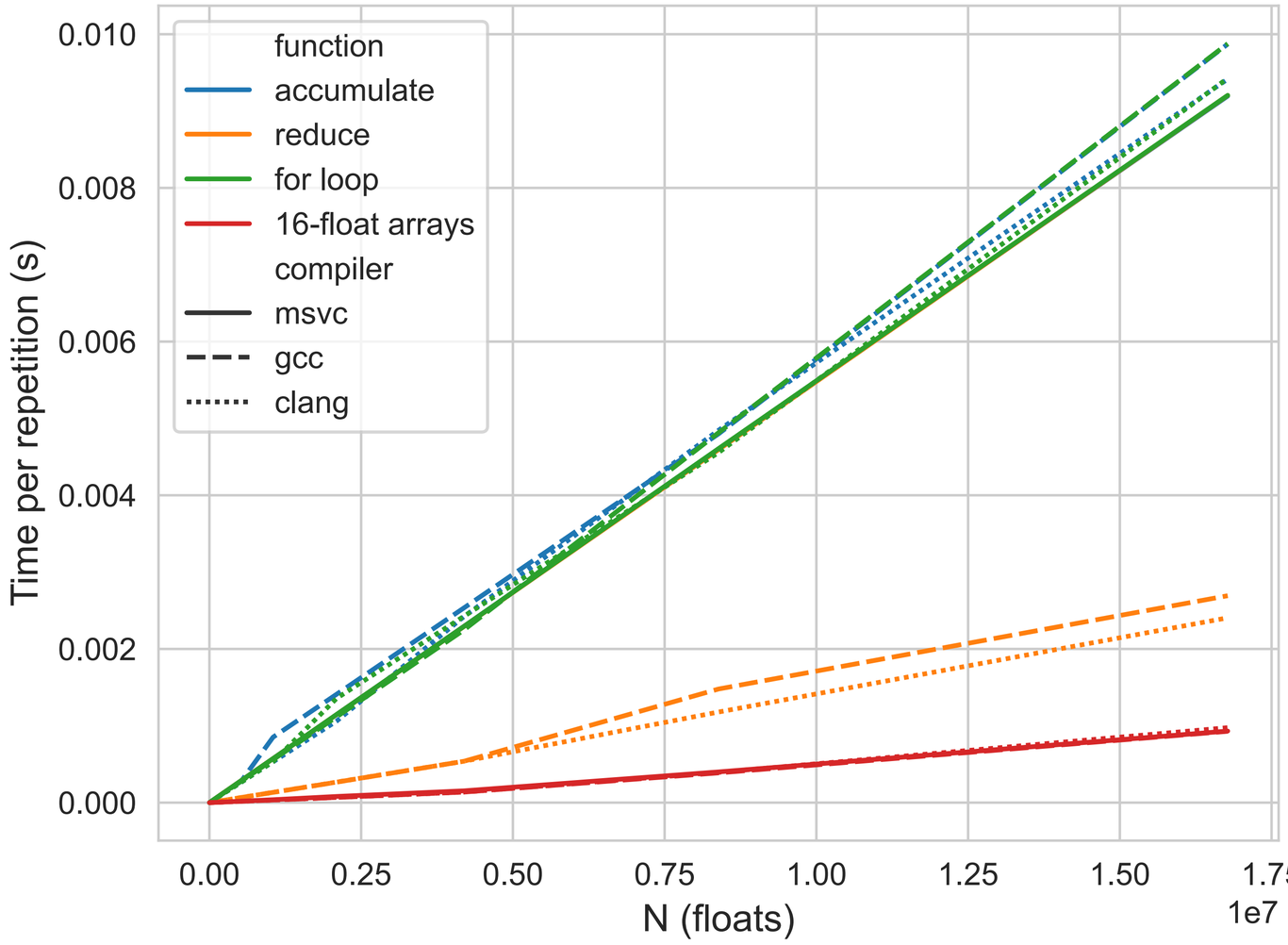

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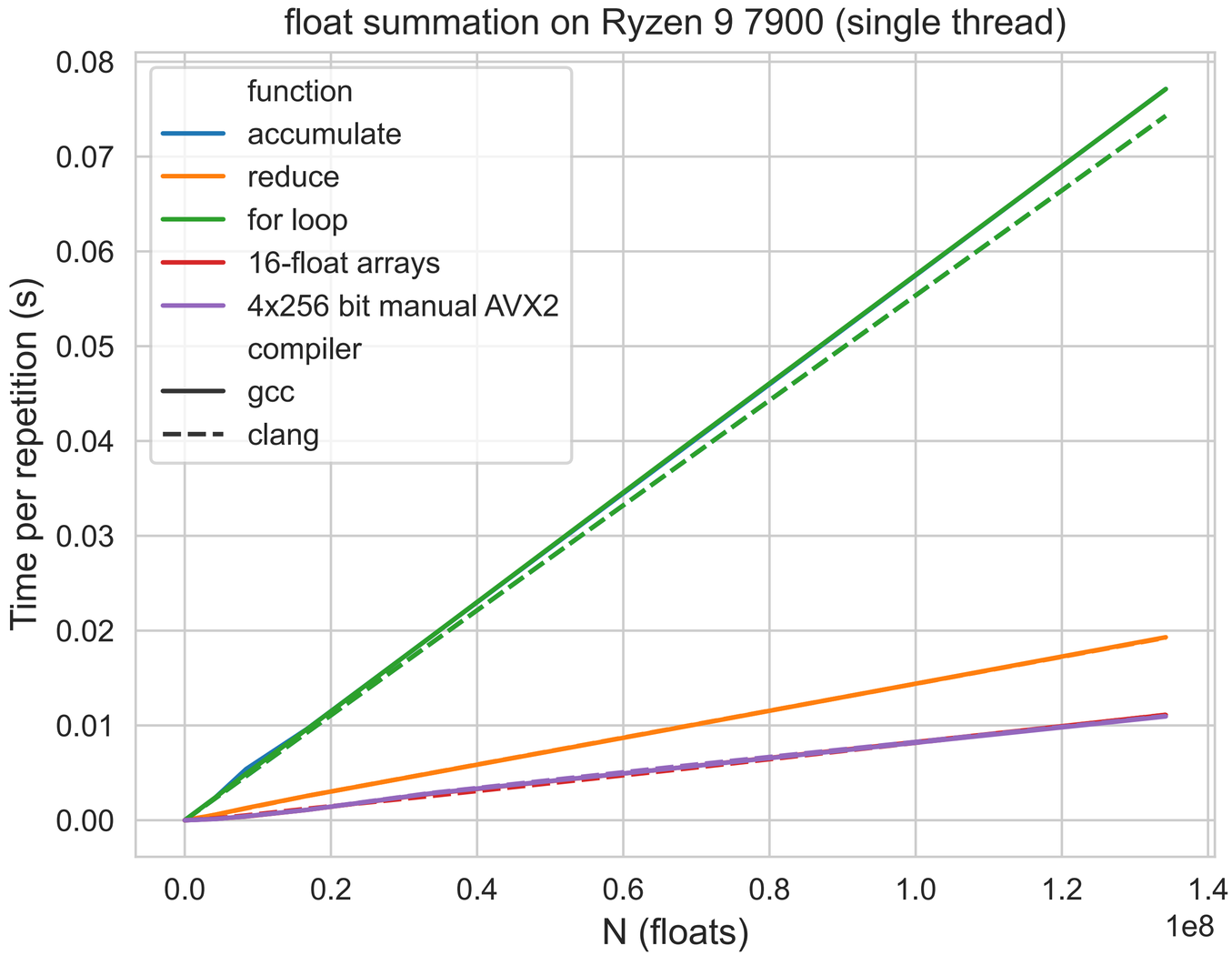

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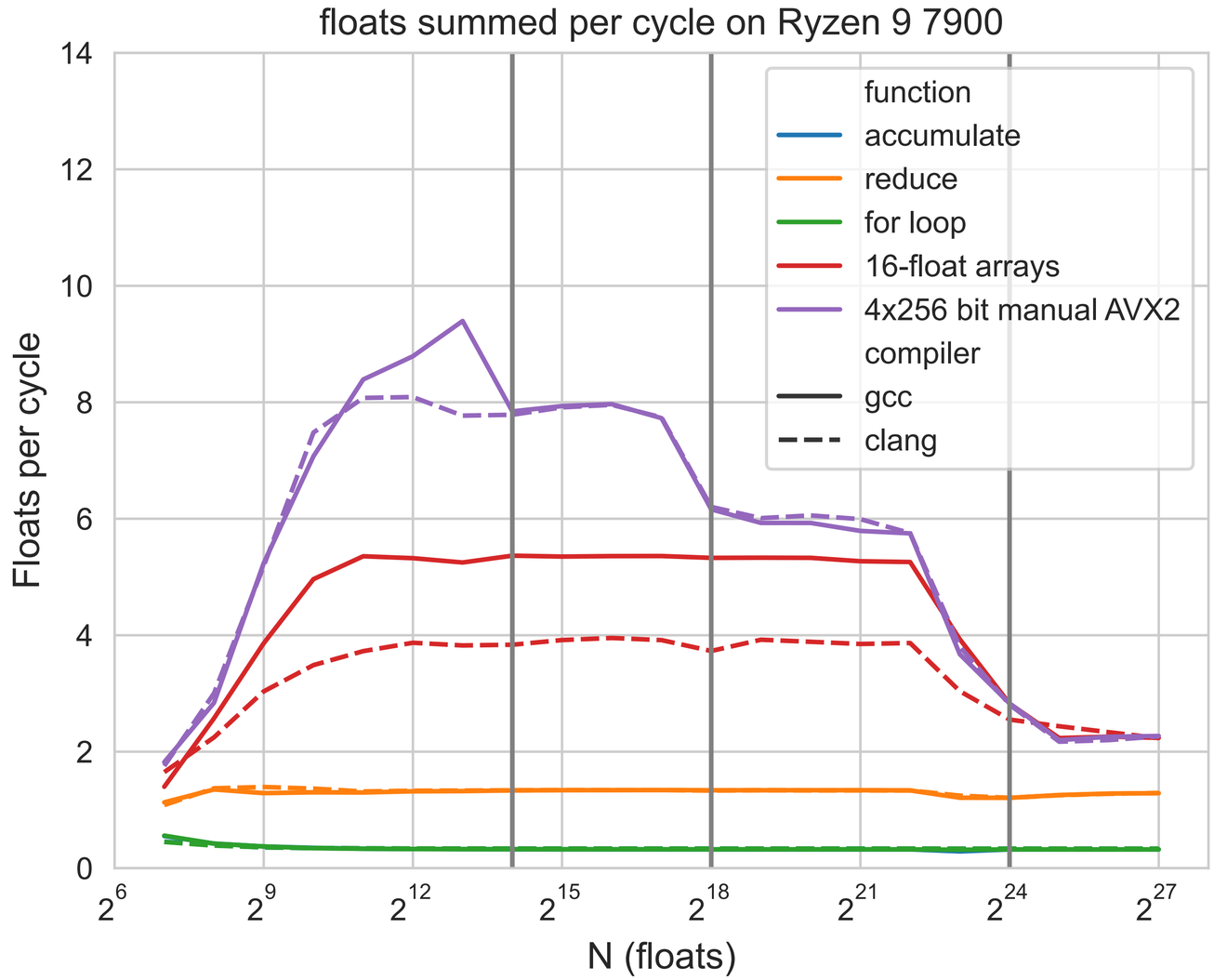
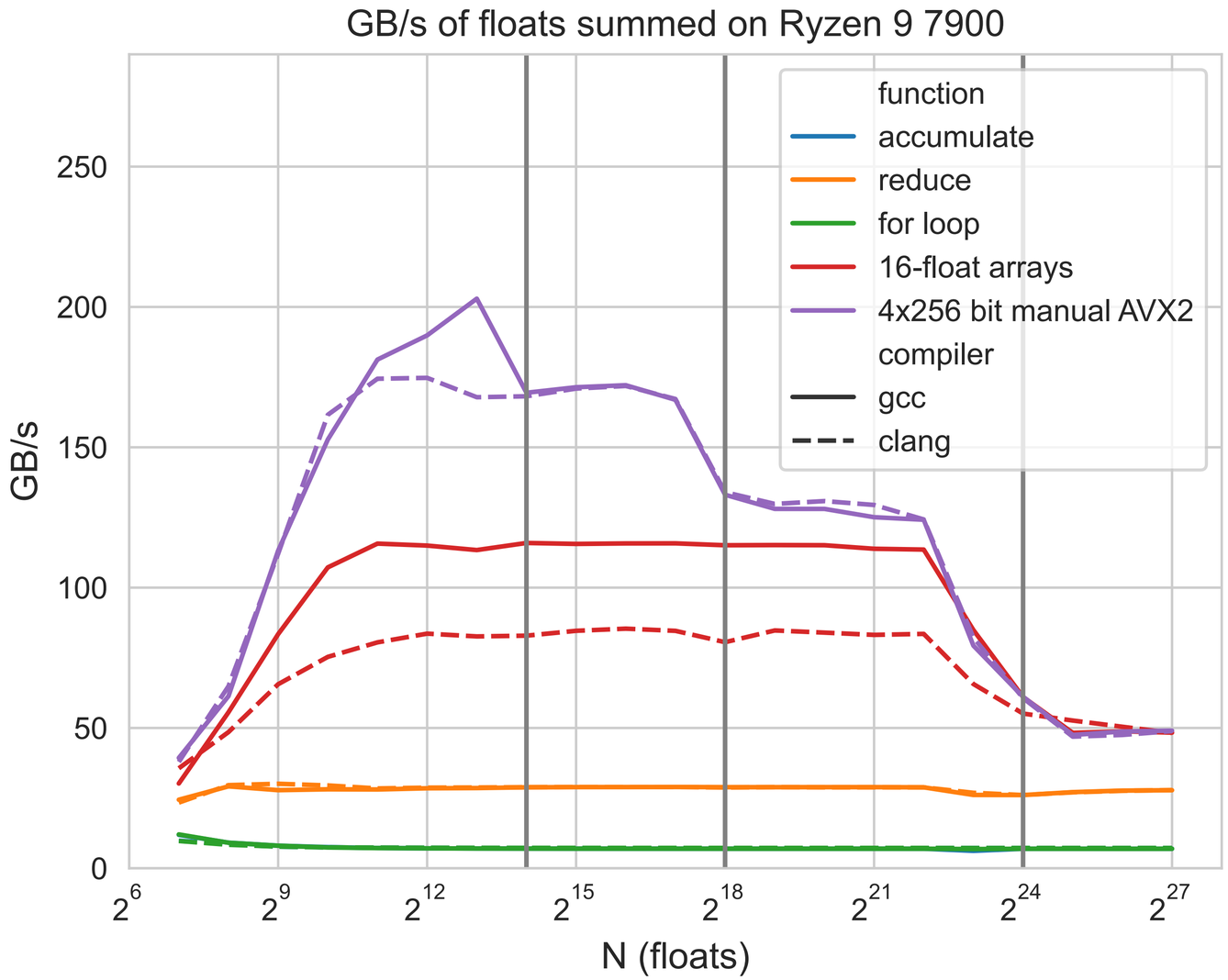


Auto-vectorization: Alternative Version

```cpp
float sum4(const std::vector<float>& x) {
    const std::size_t n = x.size(), i = 0;
    if(n < 32) return std::accumulate(x.begin(), x.end());
    alignas(64) std::array<float, 16> subsums, next;
    std::fill_n(&subsums[0], 16, 0.0f);
    for(; i + 15 < n; i += 16) {
        for(int j = 0; j < 16; ++j) {
            next[j] = x[i + j];
        }
        for(int j = 0; j < 16; ++j) {
            subsums[j] += next[j];
        }
    }
    // handle <= 15 remaining values
    for(std::size_t j = 0; i + j < n; ++j)
        subsums[j] += x[i + j];
    }
    // sum intermediate values
    for(int k = 8; k > 0; k /= 2) {
        for(int j = 0; j < k; ++j) {
            subsums[j] += subsums[j + k];
        }
    }
    return subsums[0];
}
```



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```
 1 struct DataUnsorted {
 2     char a;
 3     char __pad1[7];
 4     long long b;
 5     bool c;
 6     char __pad2[7];
 7     double d;
 8     int e;
 9     char __pad3[4];
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11 // sizeof(DataUnsorted) == 40
```

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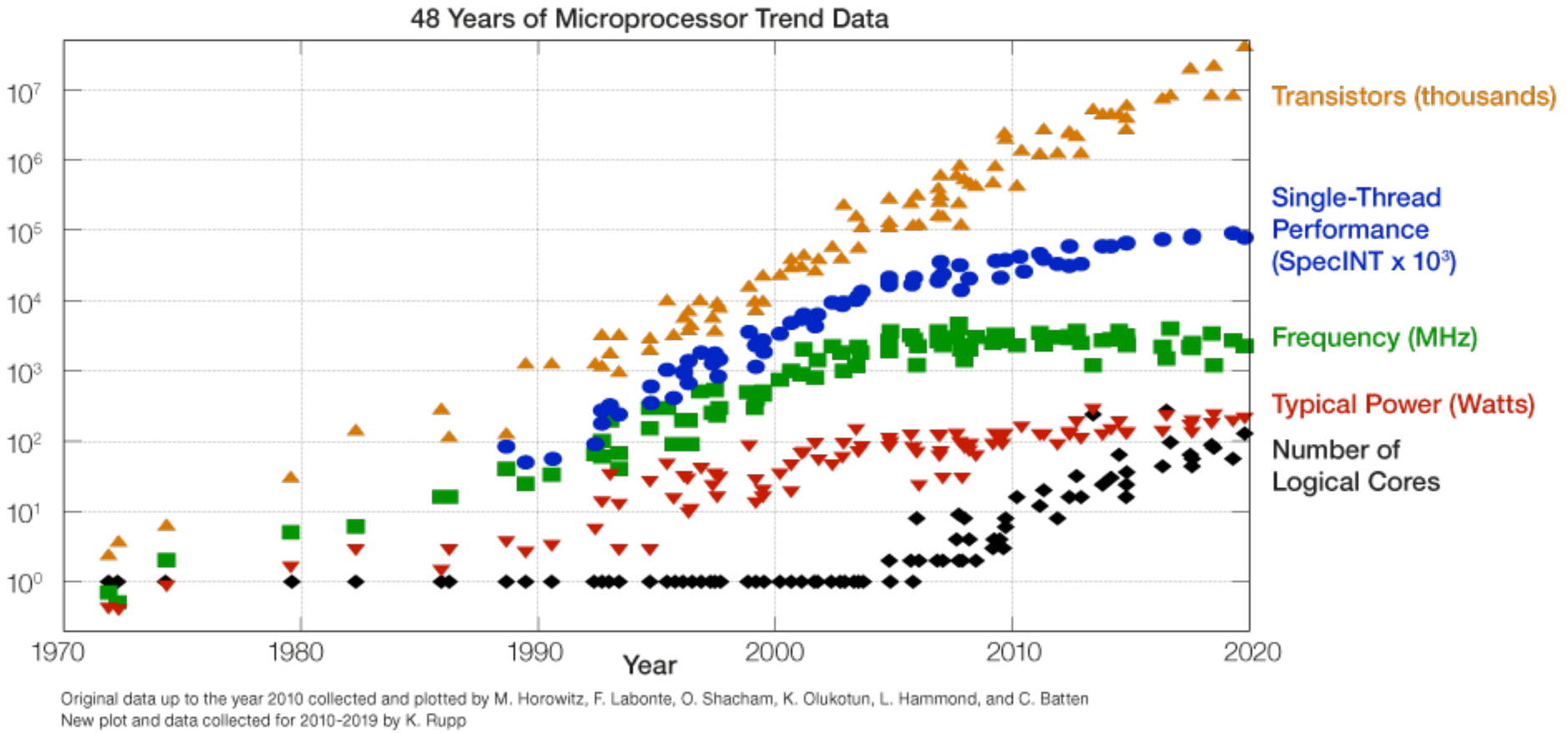
Parallelization



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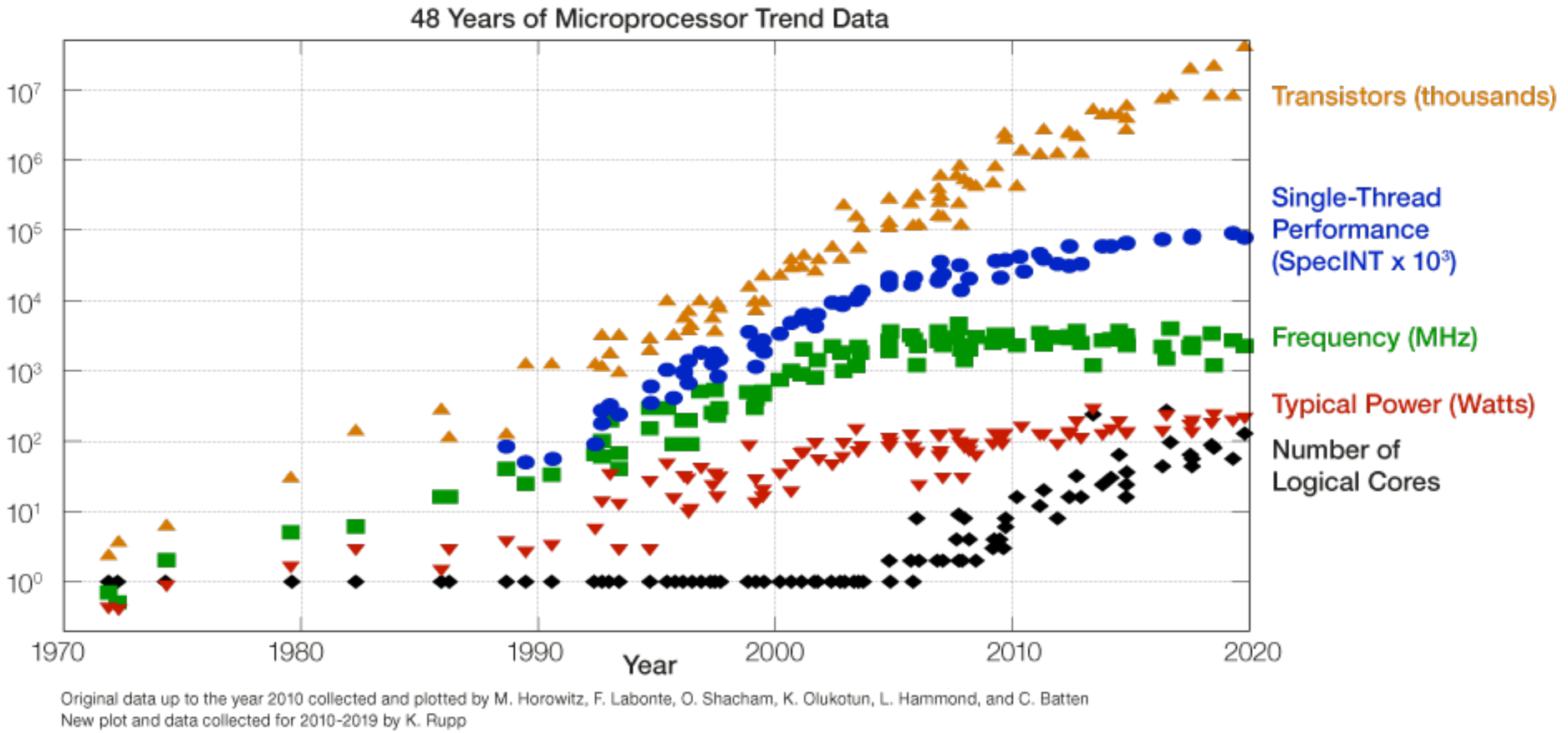

So far, everything we did used a single thread (instruction-level parallelism).
Fully utilizing a modern CPU requires parallelization!

Amdahl's Law

Usually, only a part of your program is parallelizable.

Let p be that fraction, and N be the number of processors.

Then, the best runtime reduction by parallelization you can hope for is

$$\frac{1}{(1-p)+\frac{p}{N}}.$$

Theoretical Limits: Amdahl's Law

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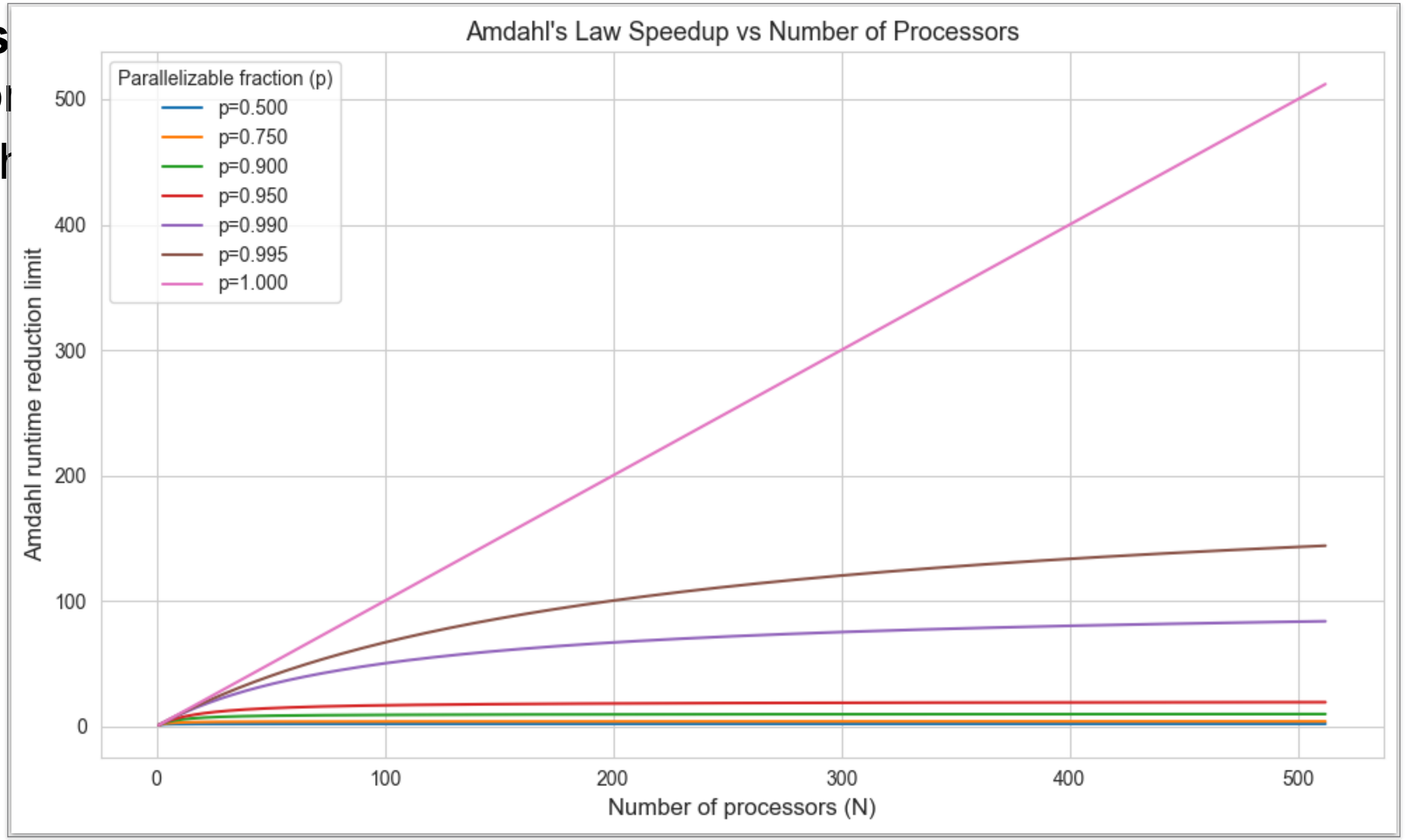

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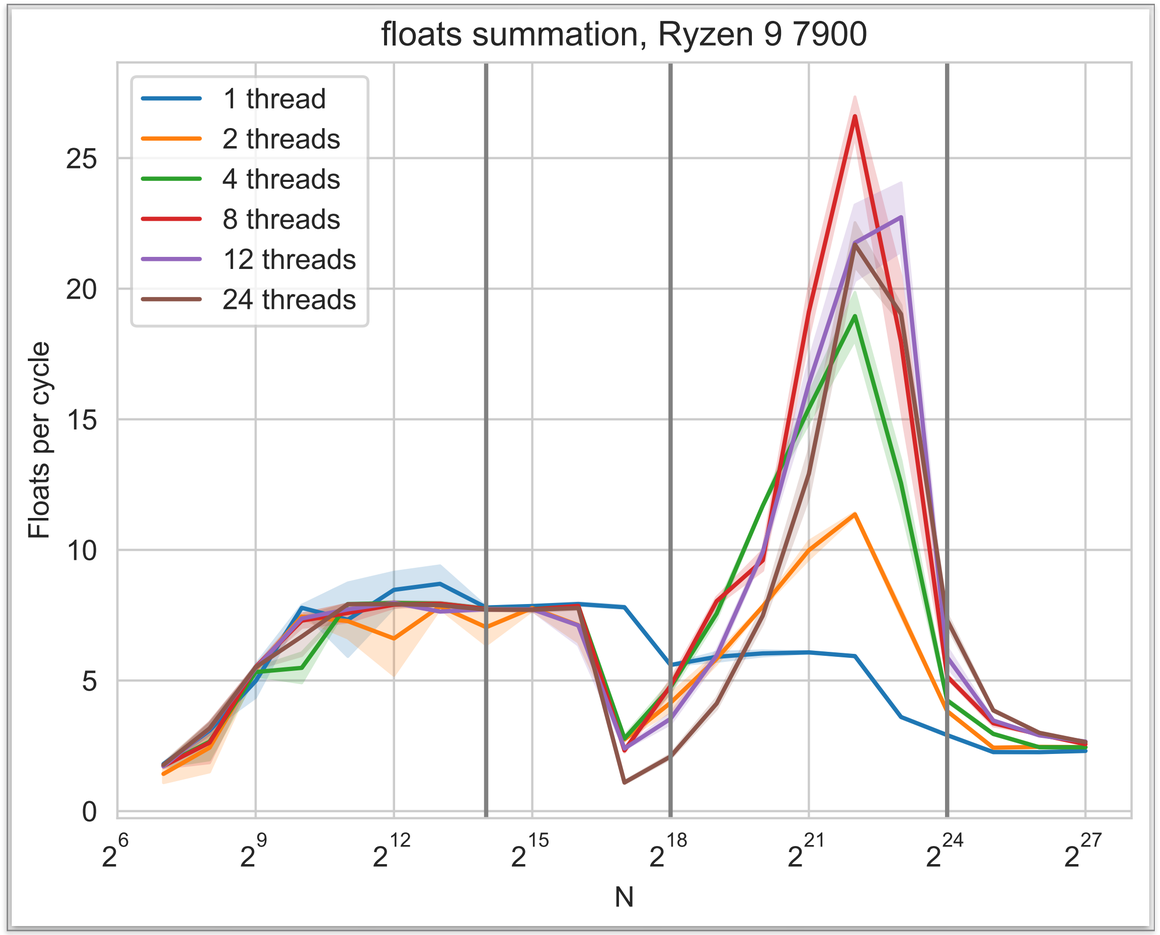

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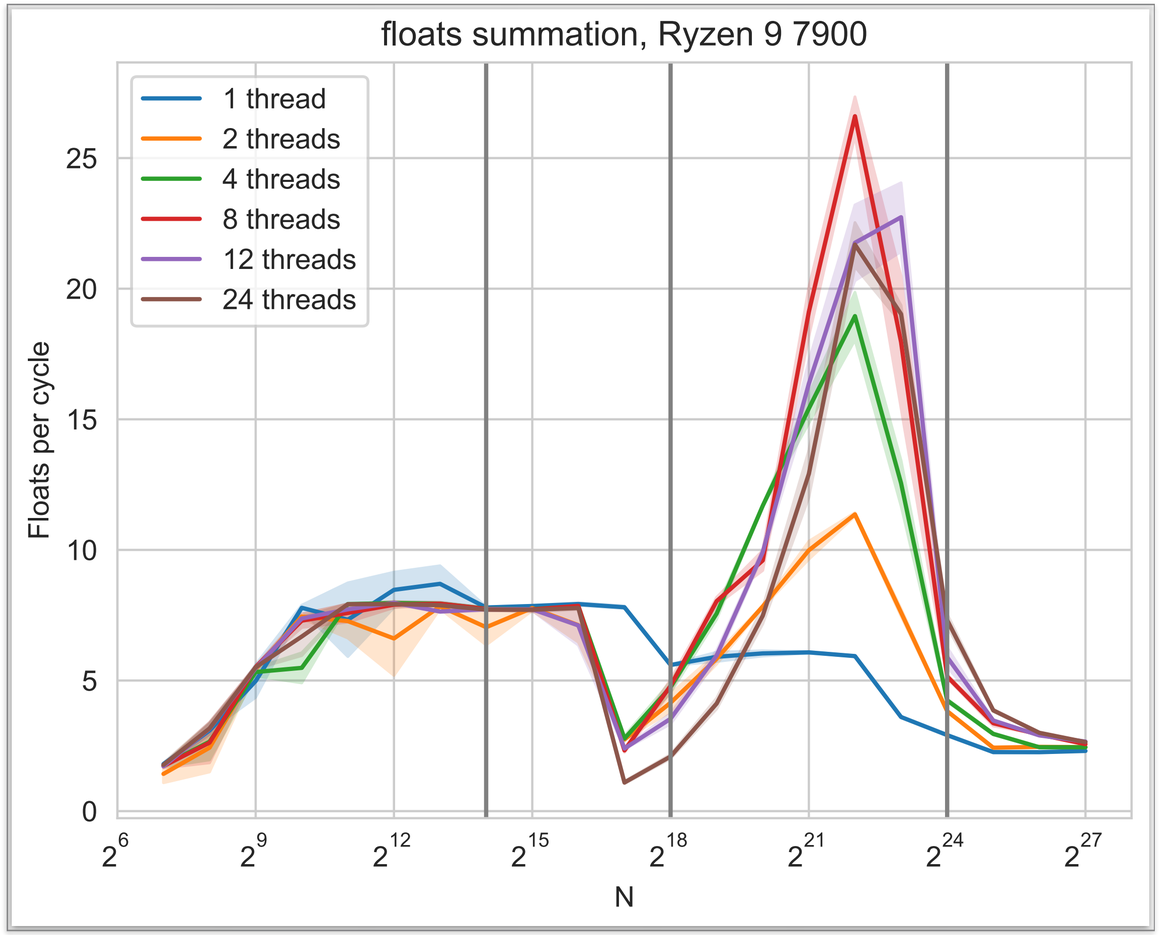

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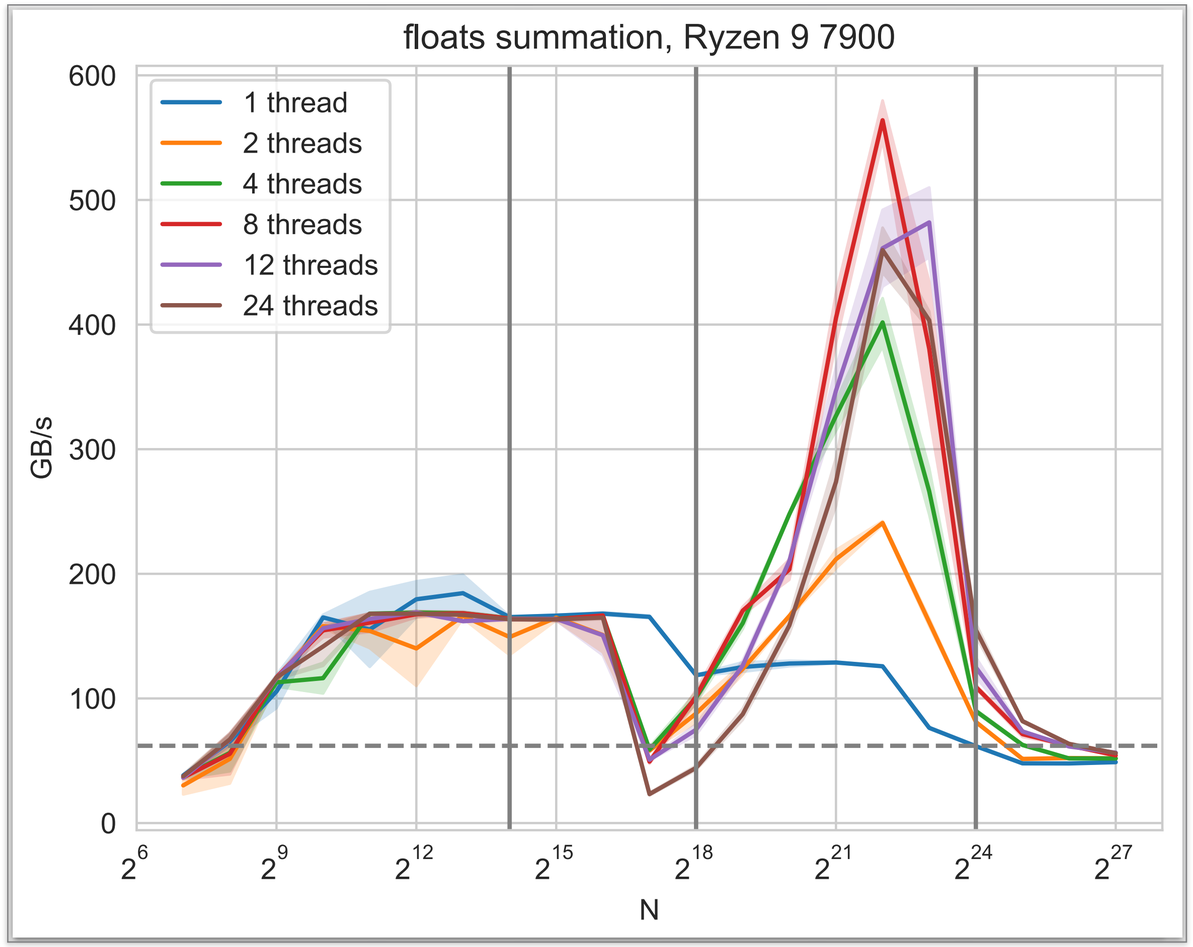

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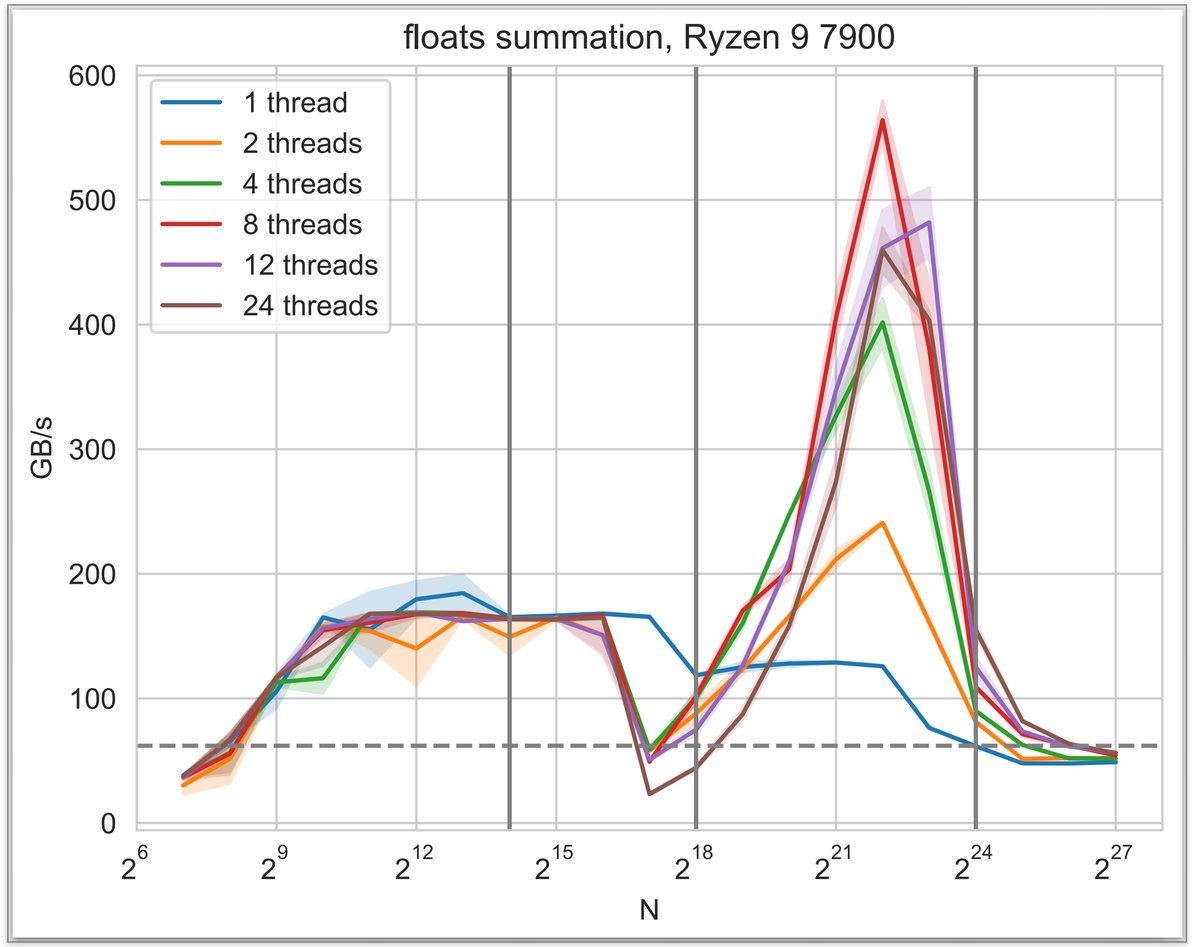

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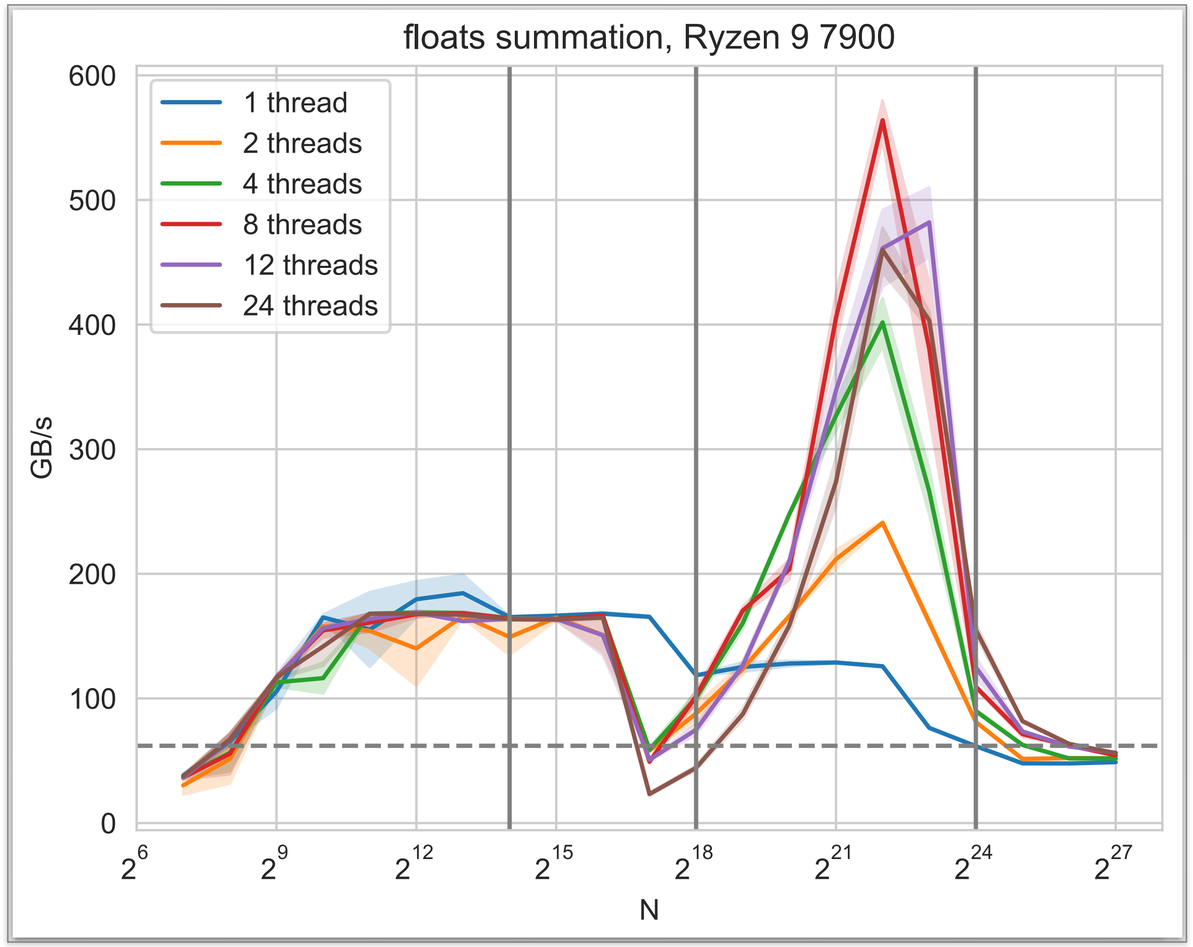

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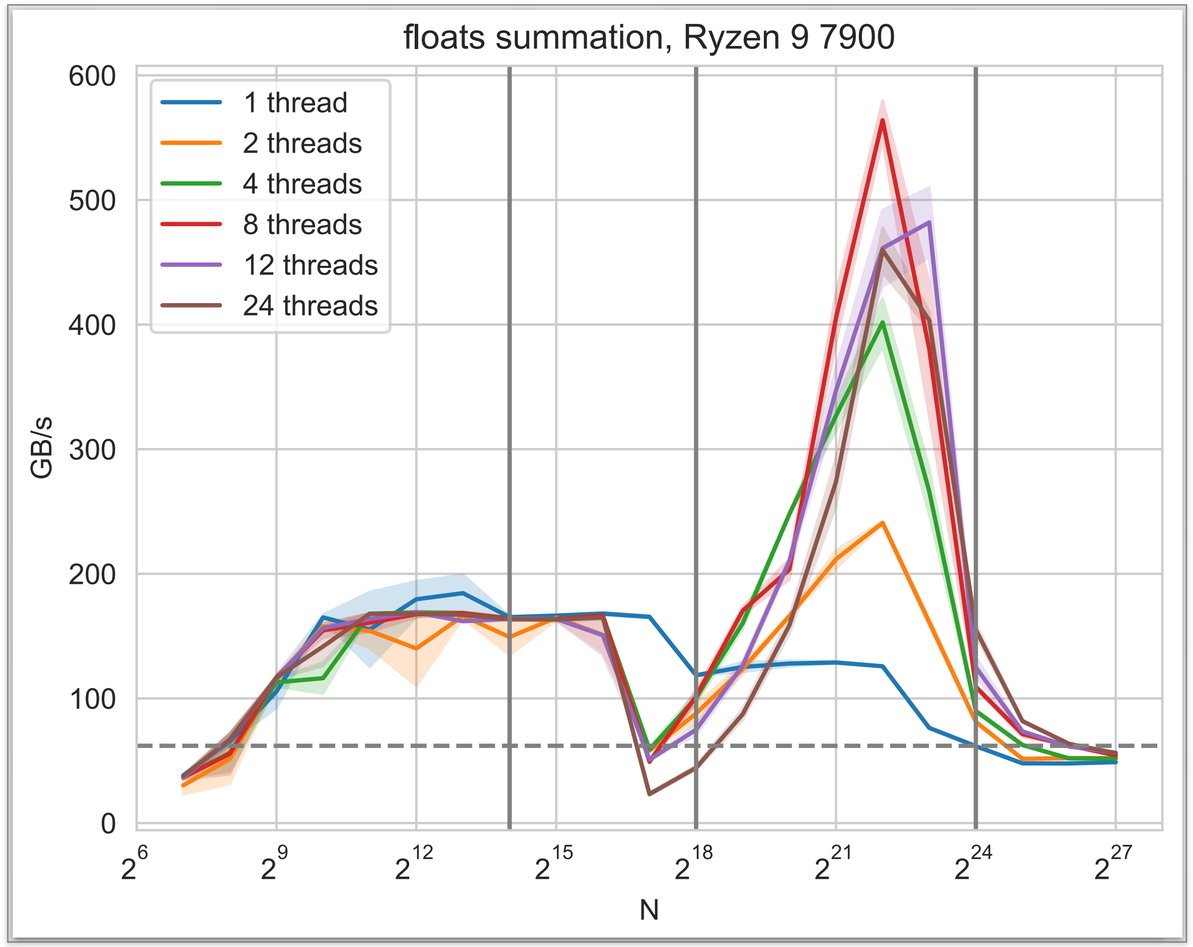

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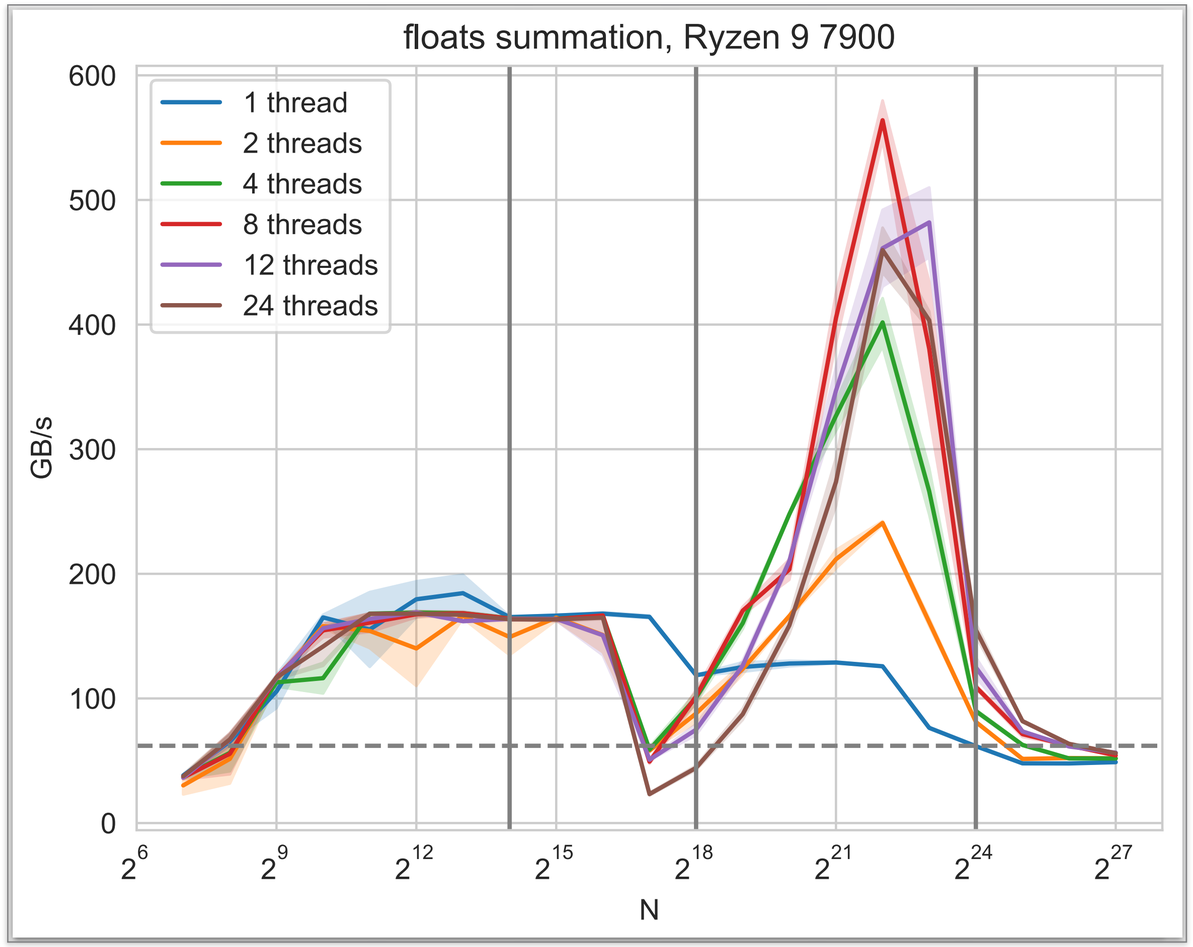

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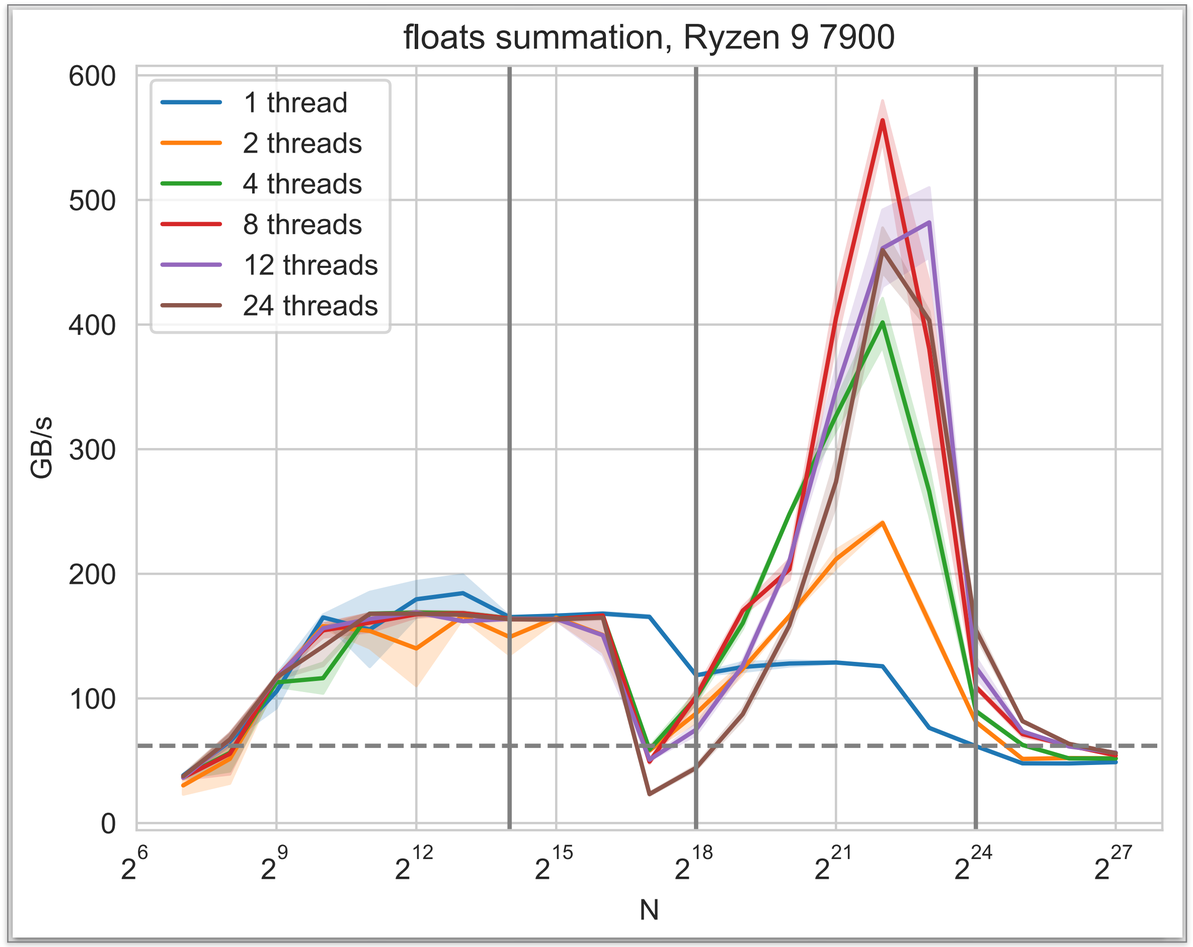

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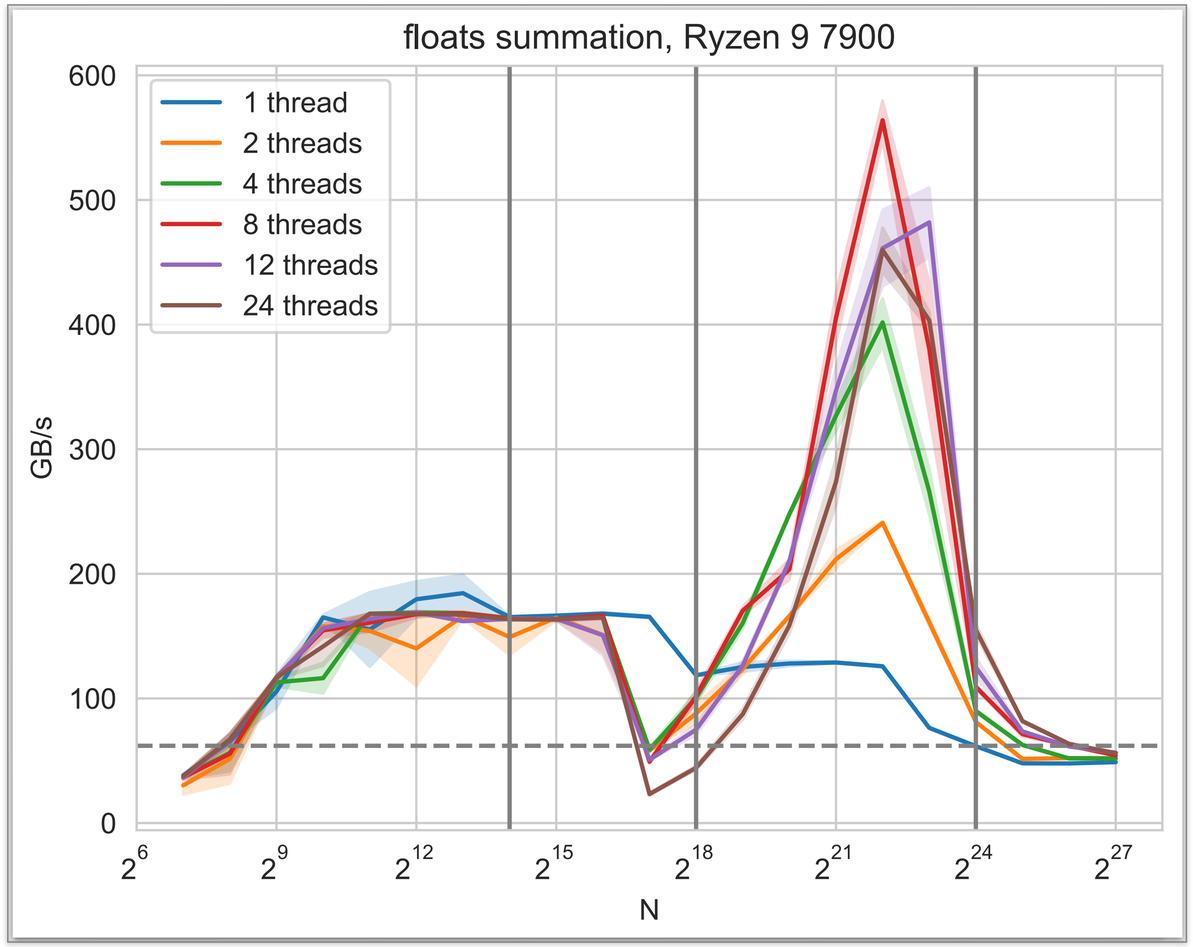

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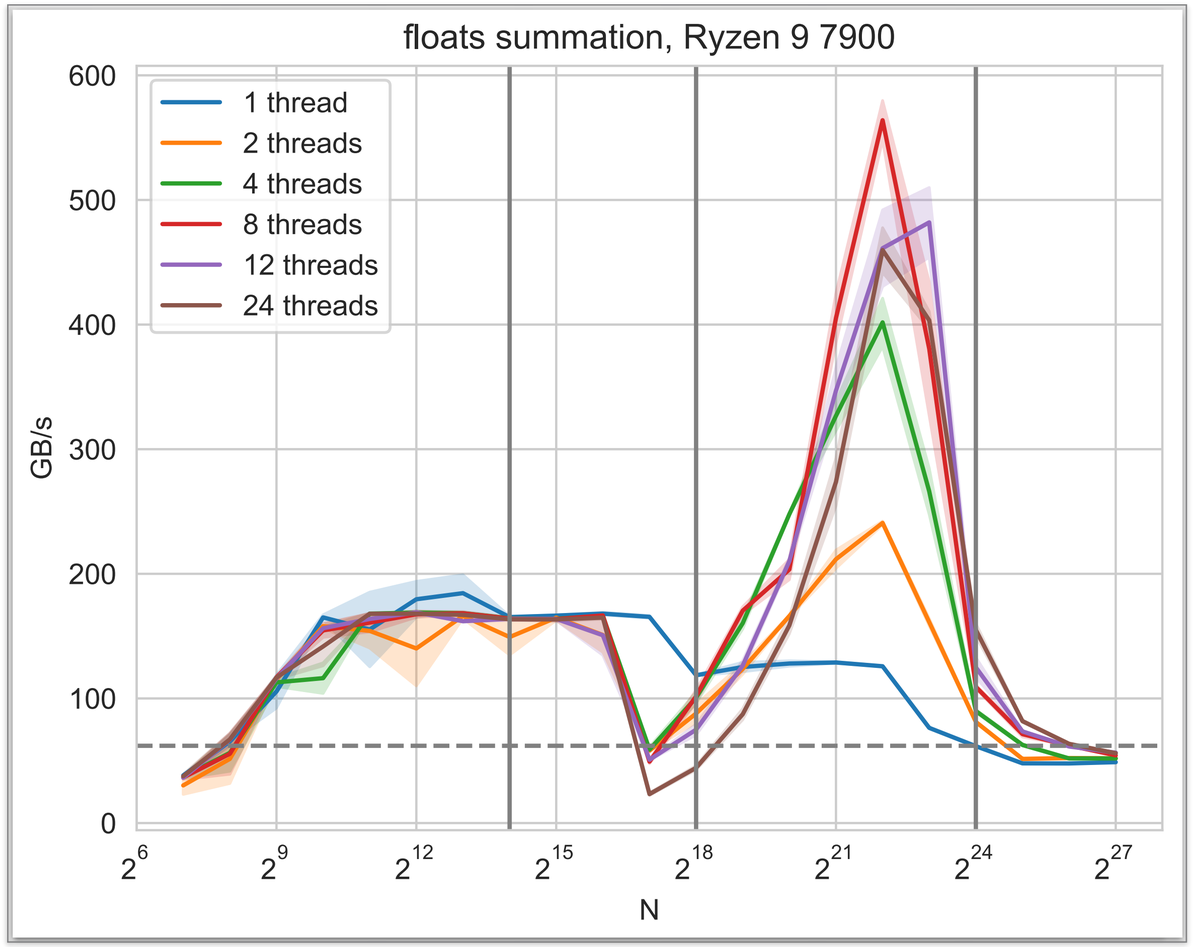

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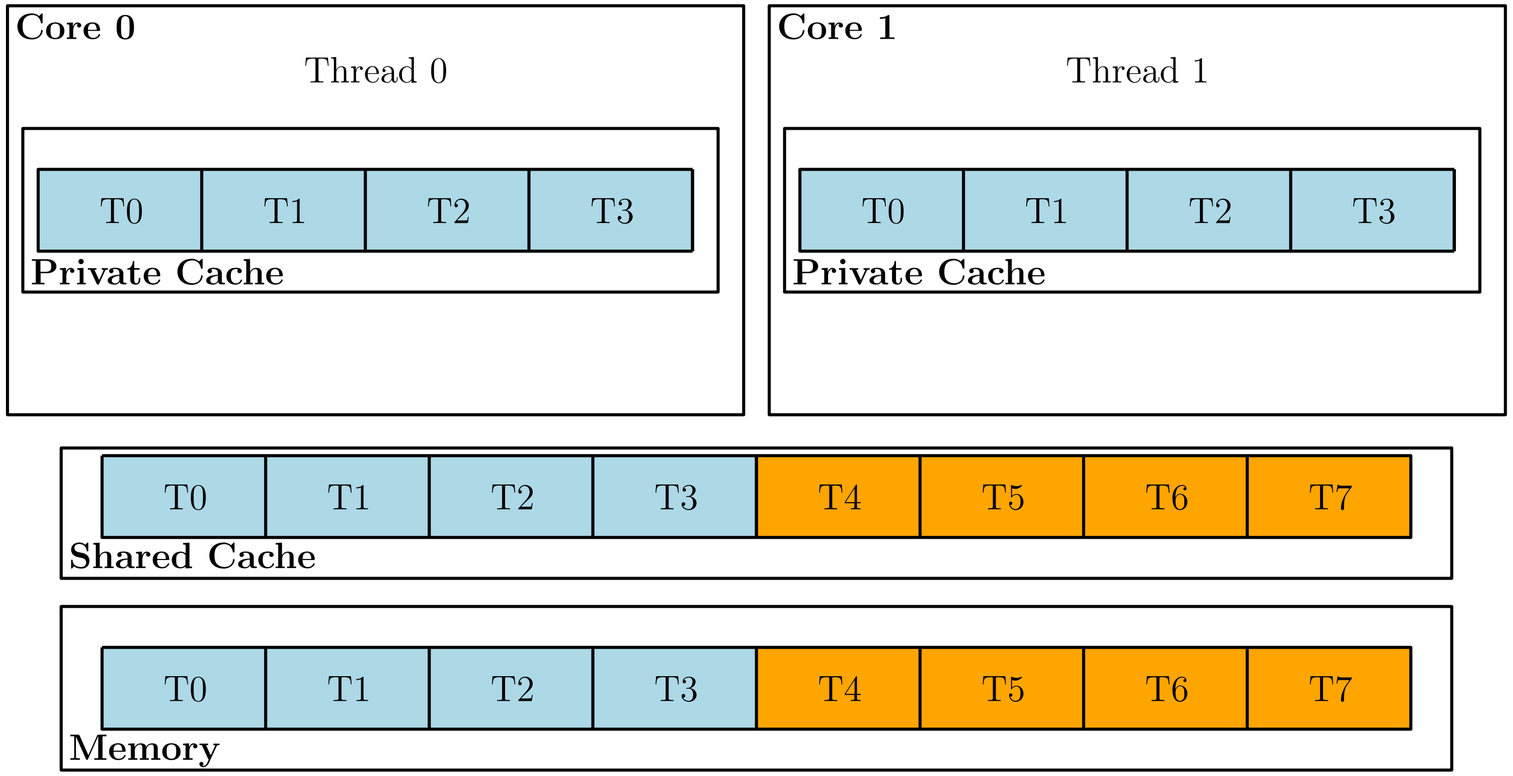

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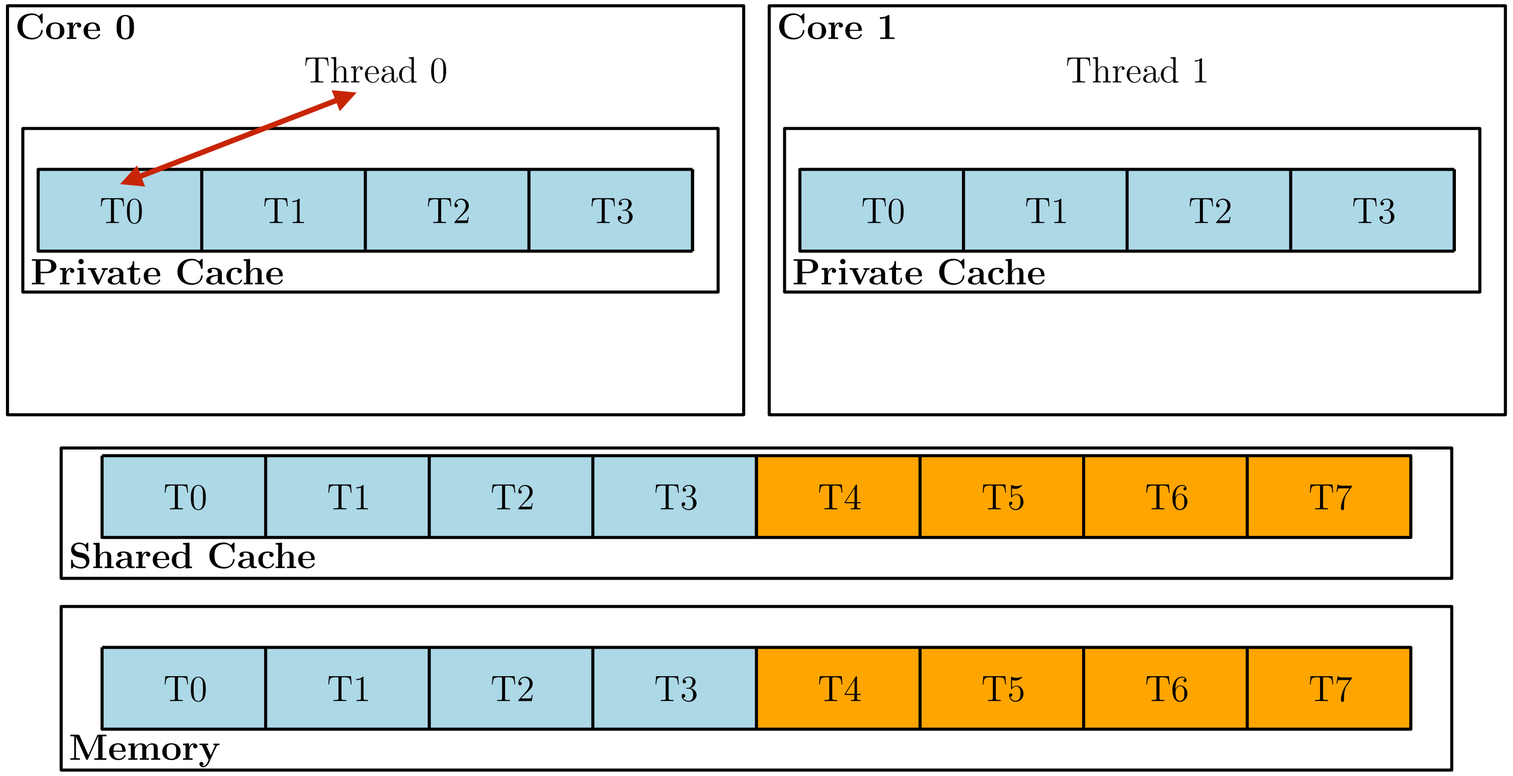

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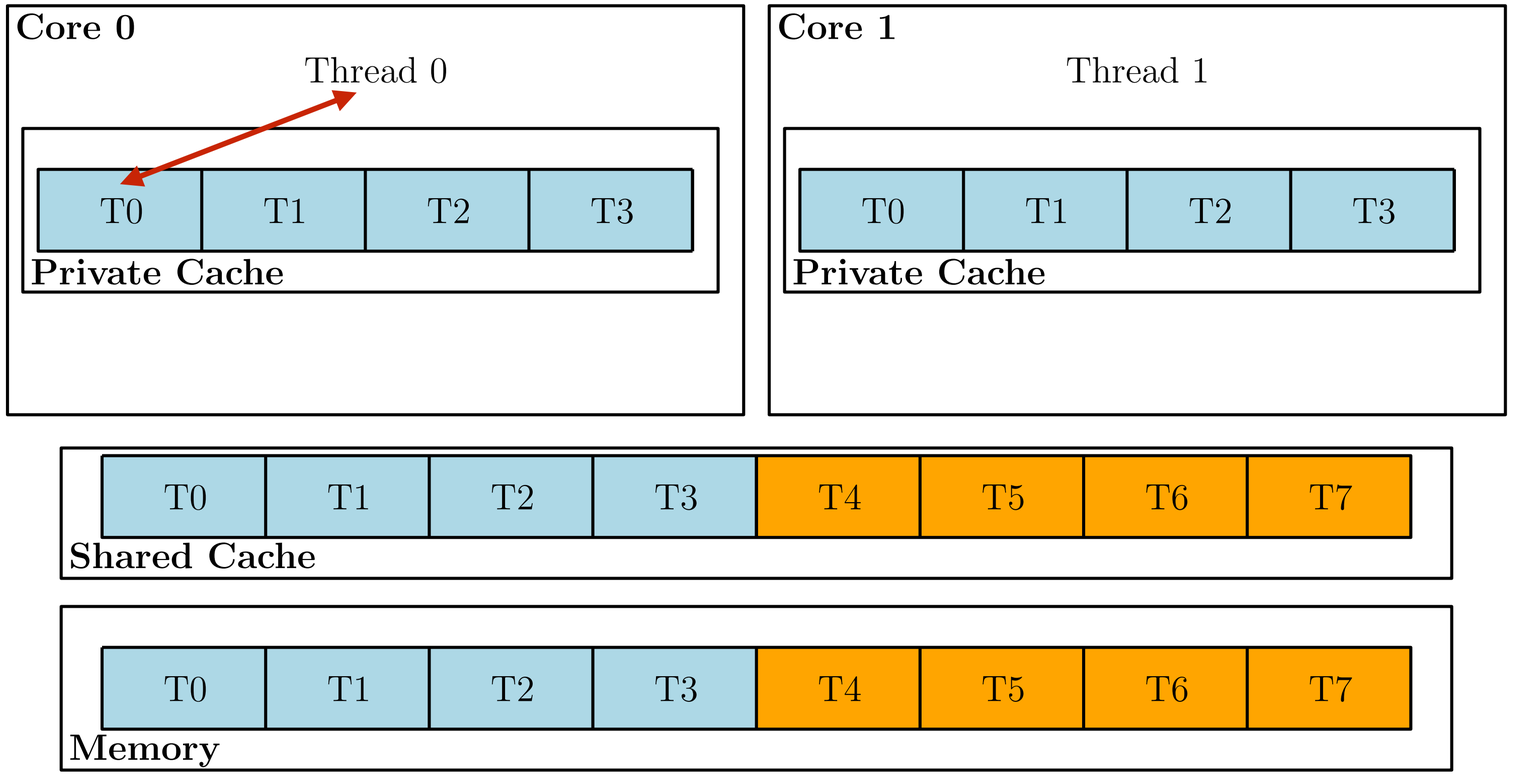

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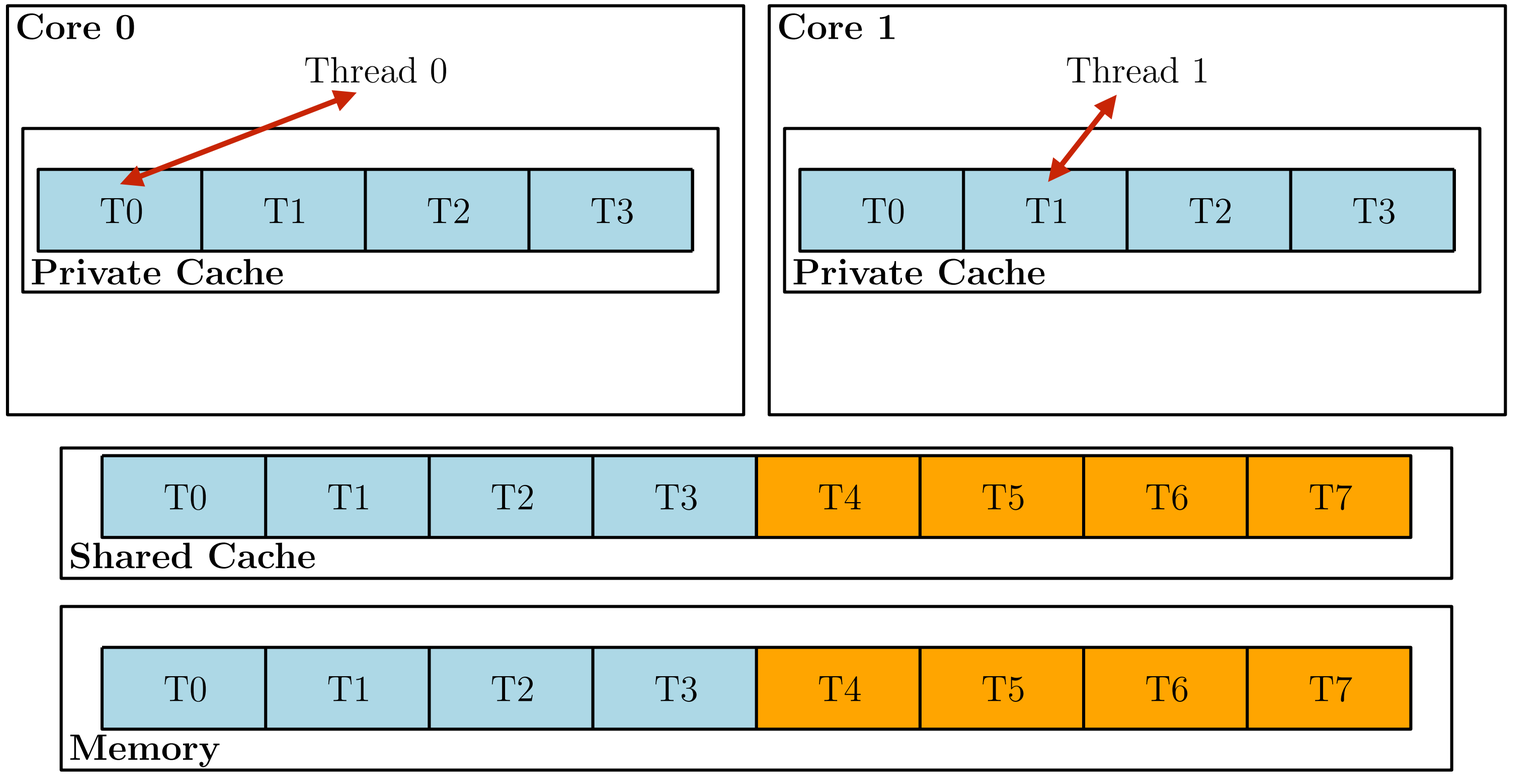

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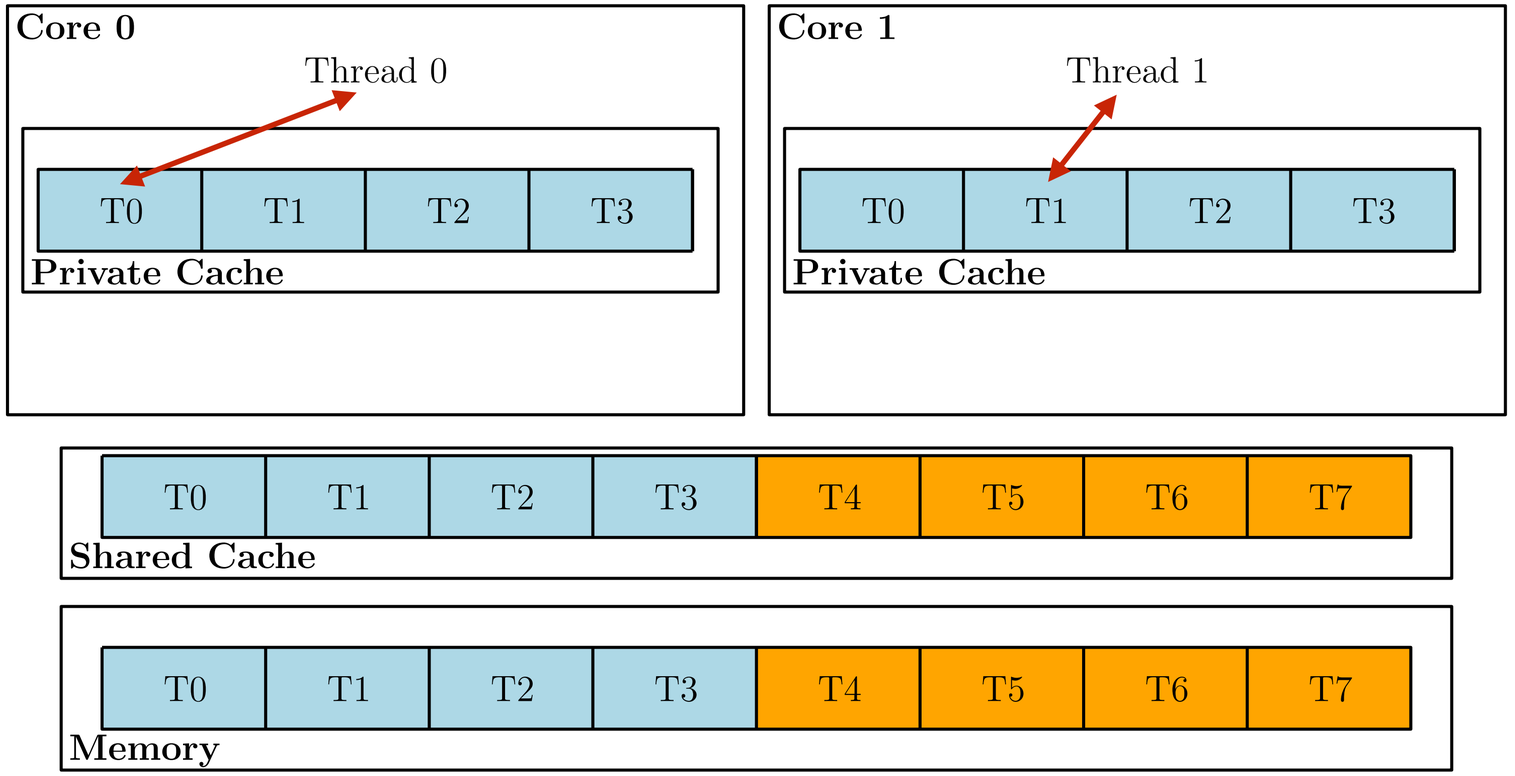

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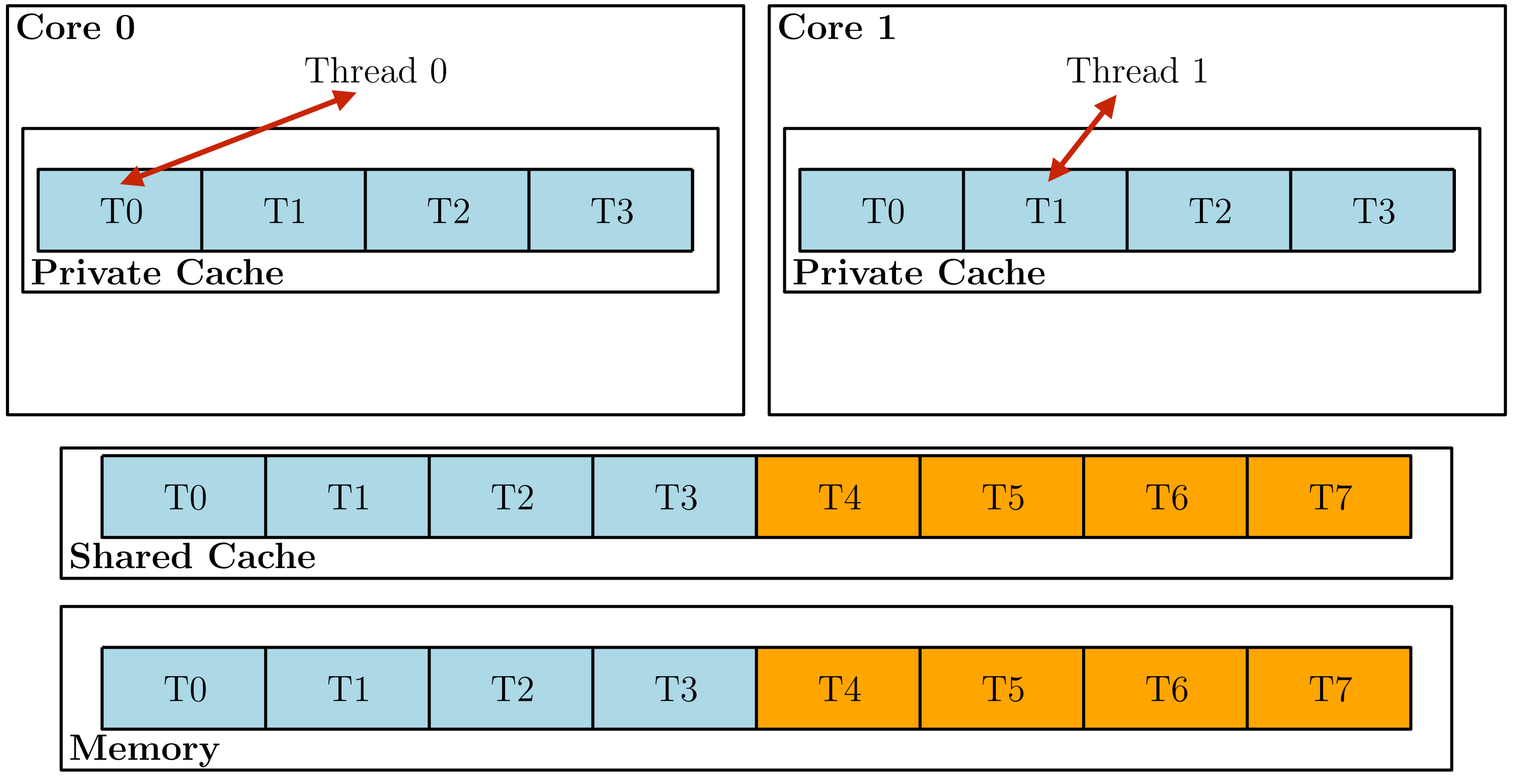

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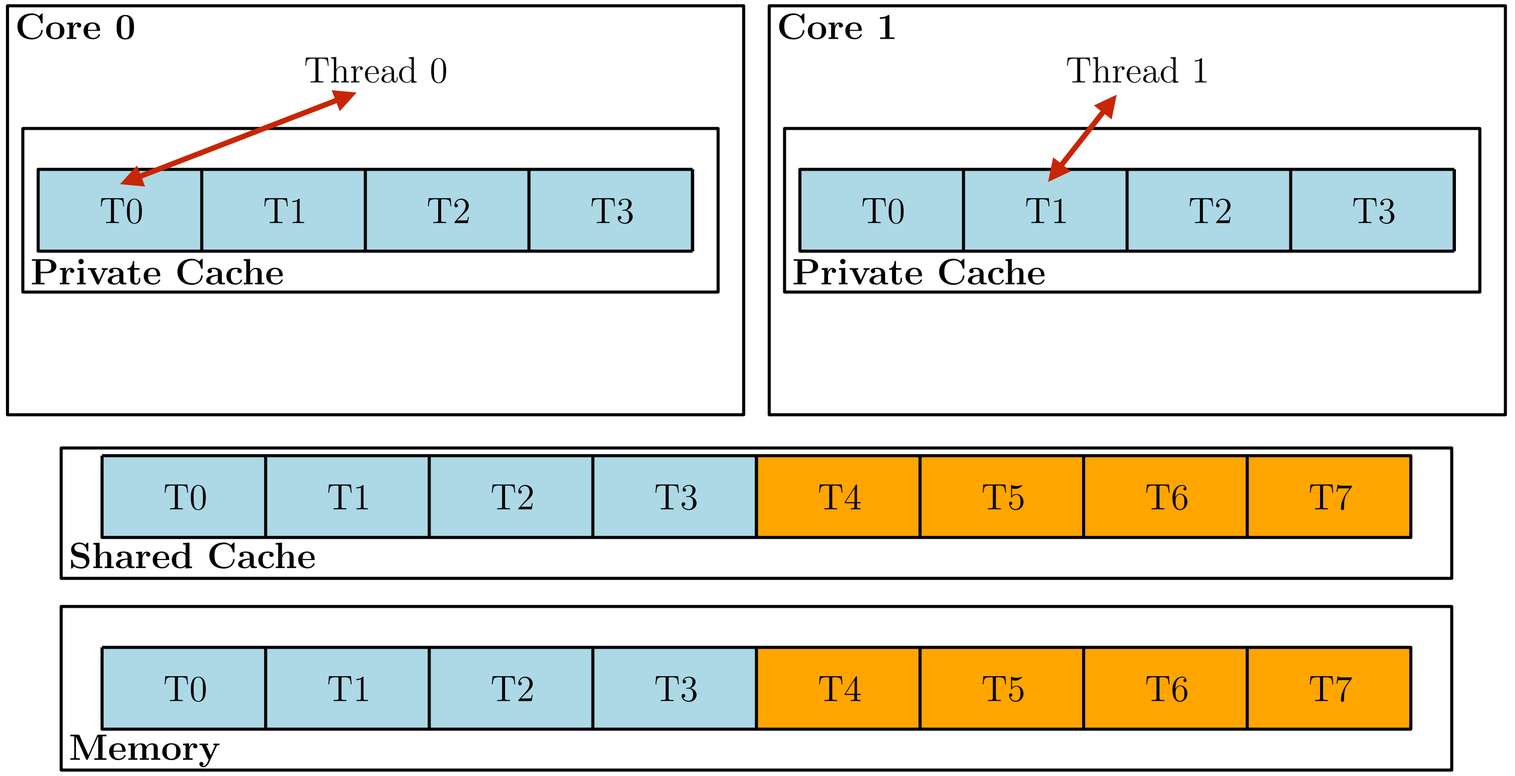

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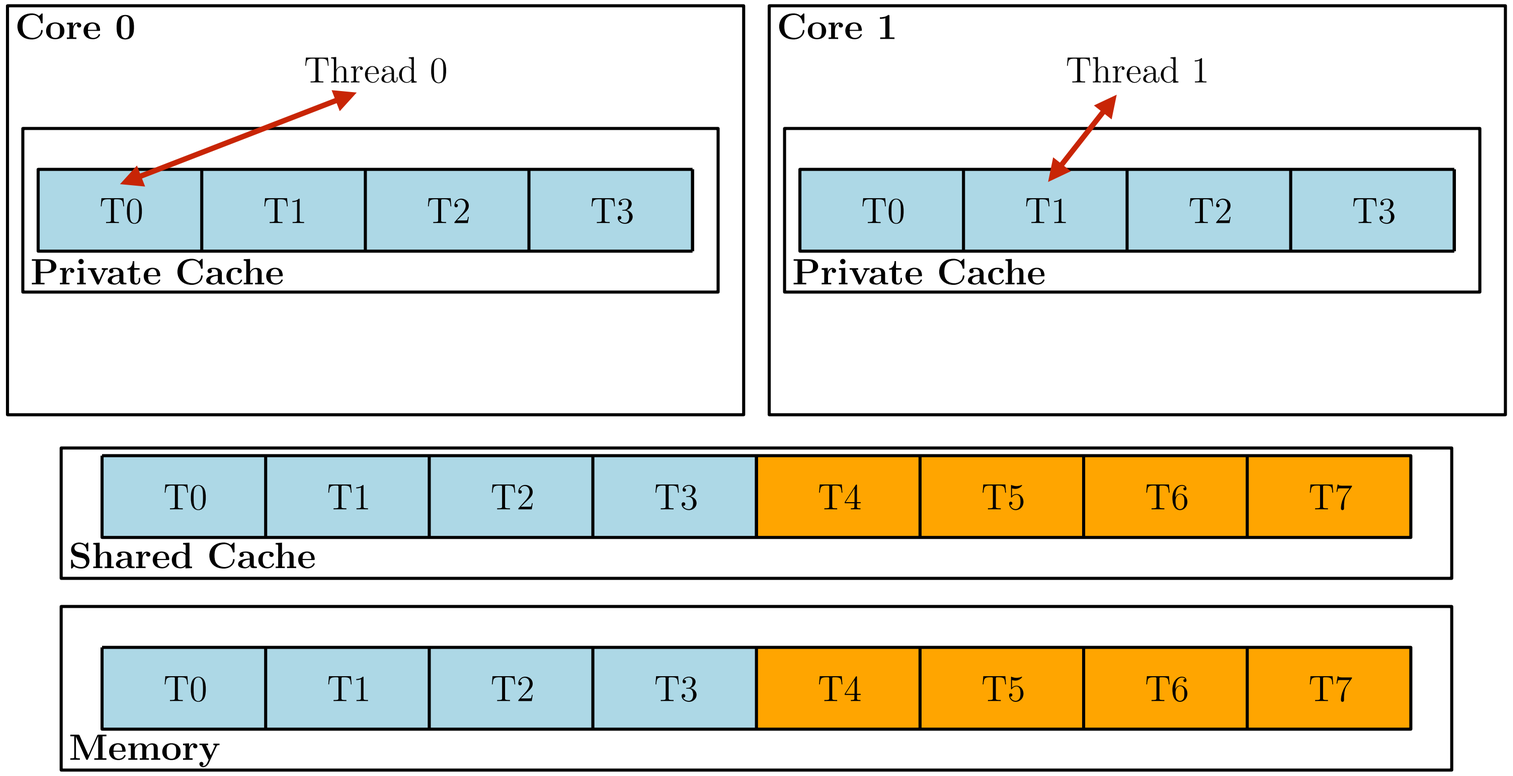

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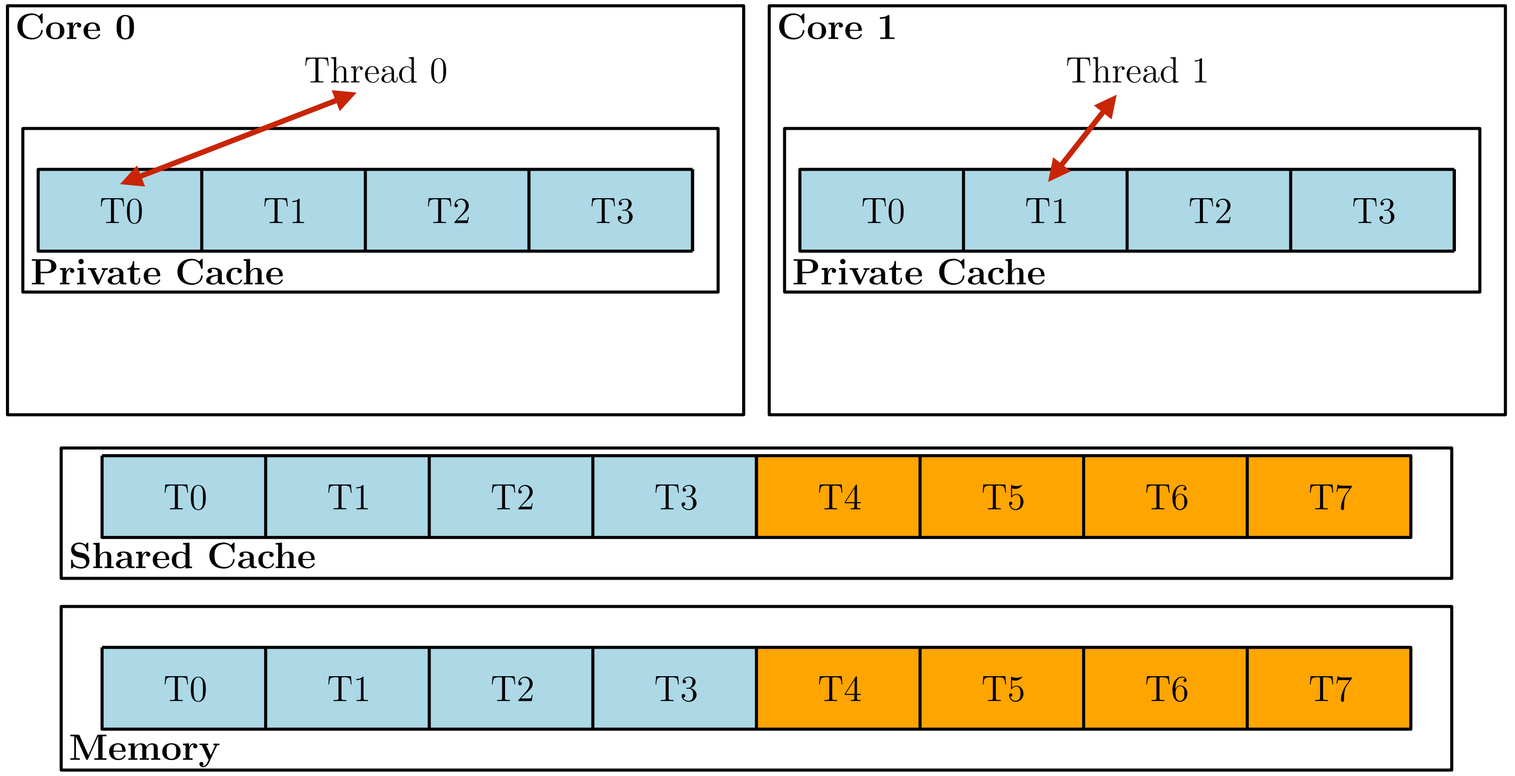

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- **Correct results!**

False Sharing

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struct ThreadOutputs {
    std::int32_t outputs[N];
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    // create N threads; thread i counts up
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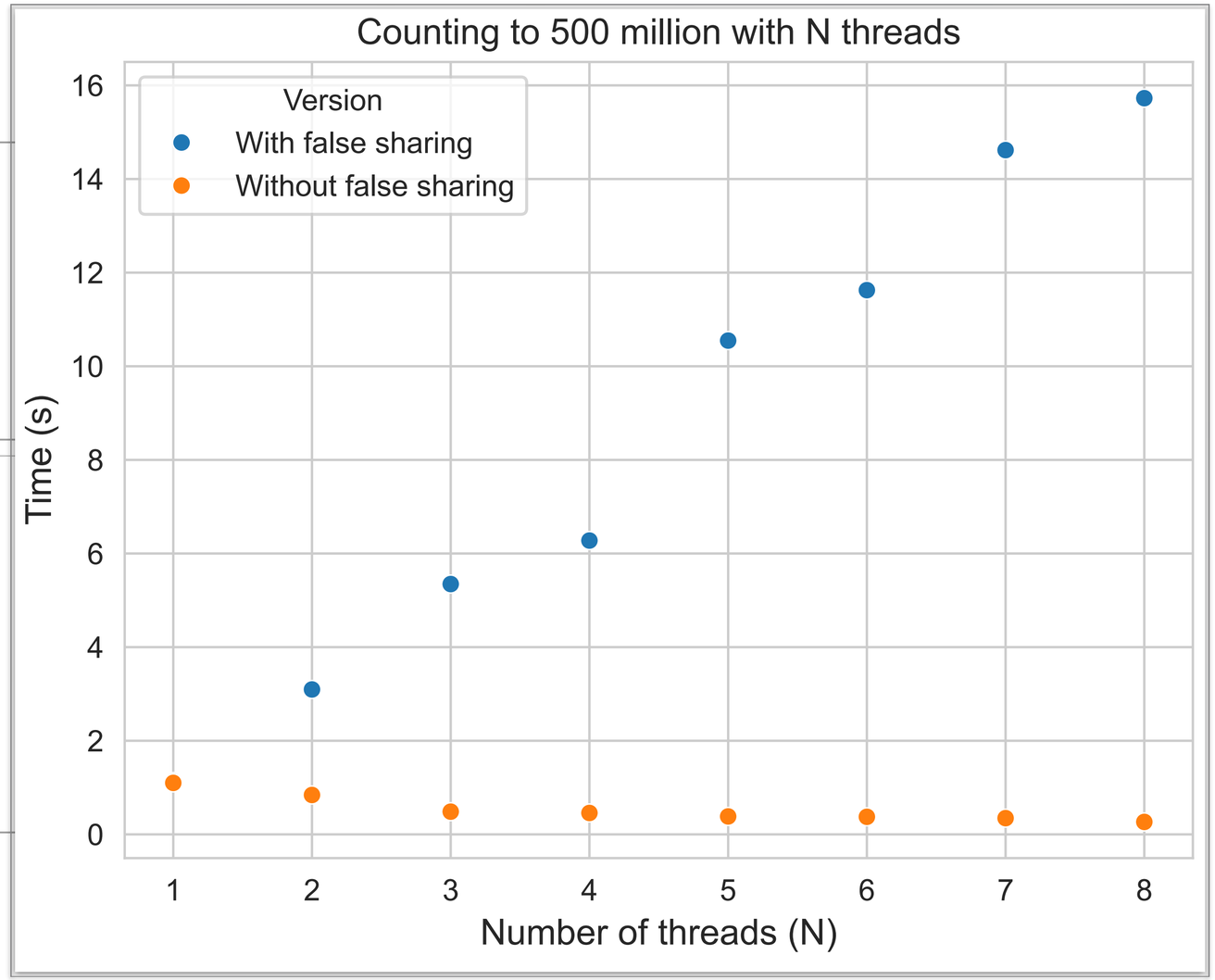

Measuring Multithreaded Performance

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Goals: find expensive locks, detect balancing issues between producers/consumers, …

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C++ alg -level p

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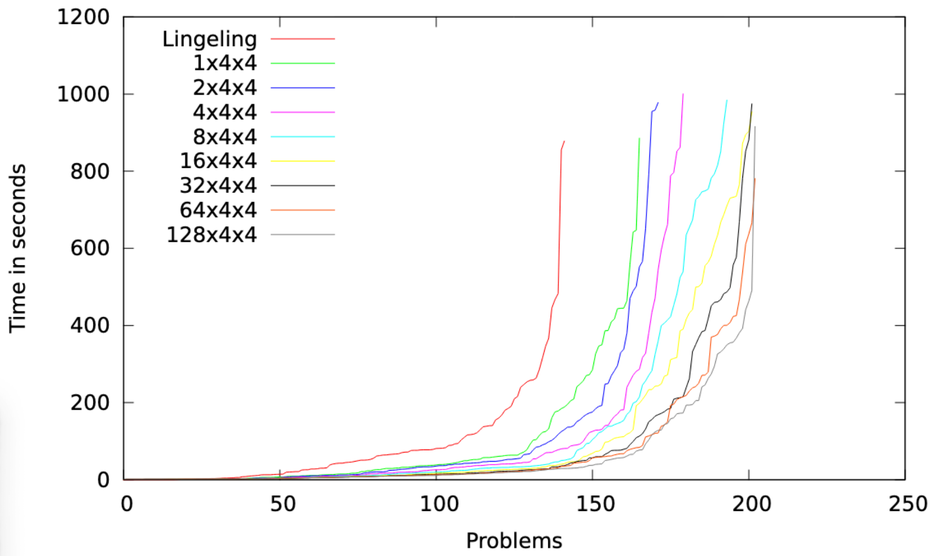
Exampl

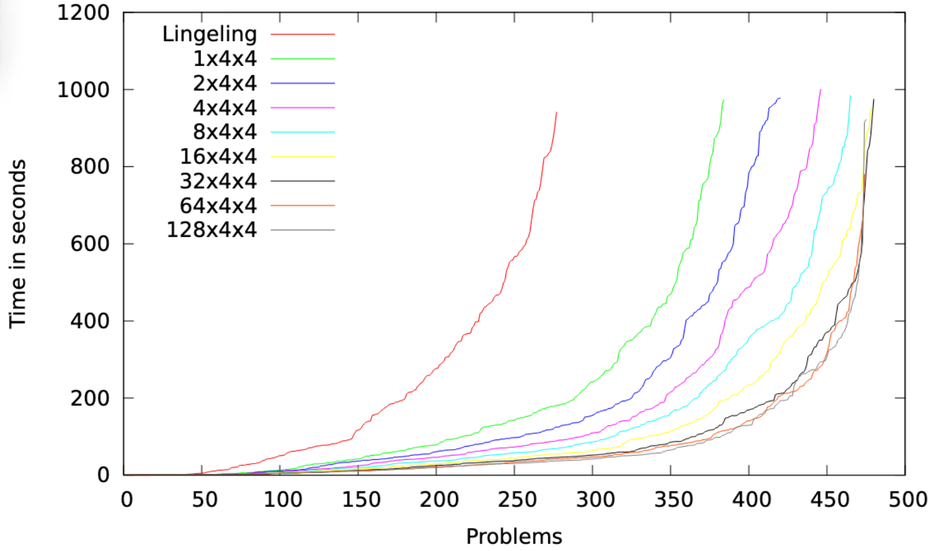
HordeSat: A Massively Parallel Portfolio SAT Solver

Tomáš Balyo, Peter Sanders, Carsten Sinz *

Karlsruhe Institute of Technology (KIT)
Karlsruhe, Germany

Experiments made using benchmarks from the application tracks of the 2011 and 2014 Sat Competitions [3] show that HordeSat can outperform state-of-the-art parallel SAT solvers on multiprocessor machines and is scalable on computer clusters with thousands of processors. Indeed, we even observe superlinear average speedup for difficult instances.





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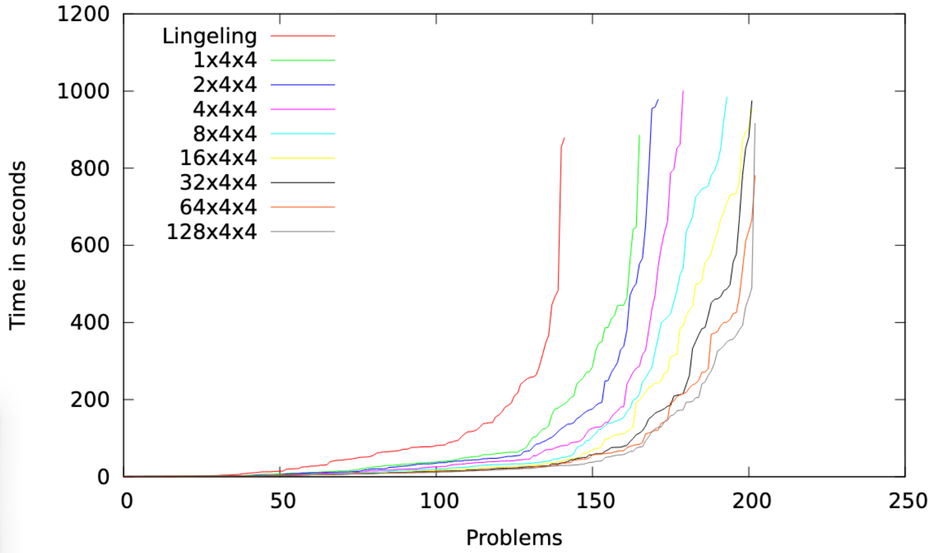

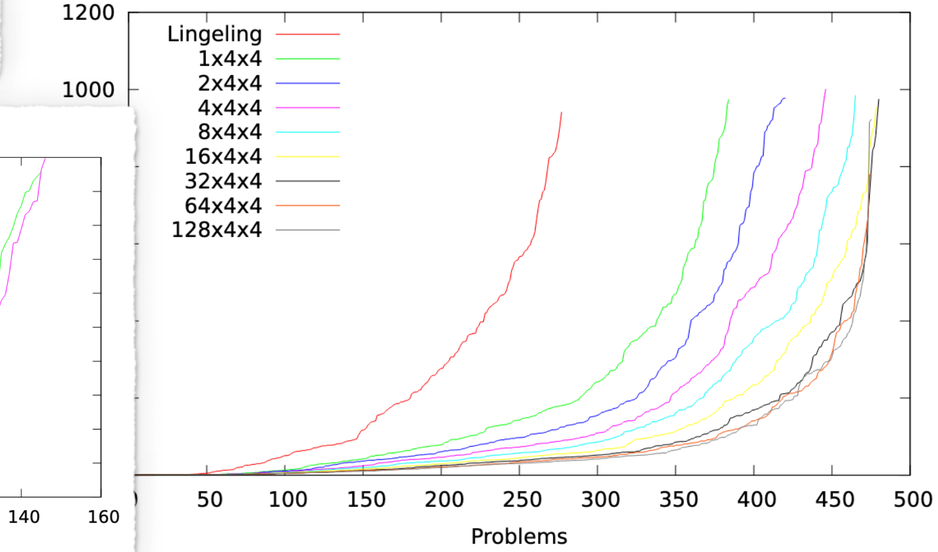

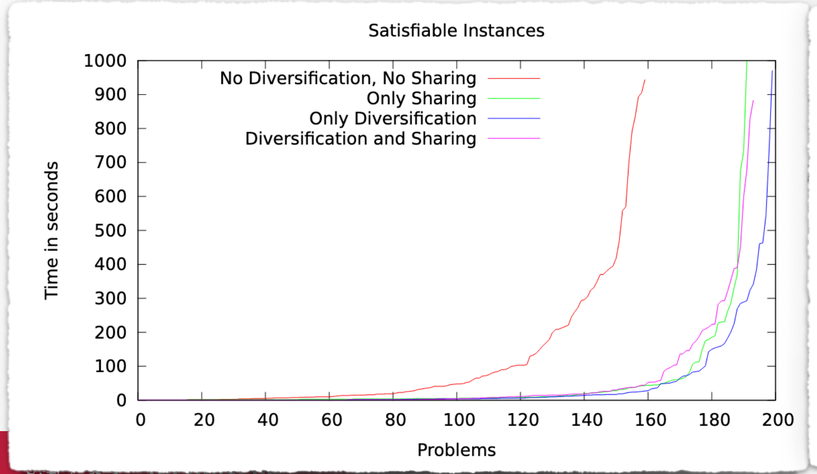

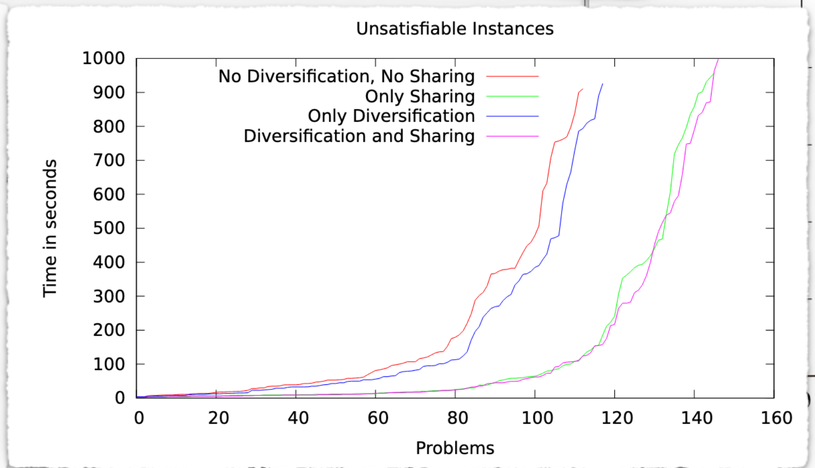

Reading

Optional further reading for a deeper dive:

- Bakhvalov, Denis. 2024.
  Performance Analysis and Tuning on Modern CPUs. 2nd (in progress).
- Drepper, Ulrich. 2007. What Every Programmer Should Know about Memory.
- Fog, Agner. 2024. Optimizing Software in C++:
  An Optimization Guide for Windows, Linux, and Mac Platforms.
- Hennessy, John L., and David A. Patterson. 2019. Computer Architecture: A Quantitative Approach. 6th ed. Morgan Kaufmann.