



703308 VO High-Performance Computing WS2021/2022

Measuring and Reporting Data

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Overview

- ▶ what and how to measure
 - ▶ time
 - ▶ time-dependent (speedup, efficiency, ...)
 - ▶ FLOPS
- ▶ use measurements to drive optimizations
 - ▶ Amdahl's law
- ▶ how to report measurements

Motivation: Optimization

- ▶ difficult to optimize without measuring
 - ▶ measurements are crucial for everything in computer science
 - ▶ How do you know whether program performance improved or not?
- ▶ difficult to measure without knowing what is measured and how
 - ▶ know your metrics!
 - ▶ performance, time, efficiency, memory footprint, energy, FLOPs, cache misses, ...
- ▶ tons of research on this topic...



Time-Related Metrics



Time

► *wall time*

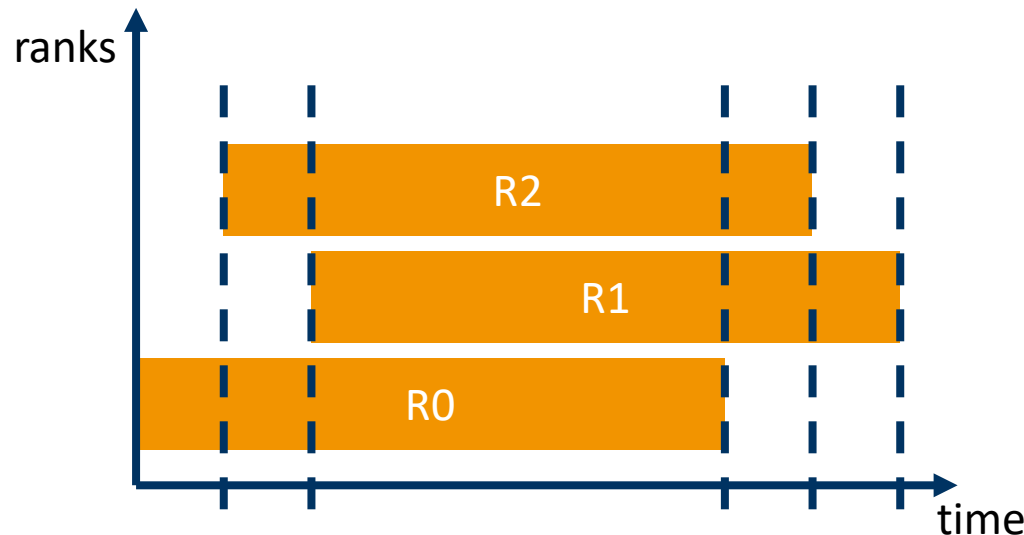
- time measured by looking at the wall clock
- disregards degree of parallelism
- the default when talking “time”

$$t_{\text{wall}} = \max_{0 \leq i < N} (t_{\text{end},i}) - \min_{0 \leq i < N} (t_{\text{start},i})$$

► *cpu time*

- wall time for each rank
- cumulative over all ranks, varies with degree of parallelism
- the default when talking “costs”

$$t_{\text{cpu}} = \sum_{i=0}^{N-1} t_i$$



Time is Parallel too

- ▶ synchronizing clocks over a large-scale system is very difficult
 - ▶ e.g. TSC: in-core TimeStamp Counter, 1 clock cycle tick rate (< 1 ns)
 - ▶ compare to network latency: 100–1000 ns, best case
 - ▶ note: CPU clock frequency scaling (DVFS) today no longer an issue
- ▶ hard to compare time measurements between processes
 - ▶ no issue if moderate accuracy and granularity requirements
 - ▶ otherwise check synchronization first (e.g. `MPI_WTIME_IS_GLOBAL`)
- ▶ also: mind the timer granularity in general
 - ▶ e.g. don't measure time intervals of 1-2 milliseconds with a 1 millisecond granularity
 - ▶ good practice: at least 10x higher granularity than shortest interval to be measured

Speedup

- ▶ speed increase of a parallel program over the sequential version
- ▶ $\text{speedup}_p = \frac{t_s}{t_p}$
- ▶ ideal: $t_p = \frac{t_s}{p}$, hence $\text{speedup}_p = \frac{t_s}{\frac{t_s}{p}} = p$ (linear)
- ▶ super-linear speedup also possible
 - ▶ e.g. problem partitioning reduces memory footprint per processor
 - ▶ enables more efficient use of memory hierarchy (caches)

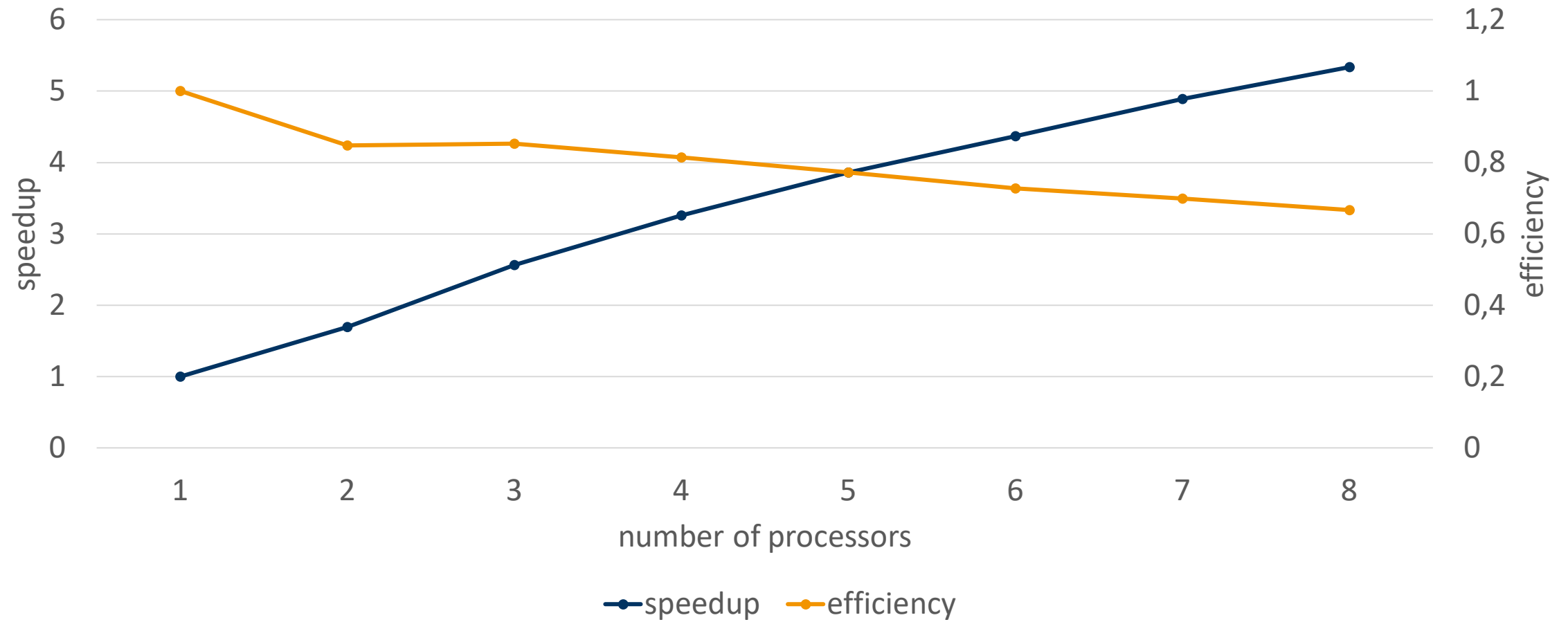
Absolute and Relative Speedup

- ▶ two kinds of speedup
 - ▶ absolute: reference t_s is the fastest sequential version
 - ▶ relative: reference t_s is the fastest parallel version run sequentially
 - ▶ bad third option: reference is $t_{p'}$, with $p' < p$ (e.g. $p' = 16$ and $p = 128$)
 - ▶ always specify your reference!
- ▶ non-trivial problem: parallelism might entail algorithmic changes and/or overheads (e.g. communication)

Efficiency

- ▶ measure of parallelization overhead
 - ▶ value range given between 0 and 1 or as a percentage
- ▶ $\text{efficiency}_p = \frac{\text{speedup}_p}{p}$
- ▶ ideal: $\text{efficiency}_p = 1$ (= linear speedup)
- ▶ worst case: $\lim_{p \rightarrow \infty} \text{efficiency}_p = 0$

Example Data for Speedup and Efficiency

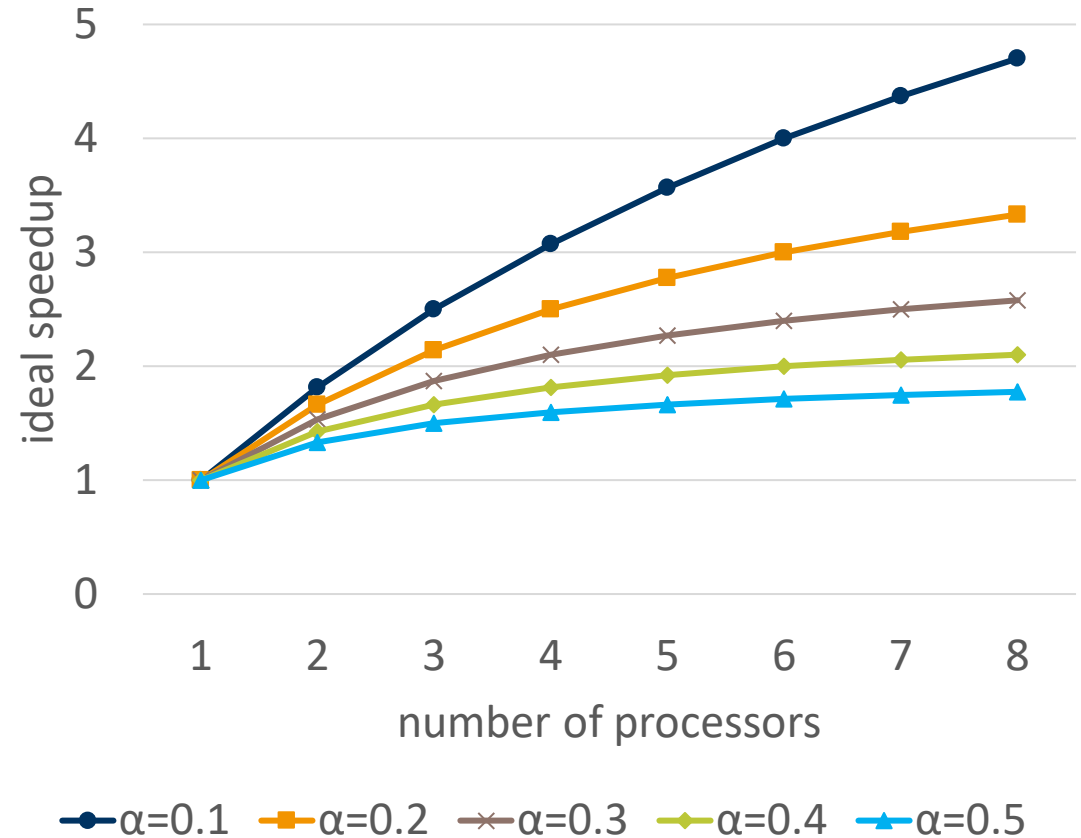


Amdahl's Law

- ▶ one of the oldest (1967) and still most important laws in parallel programming
- ▶ defines (upper limit on) speedup when dividing a parallel program into a sequential part (r_s) and a parallel part (r_p), with $r_s + r_p = 1$
- ▶ idea: r_s cannot be improved through parallelism
 - ▶ hence it must somehow pose a limiting factor for any potential speedup
 - ▶ all parallelism improvement must originate solely from improving r_p
- ▶ note: idealized perspective, does not include e.g. hardware bottlenecks

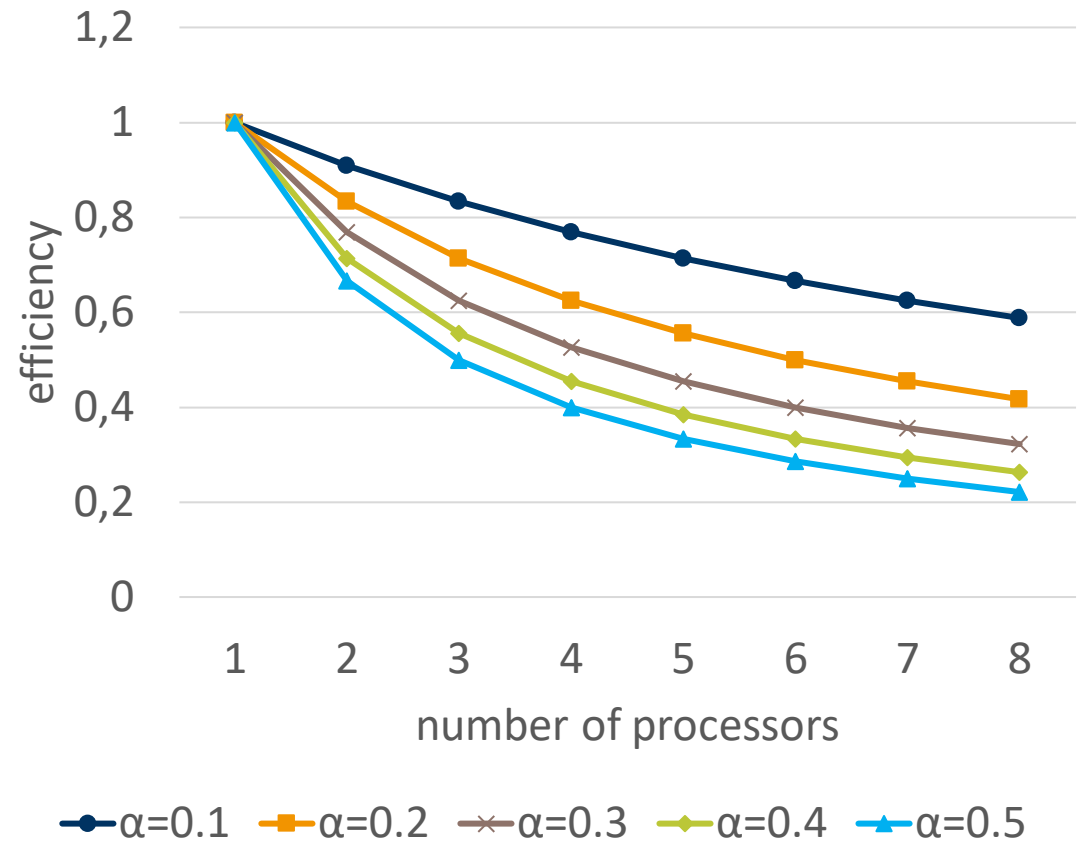
Amdahl's Law cont'd

- ▶ law: $\text{speedup}_n = \frac{1}{r_s + \frac{r_p}{n}} = \frac{1}{\alpha + \frac{1-\alpha}{n}}$
- ▶ severely limits potential speedup, even for infinite parallelism
- ▶ example: $\alpha = 0.2$ (=20 % sequential)
 - ▶ ideal speedup on 8 processors is 3.33
 - ▶ ideal speedup on ∞ processors is 5



Amdahl's Law: Efficiency

- ▶ the same principle applies to parallel efficiency
- ▶ example: $\alpha = 0.2$ (=20 % sequential)
 - ▶ max. efficiency on 8 processors is 0.42
 - ▶ max. efficiency on ∞ processors?



Amdahl's Law: Implications

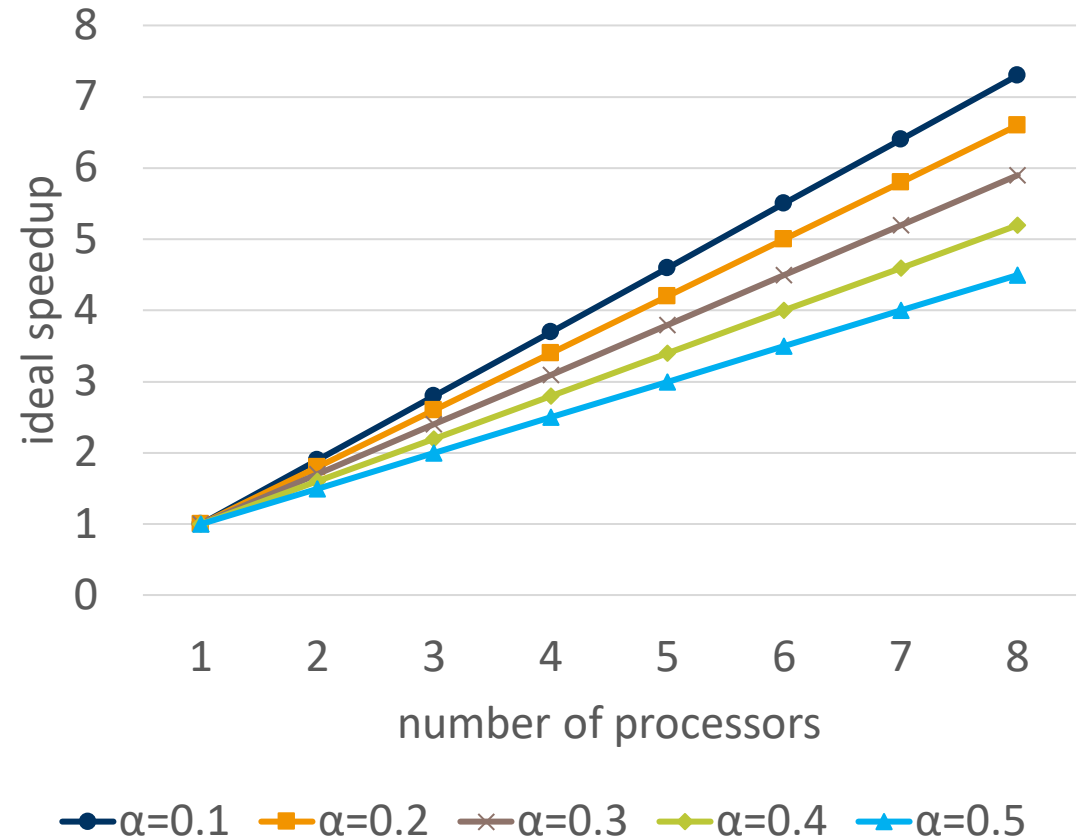
- ▶ first order of business: minimize α !
 - ▶ change algorithm to reduce amount of sequential code
 - ▶ careful, changes reference for relative speedup
 - ▶ optimize sequential code as much as possible
- ▶ don't spend excessive effort on optimizing parallel portion
- ▶ consider a sensible maximum degree of parallelism
 - ▶ don't allocate 1024 processors when using 128 is equally fast
 - ▶ also consider other users, power consumption, cpu time budgets, ...!

Amdahl's Law: Shortcomings

- ▶ Noticed, that it assumes the amount of work to be fixed?
 - ▶ not realistic for many use cases, problem size often scales with machine size
 - ▶ some problems are solved in real-time (e.g. rendering)
but at the highest problem size (e.g. image quality) possible
 - ▶ more resources (=processors) can indeed help here
- ▶ John Gustafson reevaluated this issue in 1988
 - ➔ Gustafson's Law

Gustafson's Law cont'd

- ▶ Assume a sequential portion α and a parallel portion $(1 - \alpha)$
- ▶ Assume that α is fixed or scales very slowly with the number of processors
- ▶ $\text{speedup}_p = \alpha + (1 - \alpha) \times P$



Strong vs. Weak Scalability

- ▶ *scalability* is (sort-of) a description for speedup and efficiency
 - ▶ “program scales (linearly)” = program achieves linear speedup
 - ▶ “program does not scale” = program doesn’t get any faster (maybe even slower)
- ▶ strong scalability
 - ▶ how the program scales with a fixed problem size
- ▶ weak scalability
 - ▶ how the program scales when keeping the problem size proportional
 - ▶ important: how to scale the problem in proportion?

Weak Scalability

- ▶ consider an application with a two-dimensional domain of size $n \times m$ (e.g. 2D heat stencil)
 - ▶ scale n , or m , or both?
 - ▶ scale timesteps?
- ▶ consider a 3D/4D/5D/... problem?
- ▶ consider a blackbox problem?



Additional Metrics



FLOPS

- ▶ floating point operations (FLOP/s: per second)
 - ▶ only operations with floating point semantics
 - ▶ does not count load/store/bitwise/...
- ▶ main measure for useful performance of software and hardware (work processed per time)
 - ▶ time not necessarily useful: can be wasted in waiting states...
- ▶ not applicable to every problem
 - ▶ consider integer-heavy problems (e.g. combinational logic, dynamic programming, ...)
 - ▶ also: memory-heavy, I/O-heavy, etc...

FLOPS cont'd

- ▶ What's the number of floating point instructions in x86 on the right?
 - ▶ 2 operations: mul, add
 - ▶ 1 instruction: fused multiply-add (FMA)
- ▶ Don't confuse *operations* and *instructions*
 - ▶ number of instructions is hardware- and compiler-dependent
 - ▶ know your hardware, compiler, and environment (e.g. compiler flags)
 - ▶ do not blindly trust hardware peak FLOPS

```
double foo(double A, double B,  
           double C, double D) {  
    D = A * B + C;  
    return D;  
}
```

```
x86:    vfmadd132sd xmm0, xmm2, xmm1
```

Common way of Counting FLOPS: Multiply + Add

```
D = A * B + C;           // 2 Ops, 1 Ins
D = A      + C;           // 1 Op,  1 Ins
D = A * B      ;           // 1 Op,  1 Ins
D = A * A * B + C;        // 3 Ops, 2 Ins
D = A * B + C * A + B     // 4 Ops, 2 Ins
```

Measuring FLOPS

- ▶ instrumentation and profiling
 - ▶ perf, PAPI, etc.
 - ▶ requires detailed knowledge of the source code, hardware, and compiler
- ▶ modeling
 - ▶ know your algorithm and implementation
 - ▶ there are also tools to automatically build models, of varying quality...

```
FP_ARITH_INST_RETIRED.SCALAR_DOUBLE  
FP_ARITH_INST_RETIRED.SCALAR_SINGLE  
FP_ARITH_INST_RETIRED.128B_PACKED_DOUBLE  
FP_ARITH_INST_RETIRED.128B_PACKED_SINGLE  
FP_ARITH_INST_RETIRED.256B_PACKED_DOUBLE  
FP_ARITH_INST_RETIRED.256B_PACKED_SINGLE  
FP_ARITH_INST_RETIRED.512B_PACKED_DOUBLE  
FP_ARITH_INST_RETIRED.512B_PACKED_SINGLE  
UOPS_EXECUTED.X87
```

(a few floating point counters available
on Intel Ice Lake CPUs)

FLOPS: Rmax vs. Rpeak

- ▶ **Rmax: achieved by software**
 - ▶ high performance linpack (HPL) benchmark
 - ▶ linear algebra stress-testing
- ▶ **Rpeak: achievable by hardware**
 - ▶ product of: number of FP units per CPU, their FP instructions per cycle, clock frequency, and number of CPUs

Rank	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	Supercomputer Fugaku - Supercomputer Fugaku, A64FX 48C 2.2GHz, Tofu interconnect D, Fujitsu RIKEN Center for Computational Science Japan	7,630,848	442,010.0	537,212.0	29,899
2	Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM DOE/SC/Oak Ridge National Laboratory United States	2,414,592	148,600.0	200,794.9	10,096
3	Sierra - IBM Power System AC922, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband, IBM / NVIDIA / Mellanox DOE/NNSA/LLNL United States	1,572,480	94,640.0	125,712.0	7,438
4	Sunway TaihuLight - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway, NRCPC National Supercomputing Center in Wuxi China	10,649,600	93,014.6	125,435.9	15,371

Application Throughput

- ▶ FLOPS are not everything
- ▶ consider what the application does
 - ▶ lagrangian simulation (no grid, move particles around): particles/s
 - ▶ eulerian simulation (no particles, compute properties at grid points): cells/s
 - ▶ chemistry applications: molecules/s
 - ▶ business applications: stock prices/s
 - ▶ unknown application: elements/s, updates/s, queries/s, ...
- ▶ domain-specific metrics are often much more useful to users than highly technical metrics

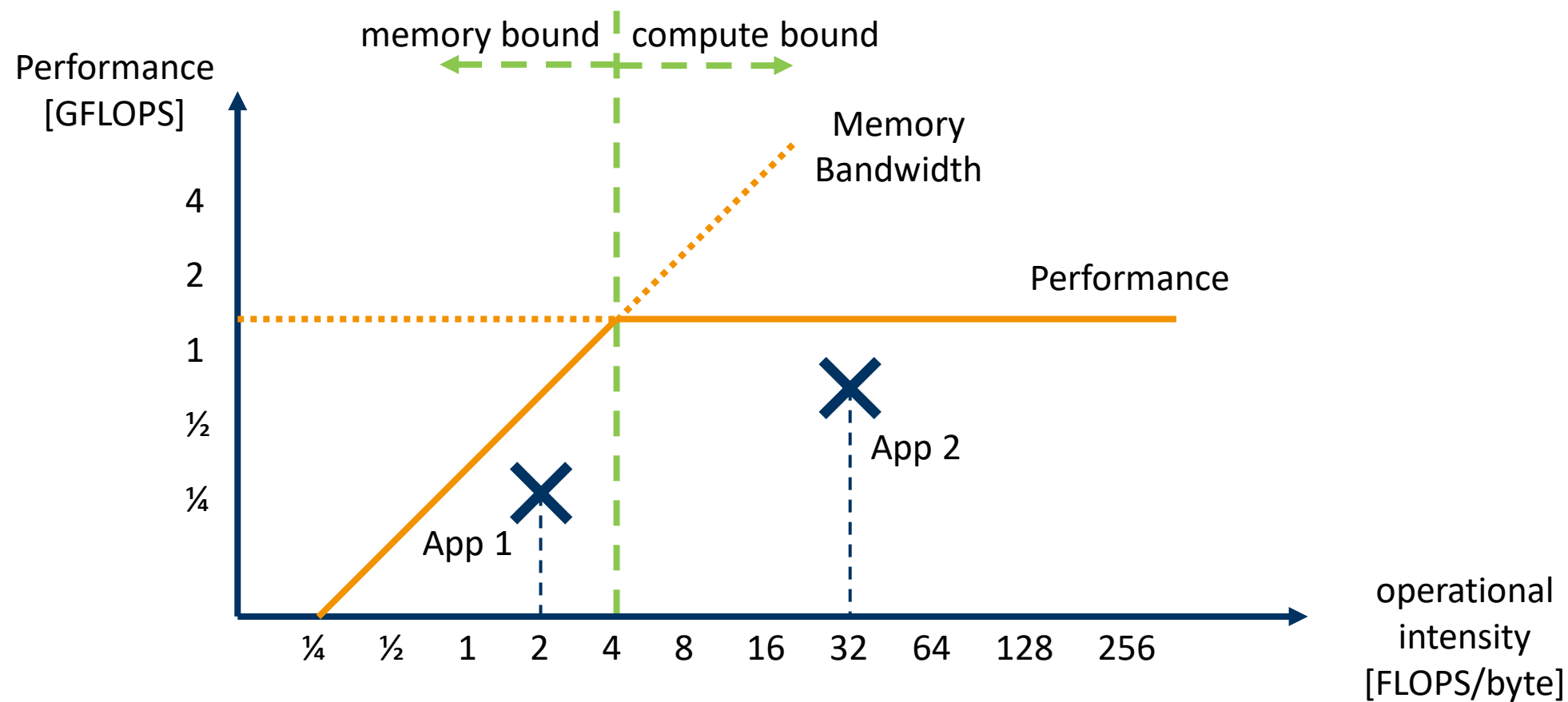
Compute Bound vs. Memory Bound (vs. Communication Bound)

- ▶ what is the bottleneck of your code X on hardware Y
 - ▶ memory accesses
 - ▶ computational throughput
 - ▶ data transfer
 - ▶ ...
- ▶ compute bound
 - ▶ no benefit in speeding up memory accesses, execution units are 100% busy
- ▶ memory bound
 - ▶ no benefit in speeding up computation, memory link is 100% busy

“Roofline” Model

- ▶ visual performance model for intra-node optimization
 - ▶ illustrates performance potential of a given hardware architecture
 - ▶ illustrates how much of this potential is used by an application
 - ▶ indicates which optimizations to apply
- ▶ indicates whether one is compute bound or memory bound

“Roofline” Model cont’d



Driving Optimizations

- ▶ Roofline model says “memory bound”
 - ▶ check cache optimality of algorithm
 - ▶ check NUMA mapping/bindings
 - ▶ check software prefetching
- ▶ Roofline model says “compute bound”
 - ▶ check vectorization (SIMD)
 - ▶ check compiler optimizations
 - ▶ check software caching (“memoization”)

Performance Counters

- ▶ originally added to CPUs for post-silicon functional debugging
 - ▶ nowadays re-purposed for performance debugging
- ▶ can be read with tools
 - ▶ command line: perf
 - ▶ library: PAPI
 - ▶ tons of additional performance tools out there...
- ▶ can be extremely useful if you know your hardware well
 - ▶ Intel: <https://perfmon-events.intel.com/>
 - ▶ AMD: <https://developer.amd.com/resources/developer-guides-manuals/> (“PPR”)

Performance Counters Example

```
[c703429@login.lcc2 ~]$ perf stat ./heat_stencil_1D_seq
...
28,826,239,136 cycles:u          #    2.471 GHz
35,220,856,783 instructions:u   #    1.22  insn per cycle
 6,711,849,029 branches:u       # 575.356 M/sec
    1,295,209 branch-misses:u   #    0.02% of all branches
      1,044 LLC-load-misses:u
        26 LLC-store-misses:u
    15,312,122 L1-dcache-load-misses:u
    476,440,489 L1-dcache-store-misses:u
```



Properly Reporting Data



How to Report Metrics? (Non-Exhaustive)

- ▶ How many repetitions of an experiment do I need to run?
 - ▶ A single run is enough, right?
 - ▶ Three runs is enough for averaging, right?
- ▶ Should I run on multiple systems?
 - ▶ Should their architecture differ?
- ▶ Should my experiments be reproducible?
 - ▶ What information is required to enable reproducibility?
- ▶ Do I show all collected data?
 - ▶ Do I select data, and if so, how?
 - ▶ Do I aggregate data, and if so, how?
 - ▶ Do I report absolute or relative values?
- ▶ Do I quantify the reliability of my data?
 - ▶ If so, how?
- ▶ ...

Experiment Repetitions

- ▶ Report whether your problem is deterministic!
- ▶ if deterministic
 - ▶ single run sufficient (should be – ideally – exactly reproducible)
 - ▶ Are performance measurements deterministic?
- ▶ if non-deterministic
 - ▶ multiple runs are required
 - ▶ report statistical measures
 - ▶ arithmetic/geometric/harmonic means
 - ▶ confidence intervals
 - ▶ ...

How Many Repetitions are Required?

- ▶ use confidence interval (CI)
 - ▶ interval around sample mean, e.g. $\bar{x} = 80$ [75; 85]
 - ▶ e.g. a 95 % CI means there's a 95 % probability it contains the true mean
- ▶ for normally distributed data
 - ▶ directly compute the number of measurements required to satisfy error e
 - ▶
$$n = \left(\frac{s \times t(n-1, \frac{\alpha}{2})}{e\bar{x}} \right)^2$$
 - ▶ check https://en.wikipedia.org/wiki/Confidence_interval#Basic_steps for details on computing CI
- ▶ for non-normally distributed data
 - ▶ re-compute CI every k experiments (choose k depending on experiment effort), stop when happy
 - ▶ at least e.g. 5 runs to compute meaningful CI

Running on Multiple Systems

- ▶ depends on how high you aim
 - ▶ “I have shown in a proof-of-concept that this might work in some selected cases”
vs.
 - ▶ “I have shown that this generally works in all cases”
- ▶ more hardware (or software!) coverage is always better
 - ▶ but trade-off between porting effort and benefits

Data Collection and Selection

- ▶ document your efforts and backup your data and documentation
- ▶ if reporting only a subset of data, clearly specify the reason and motivation
 - ▶ e.g. only 8 to 16 nodes; only 4, 9, 16, 25, and 36 nodes
 - ▶ e.g. only using half the cores per node
 - ▶ e.g. applications 1, 2, and 3 on hardware A and B, but data for 3 on B is missing
 - ▶ e.g. only measuring parts of an application

Data Aggregation

▶ costs

- ▶ usually atomic units, linear relationship
- ▶ can directly aggregate using arithmetic mean
- ▶ e.g. execution time (seconds), memory footprint (megabytes), energy consumption (joule)

▶ rates

- ▶ if able, aggregate costs first and then compute rate; otherwise use harmonic mean
- ▶ e.g. FLOP/s, MB/s, etc.

▶ ratios

- ▶ if able, don't aggregate at all; if required, aggregate base data instead
- ▶ e.g. "A is 50 % higher than B"

Reproducibility

- ▶ publish all required information, but not more than that
 - ▶ source code
 - ▶ compiler, version, flags, libraries
 - ▶ hardware architecture (detail depends on use case)
 - ▶ external factors (e.g. other users, load of the system, room temperature, ...)
 - ▶ reference data to compare against
 - ▶ aggregation methods, if used
- ▶ note: doesn't mean you need to provide a VM or container...
 - ▶ But often you can!

Four Steps to Creating an Optimized Parallel Program

- ▶ 1. devise and implement the simplest, most straight-forward parallel solution that you can think of
- ▶ 2. measure the performance (or whatever metric you are interested in) to obtain a point of reference
- ▶ 3. improve your program based on your measurements
- ▶ 4. `while(!☺) { step2(); step3(); }`

Sequential Equivalence

- ▶ **strong sequential equivalence**
 - ▶ bitwise identical results
 - ▶ requires preserving the order of computations compared to sequential version
 - ▶ potentially big impact on performance
(associativity, collective communication patterns, ...)
- ▶ **weak sequential equivalence**
 - ▶ mathematically equivalent but not bitwise identical
(IEEE 754 float arithmetic is neither associative, nor commutative)
 - ▶ does not require preserving the order of computations
- ▶ **Always check your requirements!**
 - ▶ If your algorithm doesn't require a specific order, why should its implementation?

Portability

- ▶ **functional portability**

- ▶ program runs on different hardware and produces correct results
- ▶ hardware architecture, compiler, libraries, etc.
- ▶ usually not hard to achieve (mostly x86/ARM + GPUs)

- ▶ **performance (also “non-functional”) portability**

- ▶ program runs efficiently on different hardware and is considered “fast”
- ▶ no exact definition, topic of ongoing research

Summary

- ▶ lots of metrics to choose from
 - ▶ classics are speedup and efficiency
- ▶ always consider Amdahl's law for everything you do
- ▶ measure before you optimize
 - ▶ and when you optimize, do it data-driven and not based on hunches

Image Sources

- ▶ Rmax/Rpeak: <https://www.top500.org/lists/2021/06/>