703308 VO High-Performance Computing
Measuring and Reporting Performance

Philipp Gschwandtner

Overview

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

Motivation: optimization

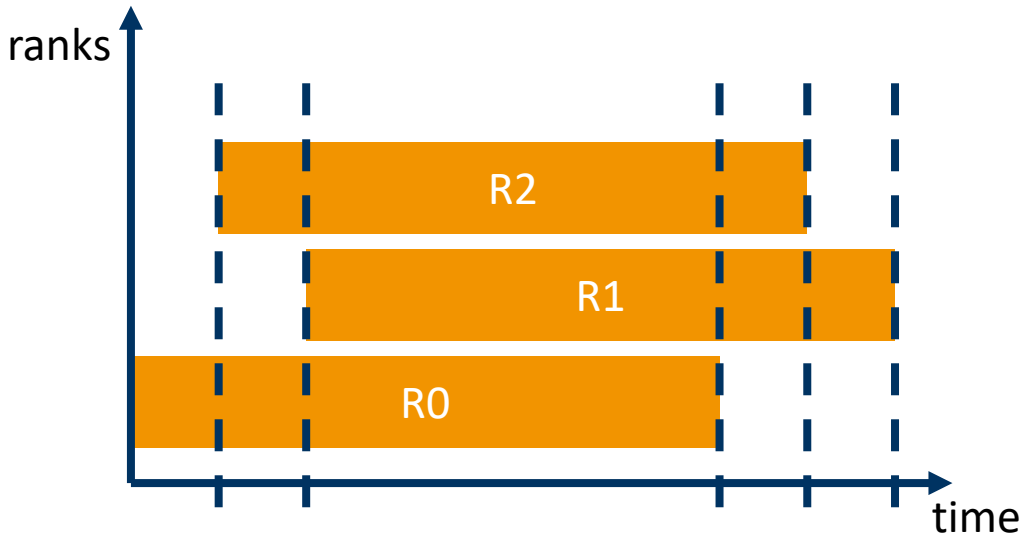
- difficult to optimize without measuring
  - measurements are crucial for everything in computer science
  - How do you know whether program performance improved or not?
  - risk of *premature optimization*
- difficult to measure without knowing what is measured and how
  - know your metrics!
    - performance, time, efficiency, memory footprint, energy, FLOPs, cache misses, cyclomatic complexity, …
- 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”
- *cpu time*
  - wall time for each rank
  - cumulative over all ranks, varies with degree of parallelism
  - the default when talking “costs”

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



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

Time is parallel too

- synchronizing clocks over a large-scale system is very difficult
  - e.g. x86' TSC: in-core **T**ime**S**tamp **C**ounter, 1 clock cycle tick rate (< 1 ns)
  - can be read with a single instruction (`rdtsc` / `rdtscp`)
  - 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 (on different nodes!)
  - no issue if moderate accuracy and resolution requirements
  - otherwise check synchronization first (e.g. `MPI_WTIME_IS_GLOBAL` using `MPI_Comm_get_attr()`)

- also: mind the timer resolution in general
  - e.g. don't measure time intervals of 1-2 milliseconds with a 1 millisecond resolution
  - good practice: at least 10x higher resolution 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: $t_p = \frac{t_s}{p}$ and 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/core
  - 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

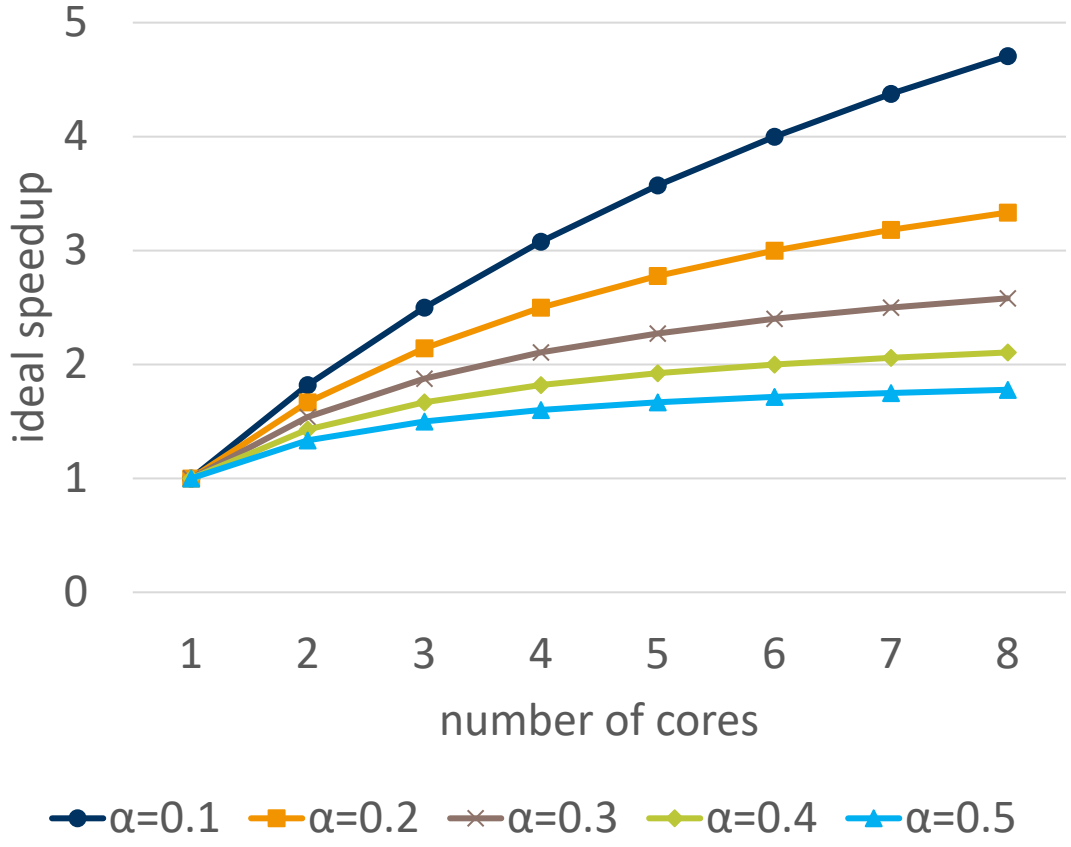
- measure of parallelization overhead
  - value range given between 0 and 1 or as a percentage
- $\text{efficiency}_p = \frac{\text{speedup}_p}{p}$
- ideal: $\text{efficiency}_p = 1$ (= linear speedup)
- worst case: $\lim_{p \to \infty} \text{efficiency}_p = 0$

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 characteristics

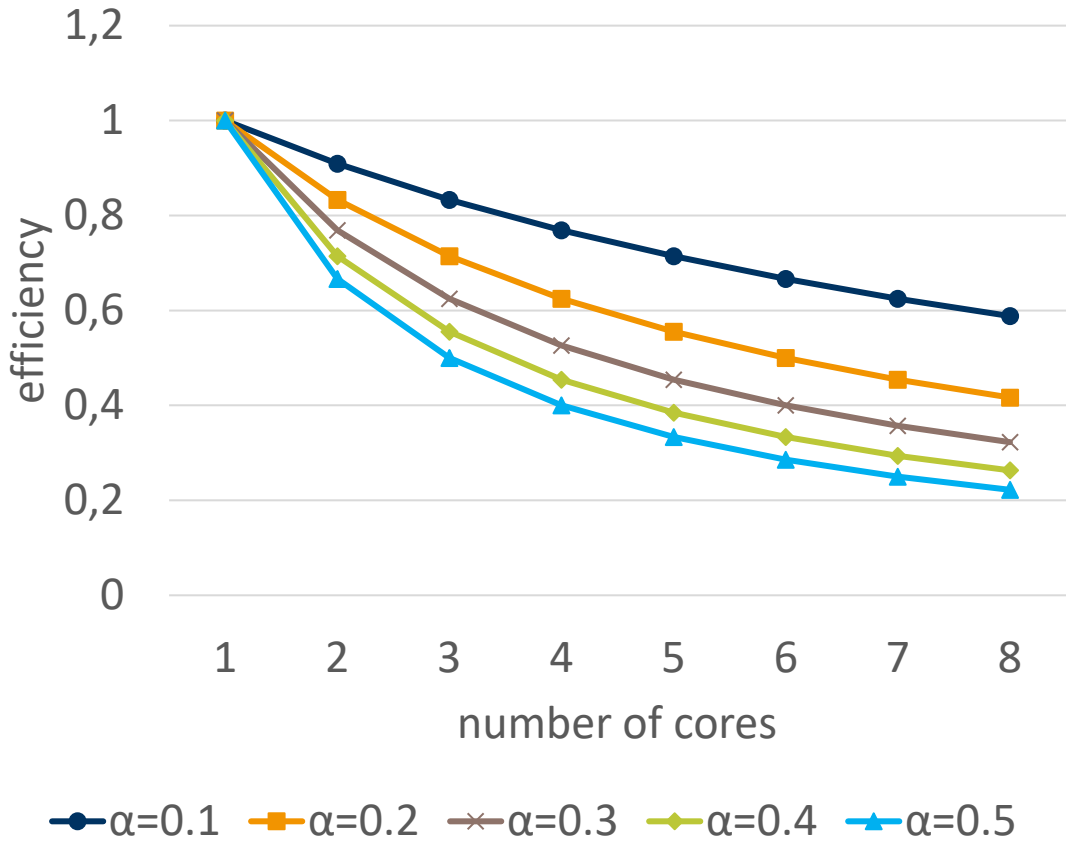
Amdahl's Law cont'd

- 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)
  - theoretical speedup on 8 cores is 3.33
  - theoretical speedup on ∞ cores is 5



Amdahl's Law: efficiency

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



Amdahl's Law: implications

- first order of business: minimize α!
  - change algorithm to reduce amount of sequential part
    - careful, changes reference for relative speedup
  - optimize sequential part as much as possible

- don't spend excessive effort on optimizing parallel part
  - 80/20 rule: diminishing benefits
  - also: risk of premature optimization

- consider a sensible maximum degree of parallelism
  - don't allocate 1024 processors when using 128 is acceptably fast
  - also consider other users, power consumption, cpu time budgets, …!

Amdahl's Law: shortcomings

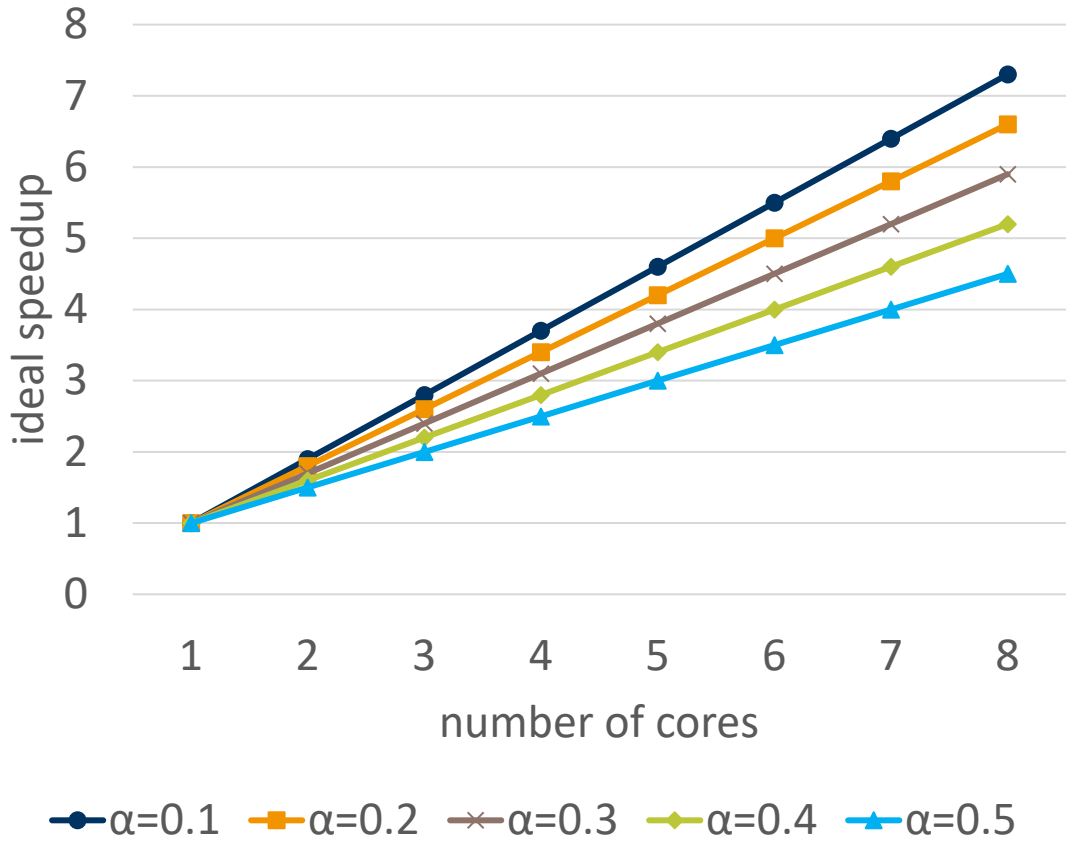
- Noticed, that it assumes the amount of work to be fixed?
  - not realistic for many use cases, problem size often scales with machine size
  - some problems are solved in real-time (e.g. rendering)
    but at the highest problem size (e.g. image quality) possible
  - more resources (=processors/cores)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

- John Gustafson reevaluated this issue in 1988

  ➔ Gustafson's Law

Gustafson's Law cont'd

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



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?
    - Consider a 2D problem: scale first dimension? Second? Both? What about in 3D/4D/5D?

Additional Metrics

FLOPS

- floating point operations (FLOP/s: per second)
  - only operations with floating point semantics (=math)
  - 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
```

Getting FLOPS data

- instrumentation and measurement
  - `perf`, `PAPI`, etc.
  - use performance counters (also “hardware counters”)
  - 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 Tiger Lake CPUs)

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: Processor Programming Reference (PPR) documentation

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
```

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 (PFlop/s)	Rpeak (PFlop/s)	Power (kW)
1	**El Capitan** - HPE Cray EX255a, AMD 4th Gen EPYC 24C 1.8GHz, AMD Instinct MI300A, Slingshot-11, TOSS, HPE DOE/NNSA/LLNL United States	11,039,616	1,742.00	2,746.38	29,581
2	**Frontier** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, HPE Cray OS, HPE DOE/SC/Oak Ridge National Laboratory United States	9,066,176	1,353.00	2,055.72	24,607
3	**Aurora** - HPE Cray EX - Intel Exascale Compute Blade, Xeon CPU Max 9470 52C 2.4GHz, Intel Data Center GPU Max, Slingshot-11, Intel DOE/SC/Argonne National Laboratory United States	9,264,128	1,012.00	1,980.01	38,698
4	**Eagle** - Microsoft NDv5, Xeon Platinum 8480C 48C 2GHz, NVIDIA H100, NVIDIA Infiniband NDR, Microsoft Azure Microsoft Azure United States	2,073,600	561.20	846.84	
5	**HPC6** - HPE Cray EX235a, AMD Optimized 3rd Generation EPYC 64C 2GHz, AMD Instinct MI250X, Slingshot-11, RHEL 8.9, HPE Eni S.p.A. Italy	3,143,520	477.90	606.97	8,461

Taken from the November 2024 list of the Top500

Application Throughput

- FLOPS are not everything
  - MB/s achieved RAM bandwidth?
  - MB/s achieved I/O bandwidth?

- consider what the application does
  - Eulerian simulation (compute properties at grid points): cells/s
  - Lagrangian simulation (no grid but moving particles): particles/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

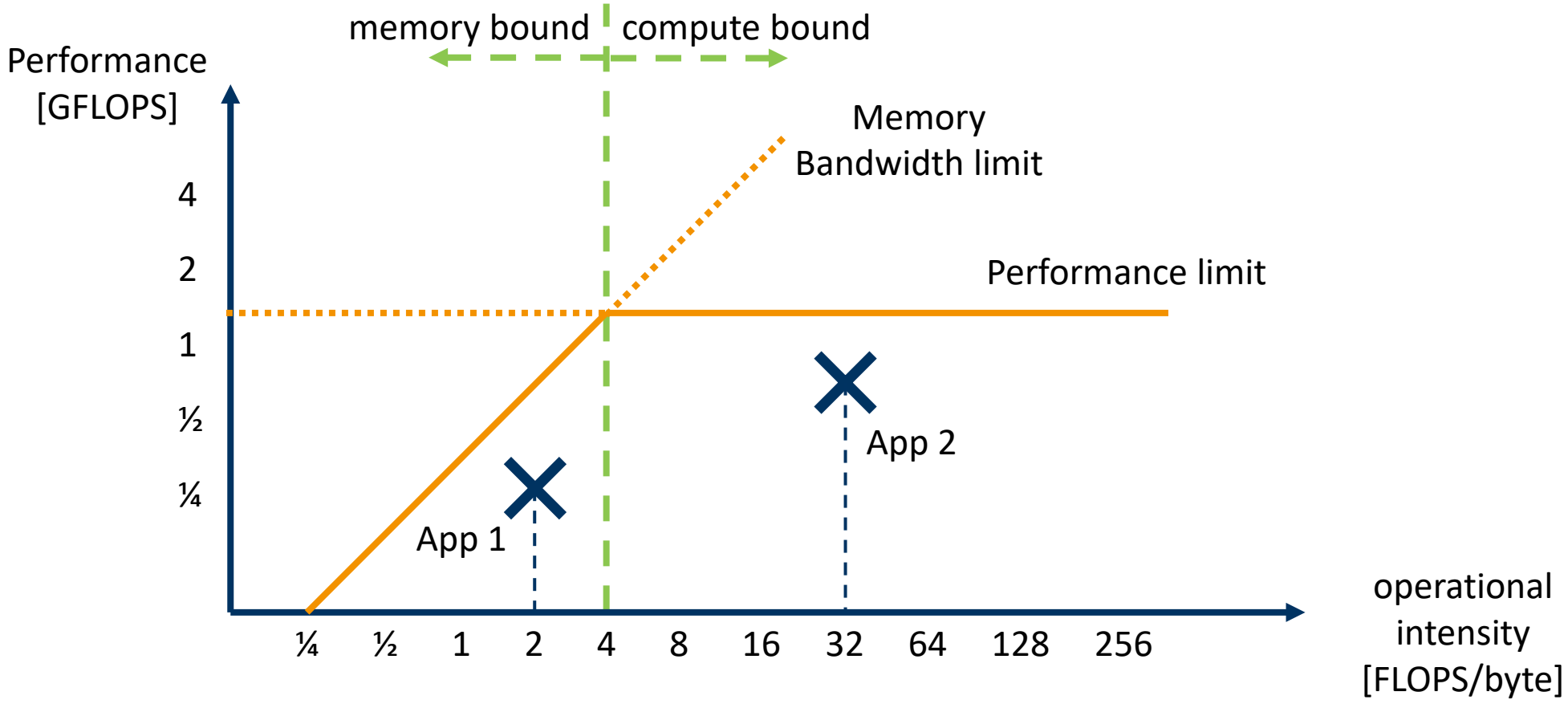
Compute bound vs. memory bound (vs. communication bound)

- 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 whether one is compute bound or memory bound
  - indicates which optimizations to apply

“Roofline” model cont’d



Driving optimizations

- If roofline model says “memory bound”, check e.g.
  - cache optimality of algorithm
  - NUMA mapping/bindings
  - software prefetching, compression, etc.

- If roofline model says “compute bound”, check e.g.
  - vectorization (SIMD)
  - compiler optimizations
  - software caching (“memoization”)

Properly Reporting Data

How to report metrics? (very brief, non-exhaustive)

- Number of repetitions?
  - Just a single run?
  - Three runs for averaging?
- Multiple hardware platforms?
  - Same or different architecture?
- Reproducibility of measurements?
  - What information is required to enable reproducibility?
- Show all collected data?
  - Select data, and if so, how?
  - Aggregate data, and if so, how?
  - Report absolute or relative values?
- …

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?

- One approach: 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
  - $n = \left(\frac{s \times t\left(n-1, \frac{\alpha}{2}\right)}{e\bar{x}}\right)^2$
  - 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
  - requires at least a couple of runs to compute first 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
  - ideally, backup raw data!
- 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 (degree of 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!

Reading recommendations

Twelve Ways to Fool the Masses When Giving Performance Results on Parallel Computers

David H. Bailey

June 11, 1991

Ref: Supercomputing Review, Aug. 1991, pg. 54--55

Abstract

Many of us in the field of highly parallel scientific computing recognize that it is often quite difficult to match the run time performance of the best conventional supercomputers. This humorous article outlines twelve ways commonly used in scientific papers and presentations to artificially boost performance rates and to present these results in the "best possible light" compared to other systems.

The author is with the Numerical Aerodynamic Simulation (NAS) Systems Division at NASA Ames Research Center, Moffett Field, CA 94035.

Many of us in the field of highly parallel scientific computing recognize that it is often quite difficult to match the run time performance of the best conventional supercomputers. But since lay persons usually don't appreciate these difficulties and therefore don't understand when we quote mediocre performance results, it is often

Scientific Benchmarking of Parallel Computing Systems

Twelve ways to tell the masses when reporting performance results

Torsten Hoefler
Dept. of Computer Science
ETH Zurich
Zurich, Switzerland
htor@inf.ethz.ch

Roberto Belli
Dept. of Computer Science
ETH Zurich
Zurich, Switzerland
bellir@inf.ethz.ch

ABSTRACT

Measuring and reporting performance of parallel computers constitutes the basis for scientific advancement of high-performance computing (HPC). Most scientific reports show performance improvements of new techniques and are thus obliged to ensure reproducibility or at least interpretability. Our investigation of a stratified sample of 120 papers across three top conferences in the field shows that the state of the practice is lacking. For example, it is often unclear if reported improvements are deterministic or observed by chance. In addition to distilling best practices from existing work, we propose statistically sound analysis and reporting techniques and simple guidelines for experimental design in parallel computing and codify them in a portable benchmarking library. We aim to improve the standards of reporting research results and initiate a discussion in the HPC field. A wide adoption of our minimal set of rules will lead to better interpretability of performance results and improve the scientific culture in HPC.

Categories and Subject Descriptors

D.2.8 [**Software Engineering**]: Metrics—*complexity measures, performance measures*

Keywords

Benchmarking, parallel computing, statistics, data analysis

Reproducing experiments is one of the main principles of the scientific method. It is well known that the performance of a computer program depends on the application, the input, the compiler, the runtime environment, the machine, and the measurement methodology [20, 43]. If a single one of these aspects of *experimental design* is not appropriately motivated and described, presented results can hardly be reproduced and may even be misleading or incorrect.

The complexity and uniqueness of many supercomputers makes reproducibility a hard task. For example, it is practically impossible to recreate most hero-runs that utilize the world's largest machines because these machines are often unique and their software configurations changes regularly. We introduce the notion of *interpretability*, which is weaker than reproducibility. *We call an experiment interpretable if it provides enough information to allow scientists to understand the experiment, draw own conclusions, assess their certainty, and possibly generalize results*. In other words, interpretable experiments support sound conclusions and convey precise information among scientists. Obviously, every scientific paper should be interpretable; unfortunately, many are not.

For example, reporting that an High-Performance Linpack (HPL) run on 64 nodes (N=314k) of the Piz Daint system during normal operation (cf. Section 4.1.2) achieved 77.38 Tflop/s is hard to interpret. If we add that the theoretical peak is 94.5 Tflop/s, it becomes clearer, the benchmark achieves 81.8% of peak performance. But is this true for every run or a typical run? Figure 1

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
  - may require 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
    (e.g. 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 exact math, 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/top500/2024/11/
- Reading recommendations: https://www.davidhbailey.com/dhbpapers/twelve-ways.pdf, https://htor.inf.ethz.ch/publications/img/hoefler-scientific-benchmarking.pdf