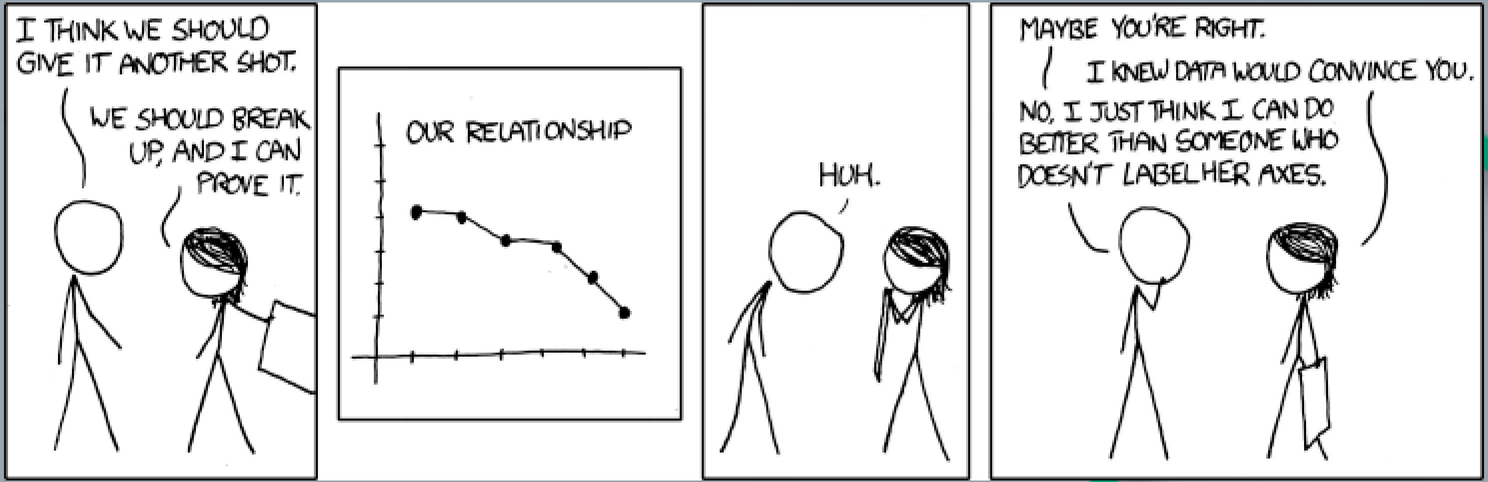
Designing experiments and presenting data



https://xkcd.com/833/

Overview

- Preliminaries
  - Questions to ask
  - Compile, run, document

- What and how to measure
  - Metrics
  - Digits
  - Variation

- How to present the data
  - Avoiding blatant mistakes
  - Exposing relevant effects

Data taking is just the beginning.

Science emerges from communication.

Preliminaries

Questions to ask

1. What is the scientific question?

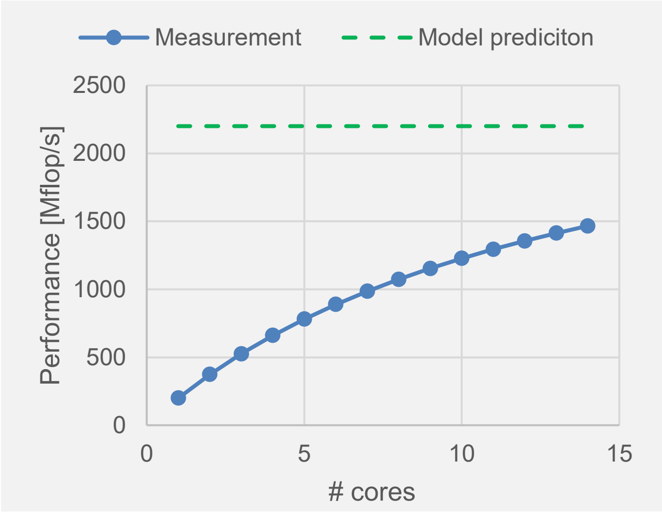
   Example: “Does this parallel loop achieve the predicted performance limit on my CPU?”

2. What measurements do I need to discuss/answer it?

   Example: Loop runtime for # of cores from 1 … max

3. How do I present the data so my conclusions are communicated clearly?

   Example: x-y plot of performance (work/time) vs. # cores, including comparison with expectation



The most important question

4. Would the audience/readers, given the resources, be able to interpret and reproduce what I did?

   Example: Specify

   - System environment
   - Compilers & compiler options
   - Library versions
   - Execution modalities (affinity, rank mapping, # of repetitions, frequency settings,…)

Some useful general hints

- Load modules with full version (`intel/2022.1.0`) and document it
- Compile code with optimization flags suitable for system
  - Intel: `-O3 -xHost` is usually a good start
  - Document the flags
- Always run with pinning and controlled CPU frequency
  - Best use base frequency (`likwid-powermeter -i`)
  - `srun --cpu-freq=X-Y:performance` or `likwid-setFrequencies`
  - Document the settings
- Capture raw output in a logfile for later analysis
  - `$ ./run.sh 2>&1 | tee $(hostname -s).log`
- Perform manual runs AND check output before thinking about scripting

What and how to measure

What and how to measure

- What to measure?
  - … depends on what you want to investigate
  - In HPC, this is often runtime (and other stuff based on it)

```
#include <time.h>

double timestamp(void) {
    struct timespec ts;
    clock_gettime(CLOCK_MONOTONIC, &ts);
    return (double)ts.tv_sec + (double)ts.tv_nsec * 1.e-9;
}

double resolution(void) {
    struct timespec ts;
    clock_getres(CLOCK_MONOTONIC, &ts);
    return (double)ts.tv_sec + (double)ts.tv_nsec * 1.e-9;
}
```

Finite resolution/granularity

```
const int N=100;

auto s = timestamp();
for(int i=0; i<N; ++i)
   sum += a[i];
auto runtime = timestamp() - s;
auto perf = N/runtime;
```

```
int NITER = 1;
for(;;) {
  auto s = timestamp();
  for(int k=0; k<NITER; ++k) {
    for(int i=0; i<N; ++i)
      sum += a[i];
    if(sum < 0.) dummy(&s,a);
  }
  runtime = timestamp() - s;
  if(runtime >= 0.1) break;
  NITER *= 2;
}
auto perf = double(N)*NITER/runtime;
```

- Runtime = raw metric
- Performance = derived metric
- Warmup iterations might be necessary
- Coarse granularity may also apply to other metrics (HW events)

Raw and derived metrics

Raw metrics/events

- wall-clock time [s]
- clock cycles [cy]
- Instructions [ins]
- floating-point instructions
- (mispredicted) branches
- cache line transfers
- cache/TLB misses
- energy consumption [Joule]
- …

Derived metrics

- clock frequency [cy/s]
- IPC [ins/cy] or CPI [cy/ins]
- FP performance [flop/cy,flop/s]
- branch misprediction ratio
- data transfer bandwidth [byte/cy,byte/s]
- cache miss ratio
- power dissipation [W]
- …

Number of digits

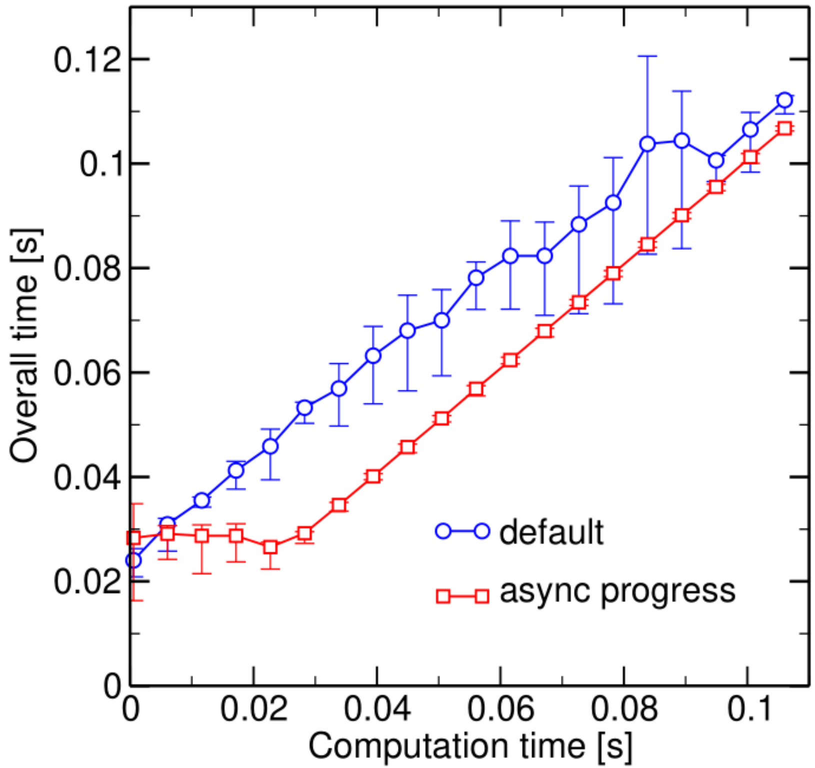
- Most measurements are not accurate to many digits
  - 3 digits mostly suffice

# cores	Time (plain) [s]	Time (optimized) [s]	Speedup [%]
1	12.0435766	8.6198441	39.71919283
2	6.1179025	5.5901951	9.439874469
3	4.9041394	4.6966098	4.418710705
4	4.7002801	4.6912042	0.193466317

Statistical variation (I)

- Although computers are supposed to be deterministic machines, measurements often fluctuate

- Communicate if fluctuations are relevant or not
  - If they are, include statistical data in your presentation!



Statistical variation (II)

Many metrics in HPC are usually not normally distributed

→ Median may be more appropriate than average

→ multi-modal distributions can be represented by violin plots

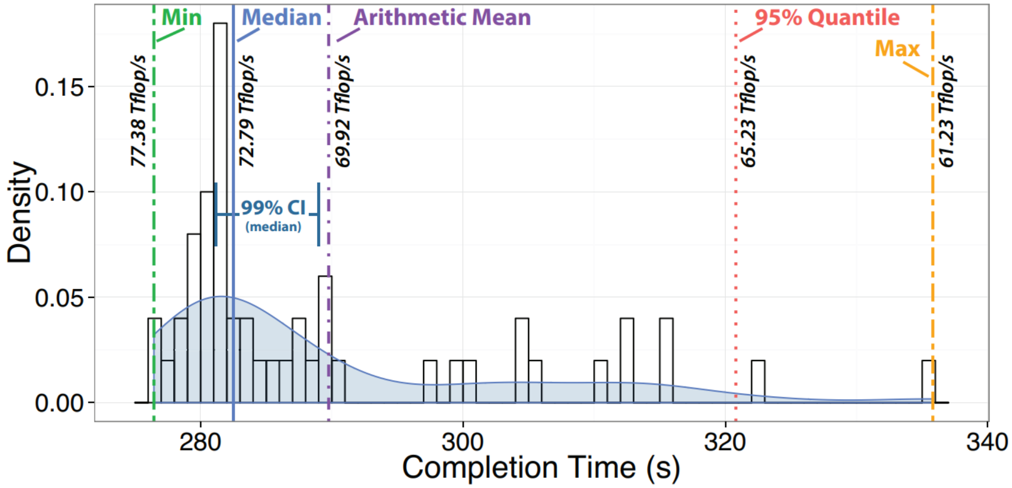
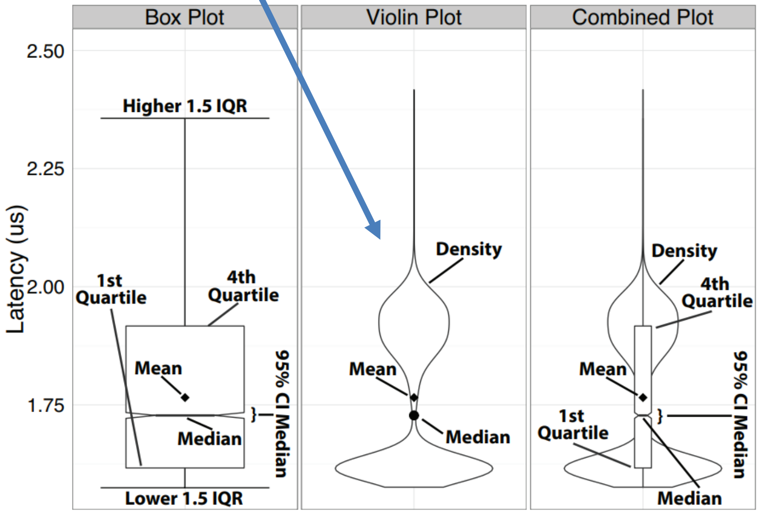
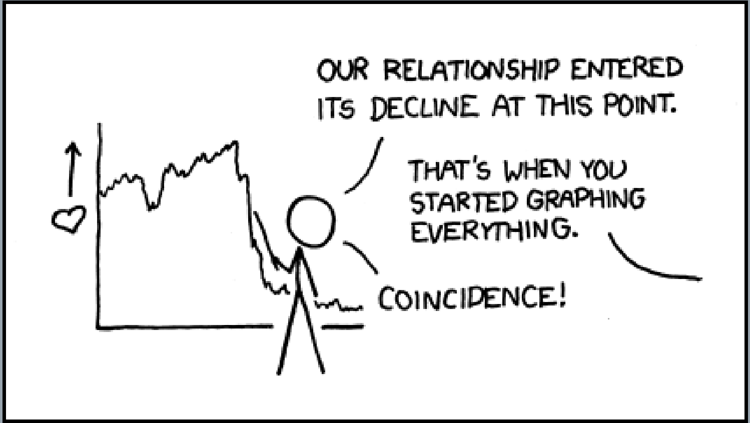


Figure 1: Distribution of completion times for 50 HPL runs.



Hoefler & Belli, DOI: [10.1145/2807591.2807644](https://doi.org/10.1145/2807591.2807644)

Presenting data with graphs



https://xkcd.com/523/

See also:
Justin Zobel: *Writing for Computer Science* (Ch. 11)
https://doi.org/10.1007/978-1-4471-6639-9

General guidelines

- X-Y plots showing measured data …
  - have meaningful labeling at the axes including units,
  - provide a meaningful caption that allows to interpret what is seen,
  - have a title describing the environment (system, settings) or provide this info in the caption,
  - have a legend if more than one data set is shown,
  - have their y-axis start at 0 unless there is a very good reason not to,
  - use log scale with care,
  - may use straight lines to connect data points to “guide the eye”

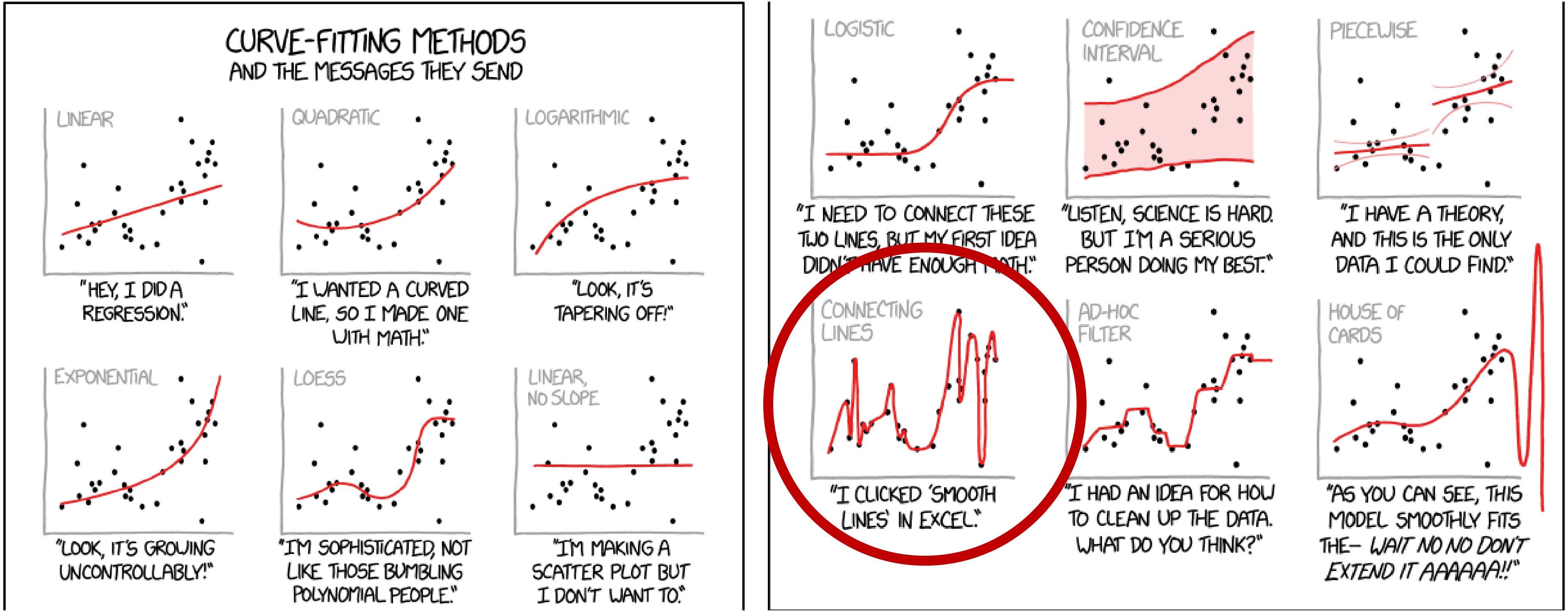
Graphs: the good, the bad, and the ugly

Figure 1: Scaling on Meggie

WTF??

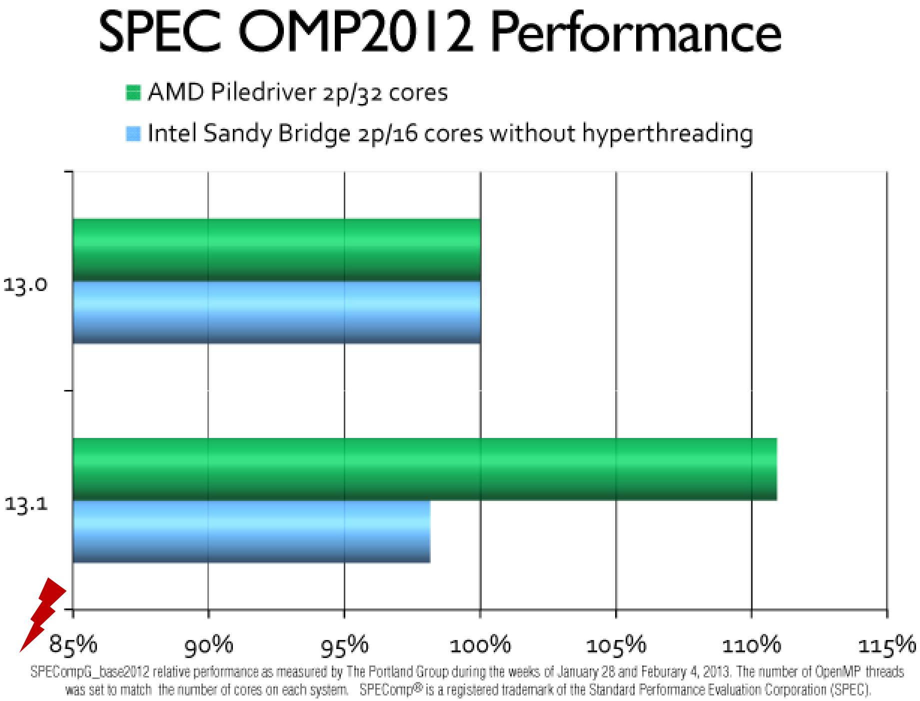
I'll have your head on a stick for such a presentation!

Curve fitting

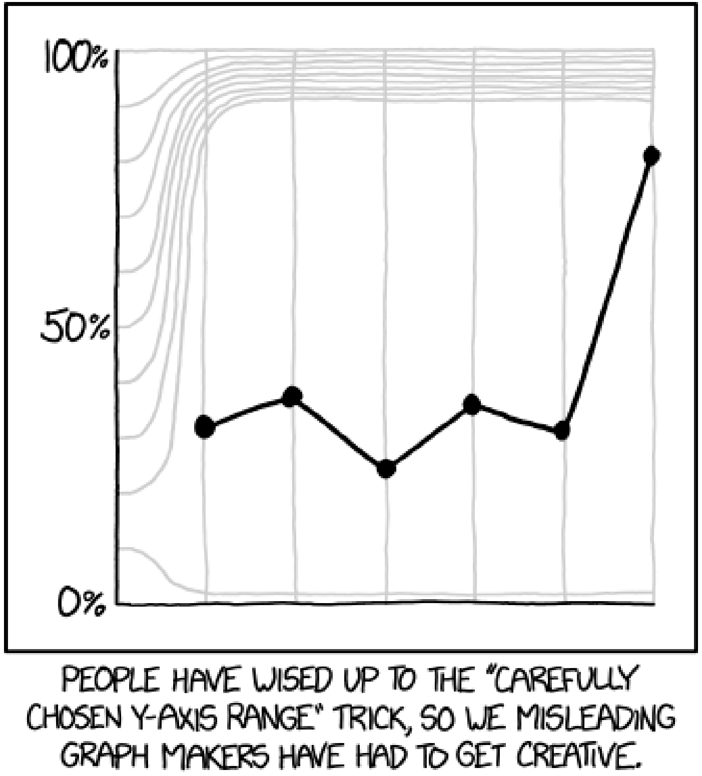


https://xkcd.com/2048

Axes



http://www.pgroup.com/images/charts/spec_omp2012_chart_big.png



https://xkcd.com/2023/

Graphs: the good, the bad, and the ugly

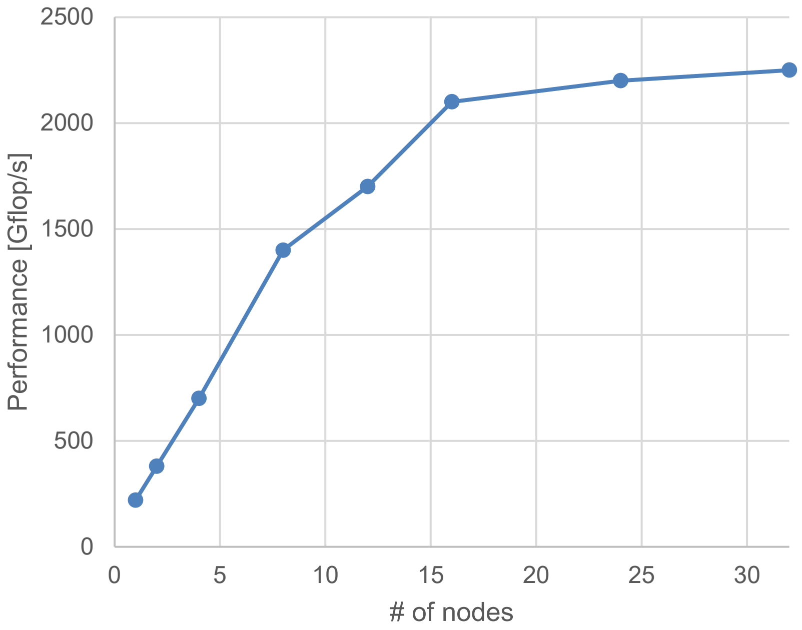


Figure 1: Performance scaling of the hybrid “CoolCFD” code on Meggie with problem set A

Provide the necessary information to allow the reader to connect the presented data to the rest of your presentation/paper

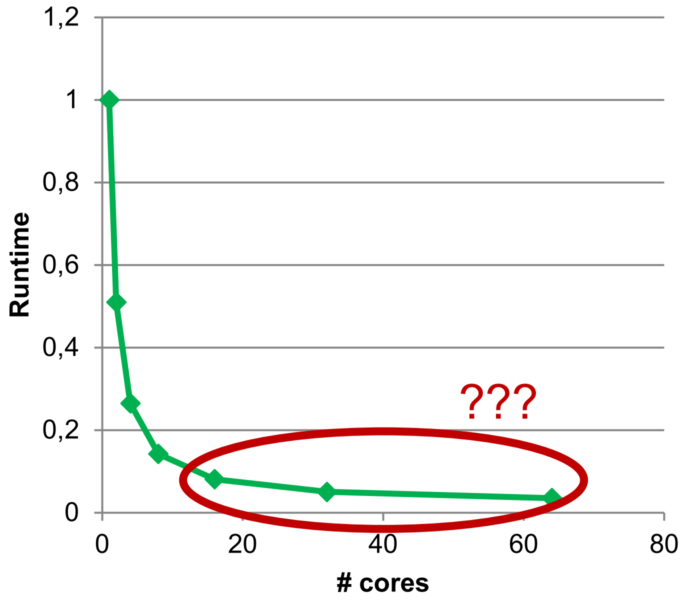
Exposing relevant effects

Showing what you want to show

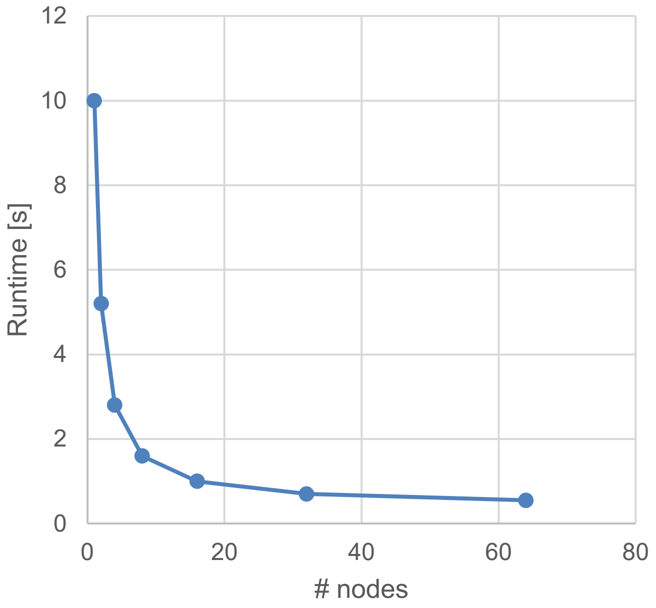
Runtime or performance scaling?

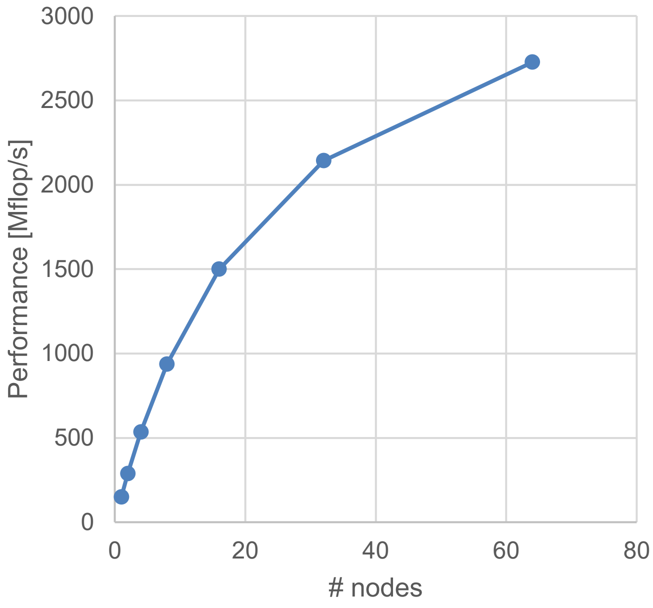
- Ultimately, the user wants to know
  "How long will my problem take to solve?"
- Plotting runtime vs. resources answers this question

- However…
  - Scaling behavior hard to visualize
  - Hard to generalize to different problem size



Runtime or performance?



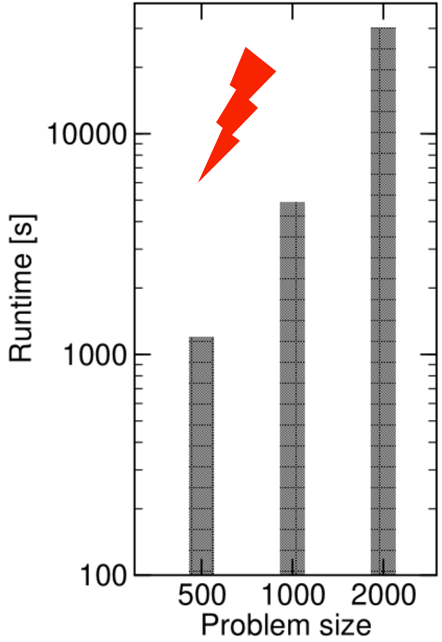


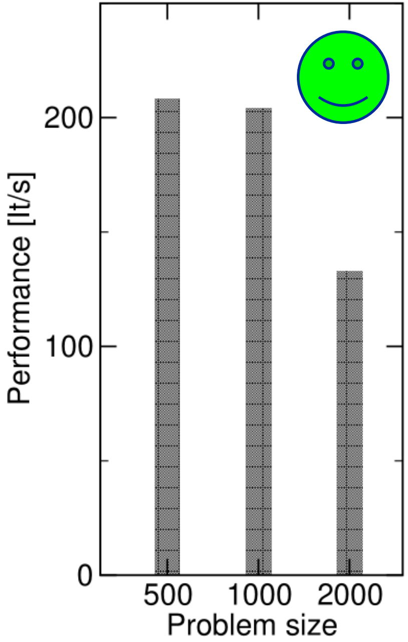
Performance is often the superior metric because it is normalized to a defined unit of work and scaling behavior is easier to read on a linear graph

Exposing the relevant effects

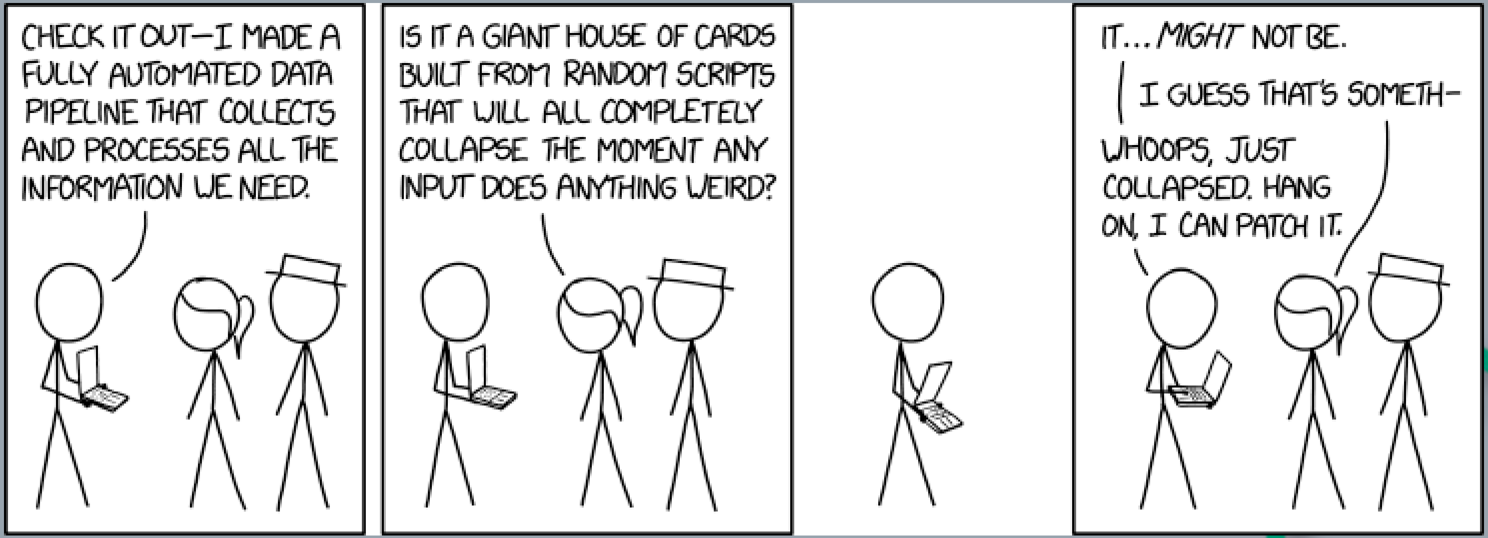
- Present data in a way that exposes the interesting correlations and ignores "trivial" dependencies
- Example: runtime or performance vs. problem size?
  - Runtime has a trivial dependence of "larger problem takes longer"
  - Performance vs. problem size shows clearly a fundamental change with larger problems

- This is highly problem specific!





Thank you.



https://xkcd.com/2054/