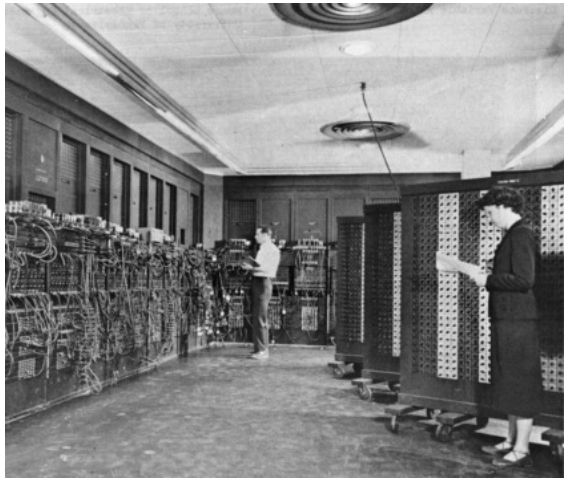
High Performance Computing: Towards Better Performance Predictions and Experiments

Tom Cornebize

2 June 2021, PhD defense

No science without computing

Arithmomètre (1851)



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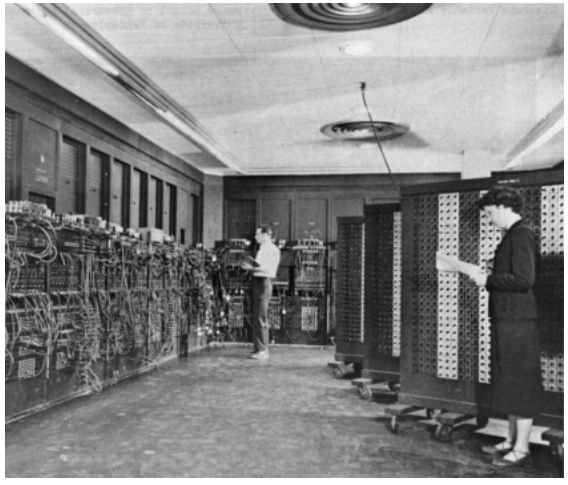

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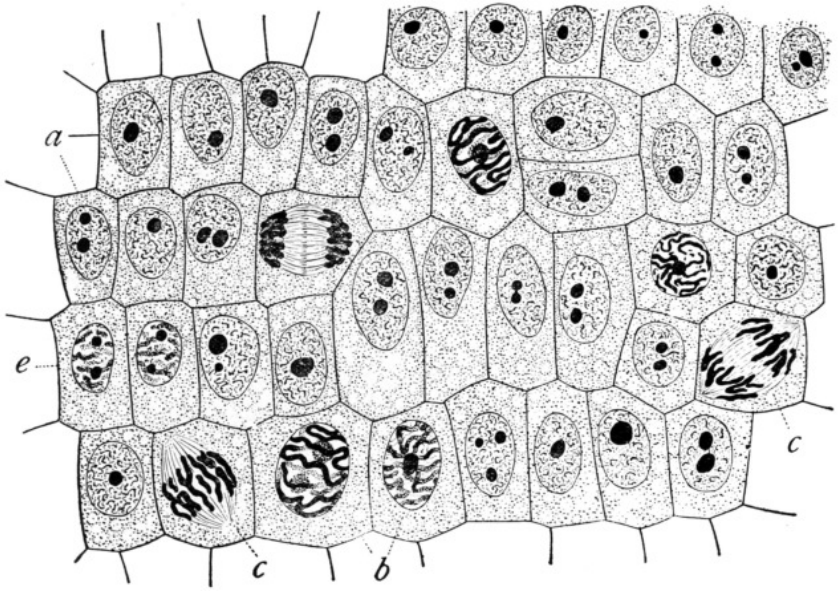
Last decades:

- Exponential performance improvements (e.g. sequencing an entire human genome costed $100,000,000 in 2001, $1000 now)
- At the price of complexity (both software and hardware)

Experimental study of computer performance



Similar to natural sciences

Complexity $\Rightarrow$ Variability and Opacity

$\Rightarrow$ No perfect model

$\Rightarrow$ Need for experiments

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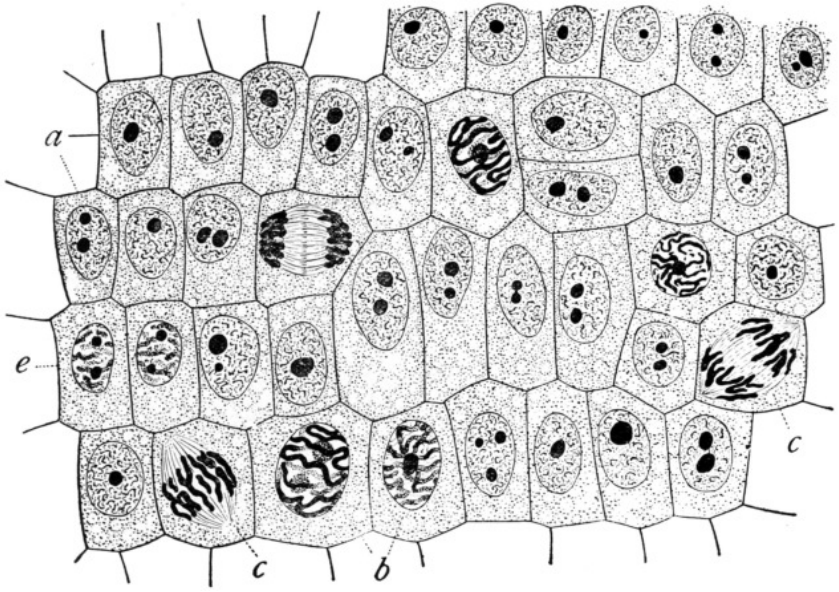

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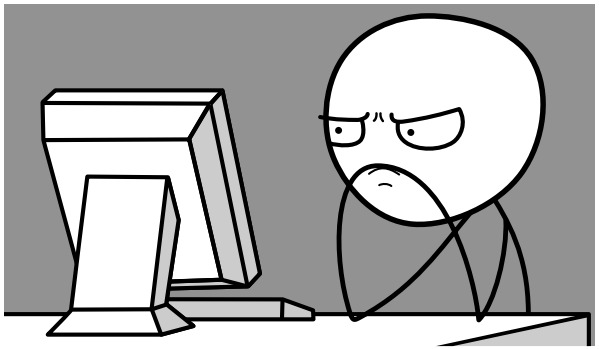
Empirical studies can be carried in reality or in simulation

Context

Typical Performance Evaluation Questions (Given my application and a supercomputer)



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  - For how long?
  - Which parameters?

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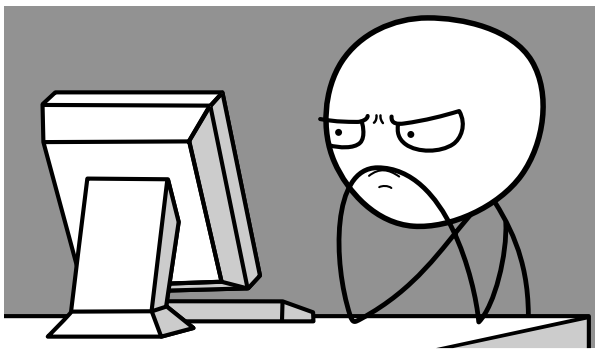

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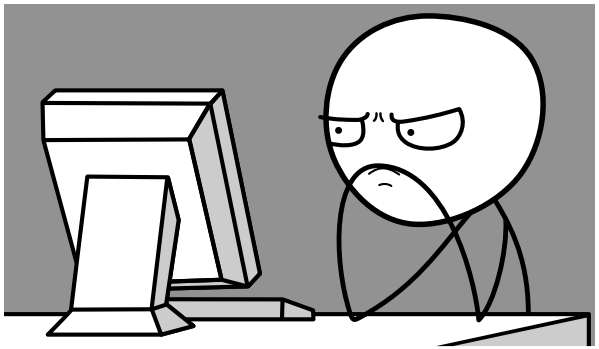

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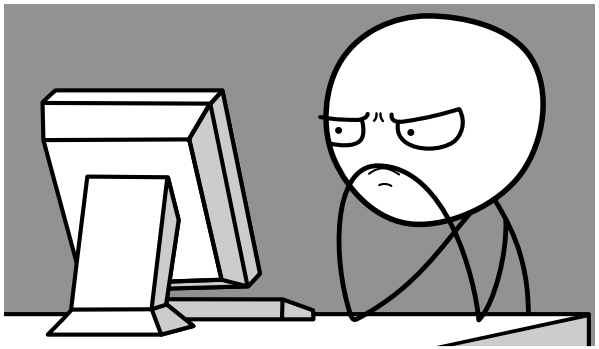

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Holy Grail: Predictive Simulation on a “Laptop”

Capture the **whole application** and **platform complexity**

Initial goal: predict the performance of a parallel application

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Thesis contributions (towards this goal)

- Case study: High Performance Linpack (HPL)
- Extensive (in)validation, comparing simulations with reality
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- Performance tests, to detect eventual platform changes

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Performance prediction through simulation

Sim(Em)ulation: The SMPI Approach

Full reimplementation of MPI on top of SIMGRID

- C/C++/F77/F90 codes run unmodified out of the box
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Emulation: how?

- Application runs for real on a laptop
- Communications are faked, good fluid network models
- Performance model for the target platform

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Contribution: Skip the expensive computations (mostly `dgemm`) and replace them by performance models

Quick word on HPL

Validations of SMPI before this thesis: simple applications without any high performance tricks

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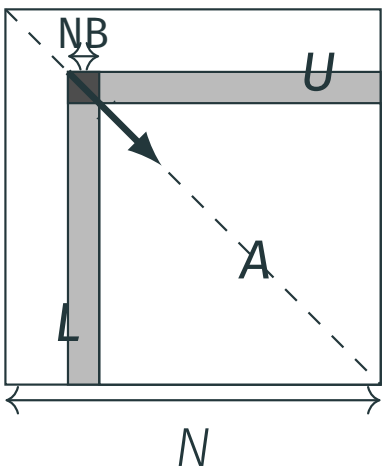

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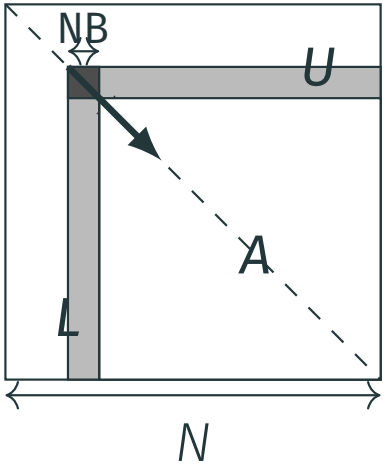

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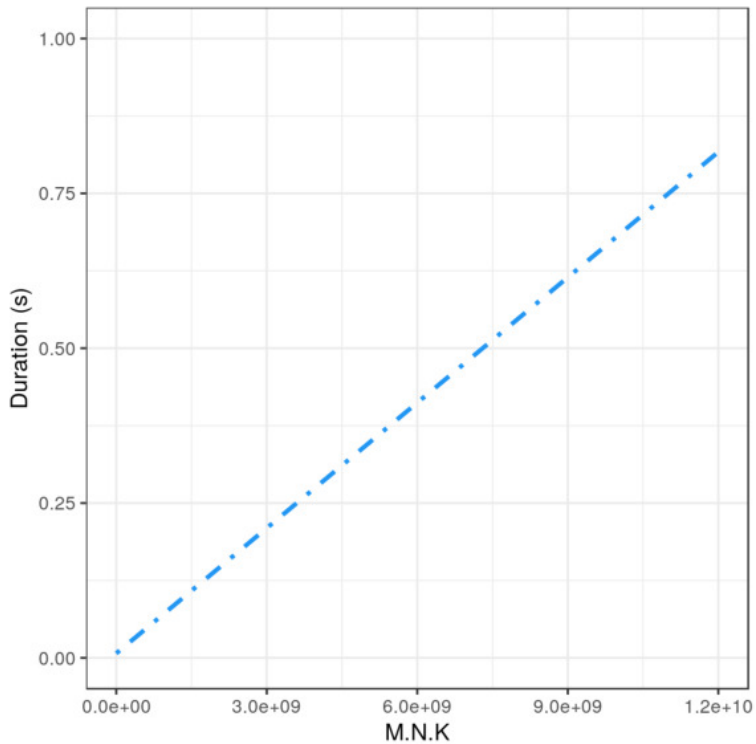
Tuning parameters

- Broadcast algorithm
- Block size
- Process grid
- etc.

Hundreds of combinations

Modeling Commputations

$$\texttt{dgemm}\,(M, N, K) = \alpha.M.N.K$$



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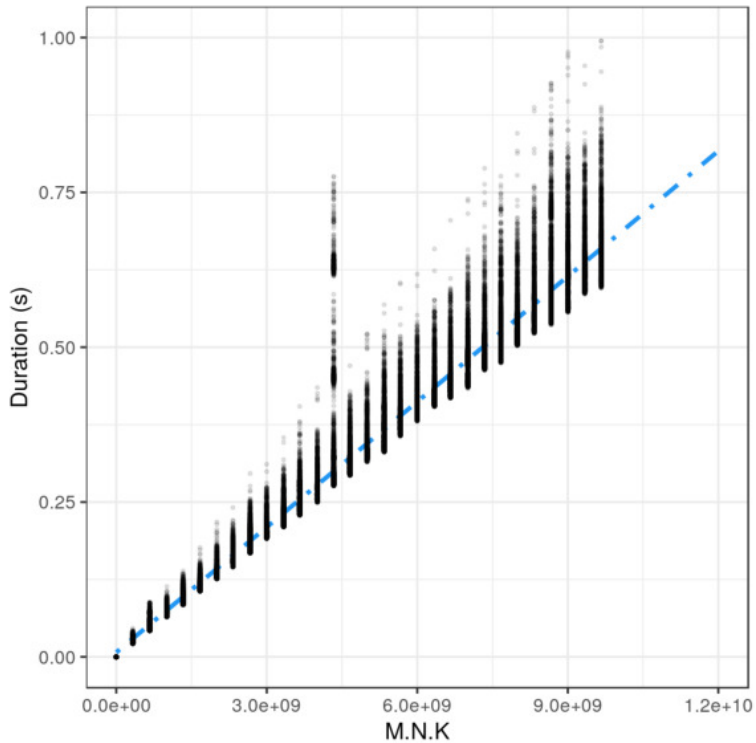

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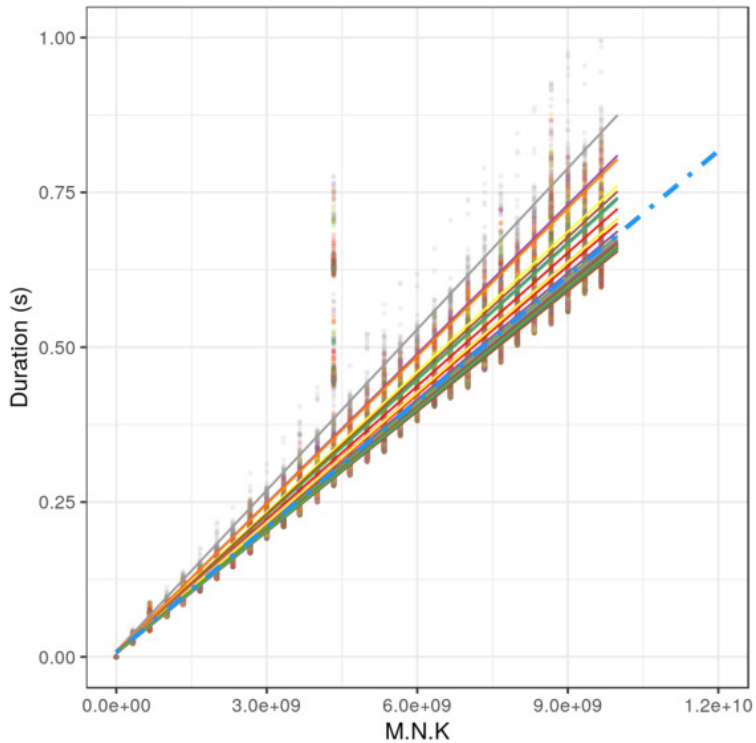
Different color $\Rightarrow$ different host



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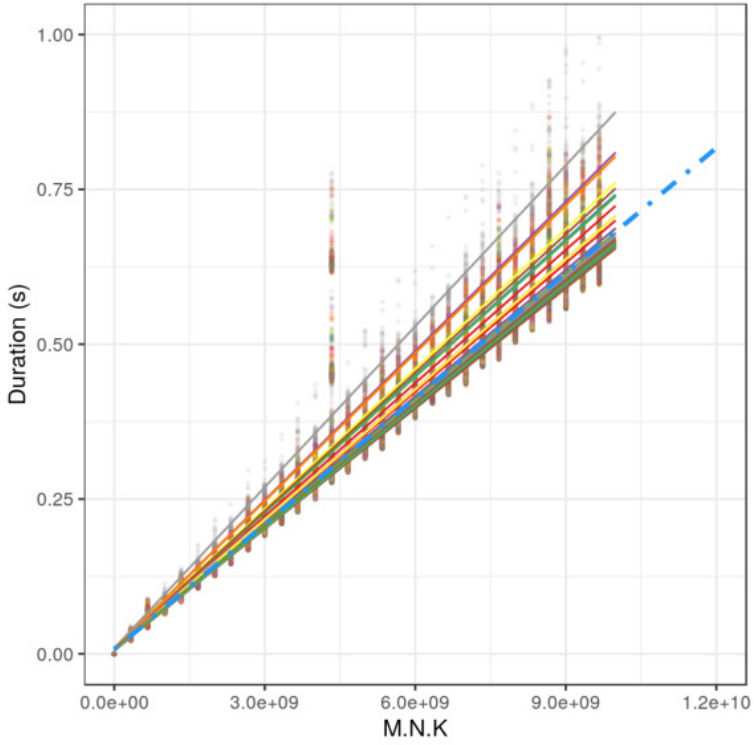

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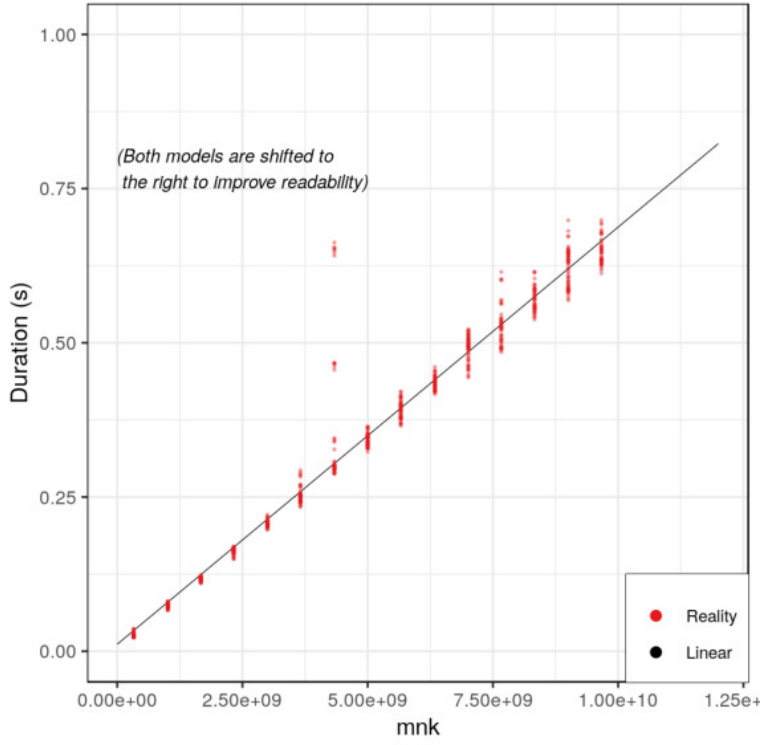

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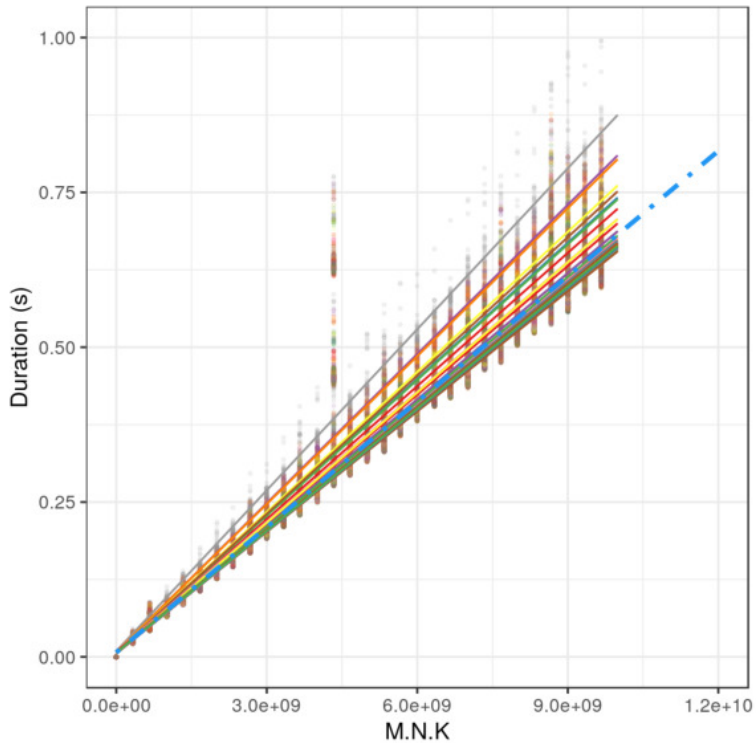

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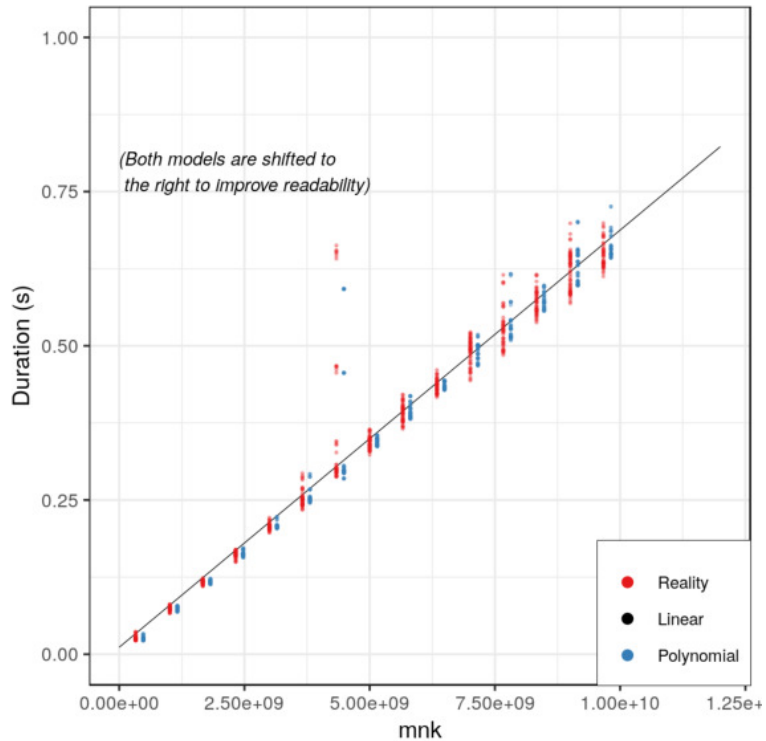

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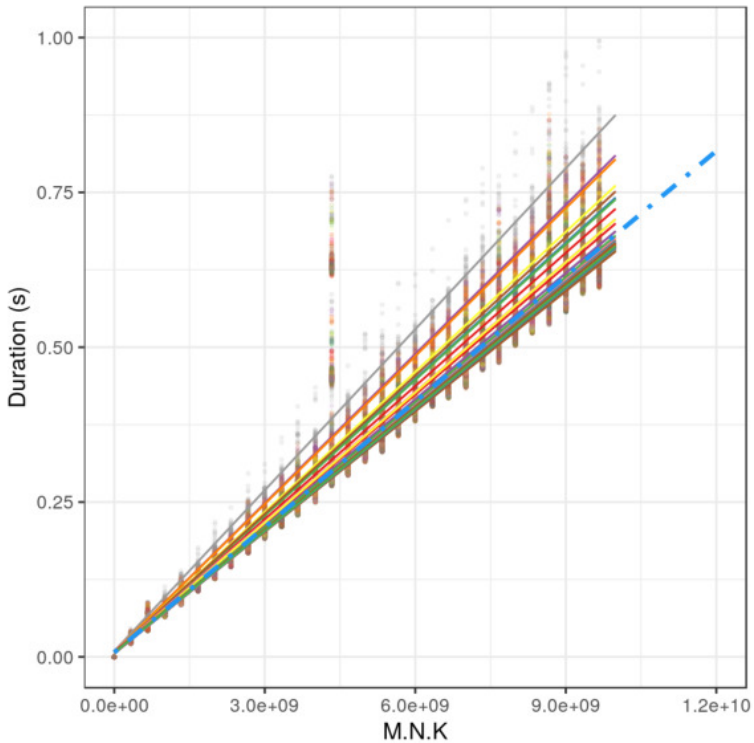

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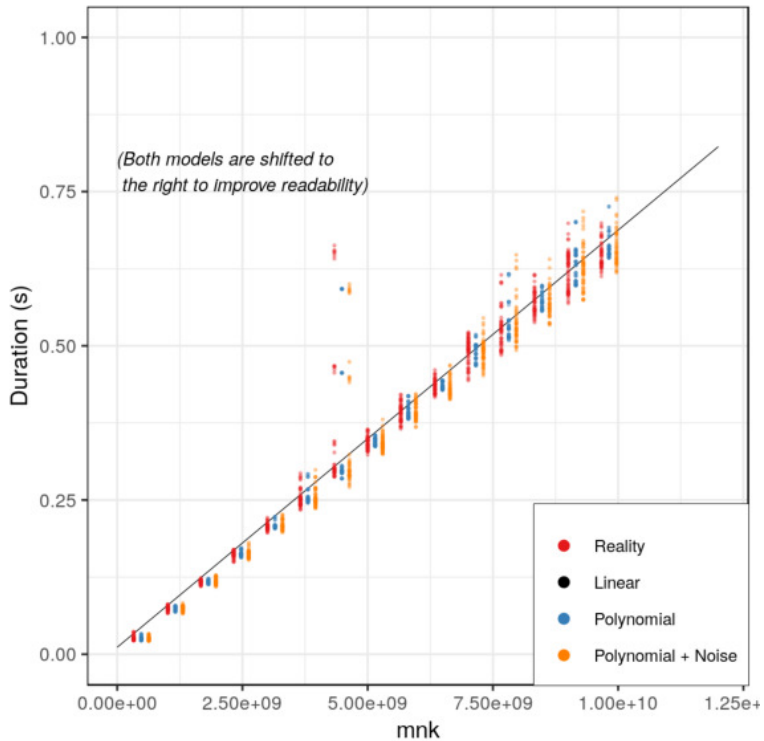

Modeling Communications

Hand-crafted non-blocking collective operations intertwinned with computations

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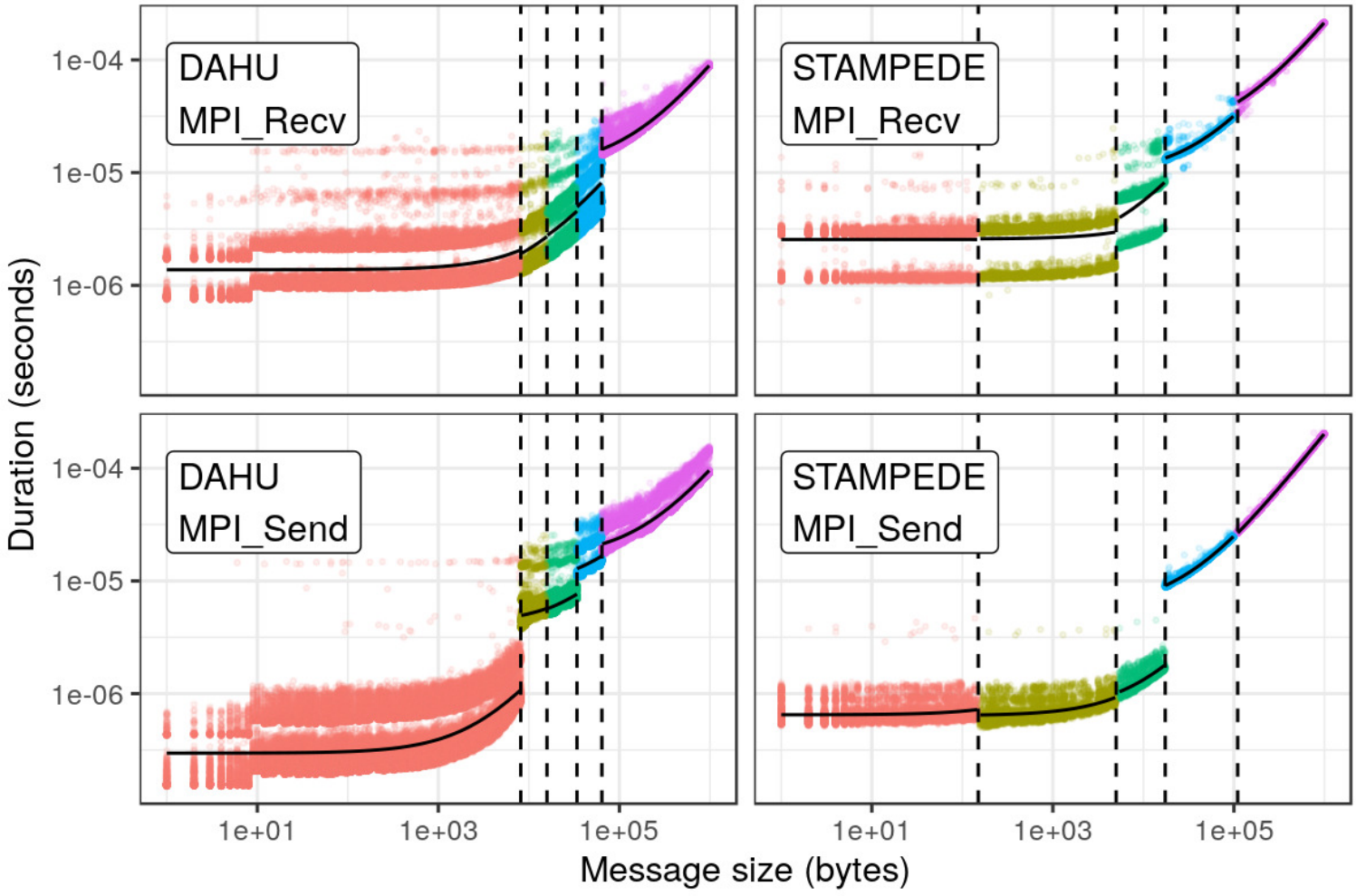
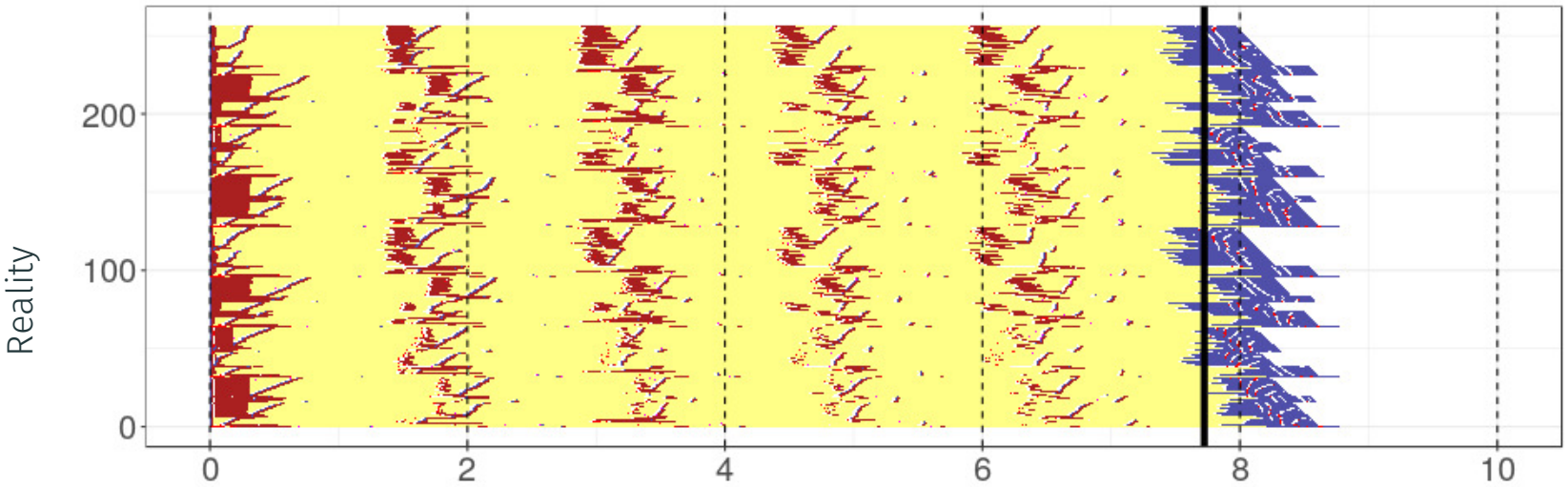


Validating the predictions

Internal behavior of the application

256 MPI ranks, interrupted after the 5^{th} iteration



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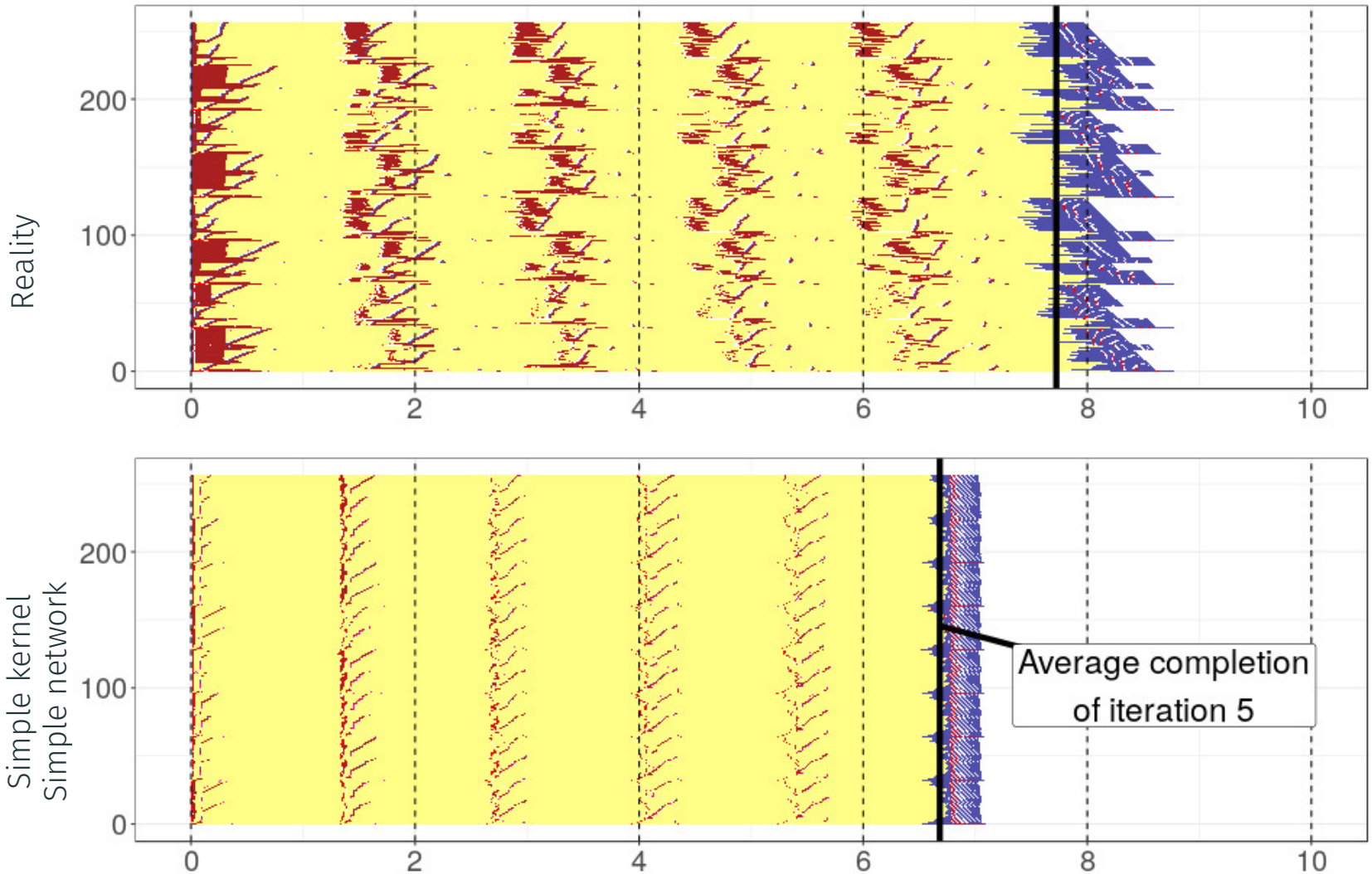

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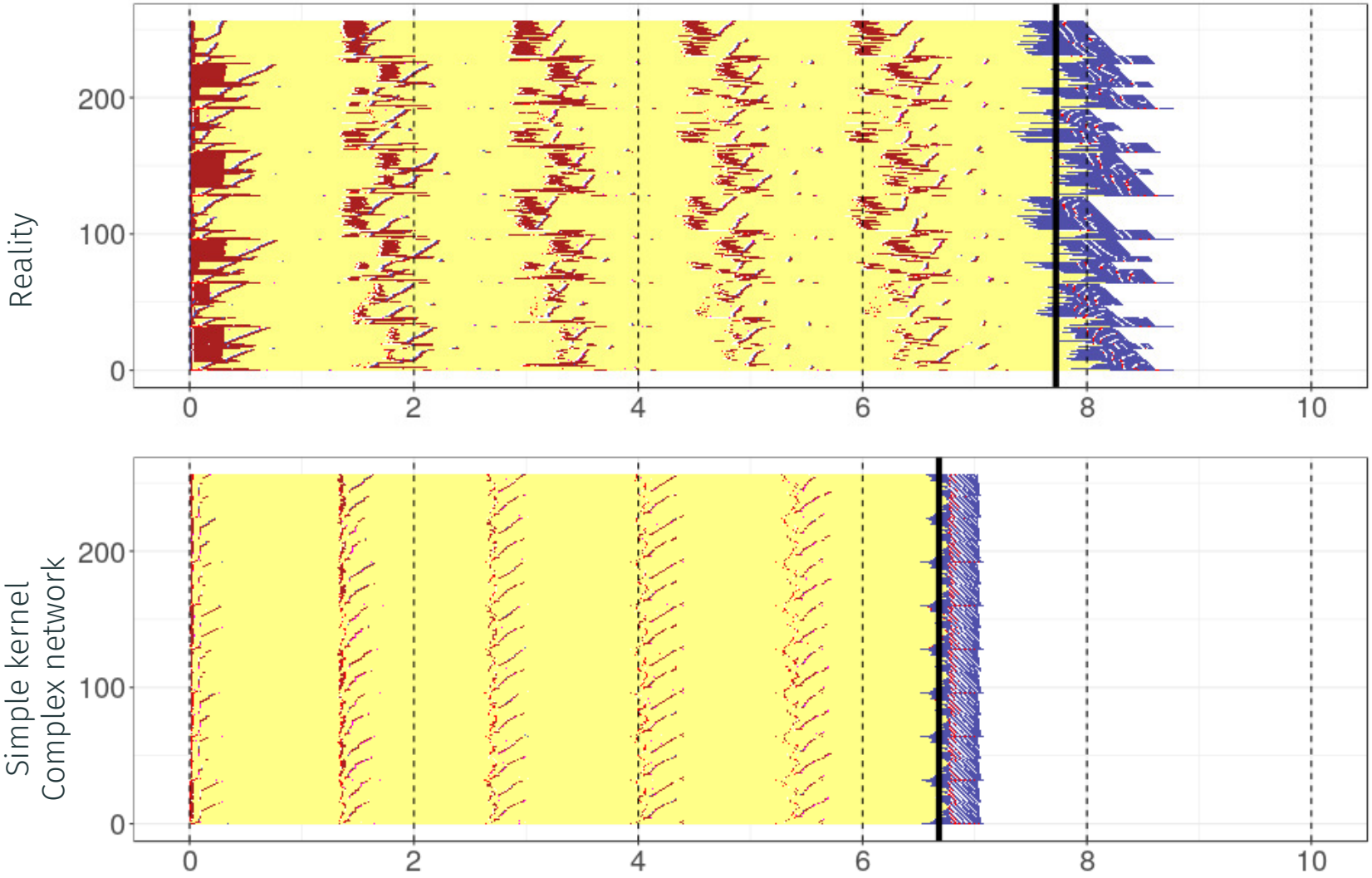

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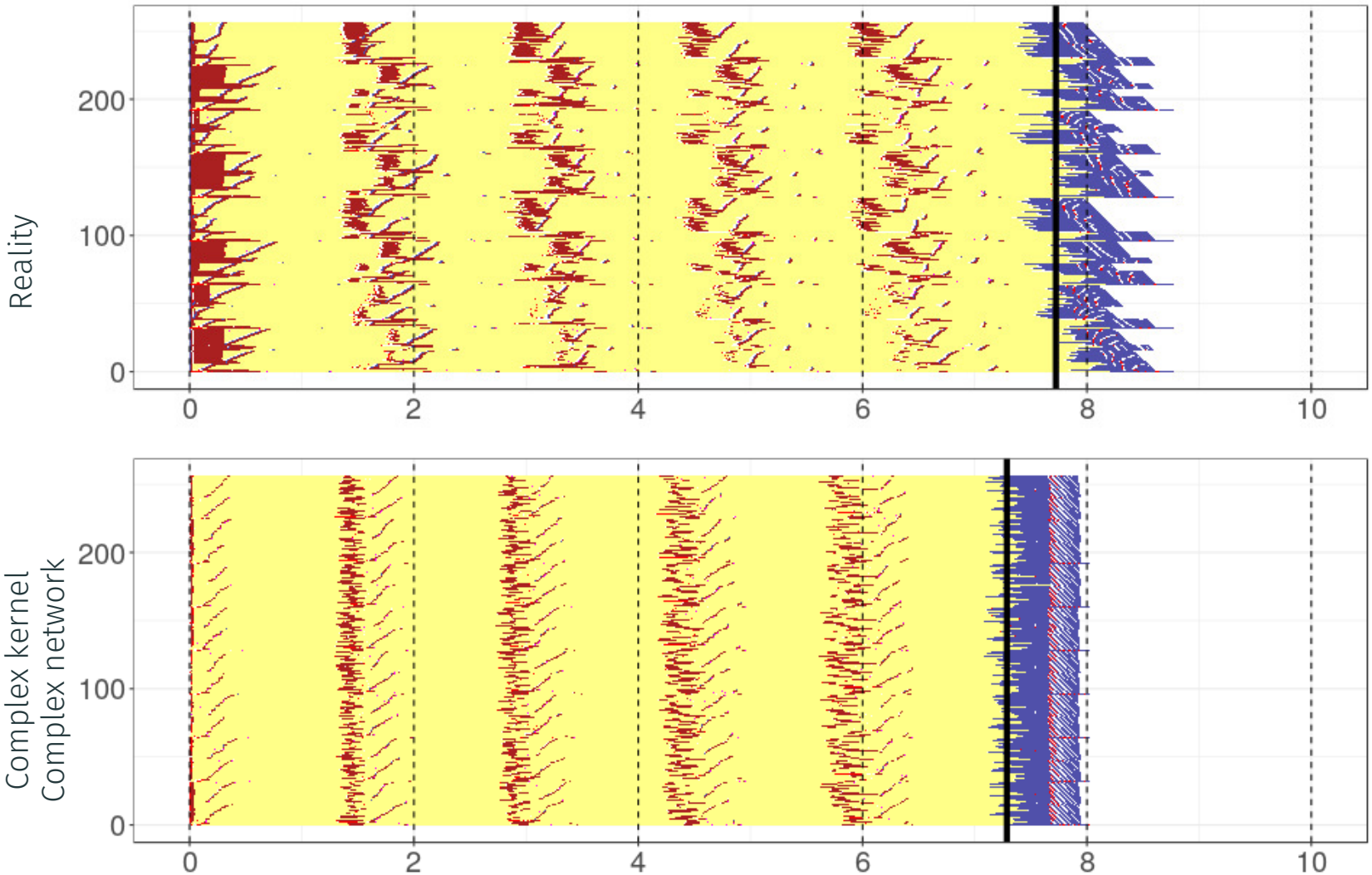
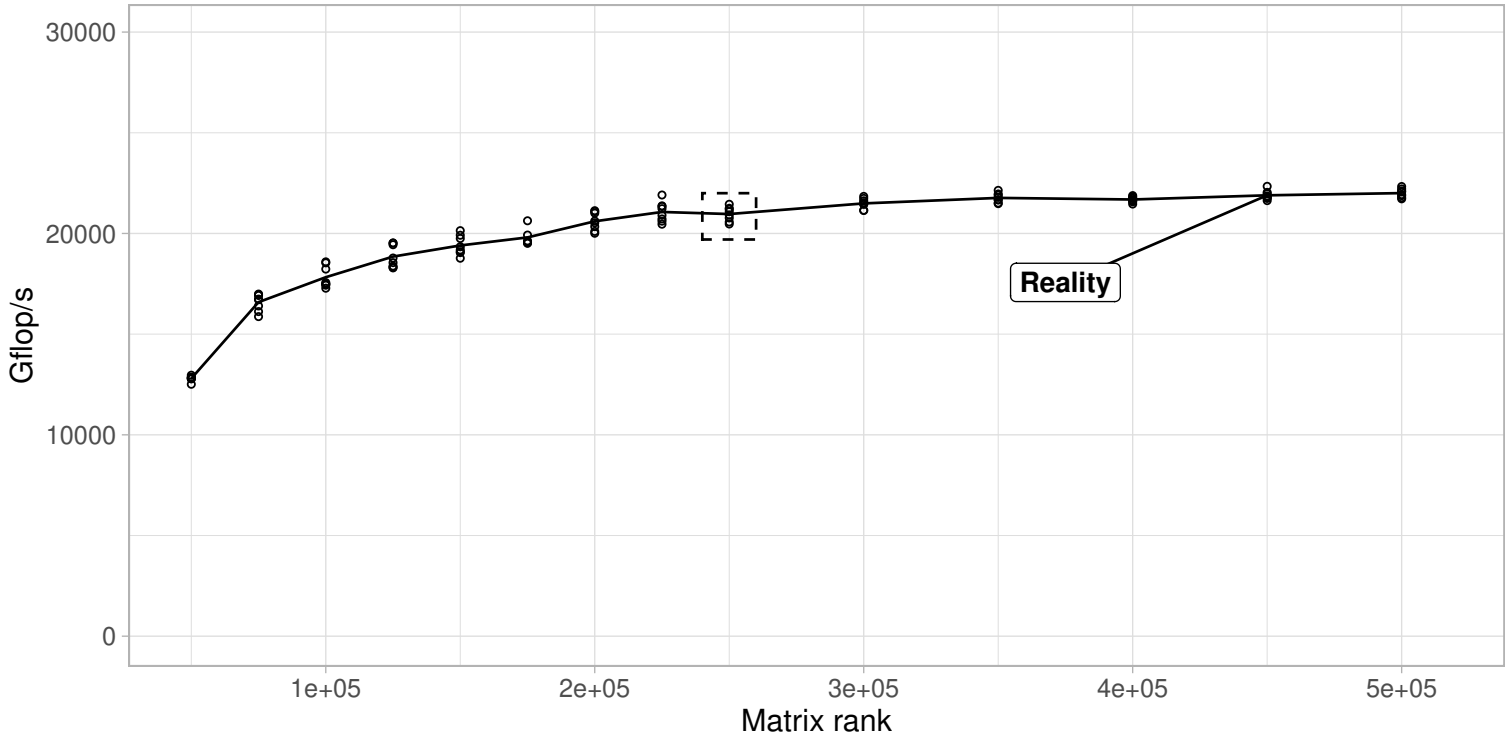


Influence of the problem size

Now the complete run, with 1024 MPI ranks



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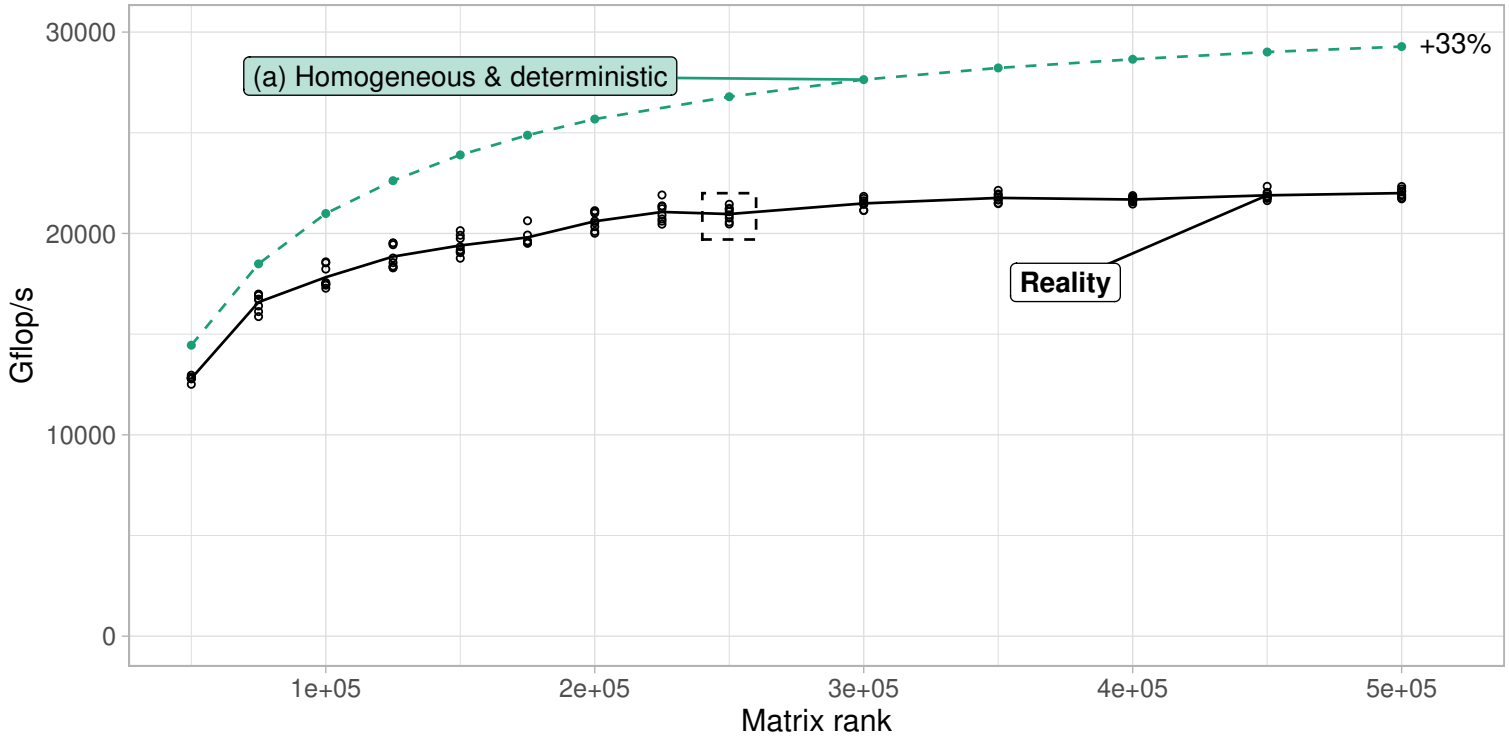

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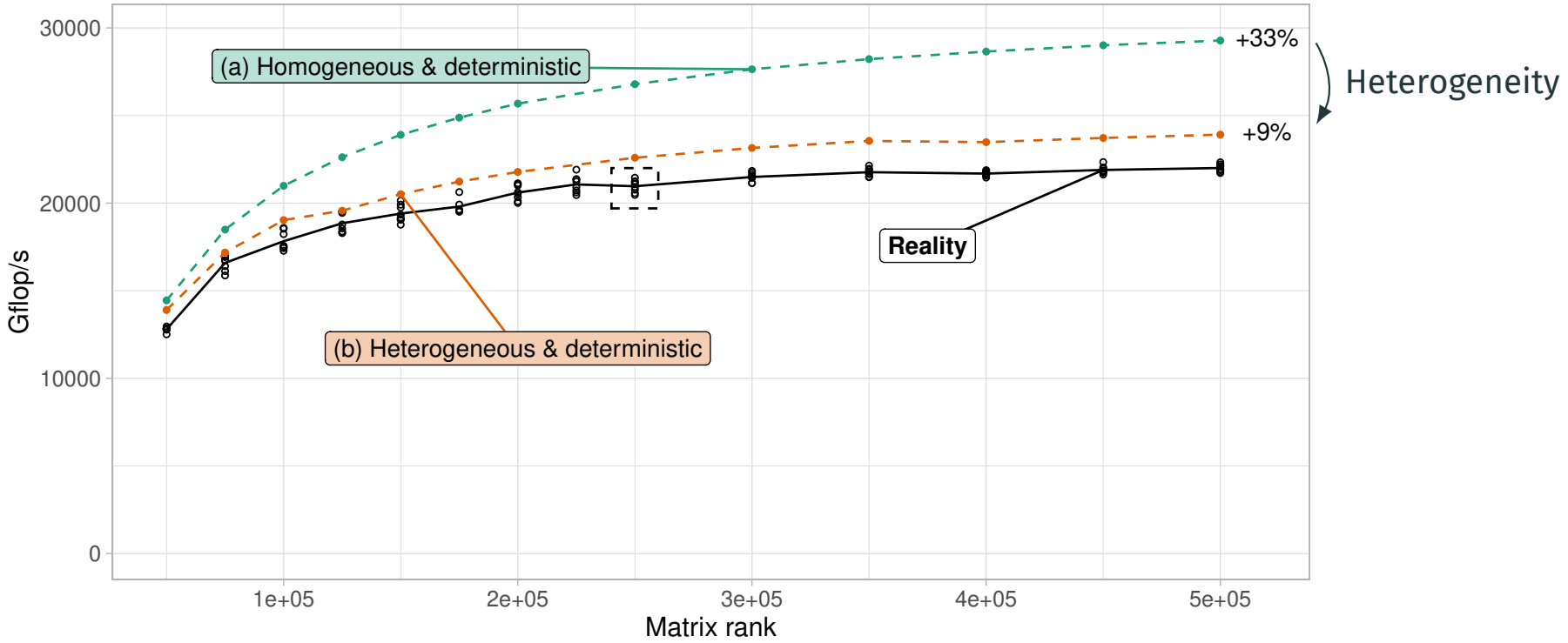

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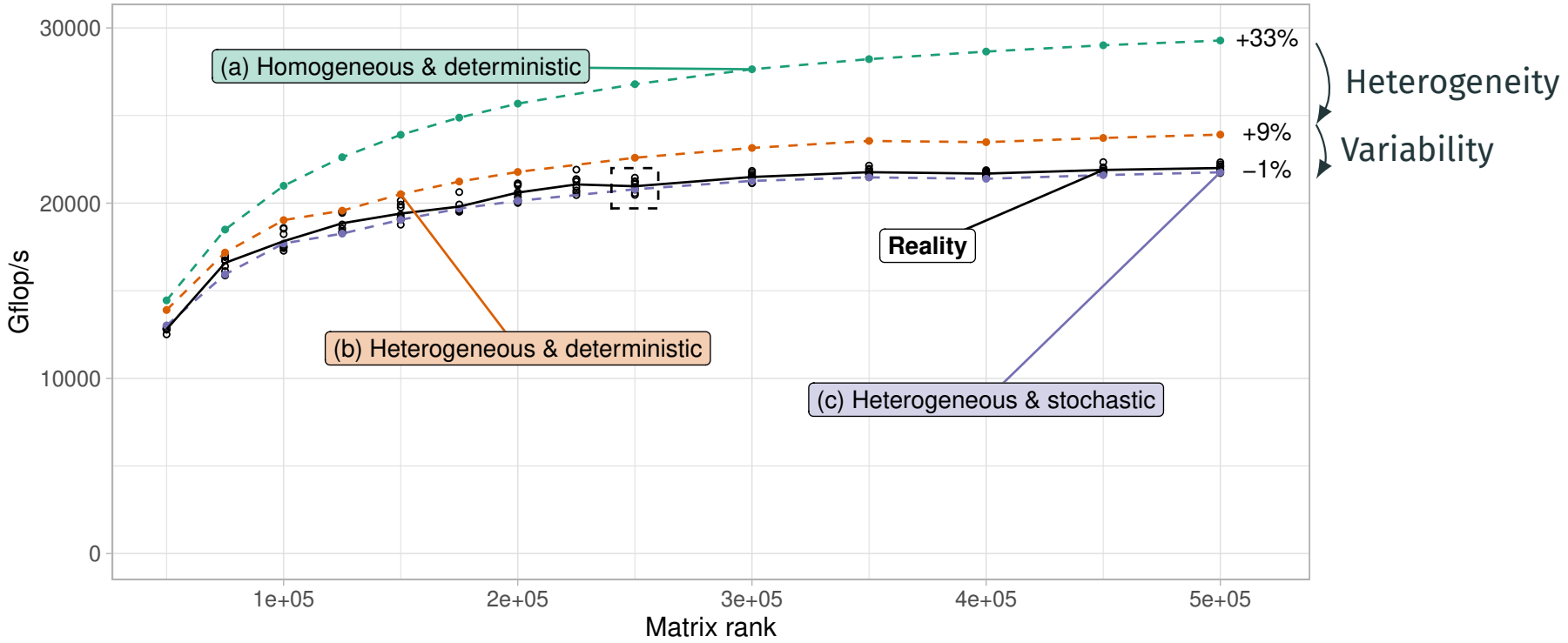

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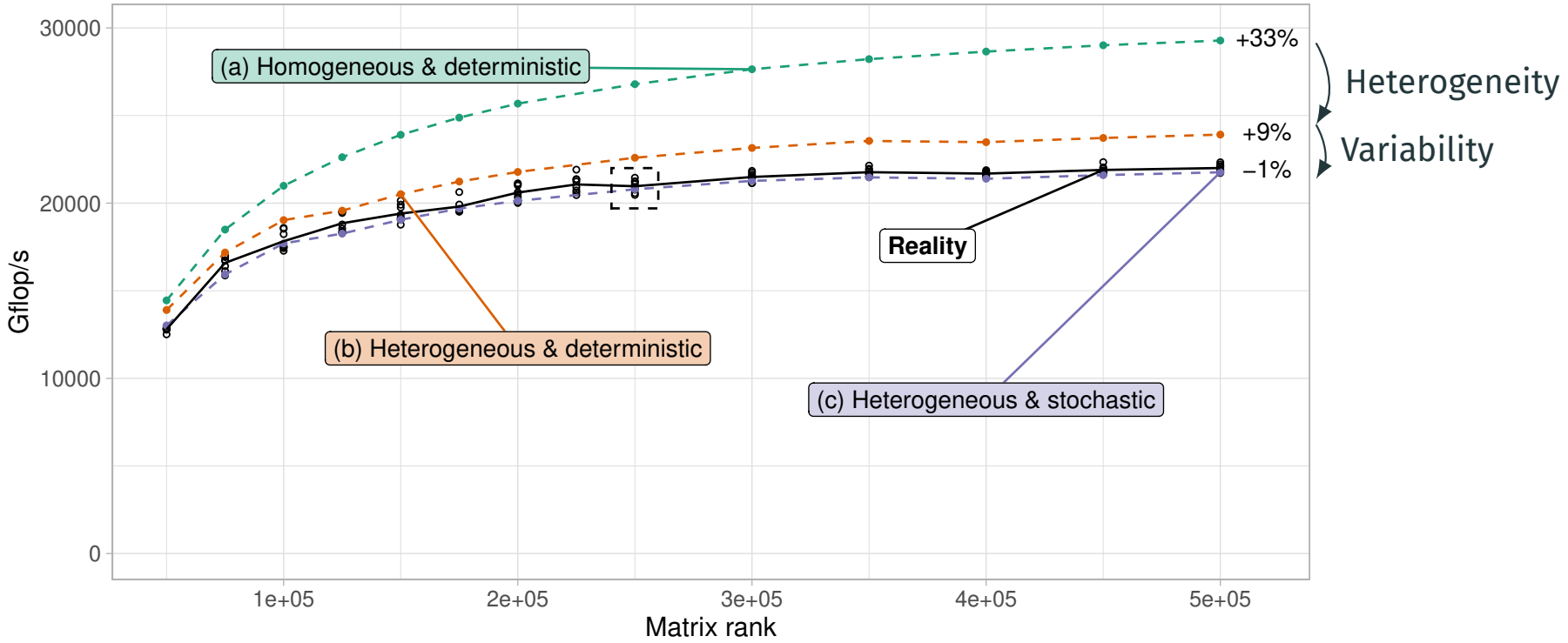
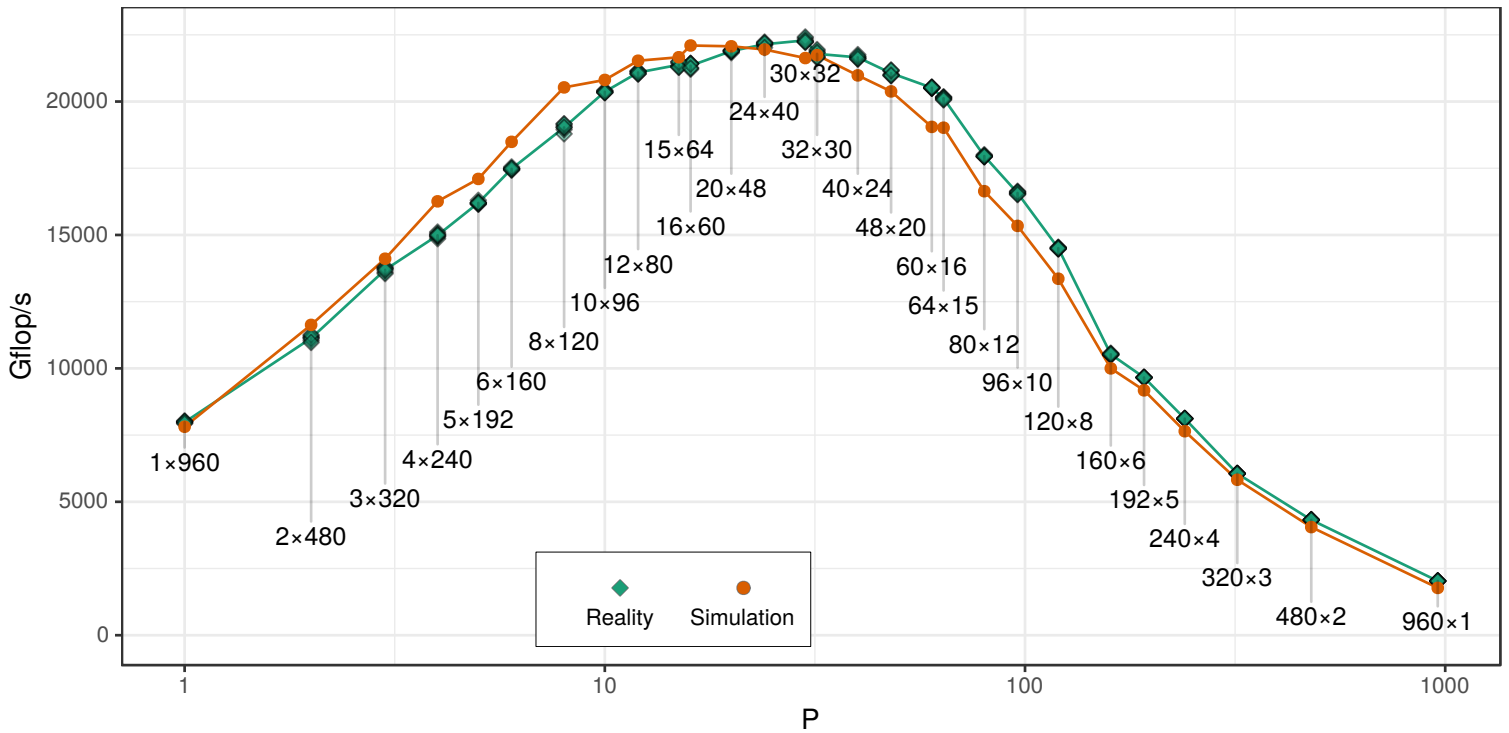


Take-Away Message: accurate prediction

Modeling both spatial and temporal computation variability is essential

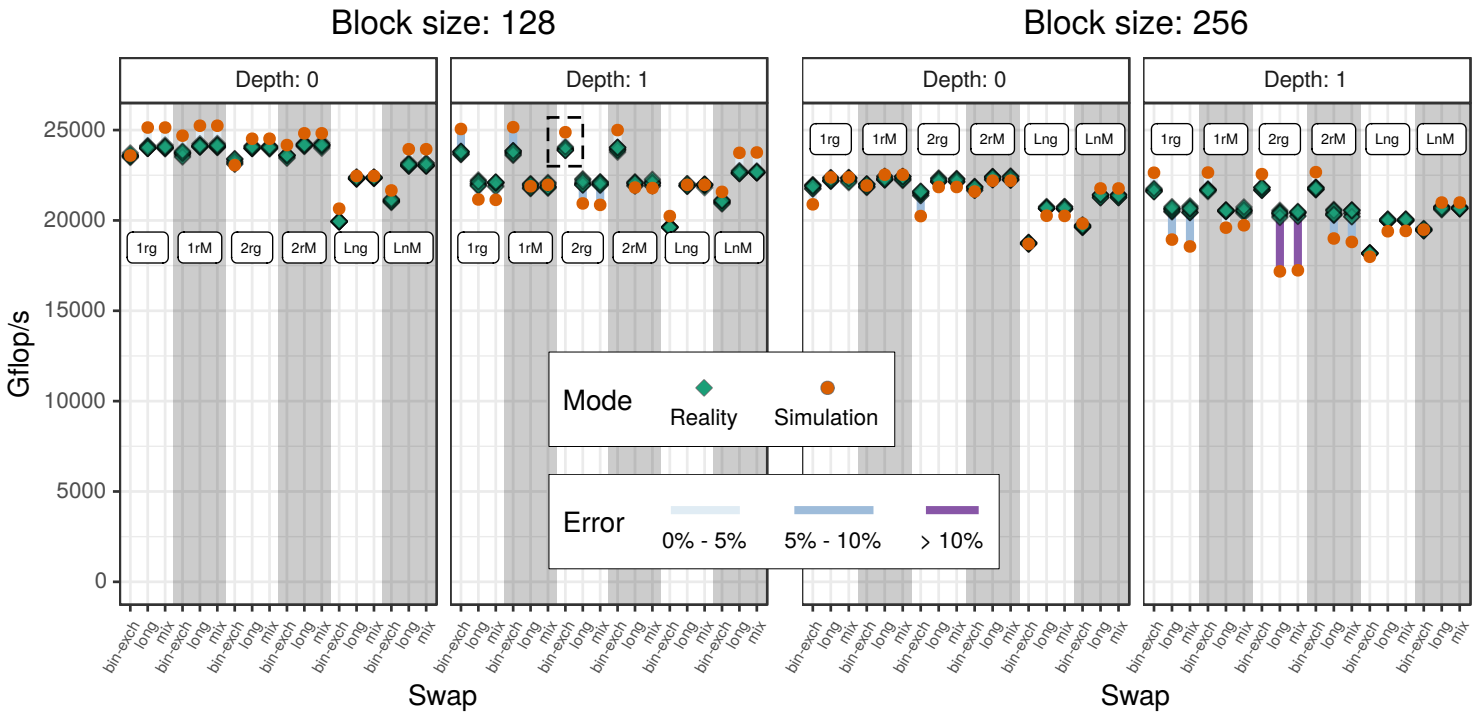
Influence of the geometry

$P \times Q$ MPI processes, organized in a 2D grid

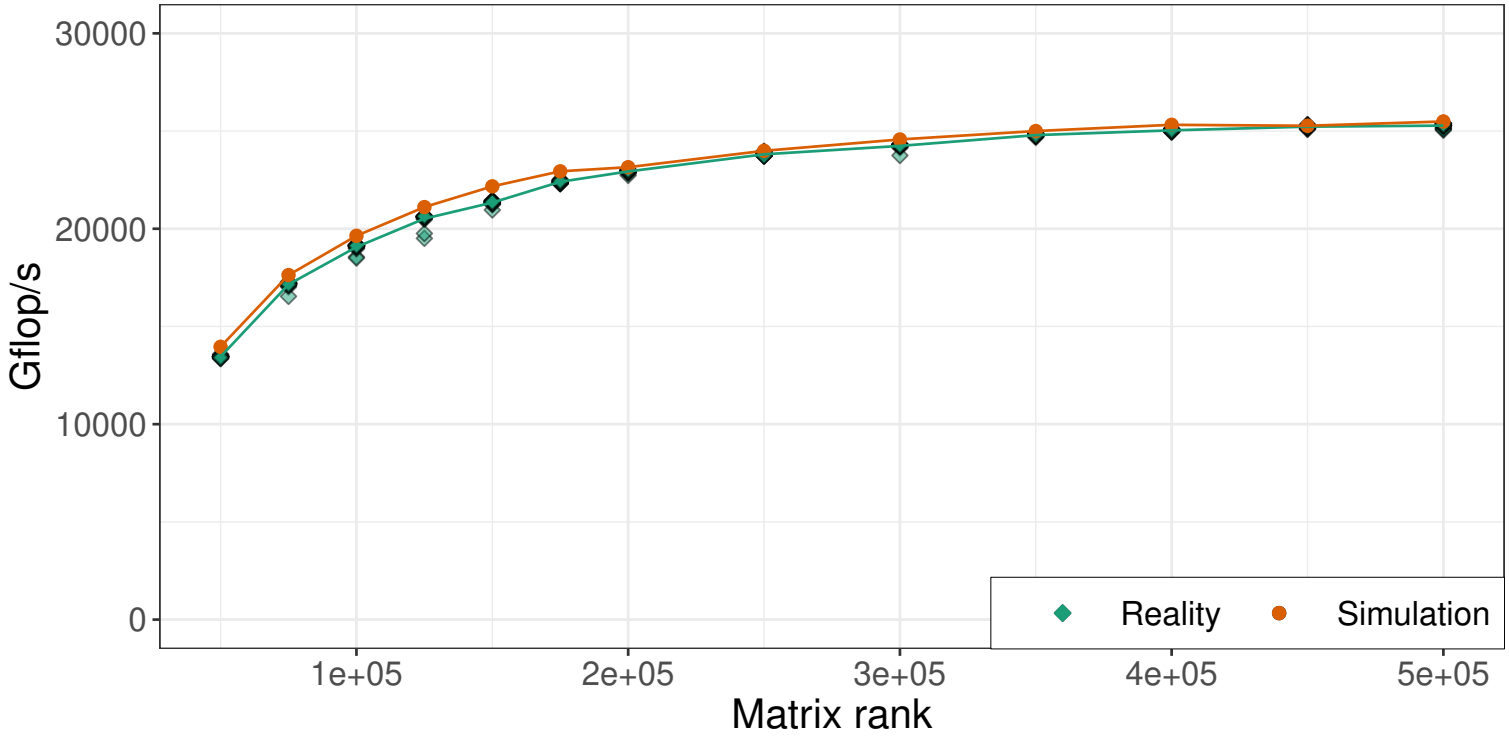


Influence of the other parameters

Tested the 72 combinations of the remaining parameters



Influence of a platform change



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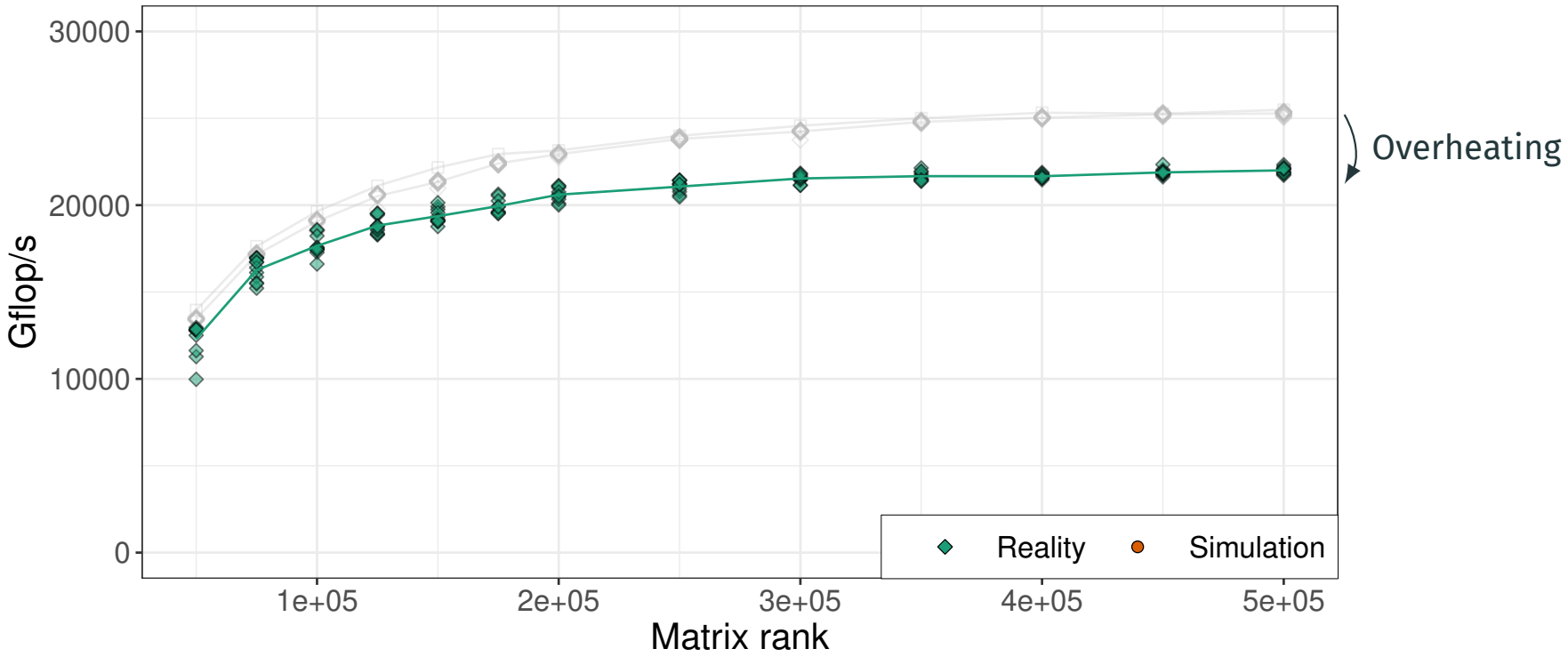

On four nodes, the cooling system malfunctionned for several weeks

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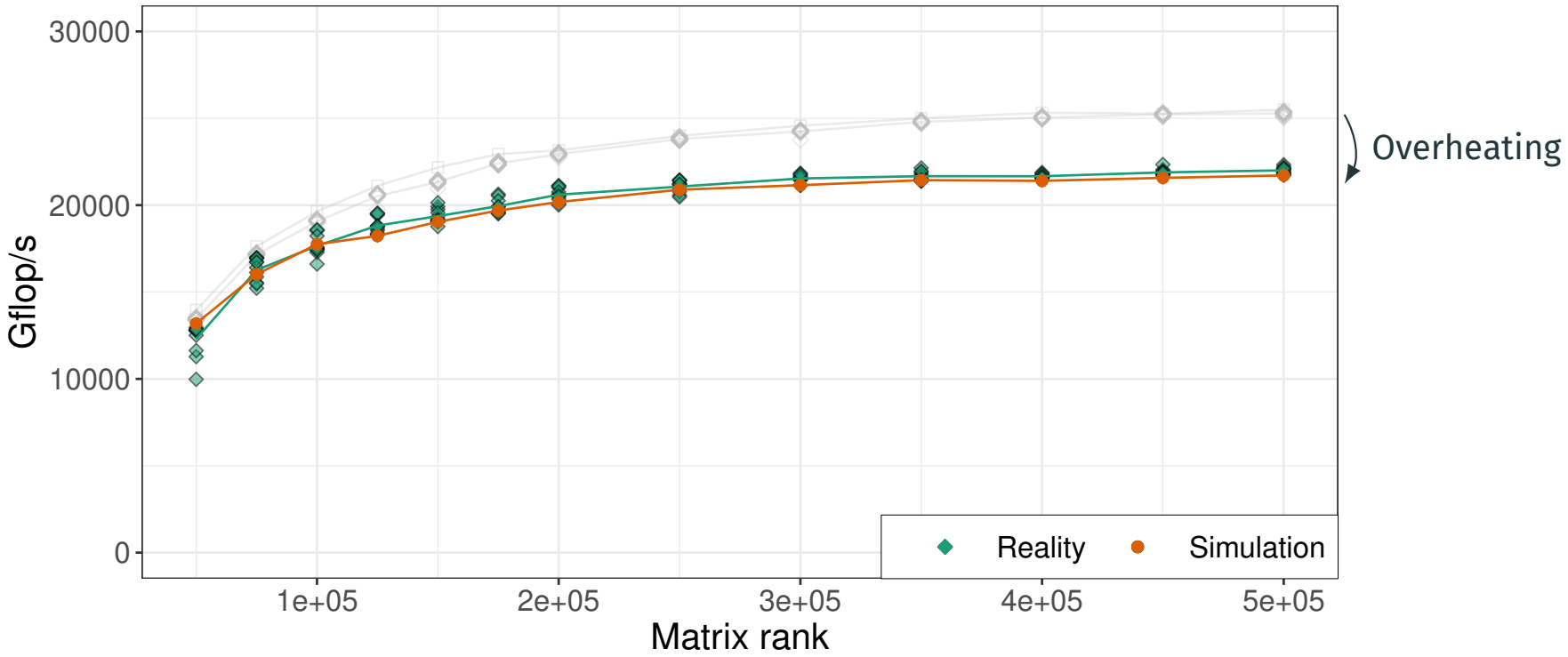

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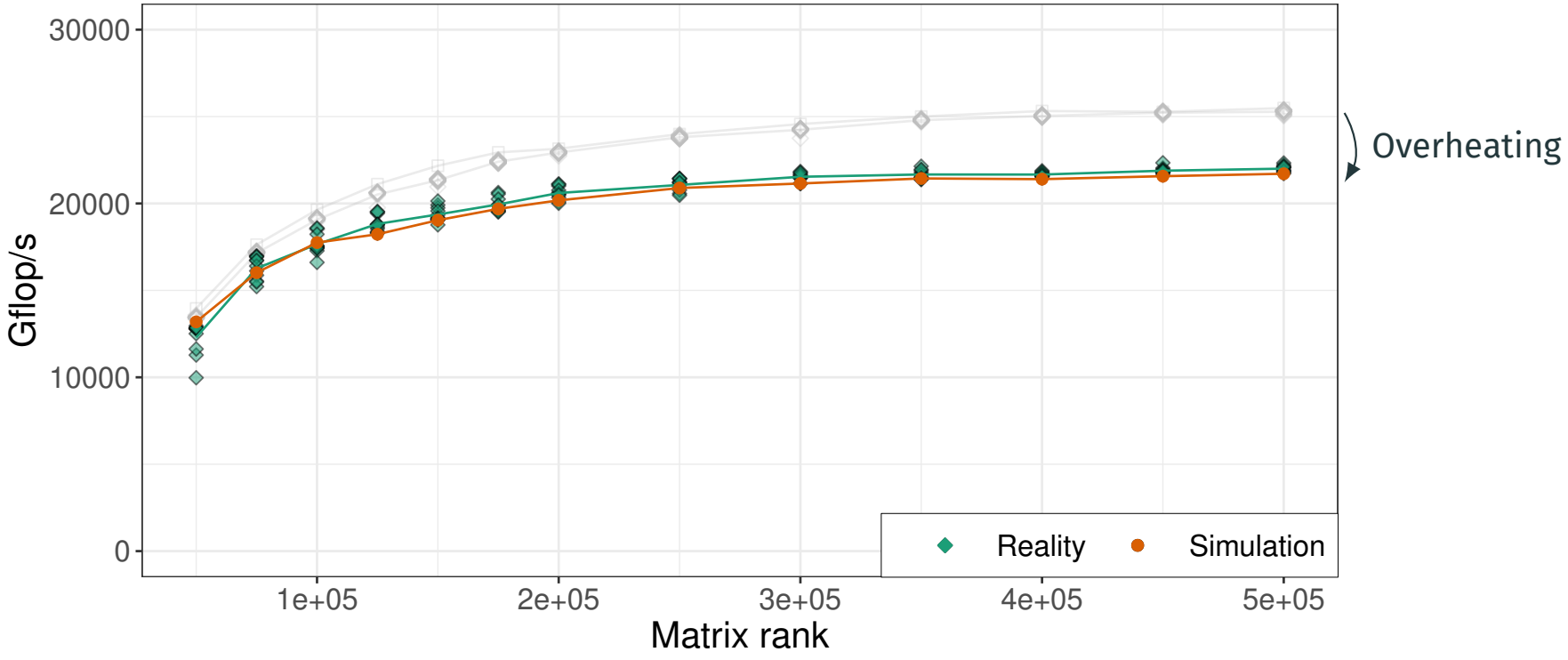

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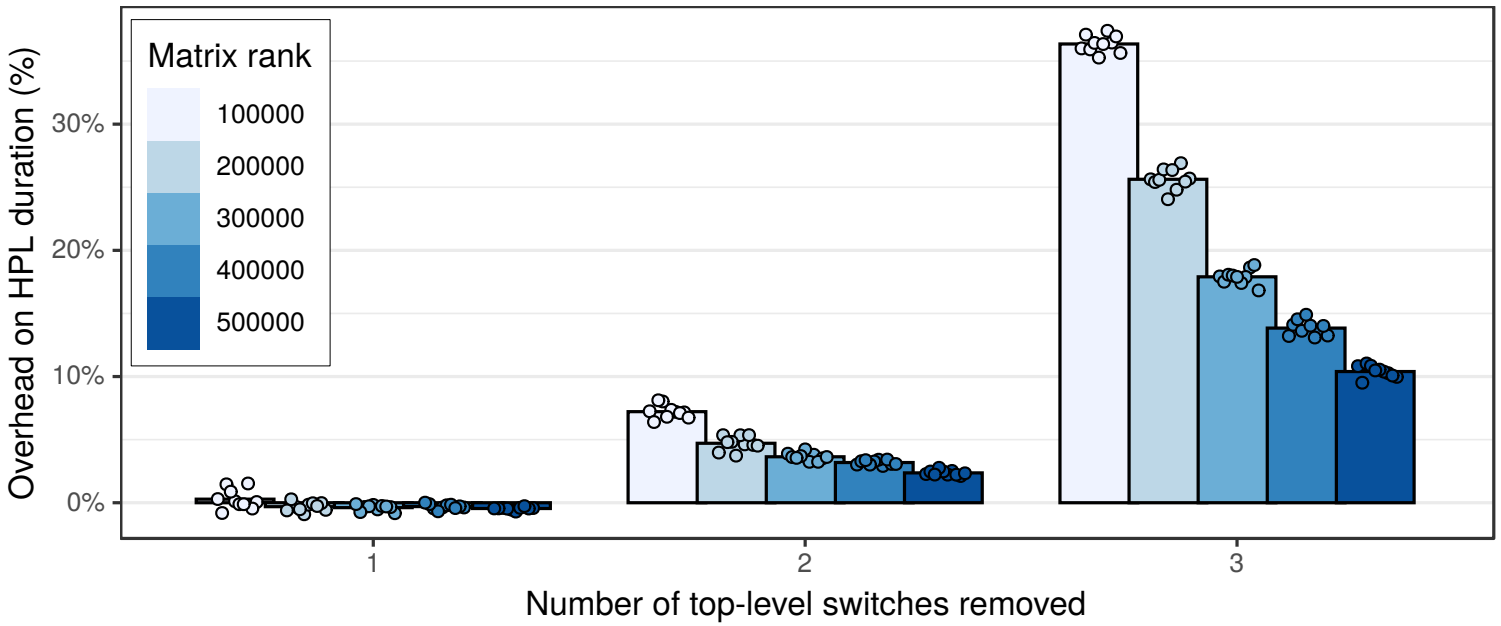
Take-Away Message: Re-measuring `dgemm` durations to generate a new model was enough to account for the platform change

Use case: sensibility analysis

What if the network topology of my cluster was different?



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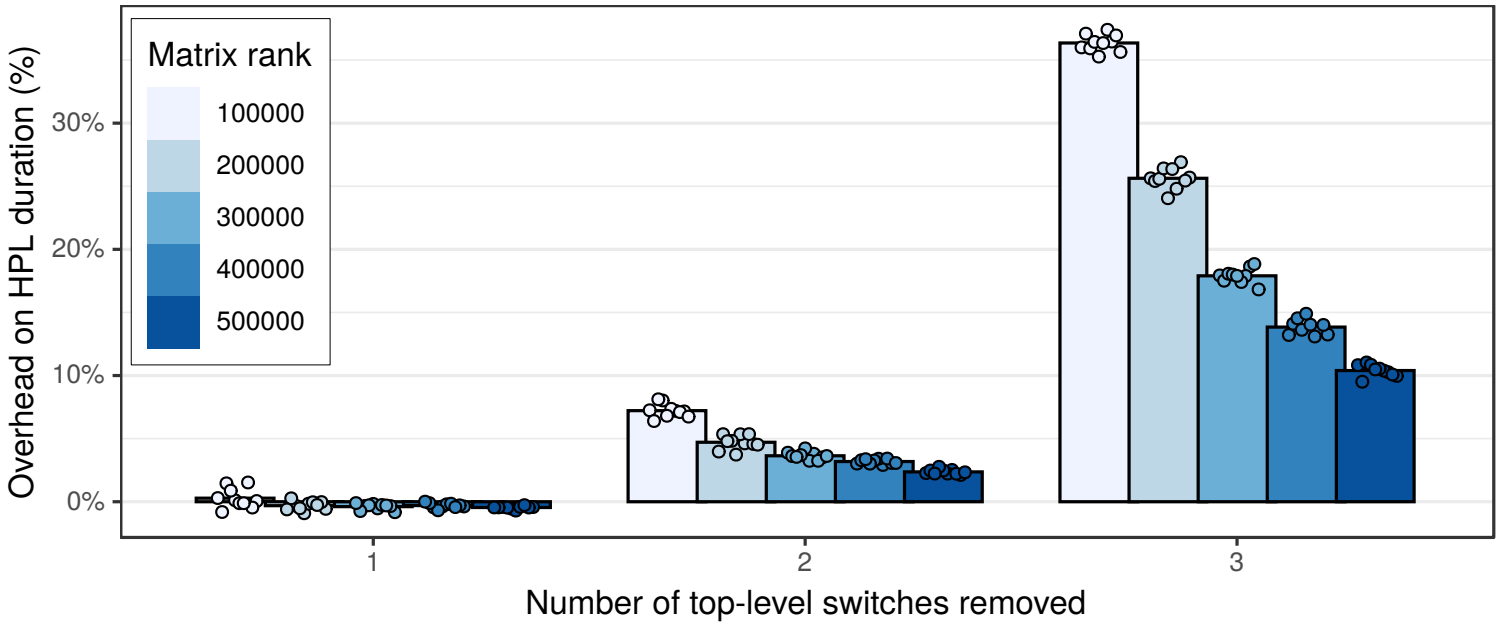

Faithful surrogate $\Rightarrow$ Empirical studies of hypothetical platforms

$\Rightarrow$ Extrapolation of existing platforms

$\Rightarrow$ Accounting for spatial and temporal variability

Goal: performance prediction ✓

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Main difficulties:

- Realistic experimental conditions
- Platform changes (e.g., the cooling issue)

Parenthesis: on the difficulties of experimentation

Experimental biases when measuring `dgemm` or MPI durations

Effect on durations, but also other metrics (e.g. CPU frequency)

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Bias may be desirable in some situations

Performance tests

Regular measures

On a near-daily basis, run the `dgemm` calibration code on Grid'5000

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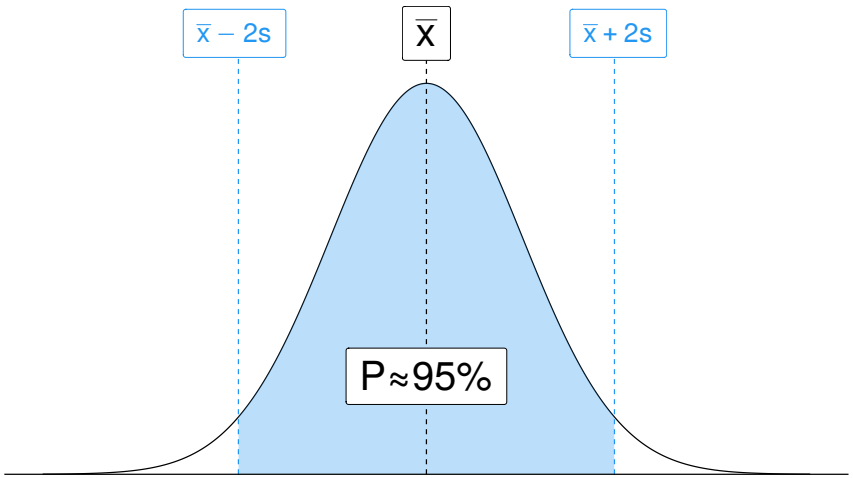
Each parameter is normally distributed (thanks to CLT)

Fluctuation interval

Given a sequence of old observations $x_1, \ldots, x_n$ and a new observation x_{n+1}, how likely was it to observe x_{n+1}?

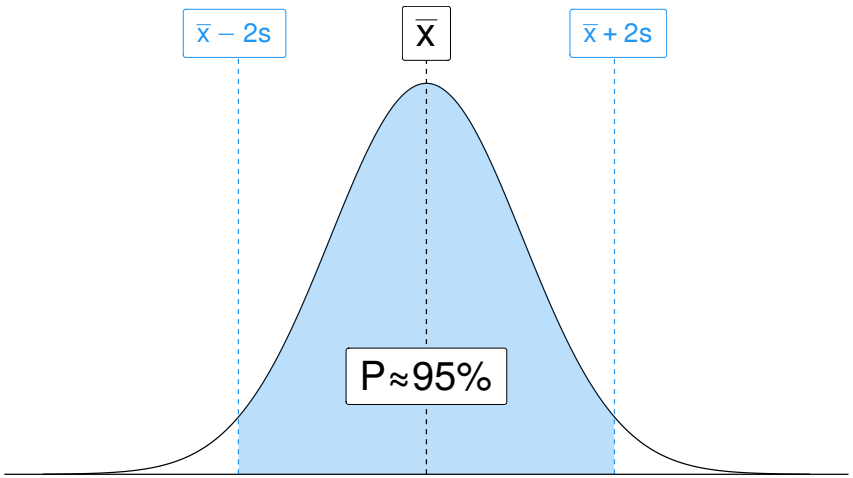


Take the sample mean $\bar{x}$ and standard deviation s of the old observations

$$\mathbb{P}\left(x_{n+1} \in [\bar{x} - 2s; \bar{x} + 2s]\right) \approx 95\%$$

Fluctuation interval

Given a sequence of old observations $x_1, \ldots, x_n$ and a new observation x_{n+1}, how likely was it to observe x_{n+1}?



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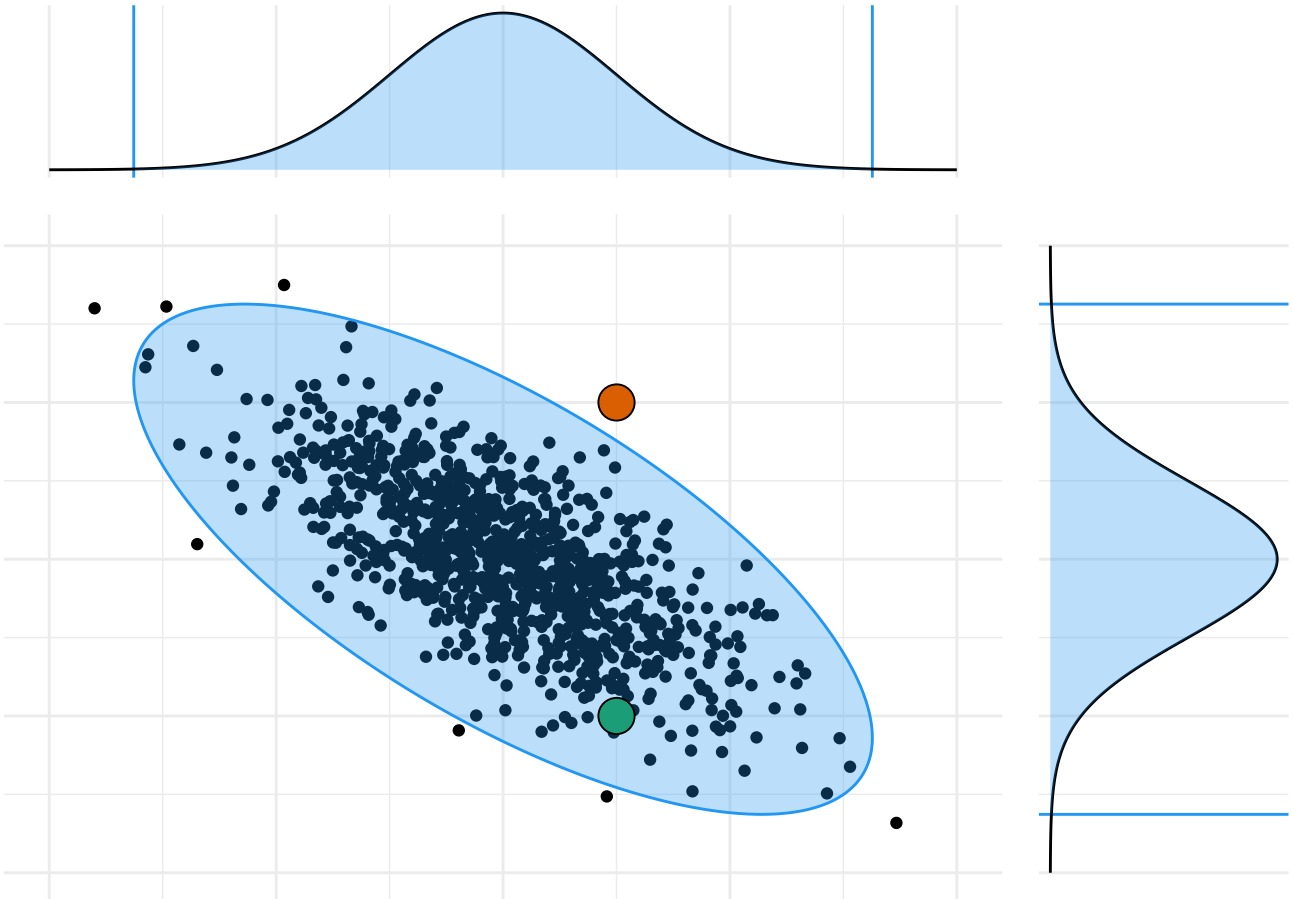
$$\mathbb{P}\left(x_{n+1} \in [\bar{x} - 2s; \bar{x} + 2s]\right) \approx 95\%$$

Note: using the F distribution instead of the normal distribution (the true mean and standard deviation are unknown)

Fluctuation interval for several variables

With several variables, using their covariance matrix

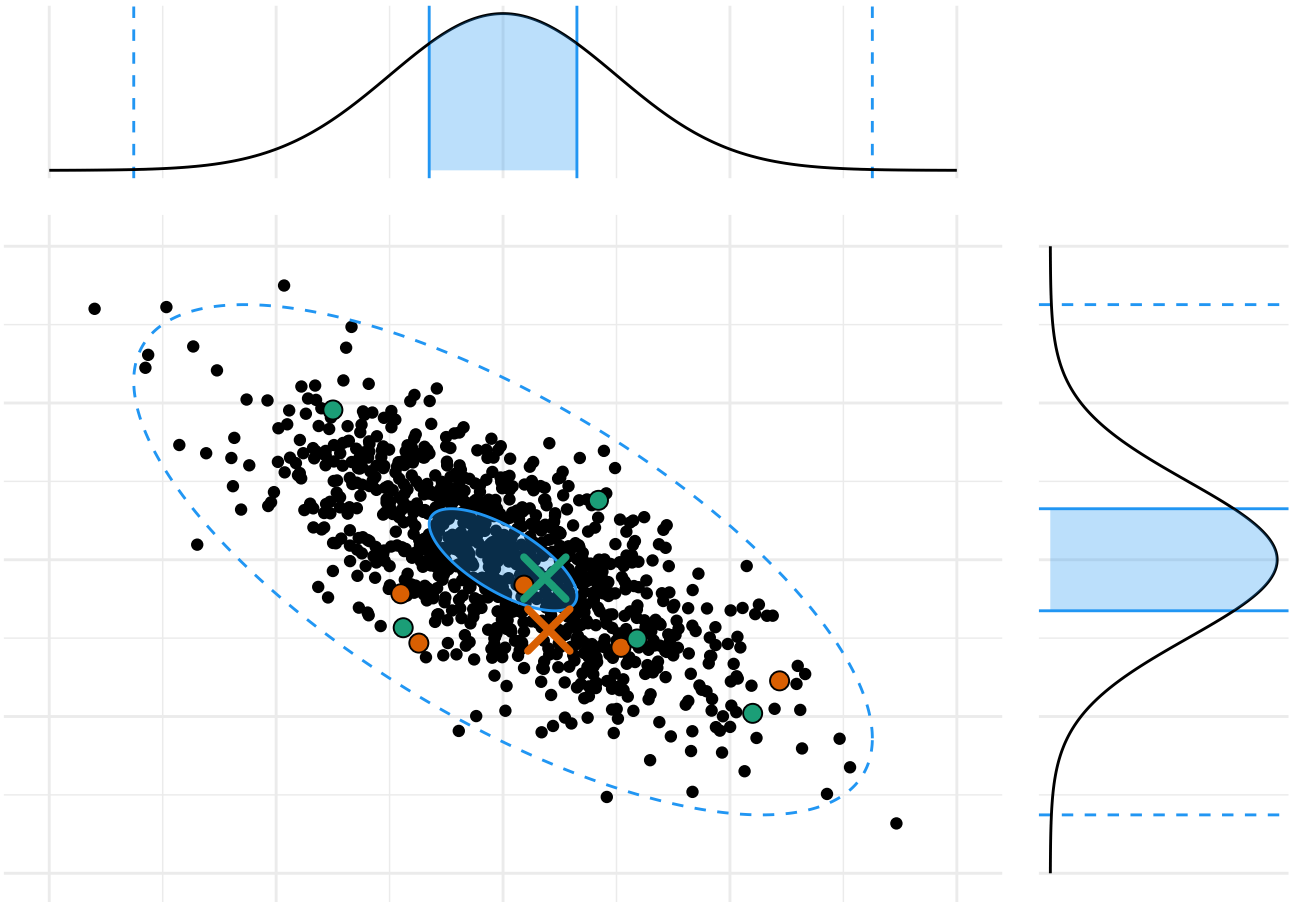
Example in dimension 2, with $\mathbb{P}(x_{n+1} \in \text{interval}) \approx 99.5\%$



Fluctuation interval for several measures

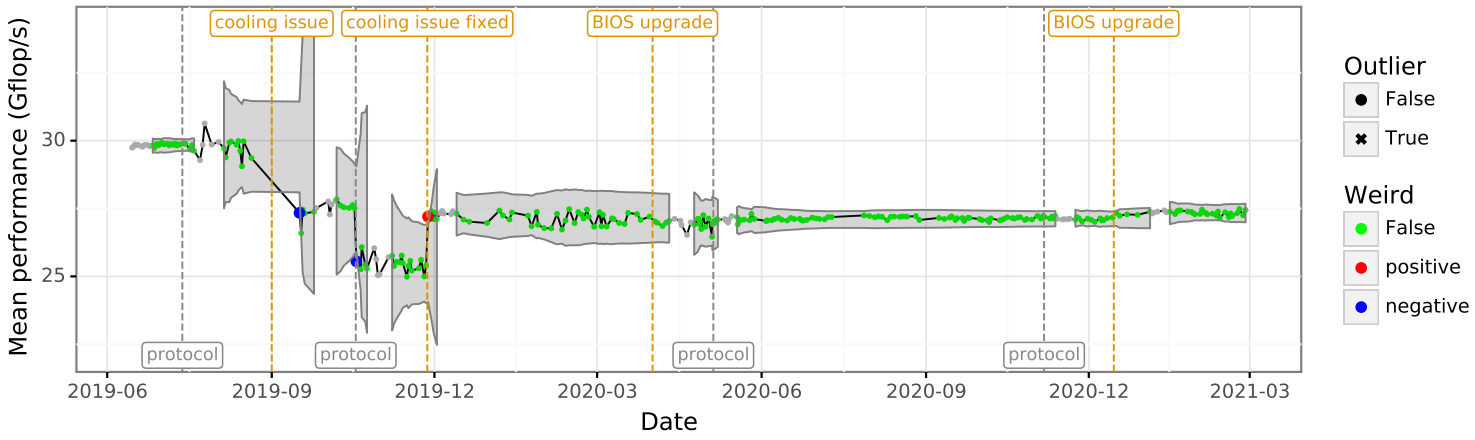
With several measures, using their average and shrinking the interval

Example with 5 measures (averages represented by crosses)



Result: performance fluctuation

Performance fluctuation of the node dahu-14



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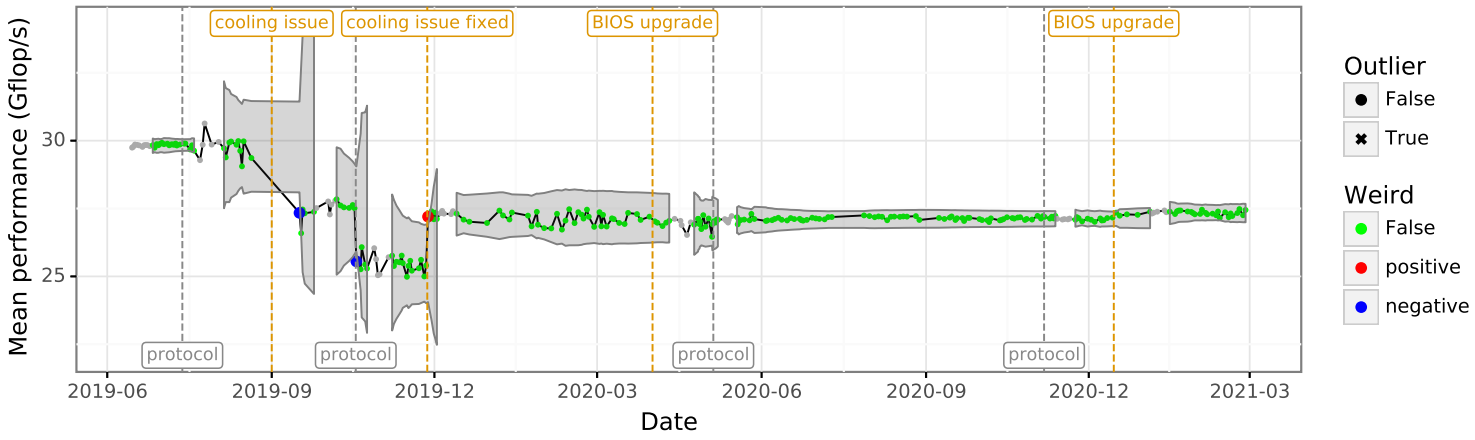
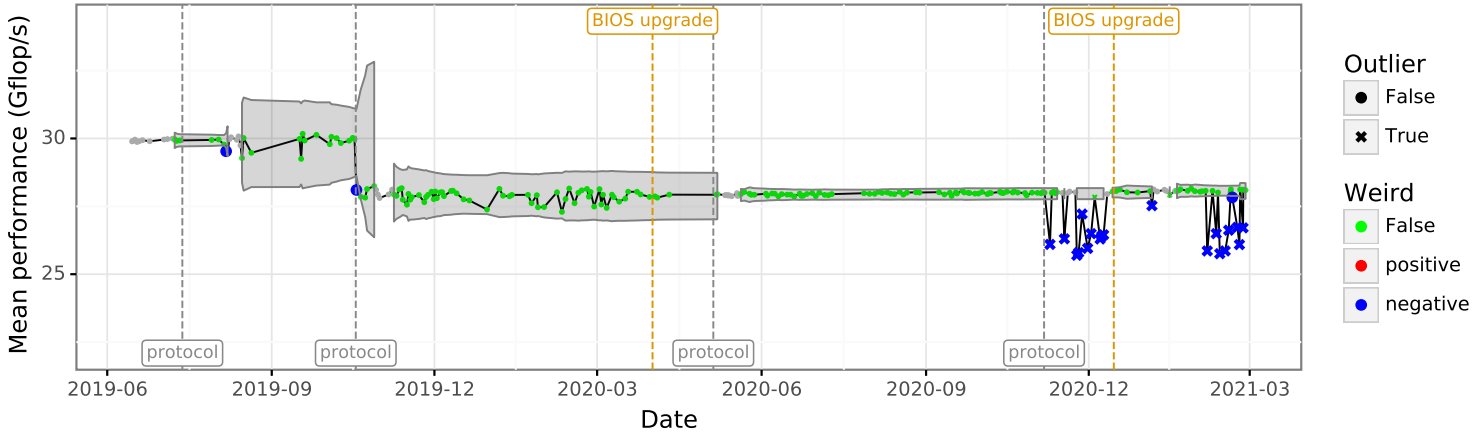
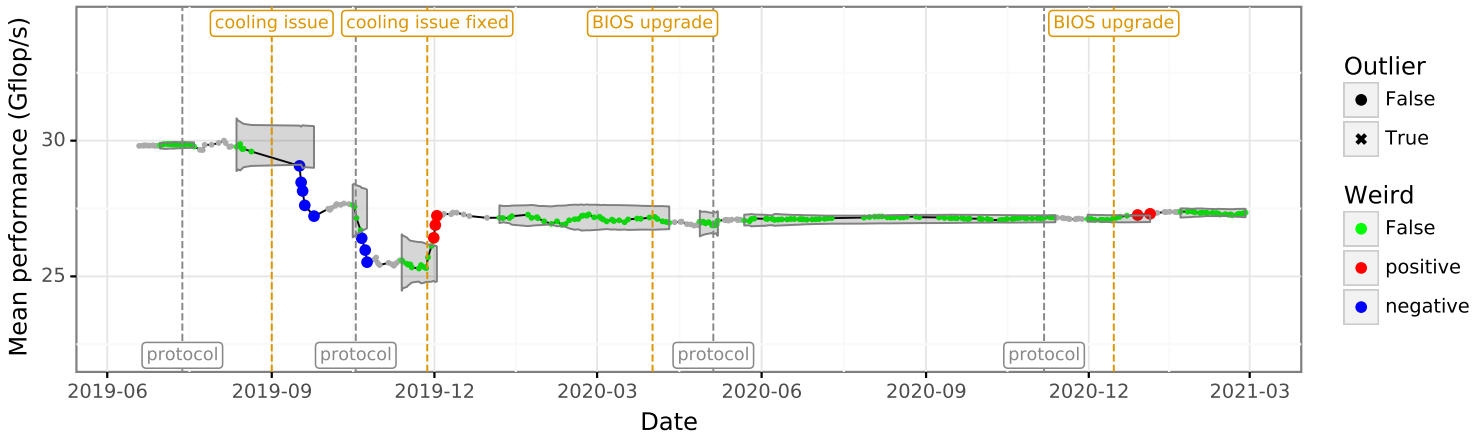


Performance fluctuation of the node dahu-32

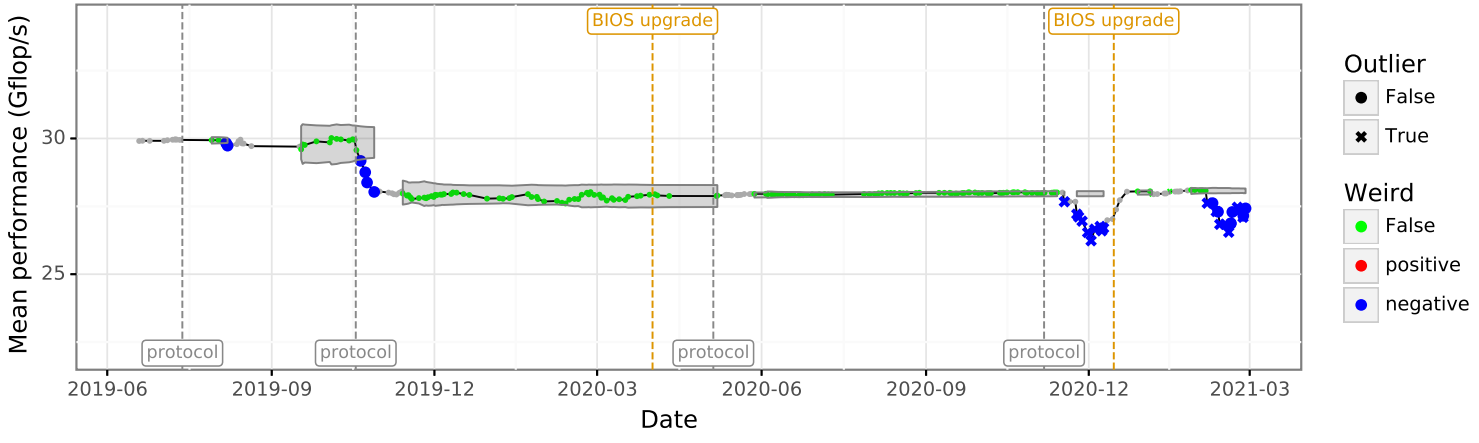


Result: performance fluctuation

Performance fluctuation of the node dahu-14 (5-day window)

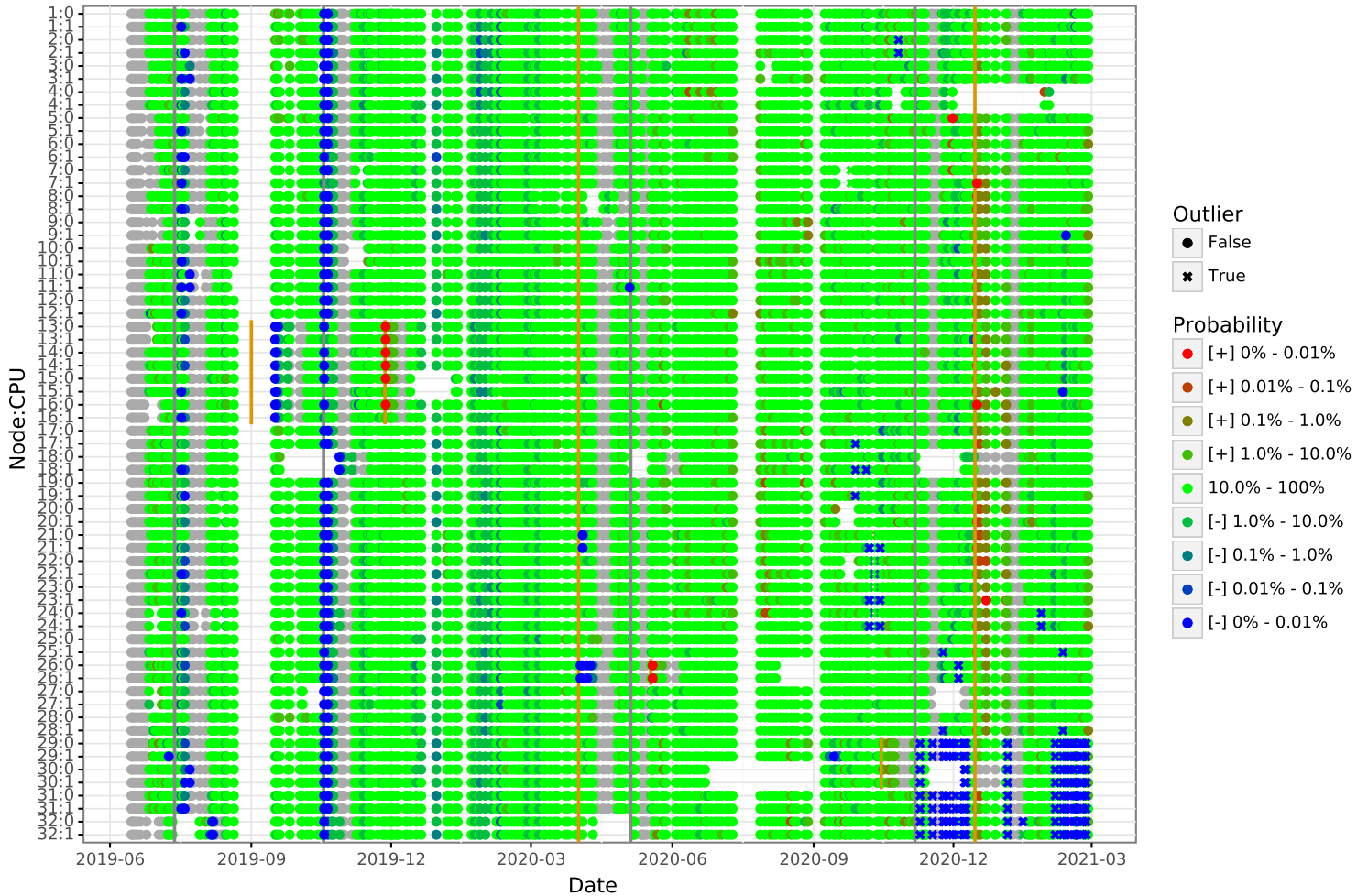


Performance fluctuation of the node dahu-32 (5-day window)



Result: performance overview

Overview of the performance on cluster dahu



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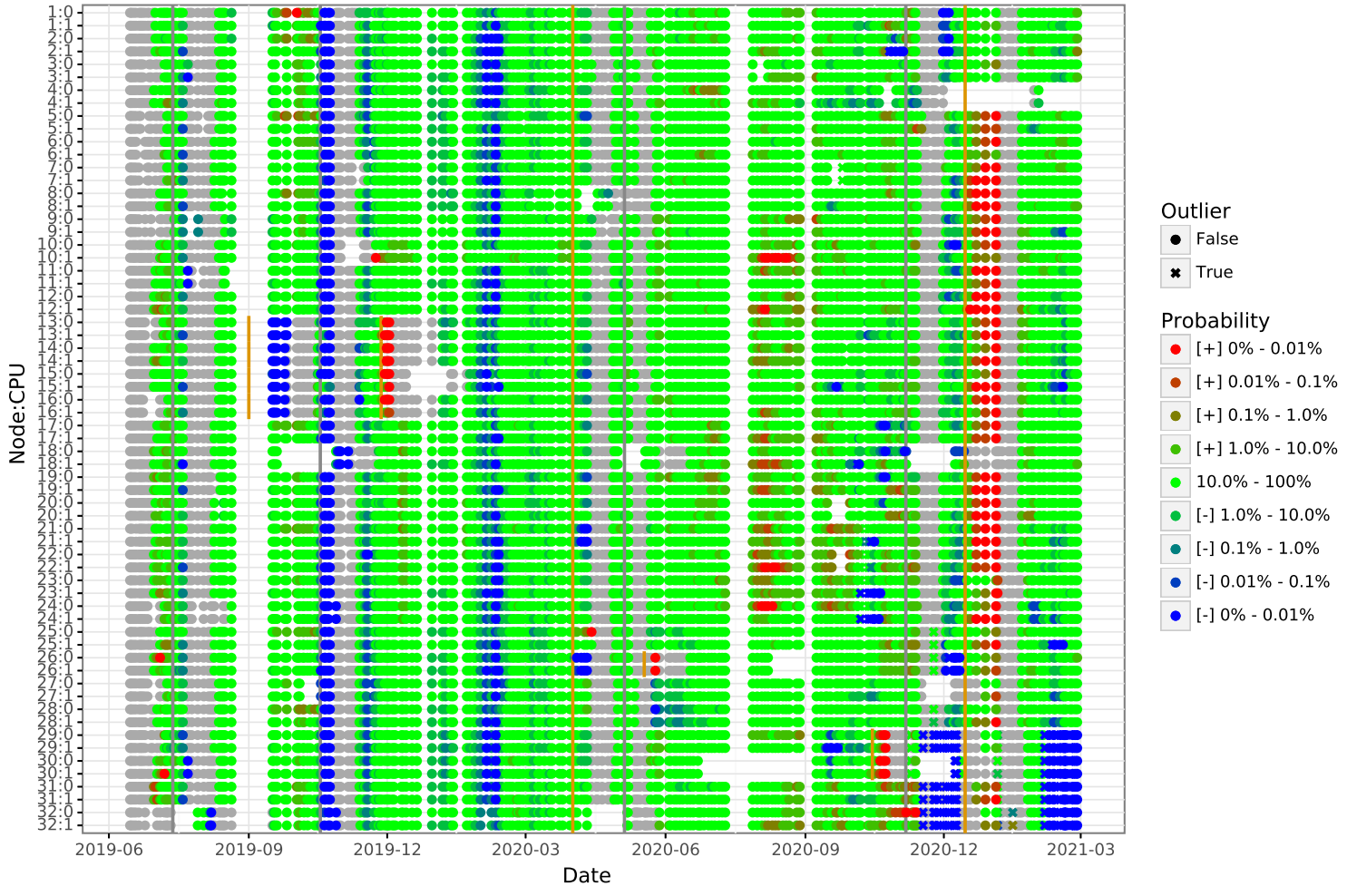

Performance tests: wraping up

Multi-variable test also implemented

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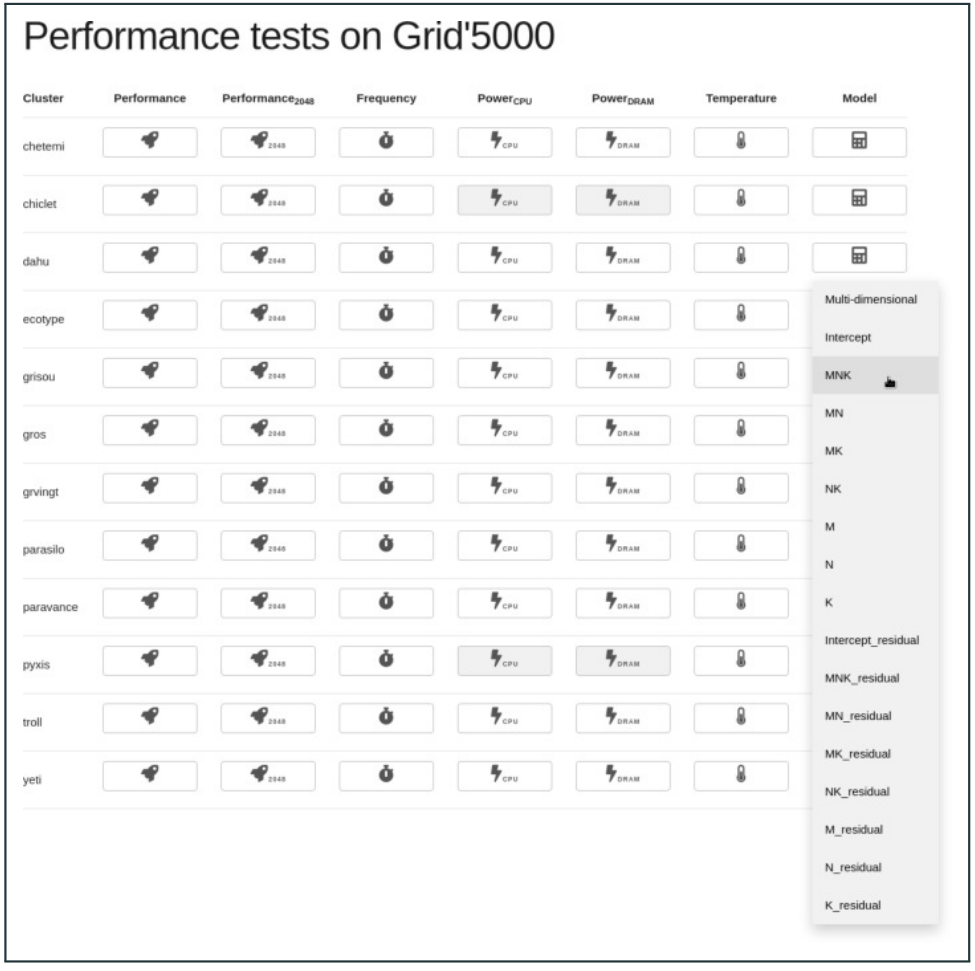
Results available on https://cornebize.net/g5k_test



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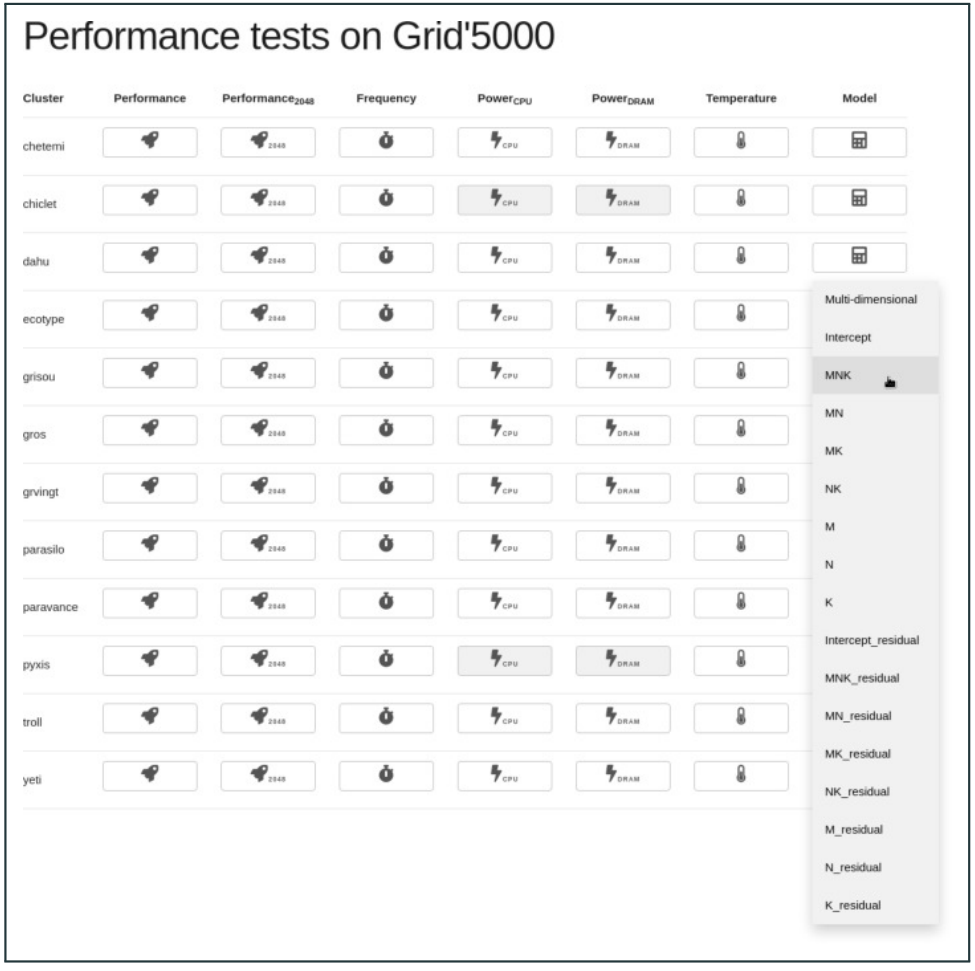

Detected events

- BIOS upgrades
- Cooling issue
- Faulty memory
- Power instability

Performance tests: wraping up

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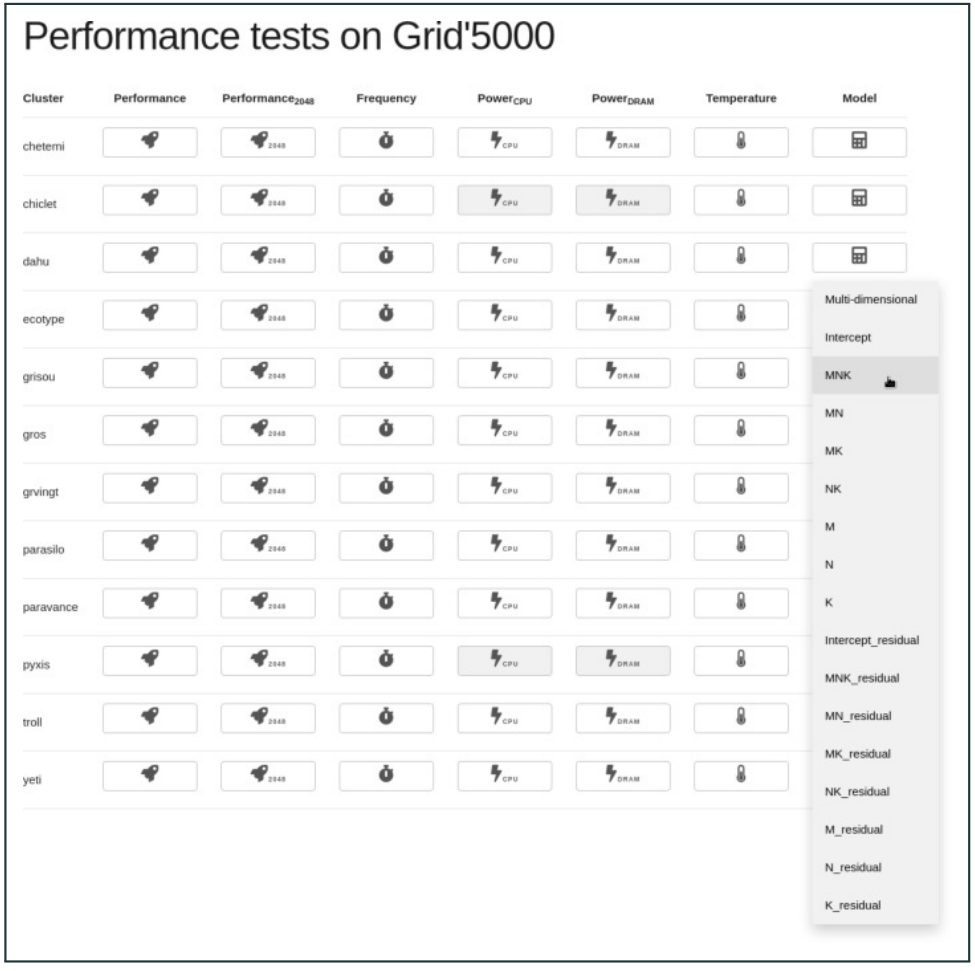


Detected events

- BIOS upgrades
- Cooling issue
- Faulty memory
- Power instability

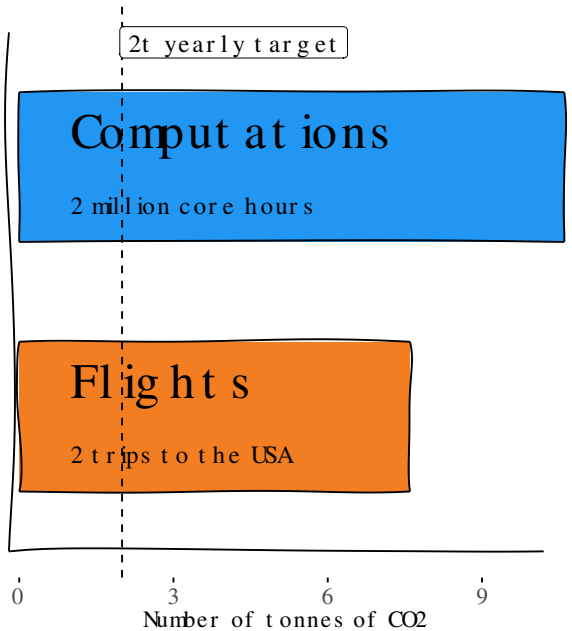
All went unnoticed by both Grid'5000 staff and users, despite significant effects

⇒ Great help potential

Concluding thoughts

There is no planet B

About 18 t of CO2eq were emitted for this thesis



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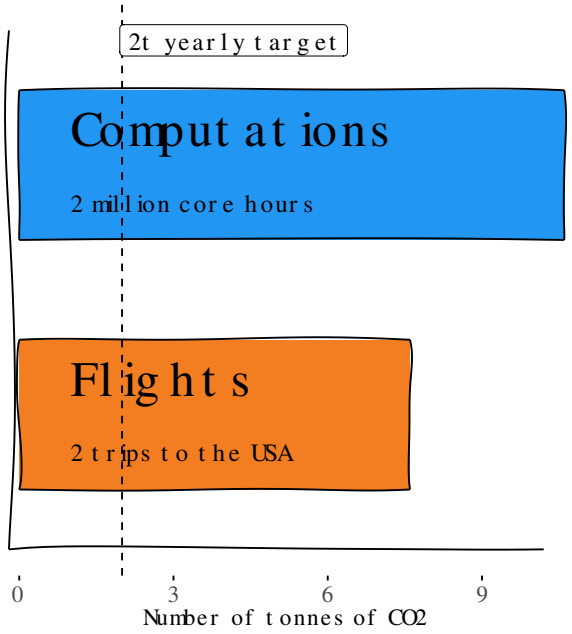

Do we really *need* to attend conferences in person?

What about computations?

Why so many computations?

More than half the total core hours were used for performance tests

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How to reduce them?

- Change the experiment procedure (e.g. no full node reinstallation, use the standard image instead)
- Test less frequently (e.g. only once a week)

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- Test less frequently (e.g. only once a week)

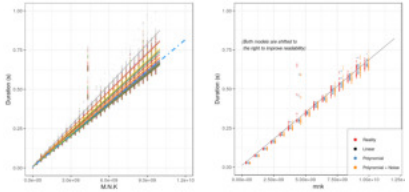
Who should be responsible of tests?

- Platform staff? But what should they test?
- Researchers? Isn't it redundant?

Modeling Commputations

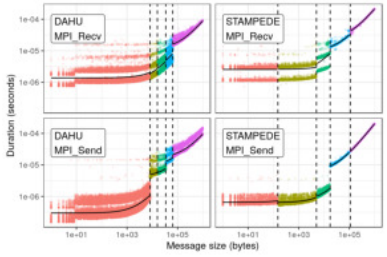
$$\texttt{dgemm}_i(M,N,K) = \underbrace{\alpha_i.M.N.K}_{\text{per host}} + \underbrace{\beta_i.M.N + \gamma_i.N.K + \ldots}_{\text{polynomial model}} + \underbrace{\mathcal{N}(0, \alpha'_i.M.N.K + \ldots)}_{\text{polynomial noise}}$$

Different color ⇒ different host For a particular host



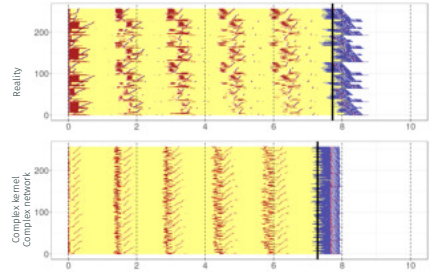
Modeling Communications

Hand-crafted non-blocking collective operations intertwinned with computations



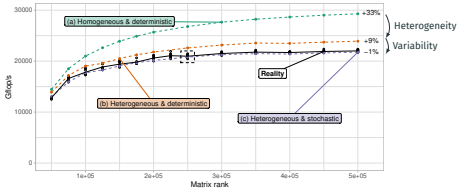
Internal behavior of the application

256 MPI ranks, interrupted after the 5th iteration



Influence of the problem size

Now the complete run, with 1024 MPI ranks

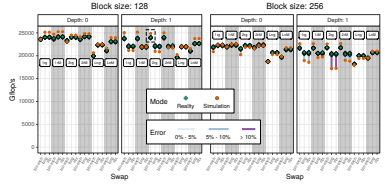


Take-Away Message: accurate prediction

Modeling both spatial and temporal computation variability is essential

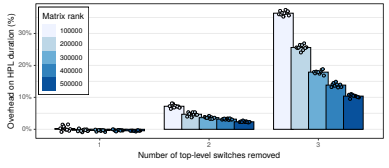
Influence of the other parameters

Tested the 72 combinations of the remaining parameters



Use case: sensibility analysis

What if the network topology of my cluster was different?

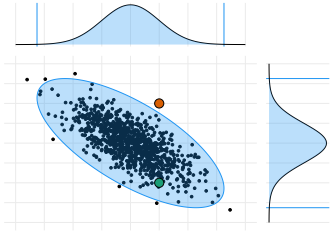


Faithful surrogate ⇒ Empirical studies of hypothetical platforms
⇒ Extrapolation of existing platforms
⇒ Accounting for spatial and temporal variability

Fluctuation interval for several variables

With several variables, using their covariance matrix

Example in dimension 2, with $\mathbb{P}(x_{n+1} \in \text{interval}) \approx 99.5\%$



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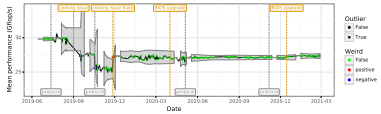

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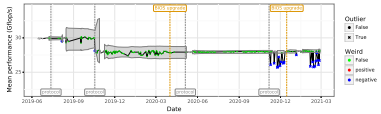

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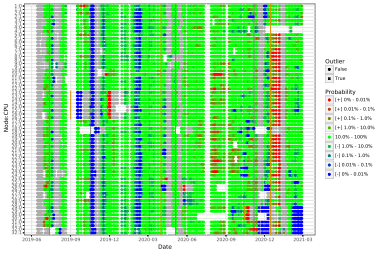

Thank you all!