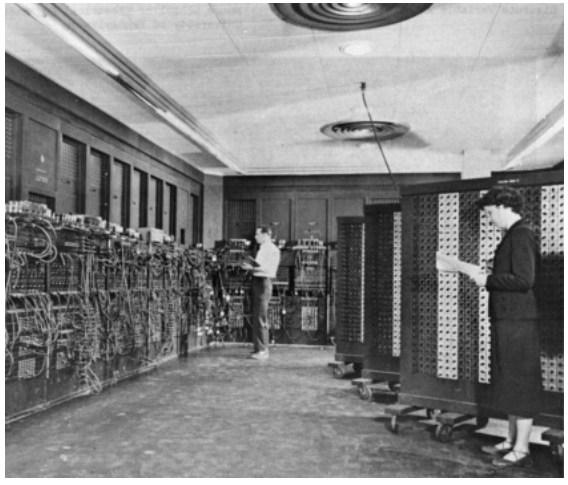
High Performance Computing: Towards Better Performance Predictions and Experiments

Tom Cornebize

2 June 2021, PhD defense

No science without computing

Arithmomètre (1851)



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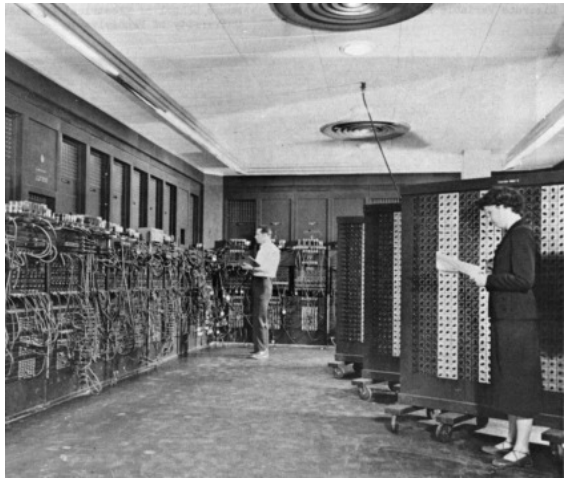

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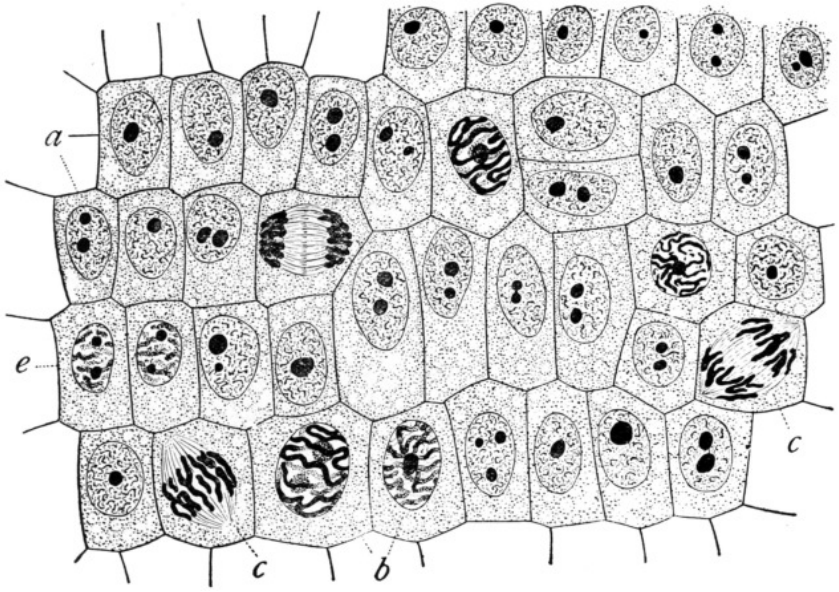
Last decades:

- 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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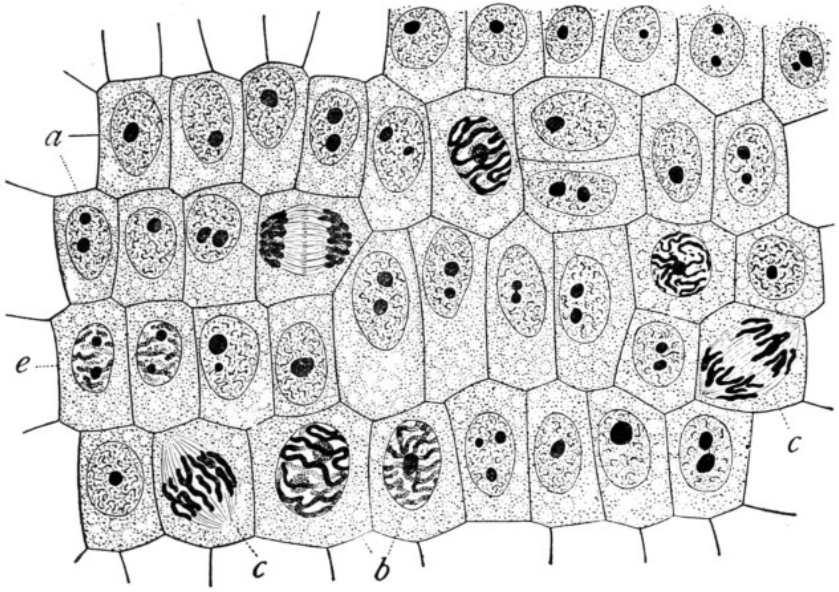

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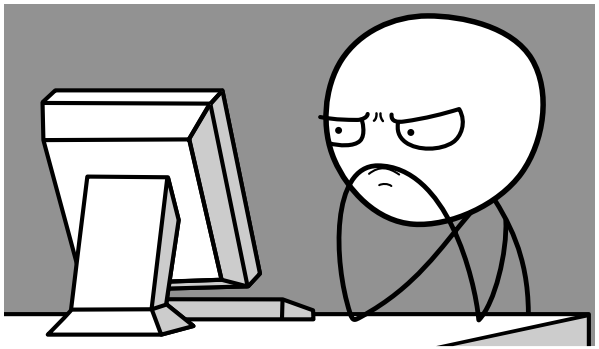
Empirical studies can be carried in reality or in simulation

Context

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



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  - How many nodes?
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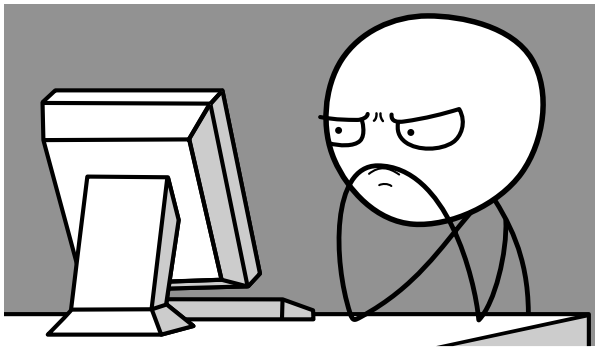

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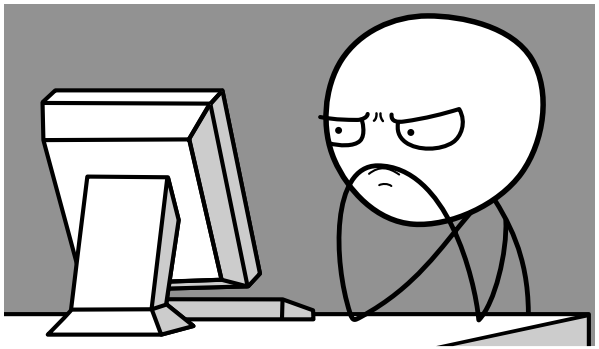

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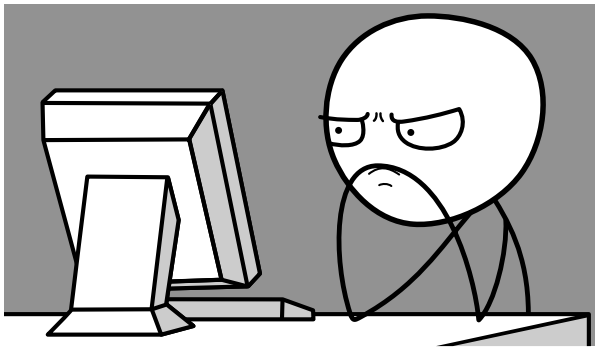

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Holy Grail: Predictive Simulation on a “Laptop”

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
- Modeling correctly the platform variability is key

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- Experiment methodology, to bias or not to bias
- 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
- Simply replace mpicc/mpirun by smpicc/smpirun

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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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Contribution: predict accurately the performance of HPL

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- More representative of some HPC applications
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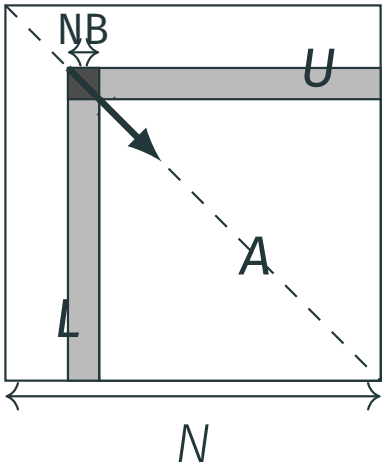

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for $k = N$ ***to*** 0 ***step*** NB **do**
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  Update the sub-matrix

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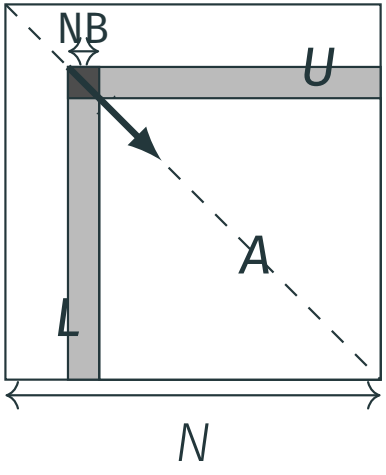

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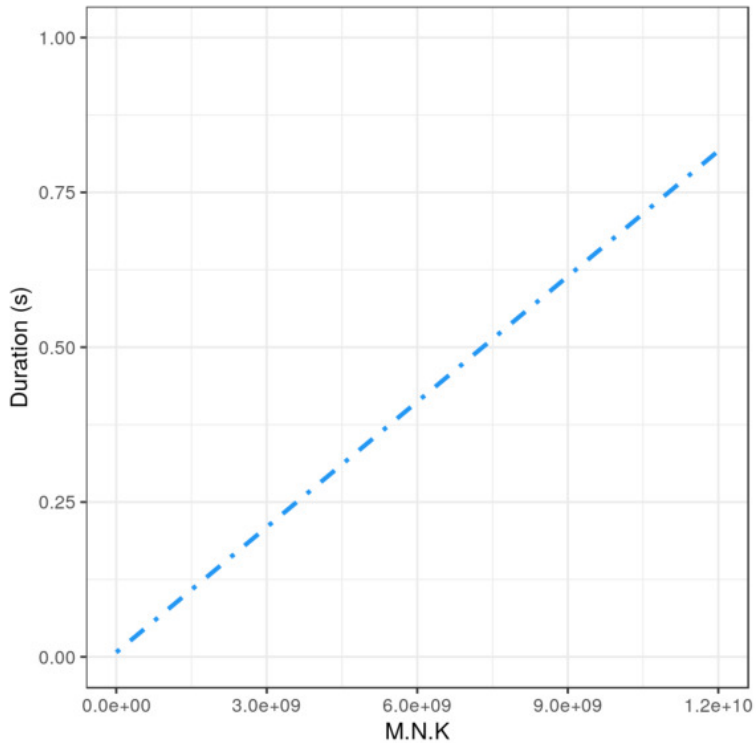
Tuning parameters

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

Hundreds of combinations

Modeling Commputations

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



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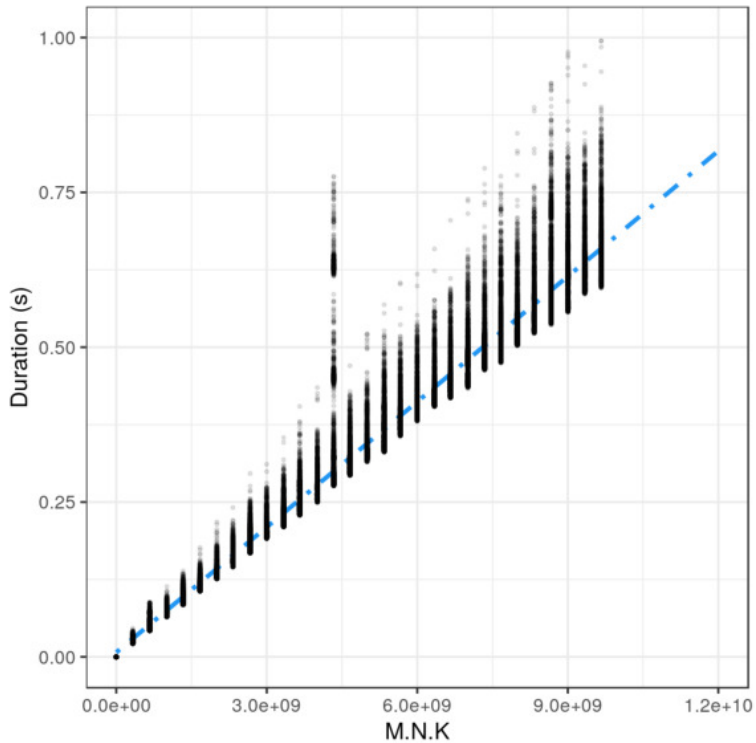

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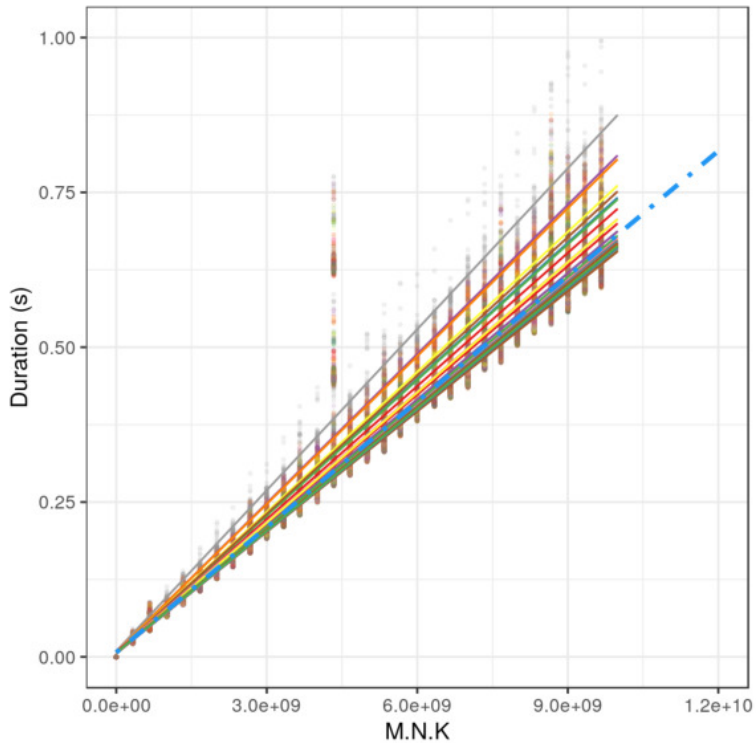
$$\texttt{dgemm}_i(M,N,K) = \underbrace{\alpha_i.M.N.K}_{\text{per host}}$$

Different color $\Rightarrow$ different host



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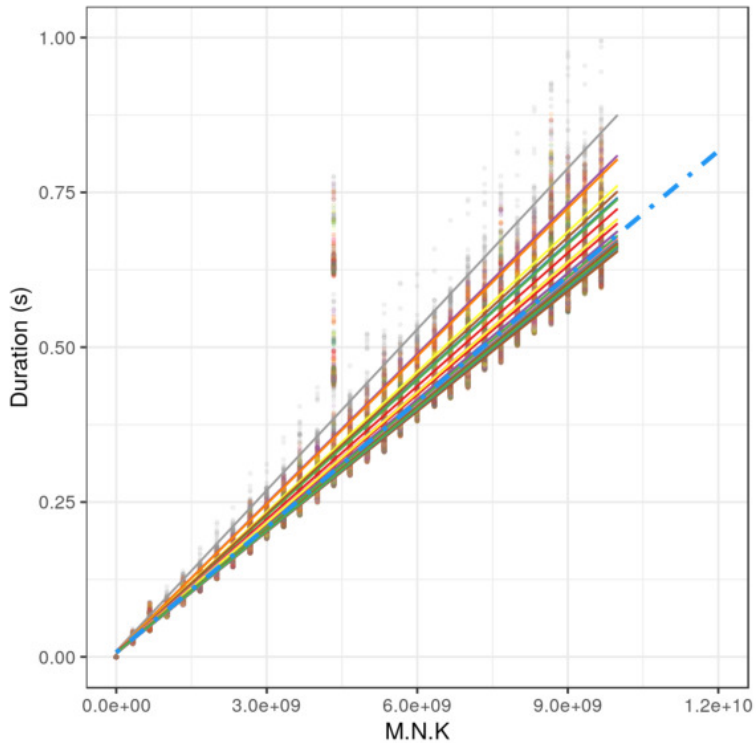
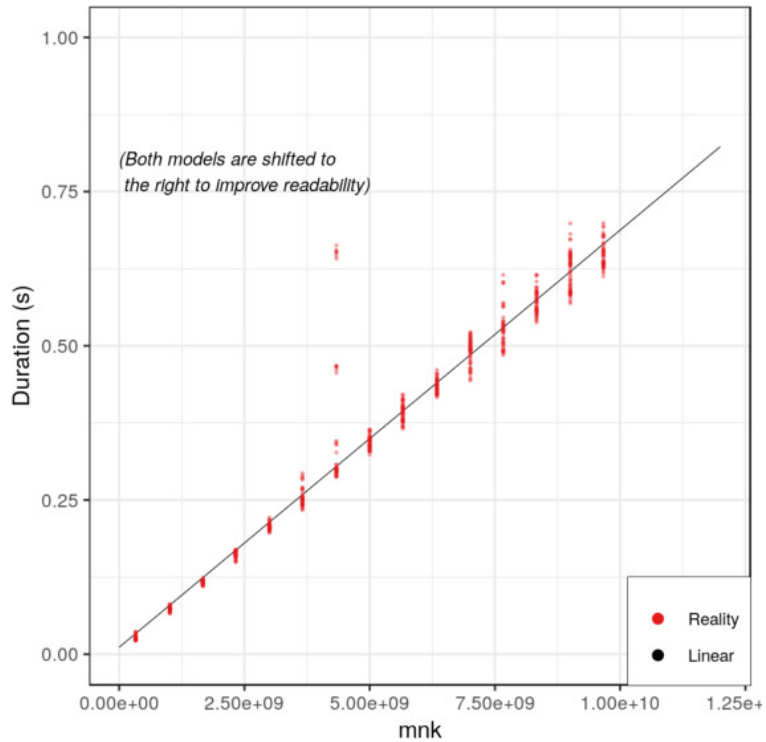


For a particular host



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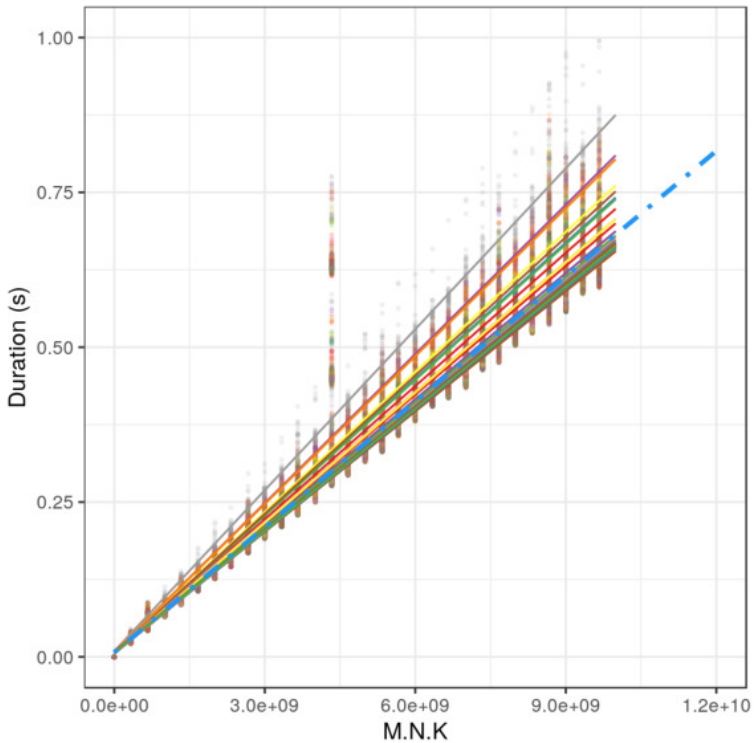

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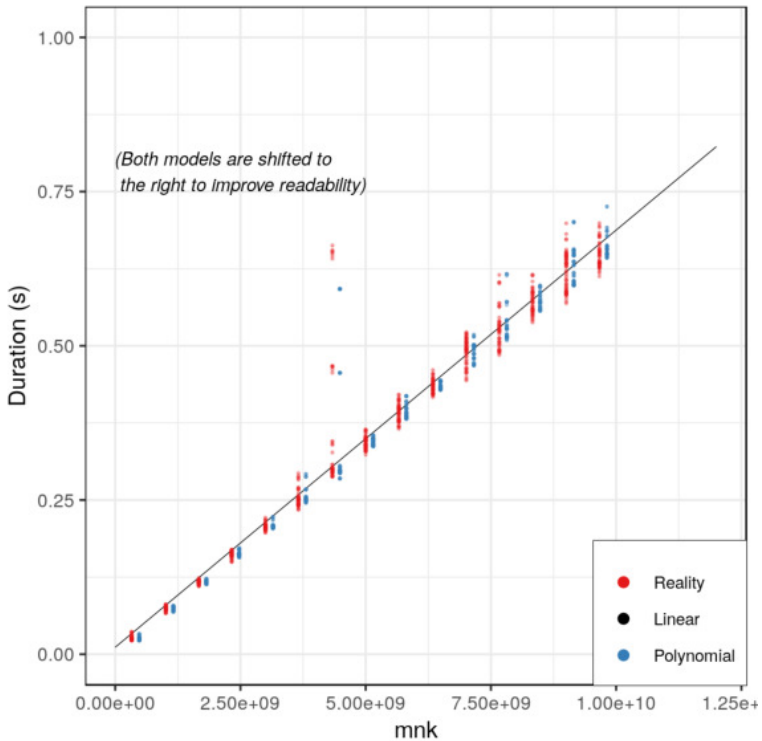

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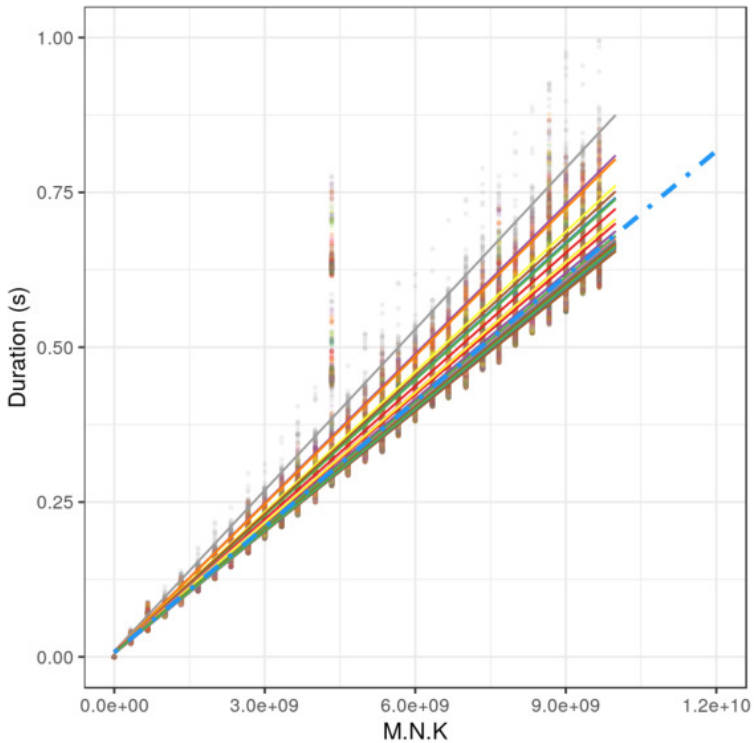

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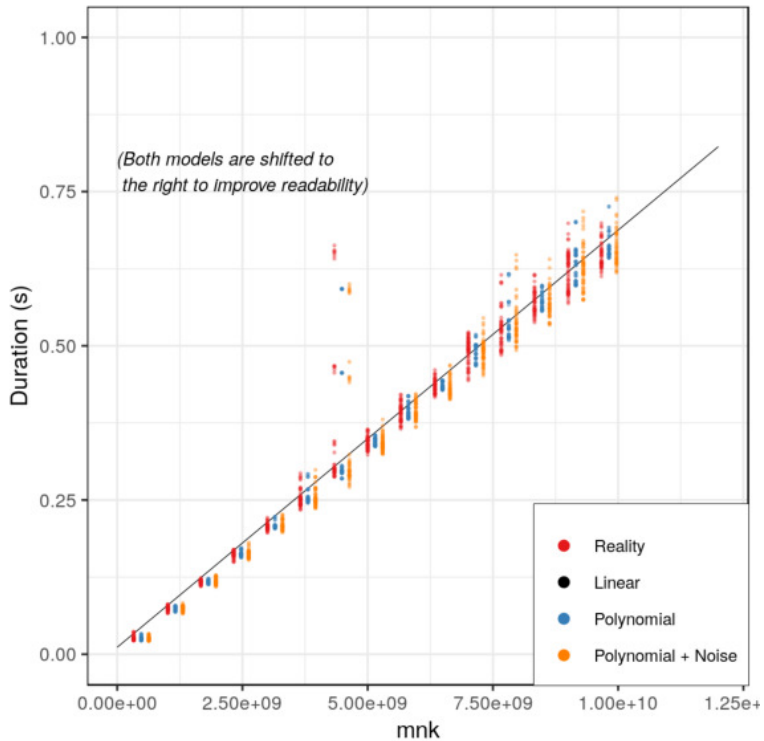

Modeling Communications

Hand-crafted non-blocking collective operations intertwinned with computations

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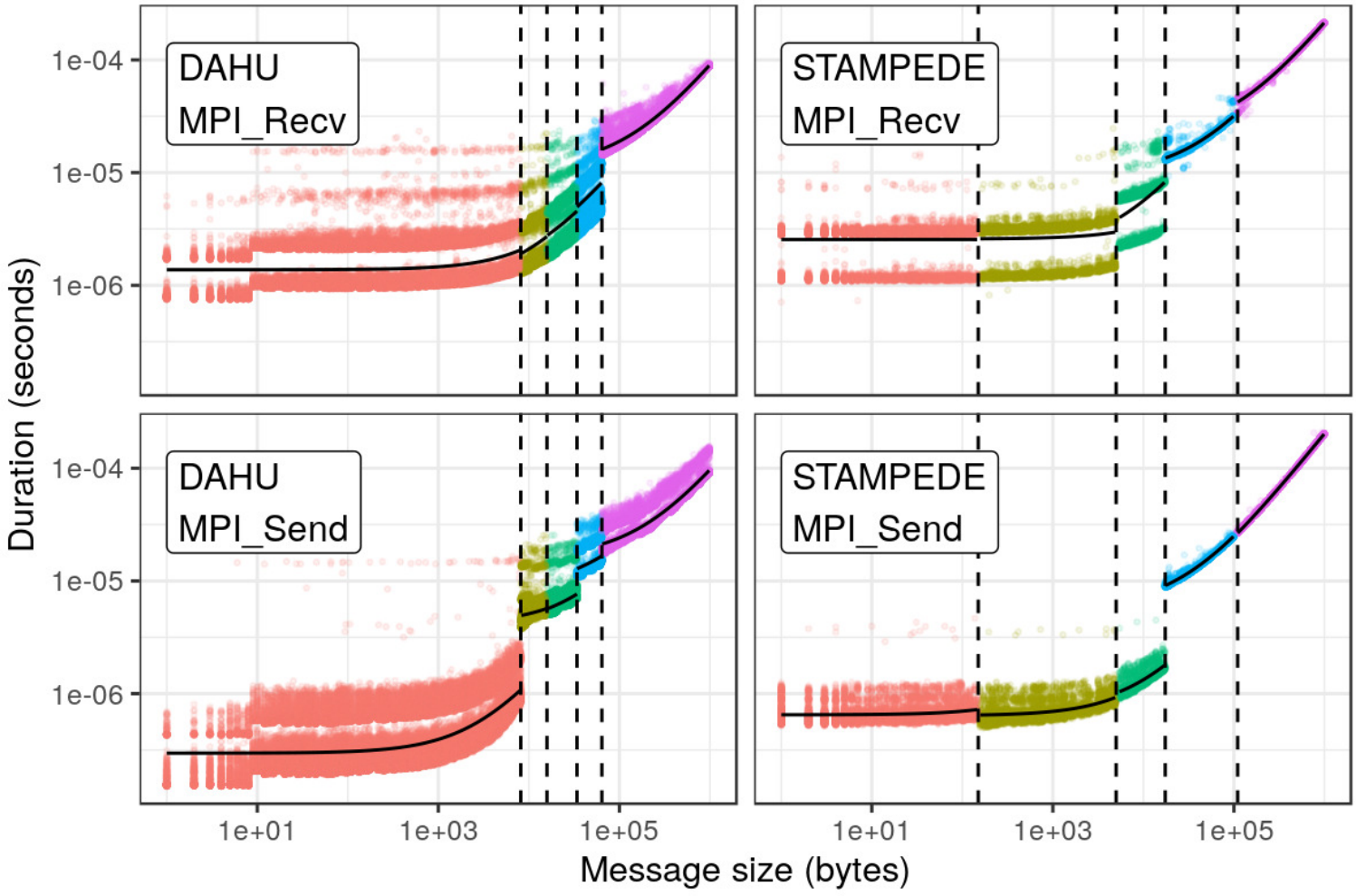
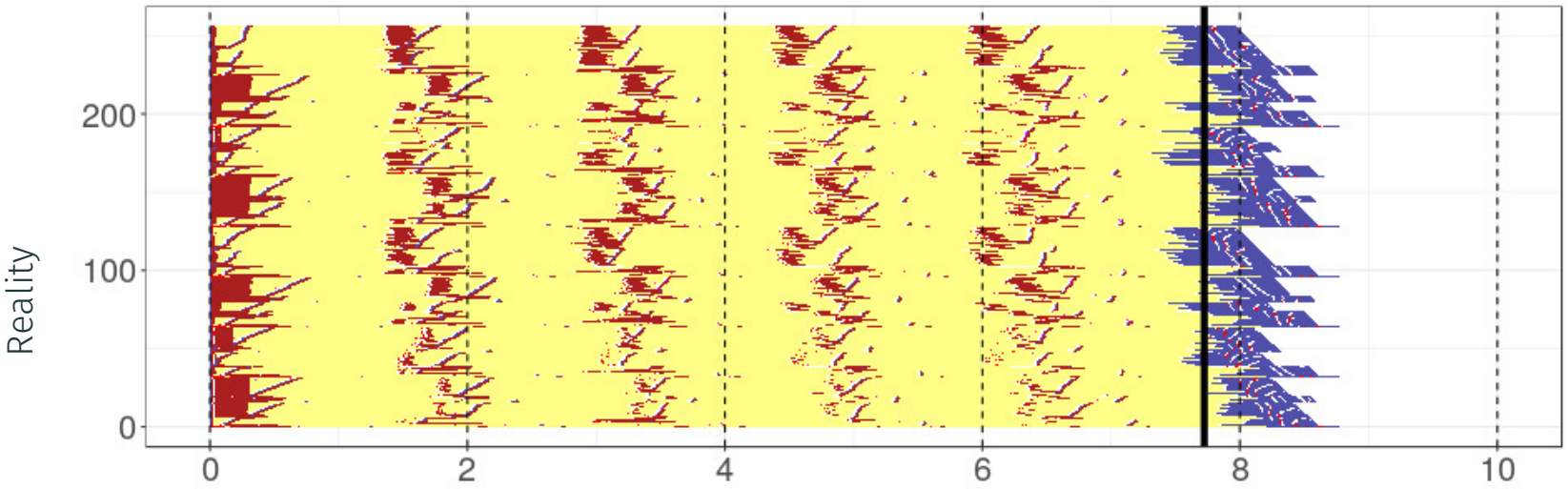


Validating the predictions

Internal behavior of the application

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



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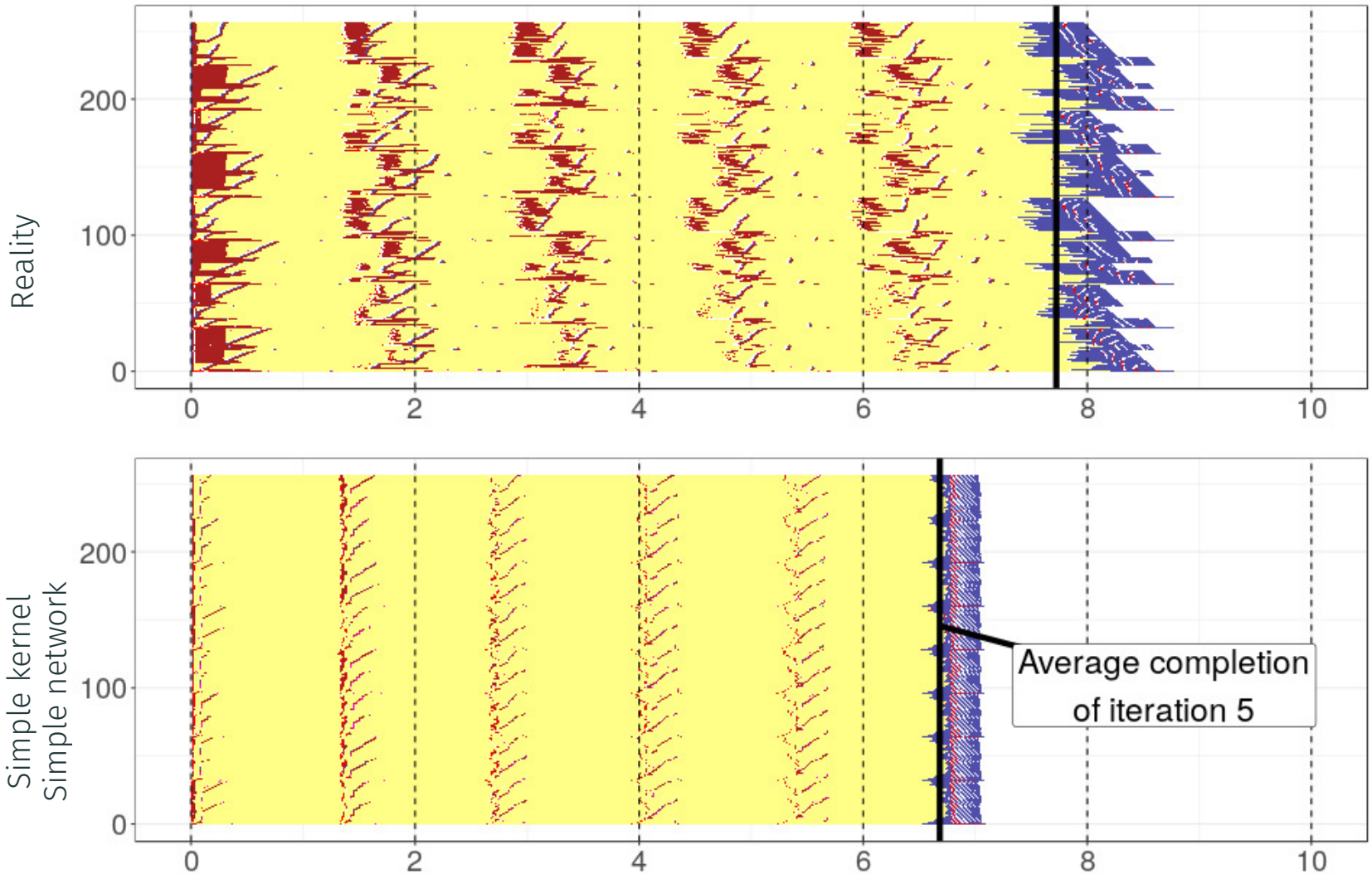

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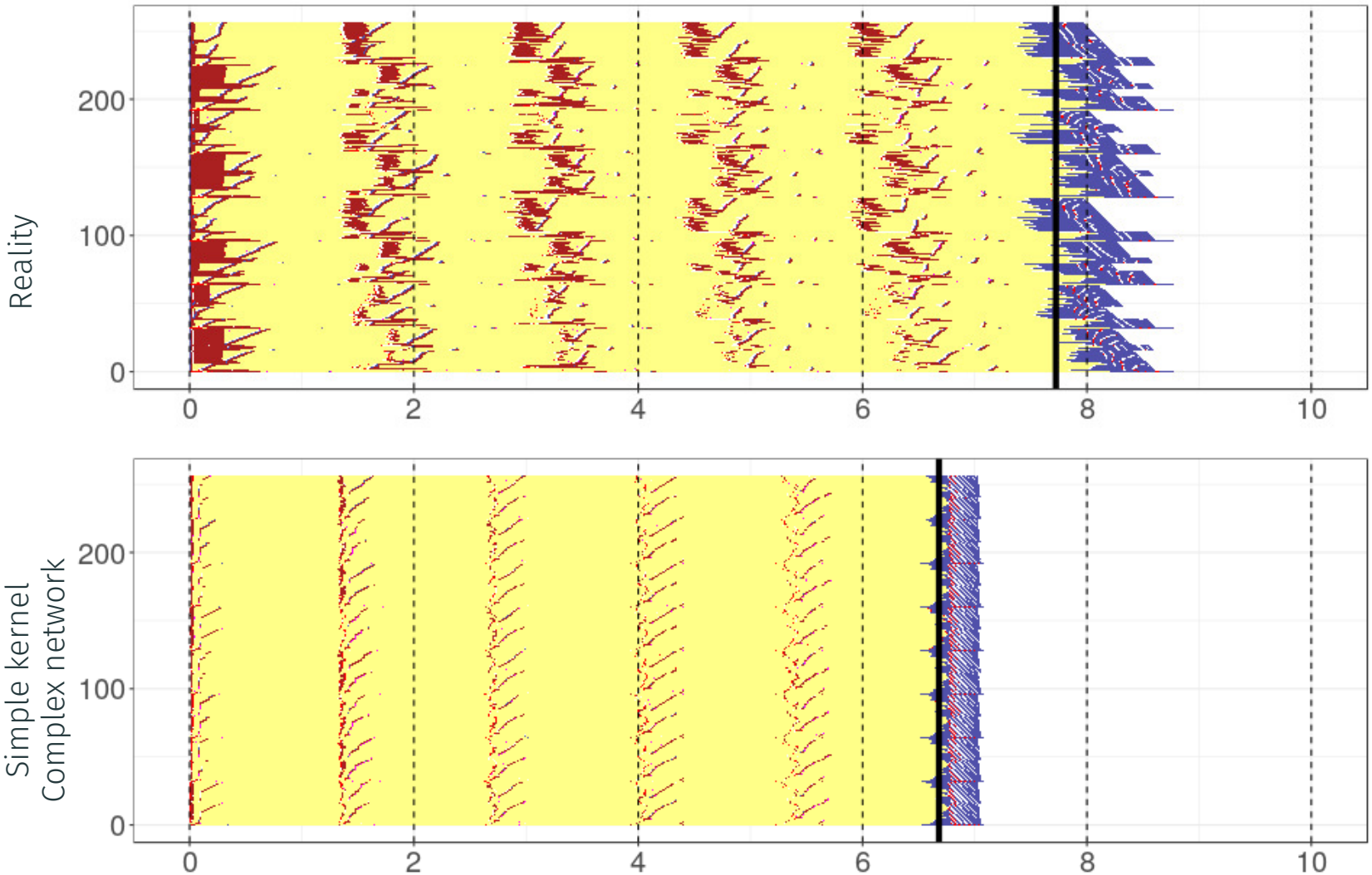

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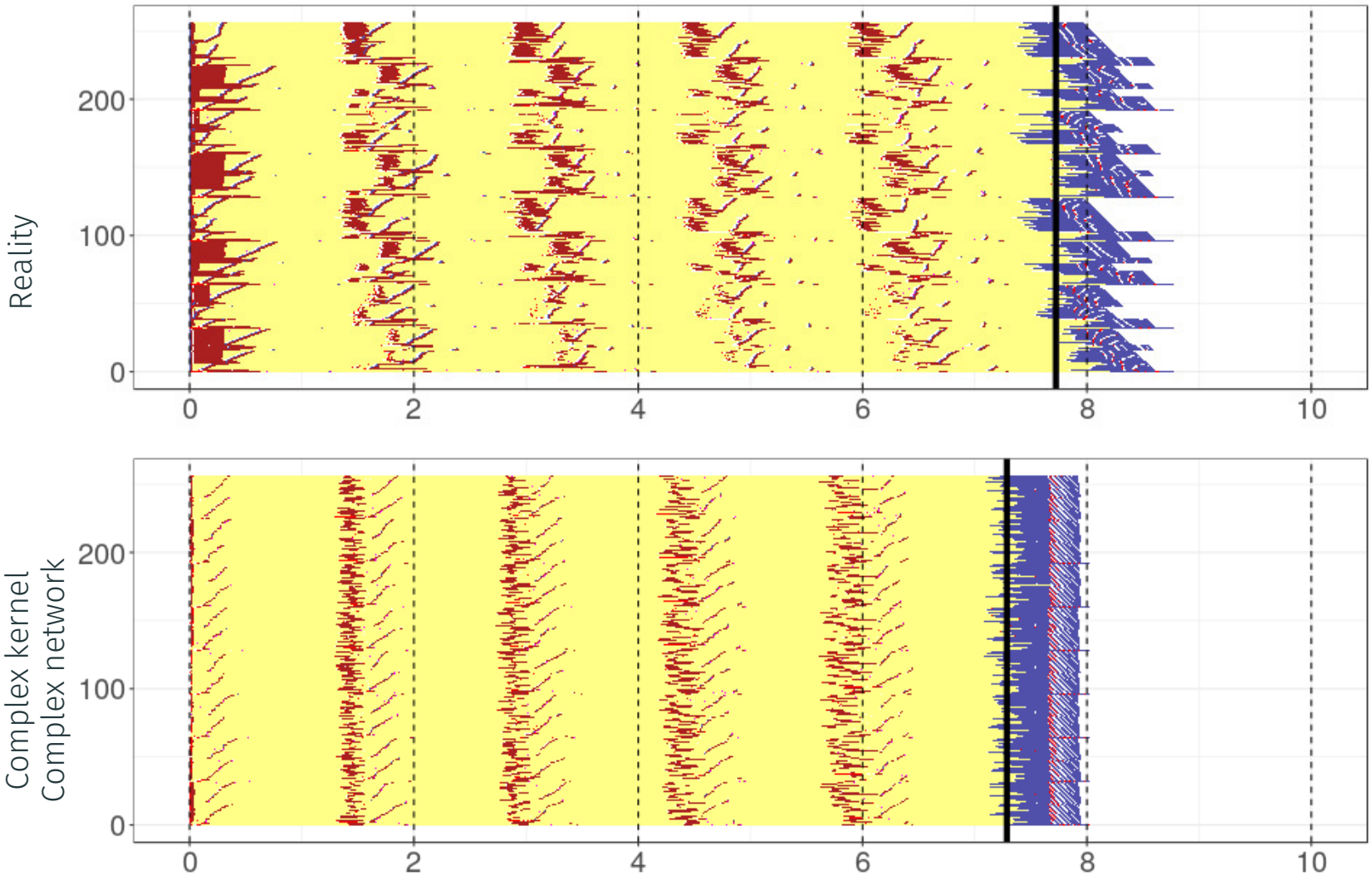
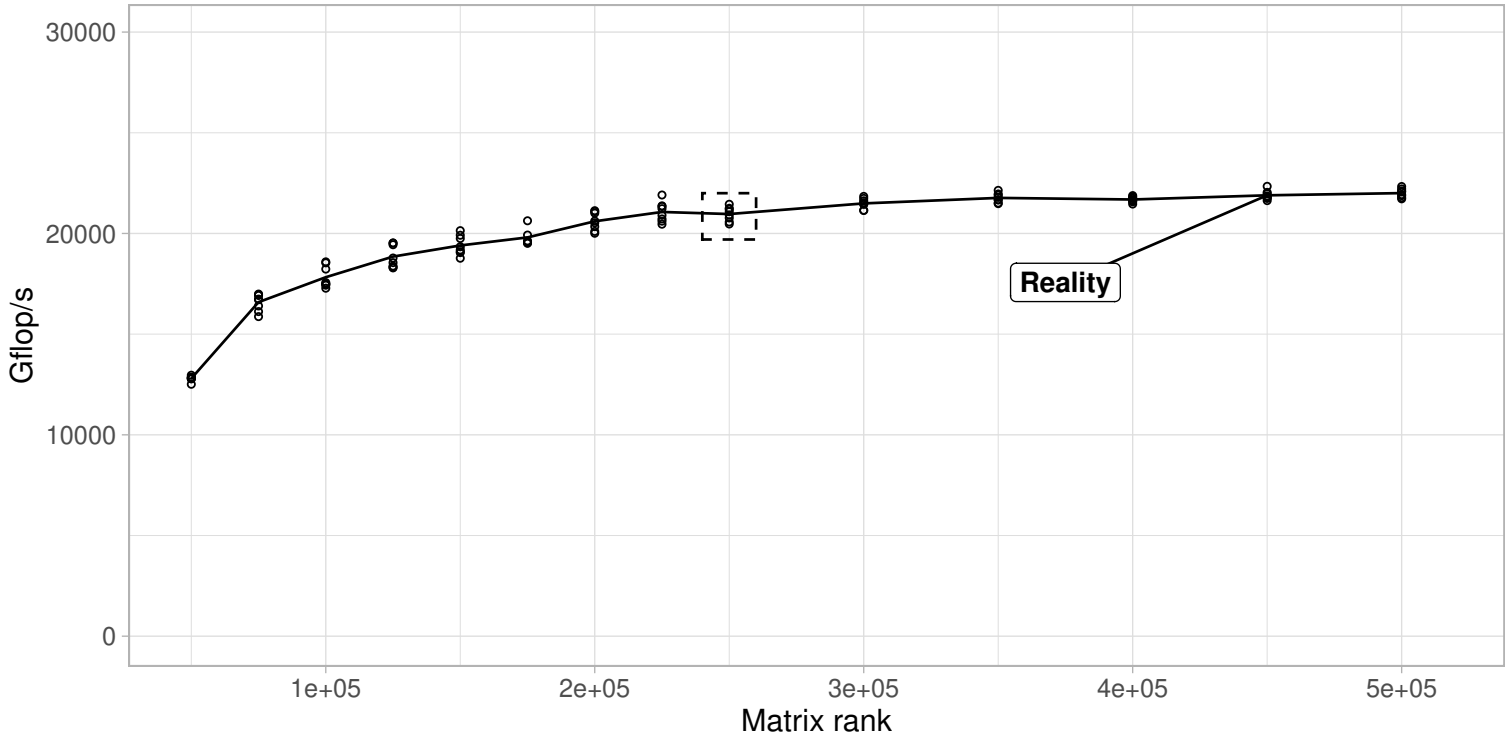


Influence of the problem size

Now the complete run, with 1024 MPI ranks



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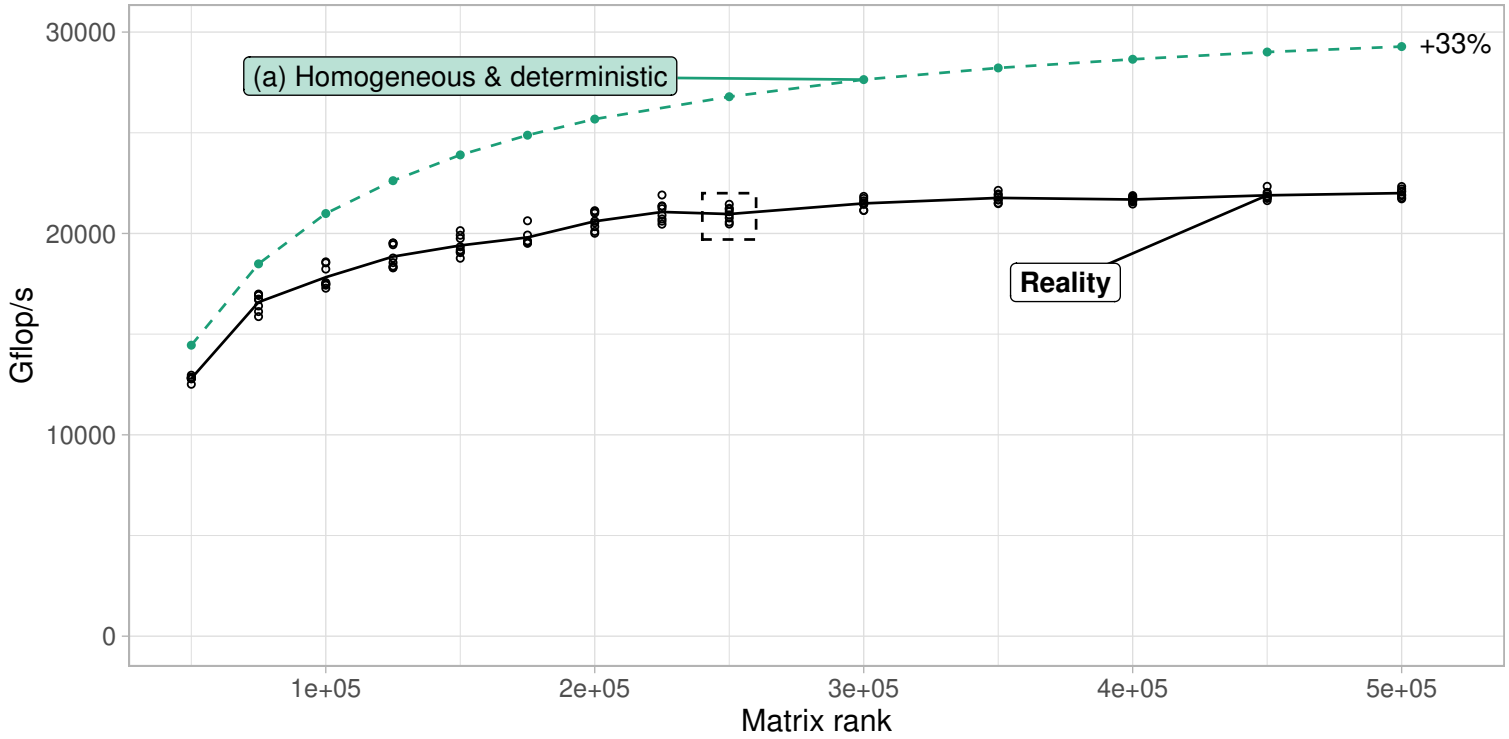

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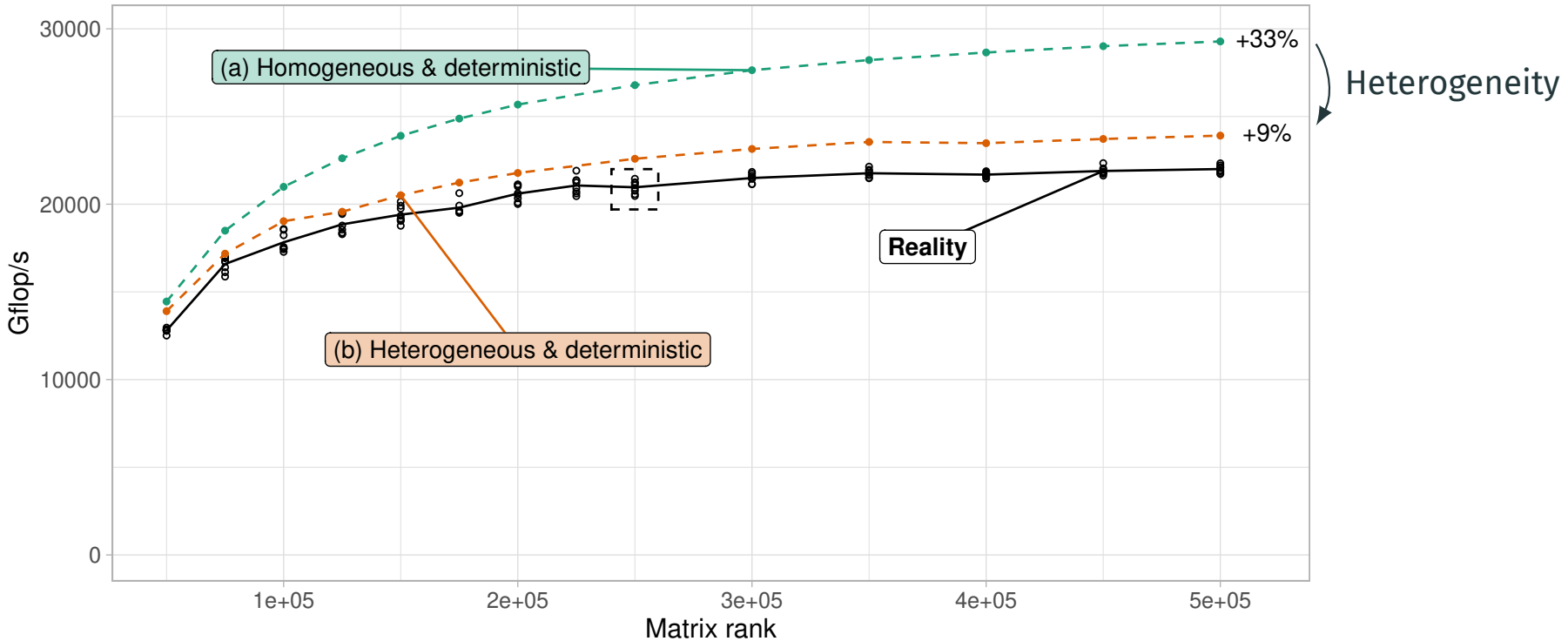

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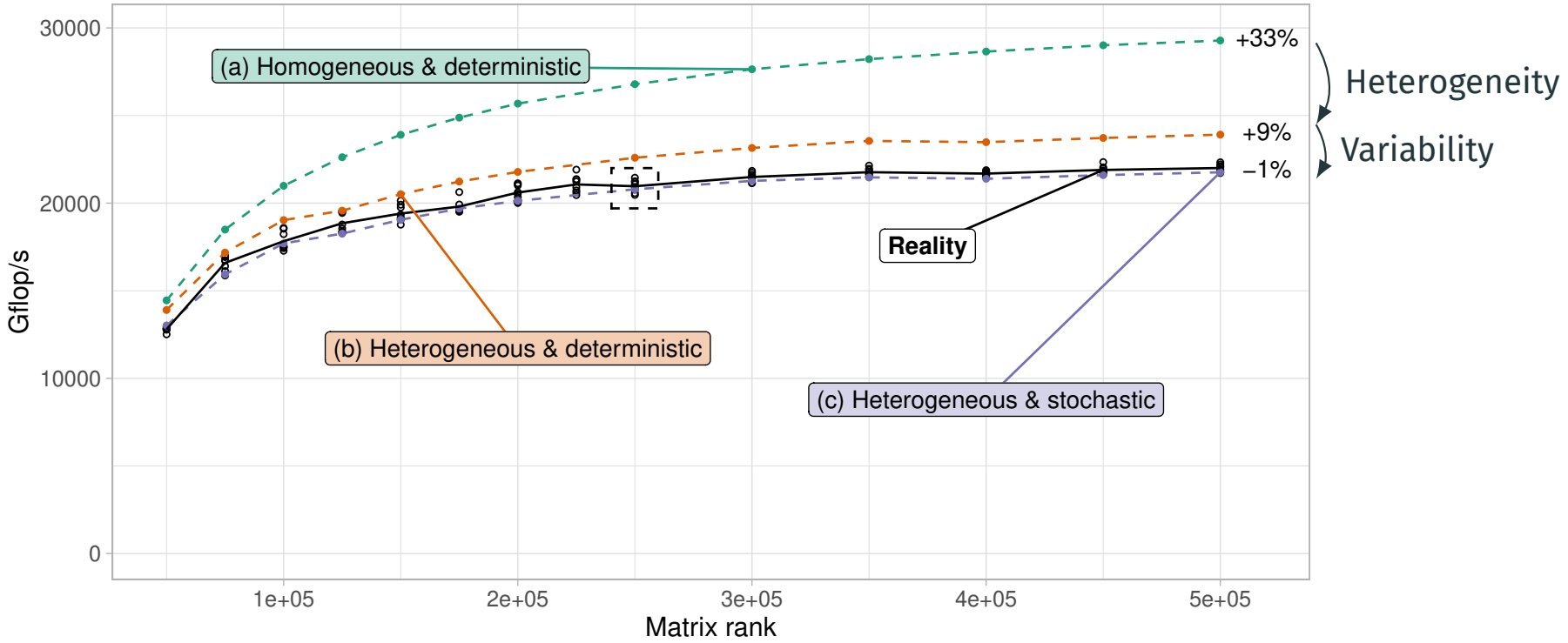

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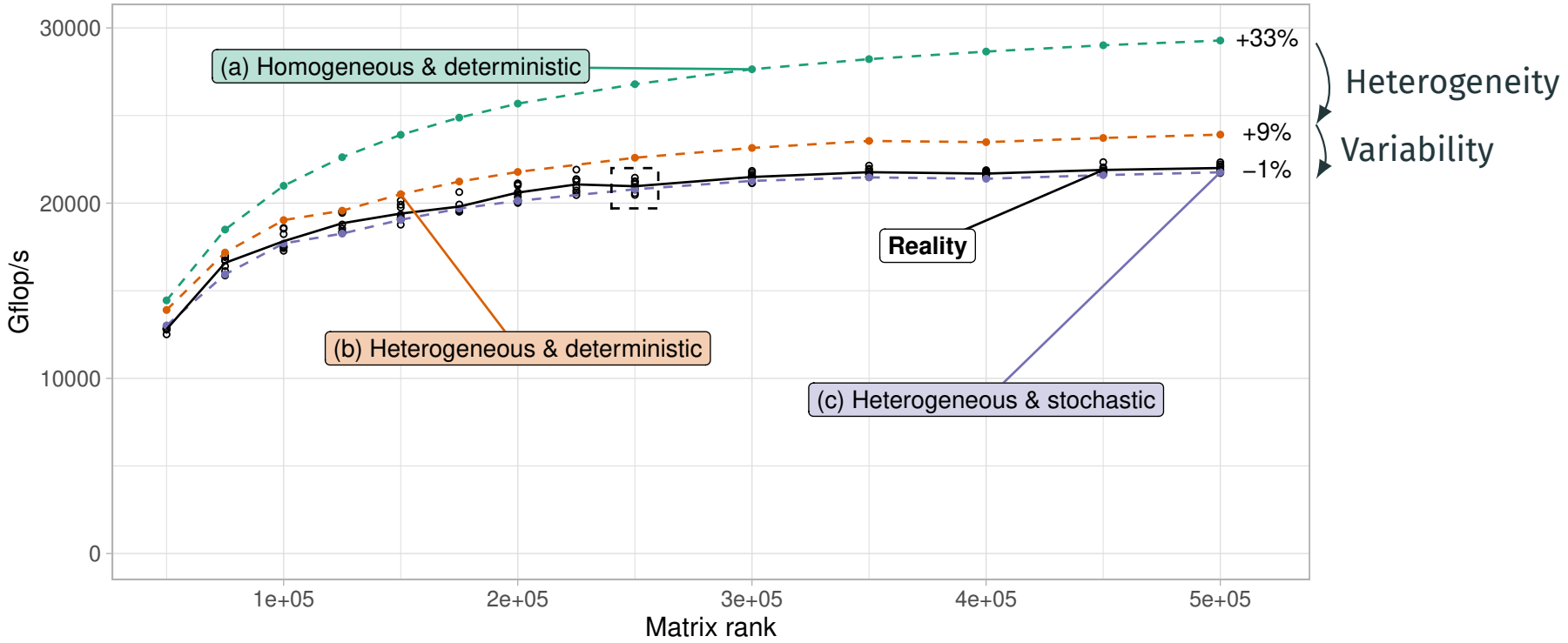
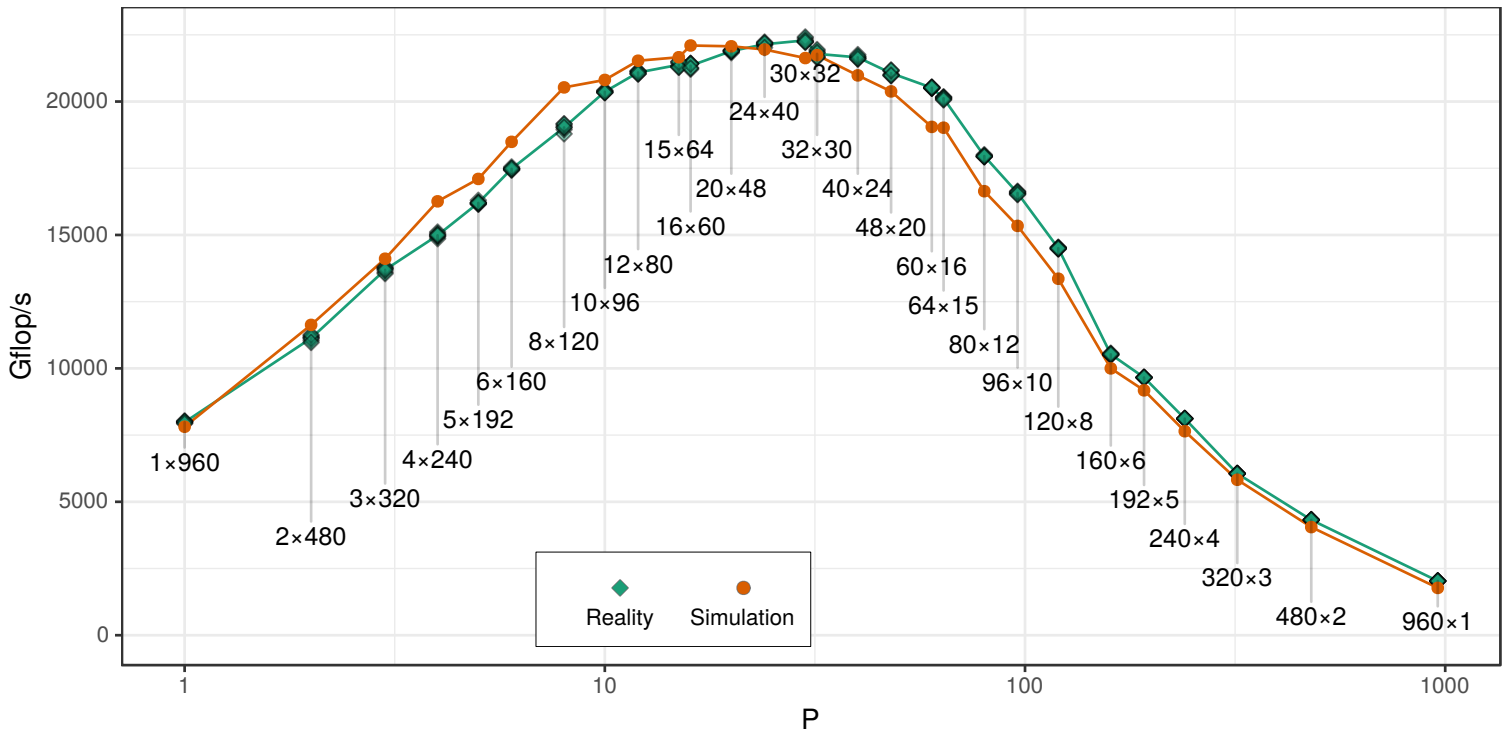


Take-Away Message: accurate prediction

Modeling both spatial and temporal computation variability is essential

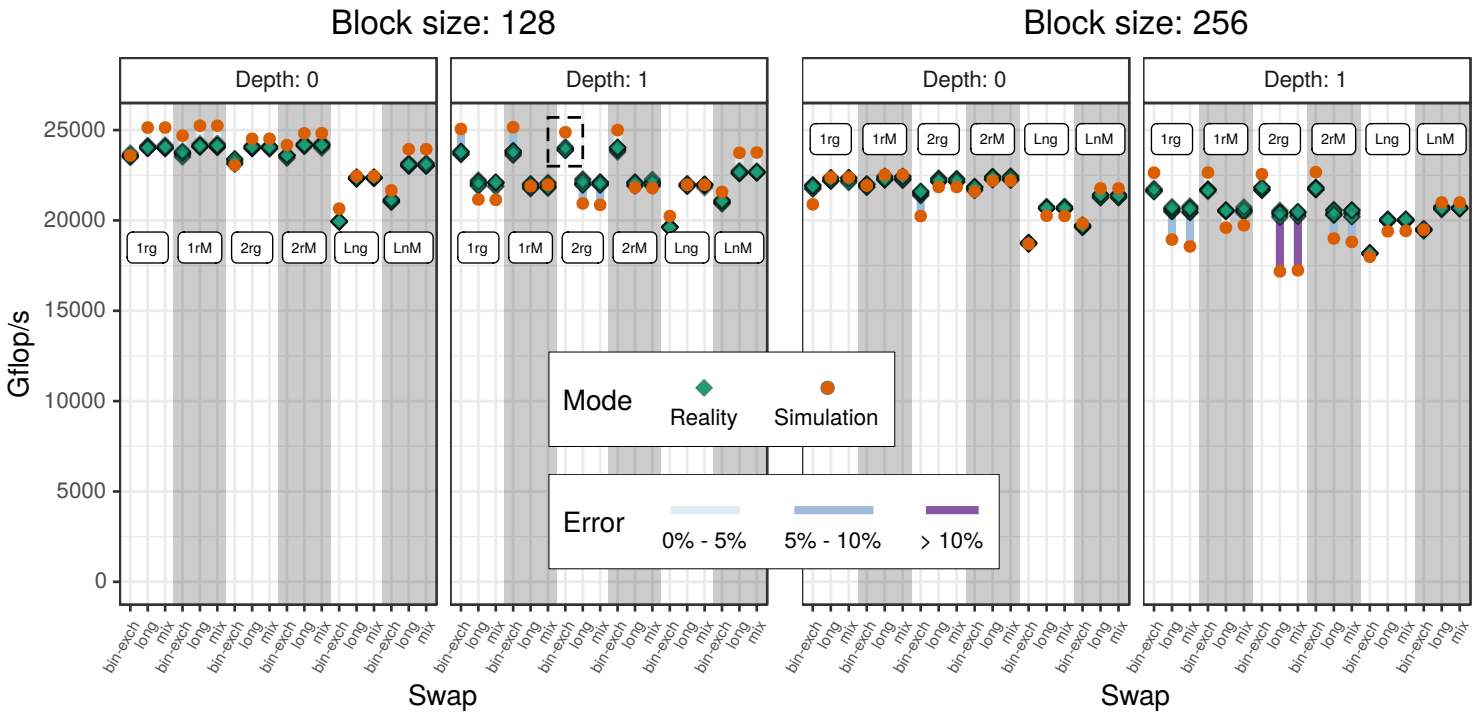
Influence of the geometry

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

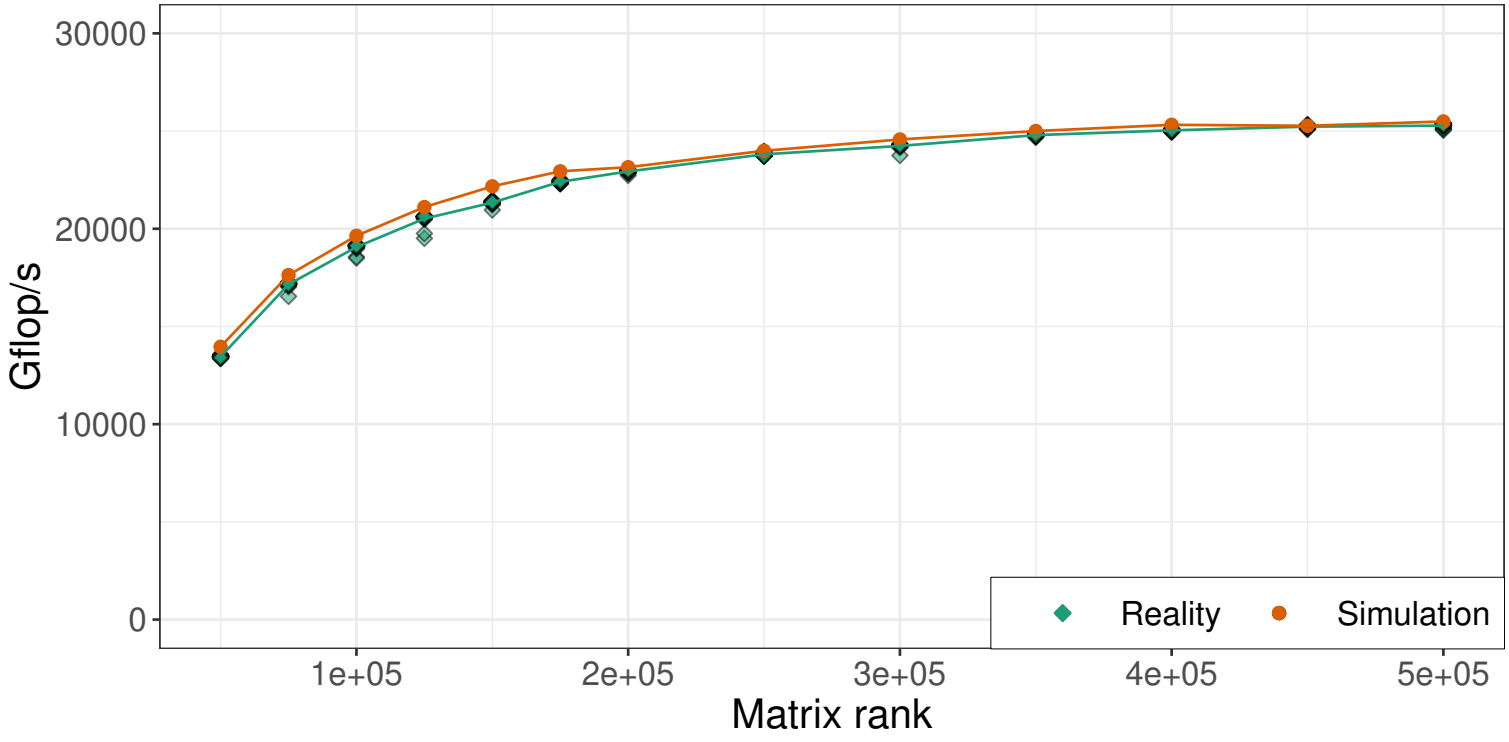


Influence of the other parameters

Tested the 72 combinations of the remaining parameters



Influence of a platform change



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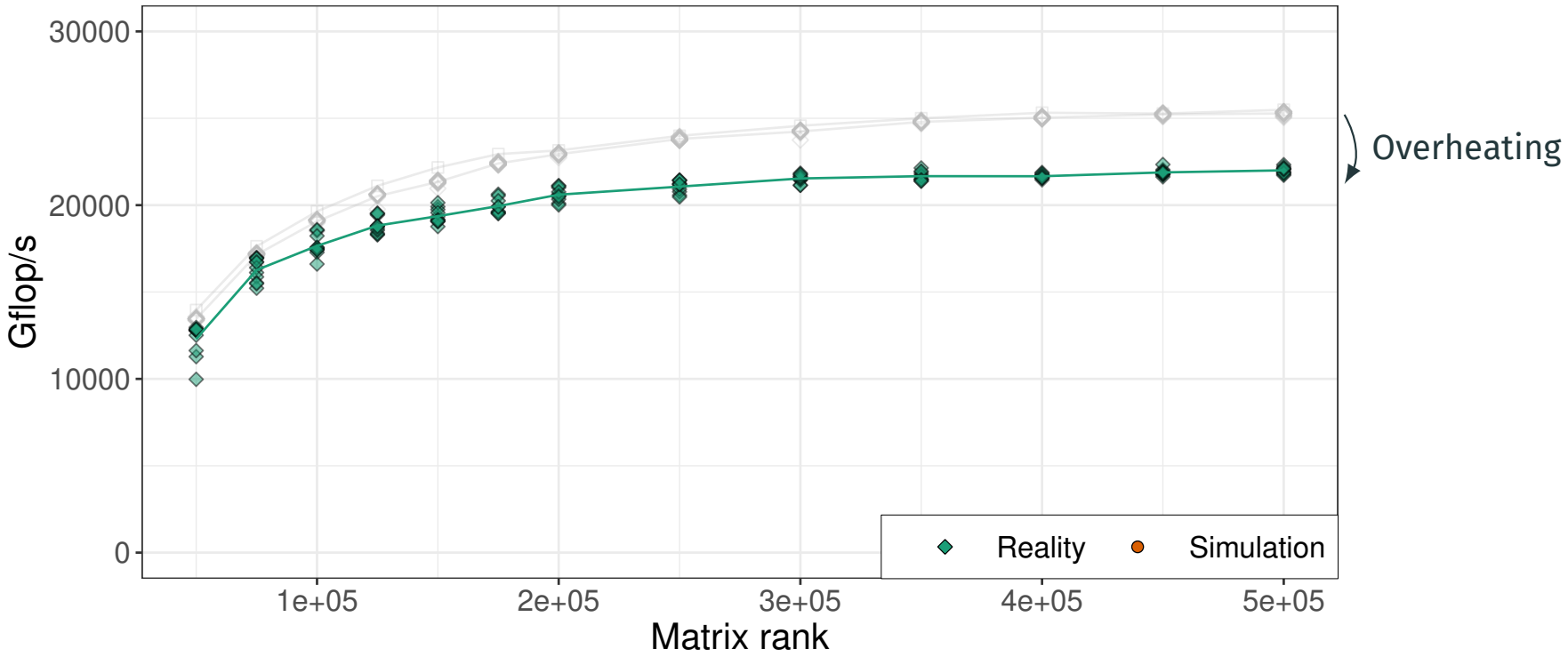
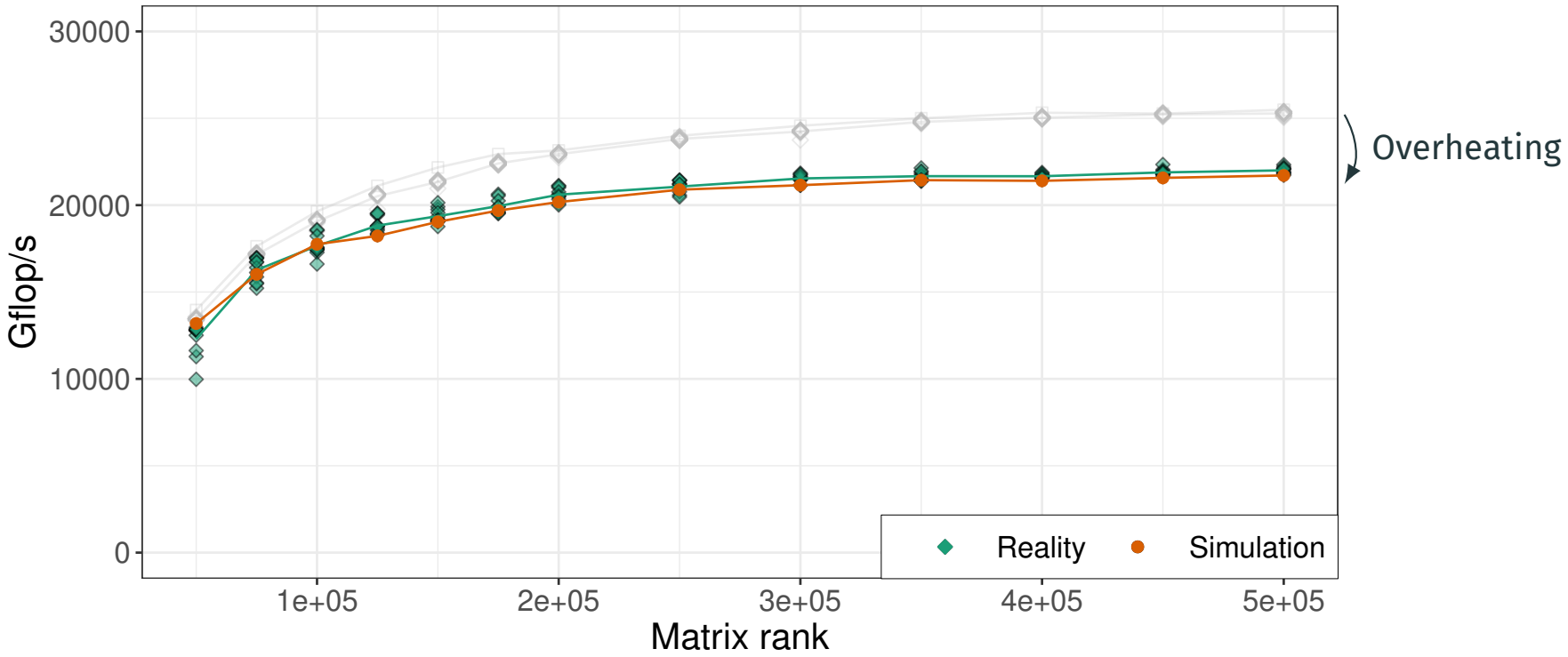


On four nodes, the cooling system malfunctionned for several weeks

Influence of a platform change



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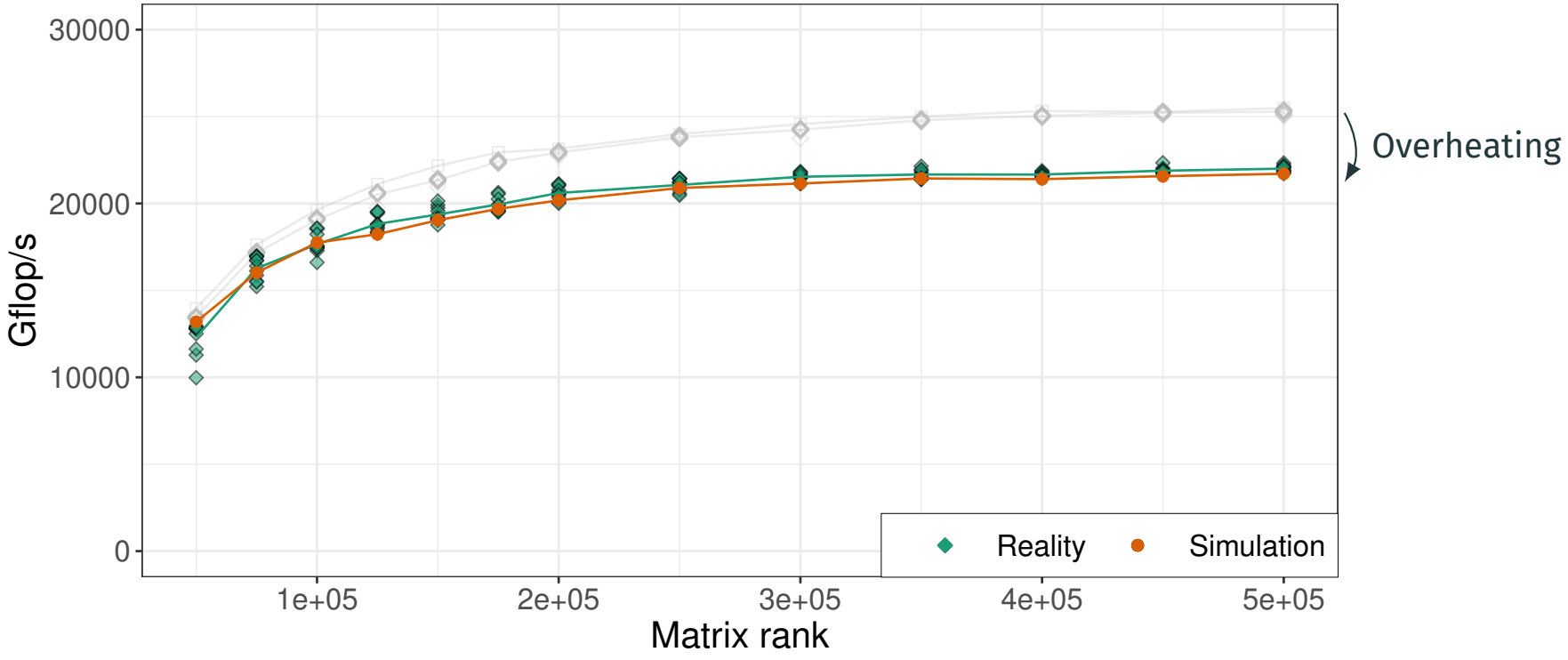

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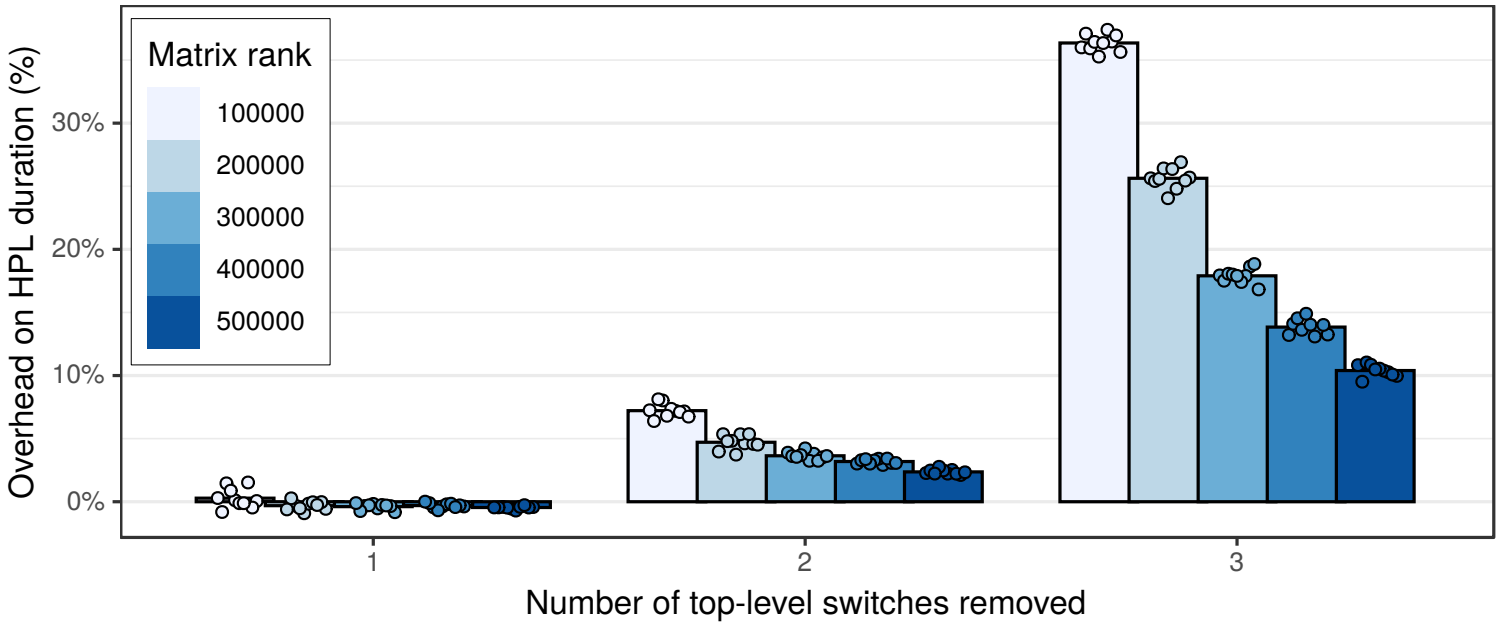
Take-Away Message: Re-measuring `dgemm` durations to generate a new model was enough to account for the platform change

Use case: sensibility analysis

What if the network topology of my cluster was different?



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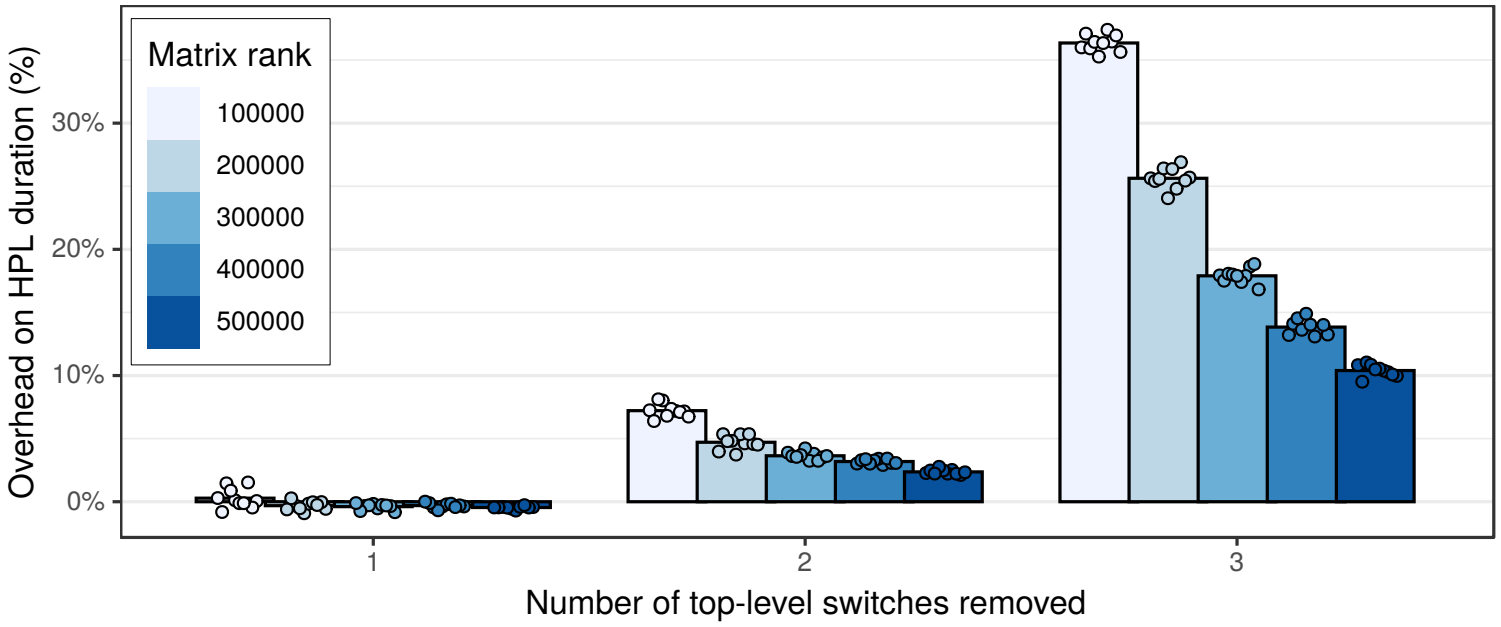

Faithful surrogate $\Rightarrow$ Empirical studies of hypothetical platforms

$\Rightarrow$ 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)

Parenthesis: on the difficulties of experimentation

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Experimental biases when measuring `dgemm` or MPI durations

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

- Sampling method for generating the sequence of calls
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Bias may be desirable in some situations

Performance tests

Regular measures

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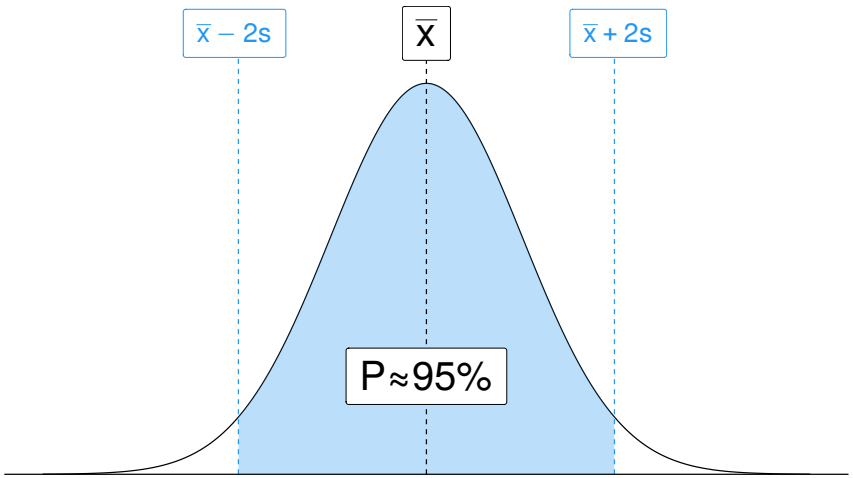
If the platform did not change, then each parameter is normally distributed (thanks to CLT)

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

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

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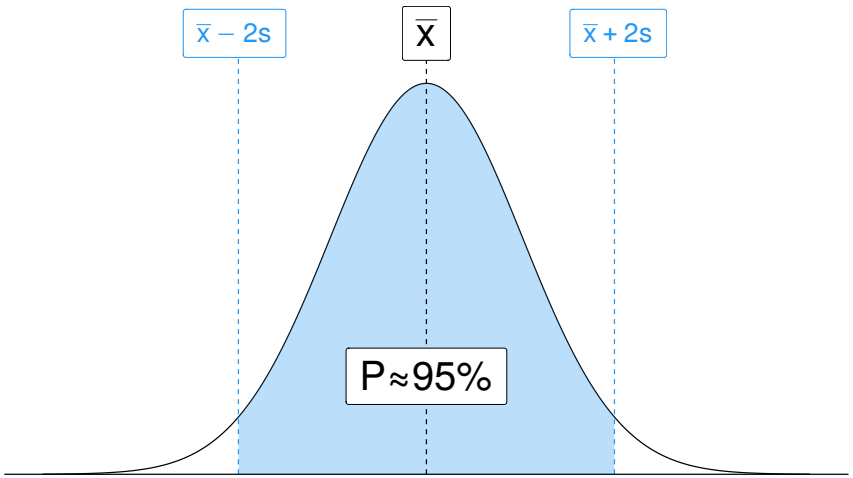

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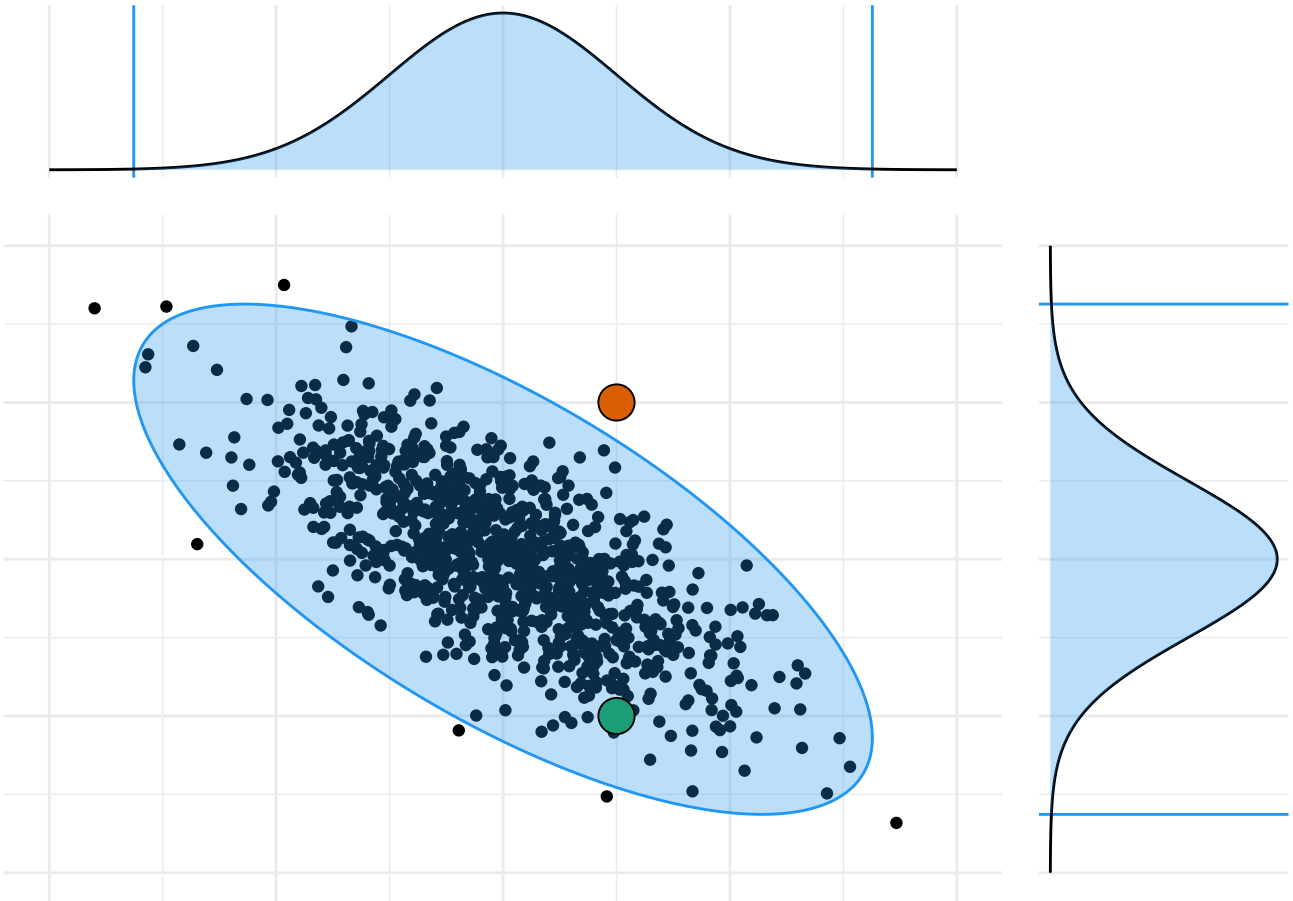
Note: using the F distribution instead of the normal distribution (the true mean and standard deviation are unknown)

Fluctuation interval for several variables

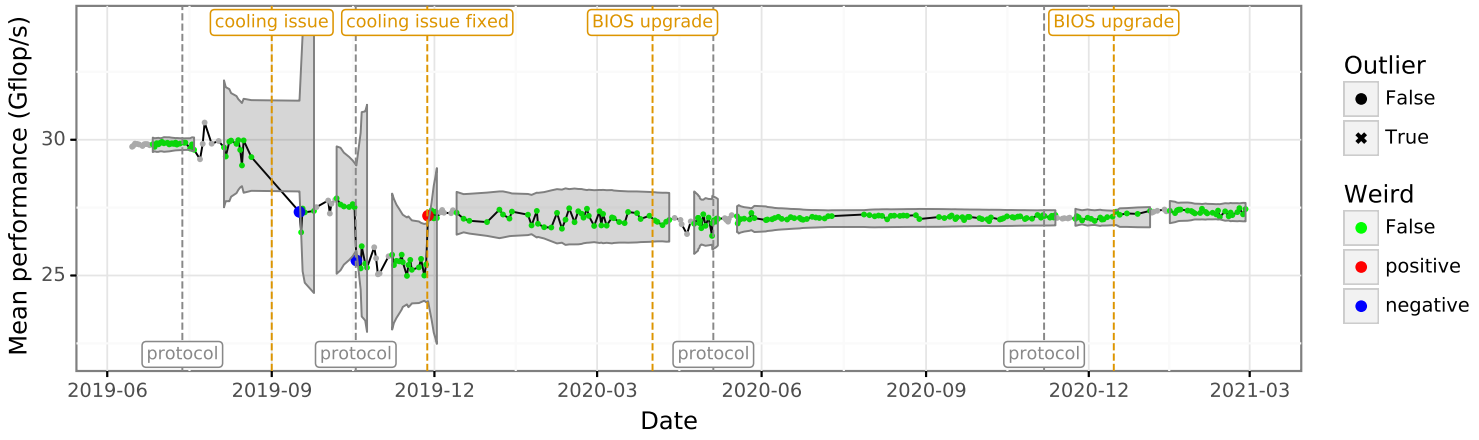
With several variables, use their covariance matrix

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



Result: performance fluctuation

Performance fluctuation of the node dahu-14



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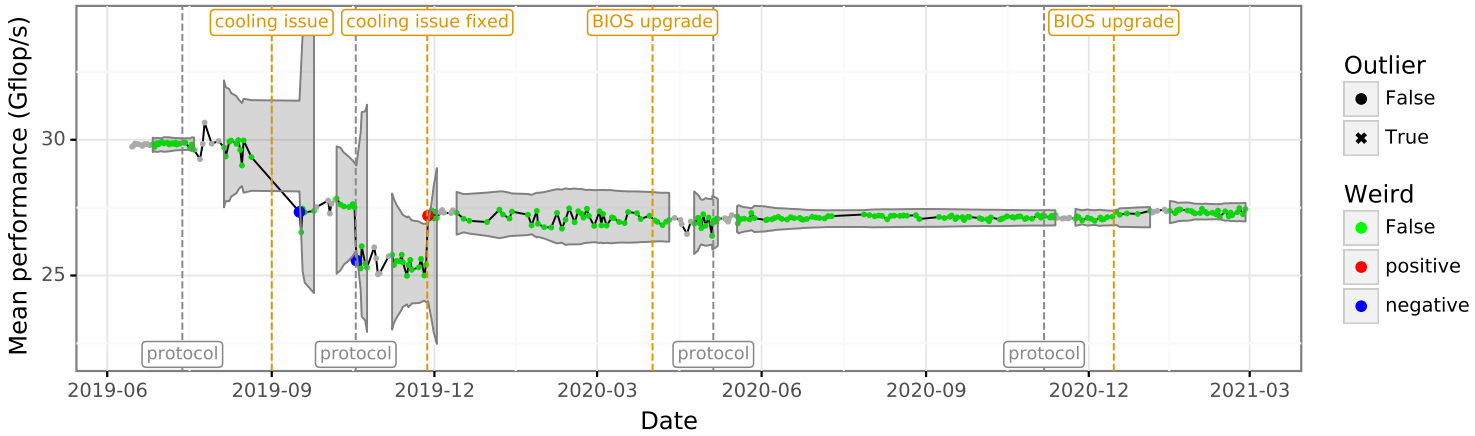
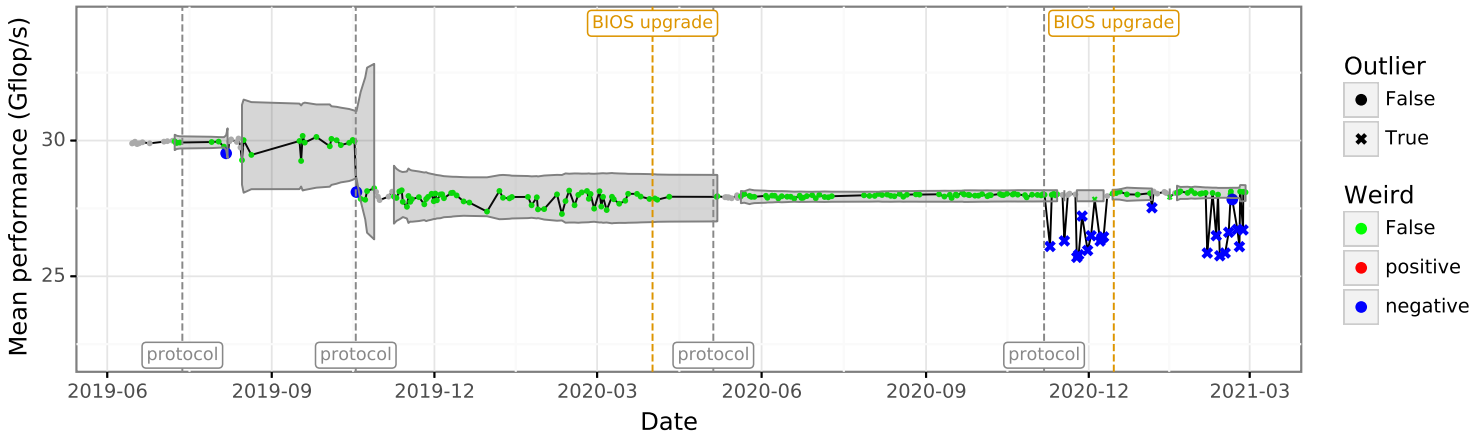


Performance fluctuation of the node dahu-32



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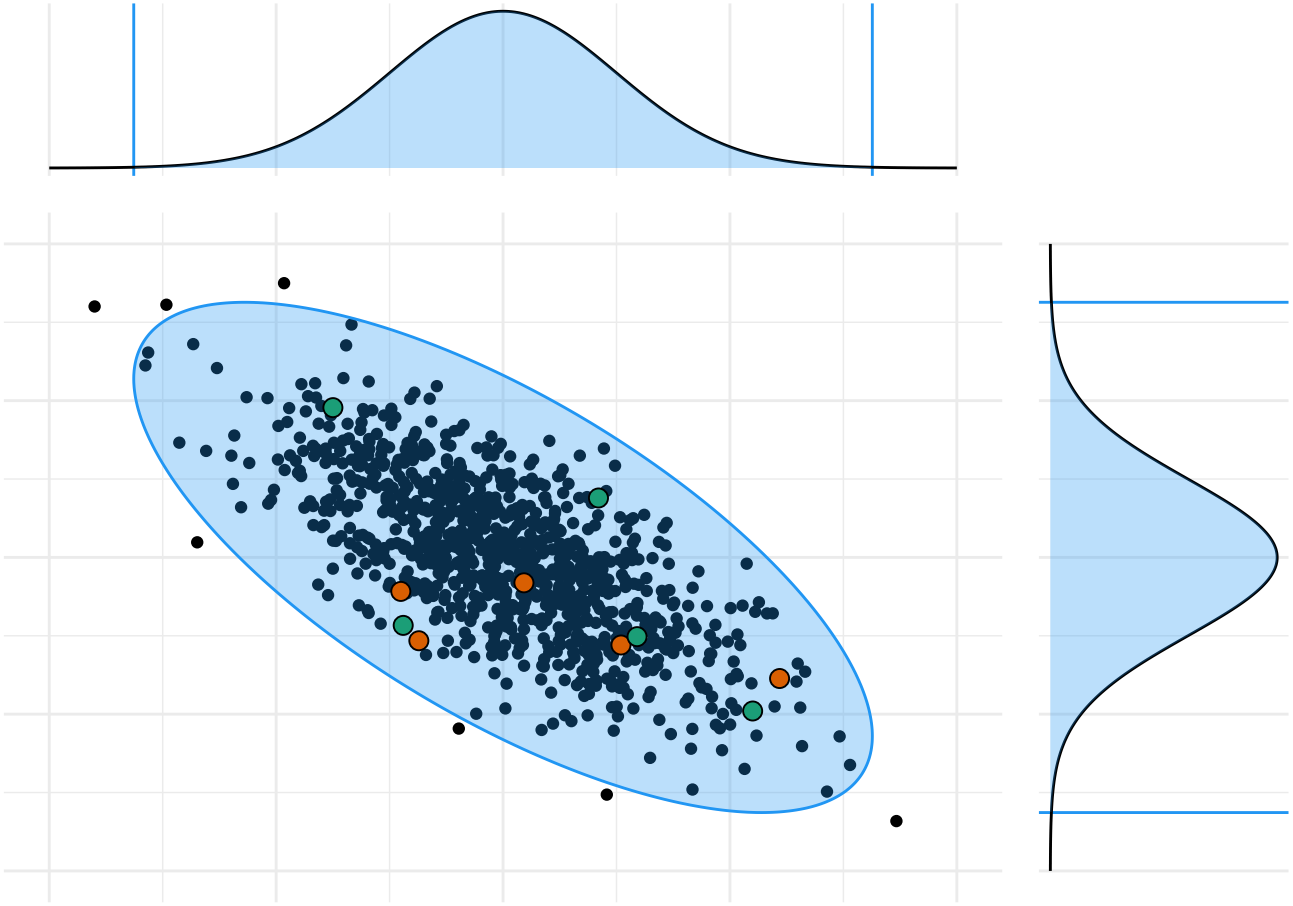
Example with 5 measures



Fluctuation interval for several measures

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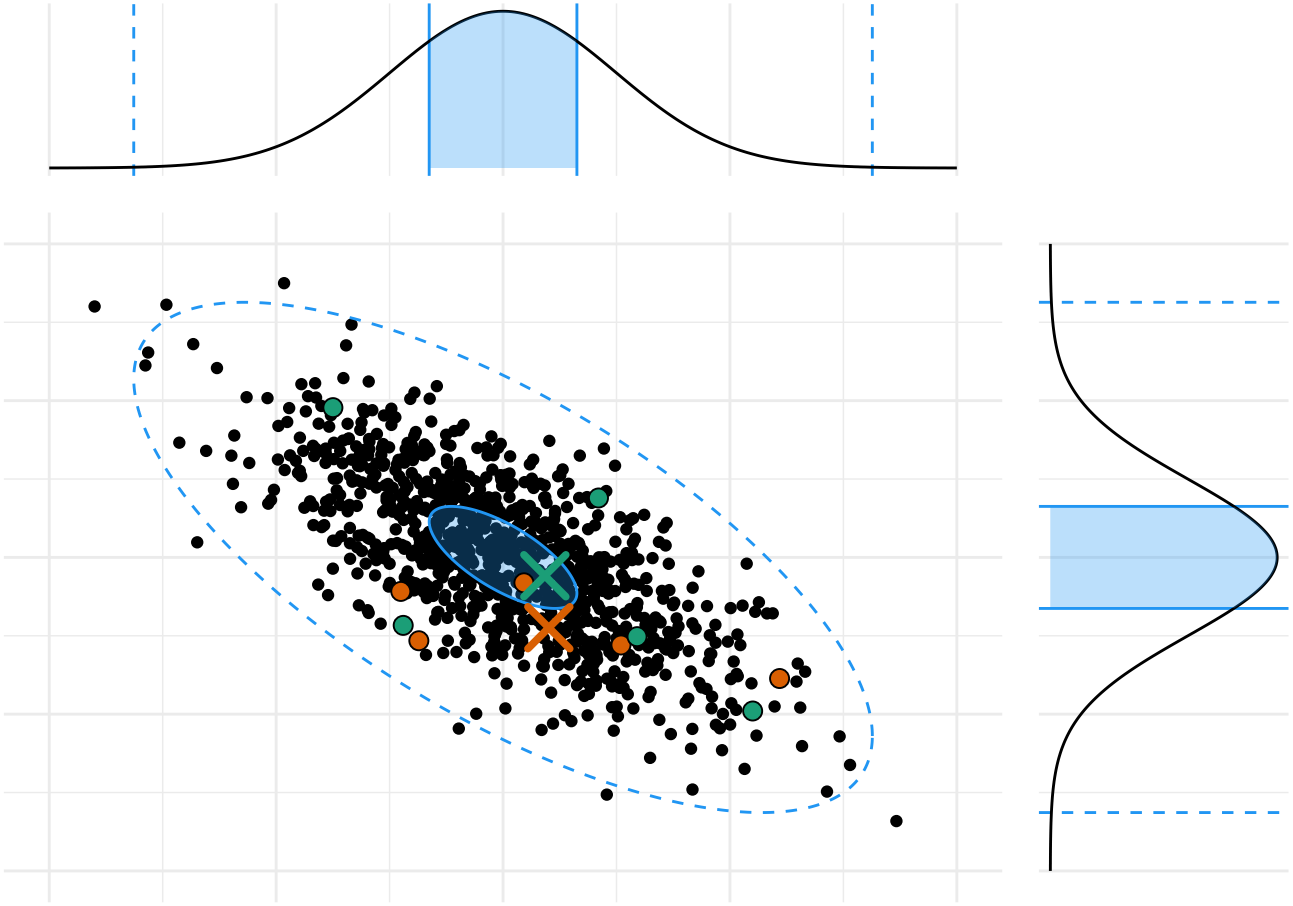
Example with 5 measures (averages represented by crosses)



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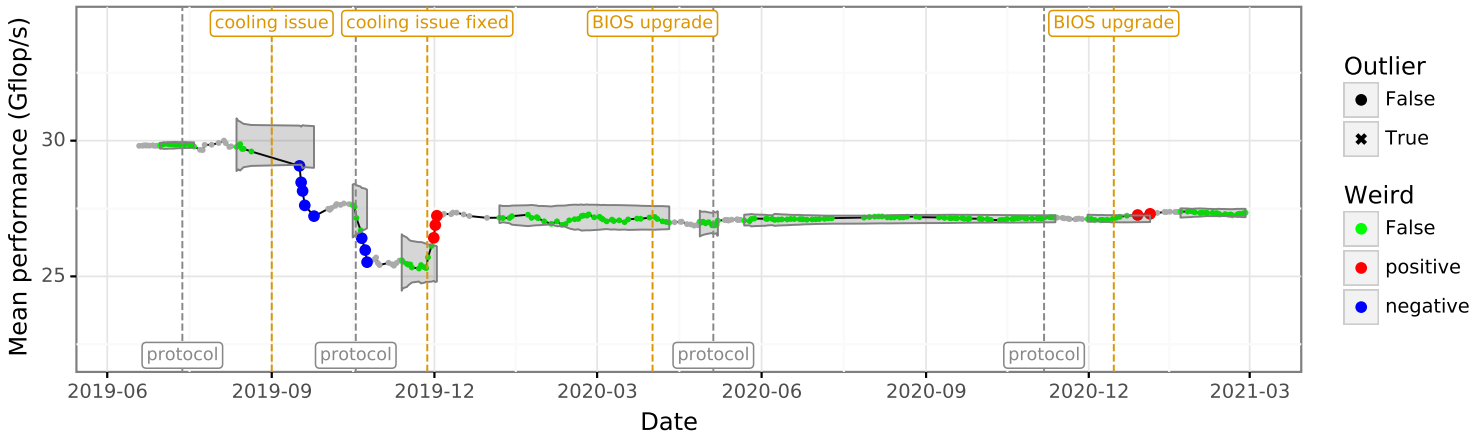
Performance fluctuation of the node dahu-14 (5-day window)



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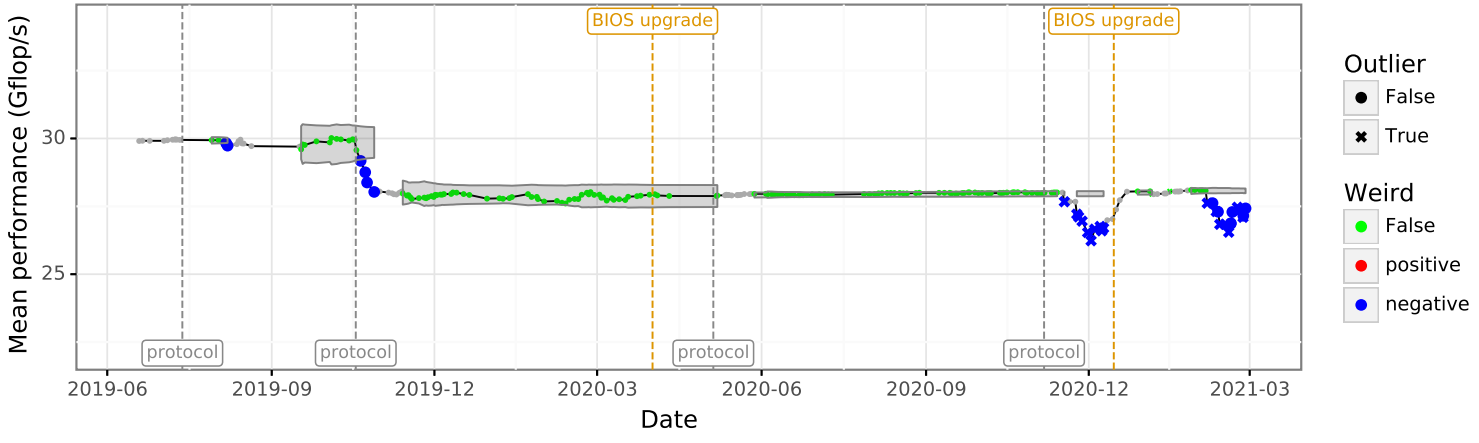
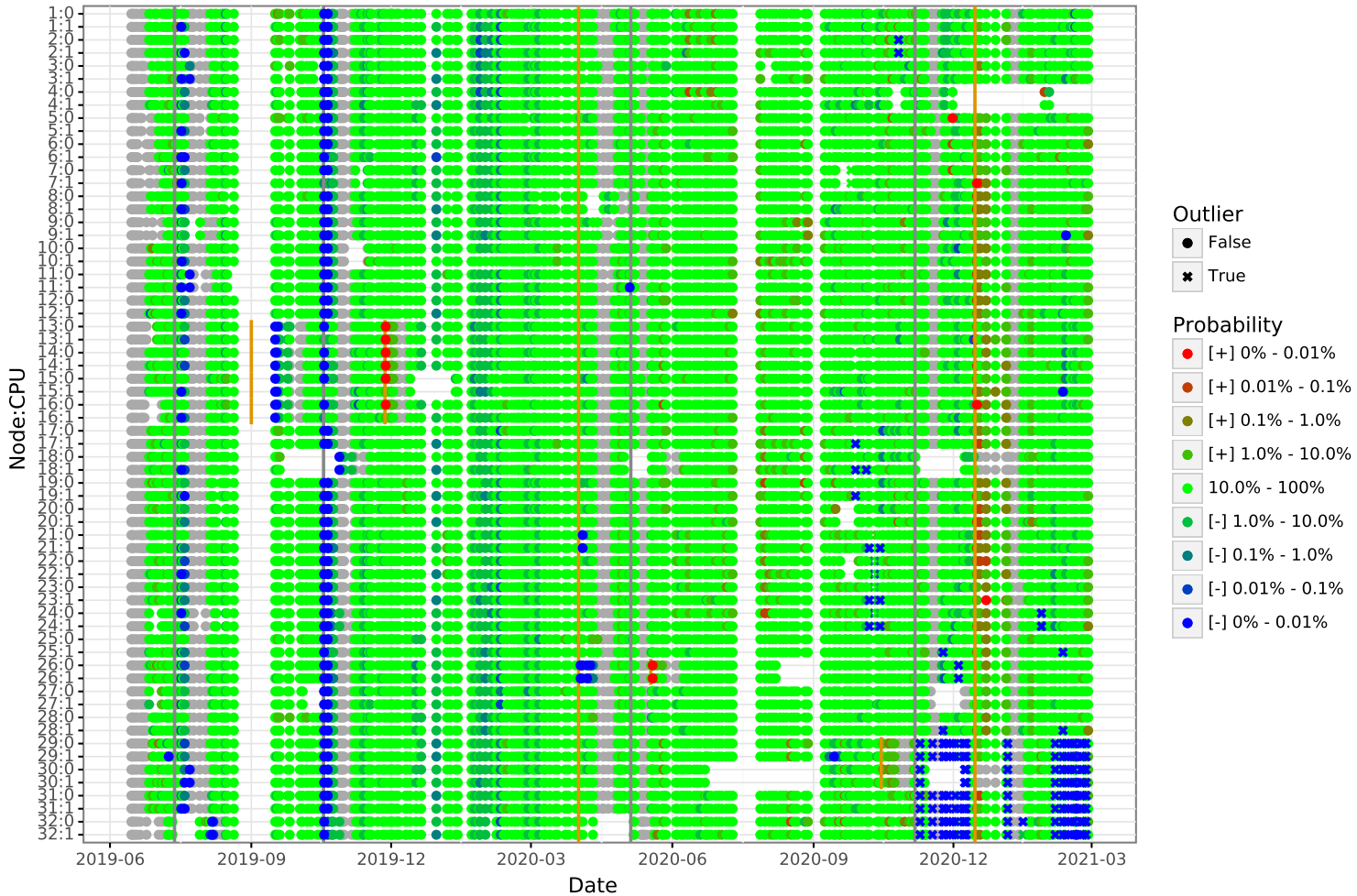


Result: performance overview

Overview of the performance on cluster dahu



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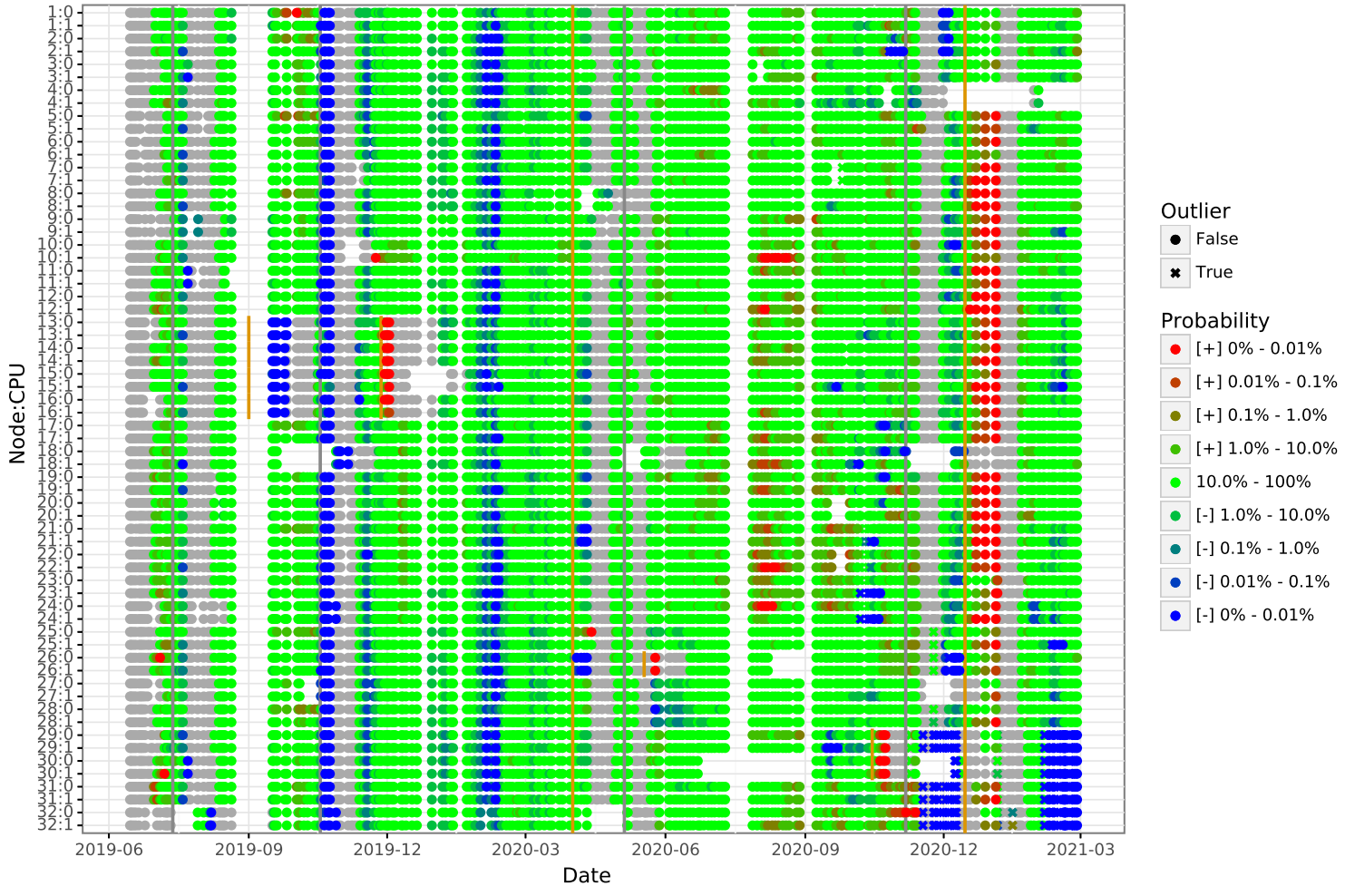

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Multi-variable test also implemented, on all the model coefficients

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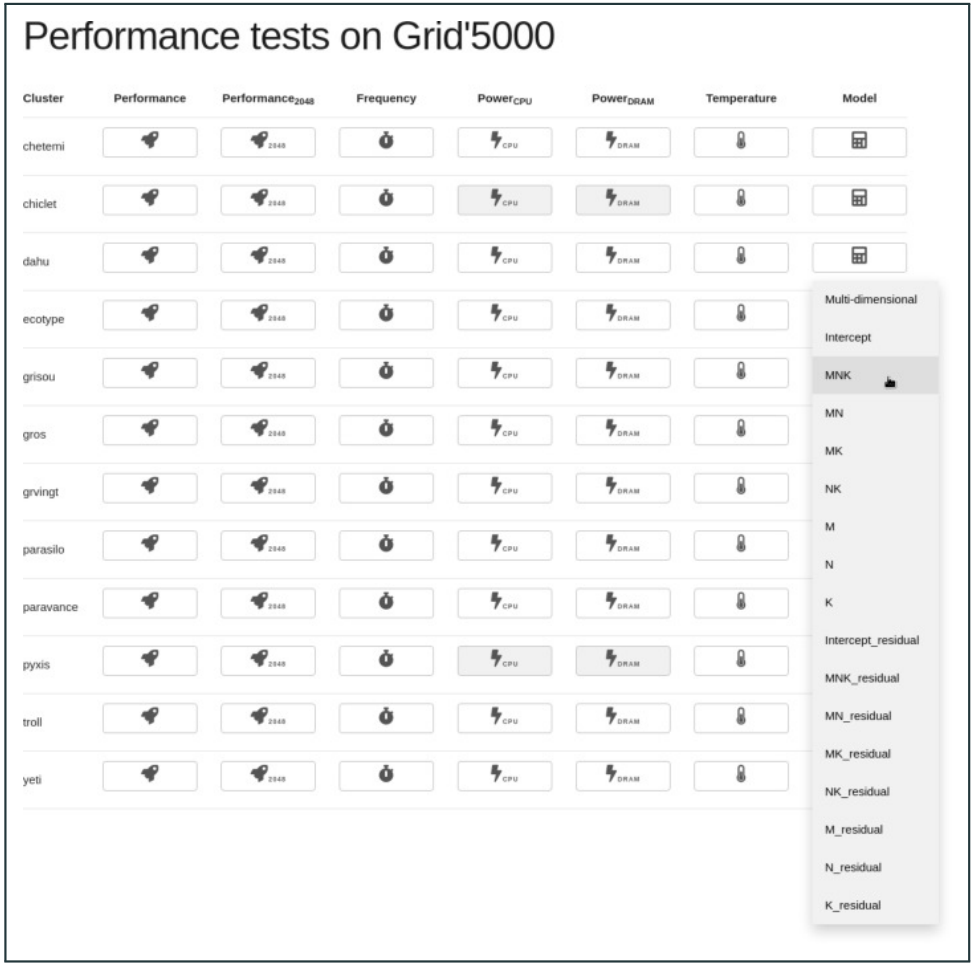

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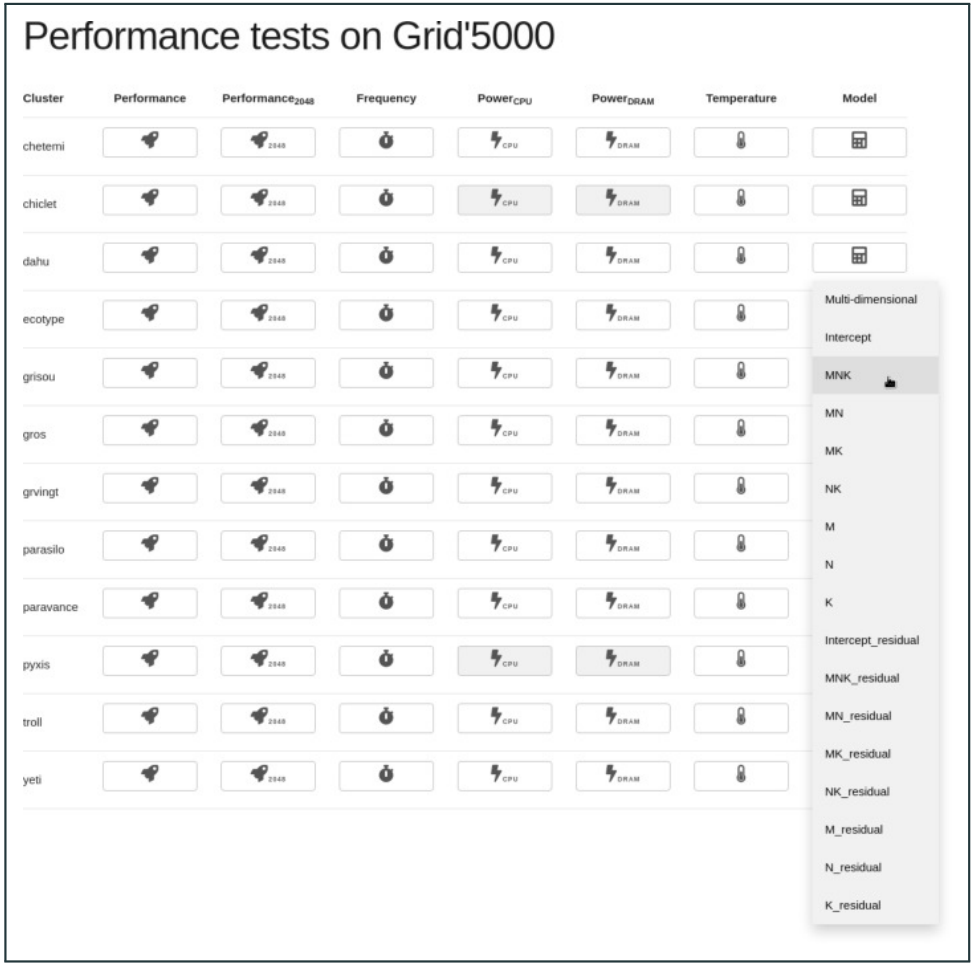

Detected events

- BIOS upgrades
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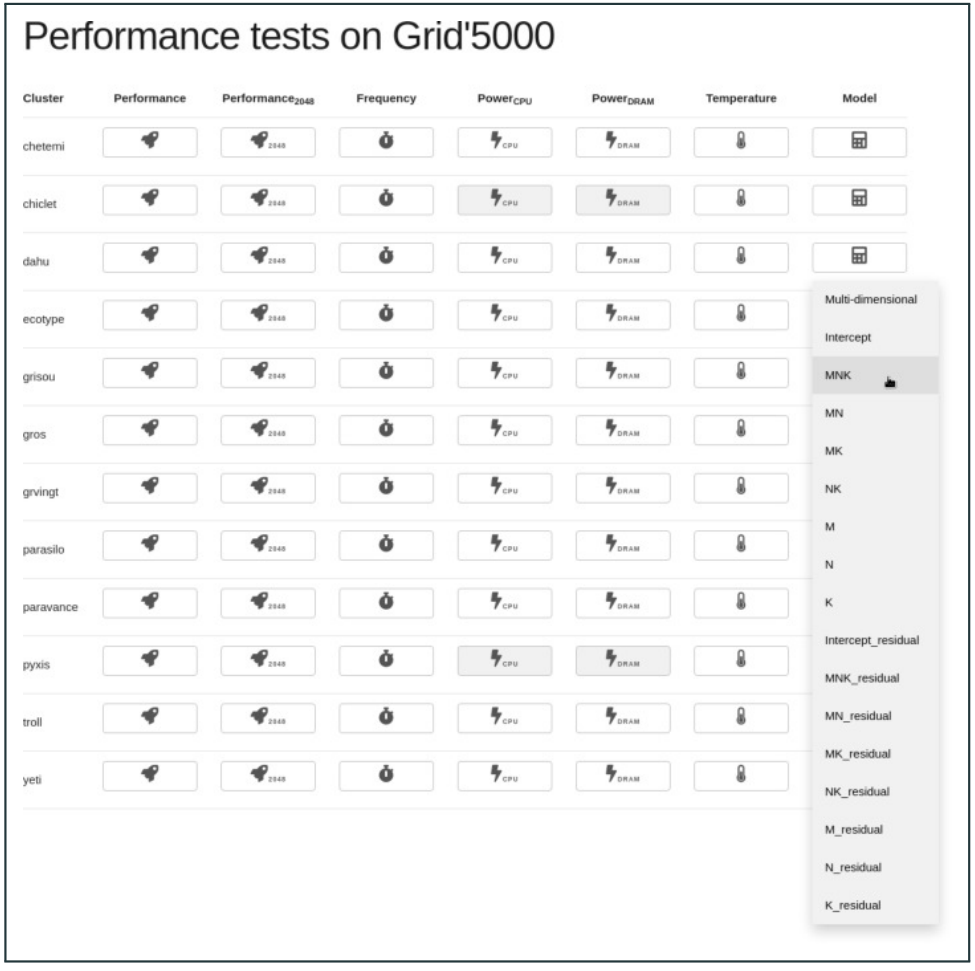

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All went unnoticed by both Grid'5000 staff and users, despite significant effects

⇒ Great help potential

Concluding thoughts

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How to know if our predictions are faithful?

There is no *correctness proof*, a model can be validated only by trying to break it

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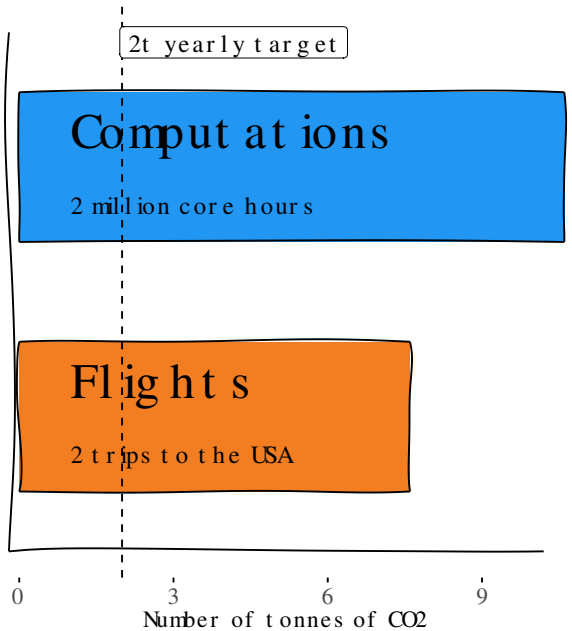
$\Rightarrow$ Often broke the simulations during the last few years

Repeated the whole study from scratch on a new cluster: ✓

Where to stop? Try all the Grid'5000 clusters? Other applications?

There is no planet B

About 18 t of CO2eq were emitted for this thesis



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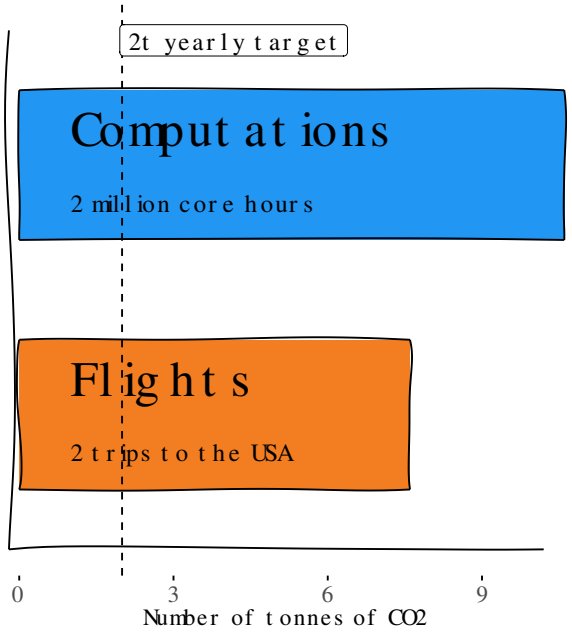

Do we really *need* to attend conferences in person?

What about computations?

Why so many computations?

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

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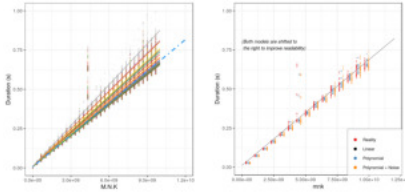
Who should be responsible of tests?

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

Modeling Commputations

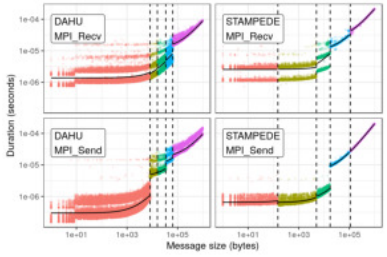
$$\text{dgemm}_i(M,N,K) = \underbrace{\alpha_i.M.N.K}_{\text{per host}} + \underbrace{\beta_i.M.N + \gamma_i.N.K + \ldots}_{\text{polynomial model}} + \underbrace{\mathcal{N}(0, \alpha'_i.M.N.K + \ldots)}_{\text{polynomial noise}}$$

Different color ⇒ different host For a particular host



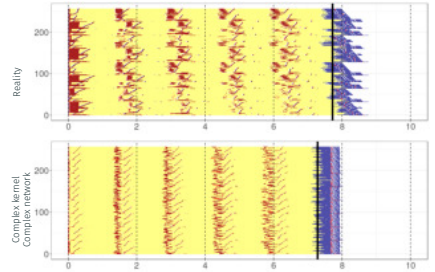
Modeling Communications

Hand-crafted non-blocking collective operations intertwinned with computations



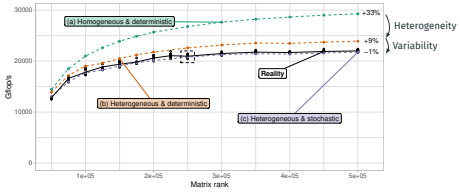
Internal behavior of the application

256 MPI ranks, interrupted after the 5th iteration



Influence of the problem size

Now the complete run, with 1024 MPI ranks

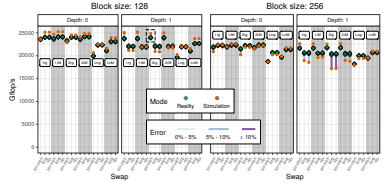


Take-Away Message: accurate prediction

Modeling both spatial and temporal computation variability is essential

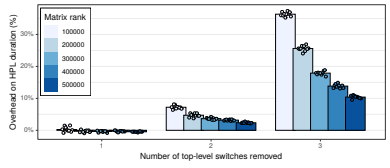
Influence of the other parameters

Tested the 72 combinations of the remaining parameters



Use case: sensibility analysis

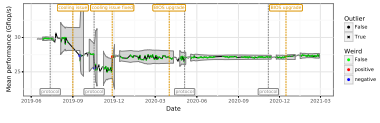
What if the network topology of my cluster was different?



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

Result: performance fluctuation

Performance fluctuation of the node dahu-14



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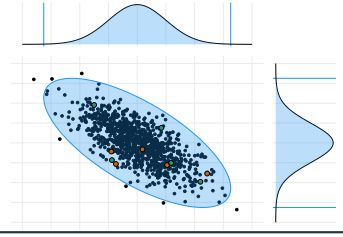

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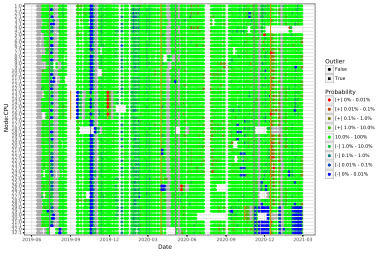

Thank you all!