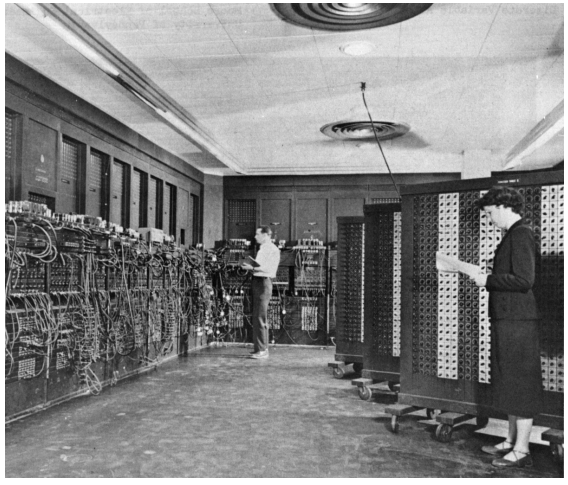
High Performance Computing: Towards Better Performance Predictions and Experiments

Tom Cornebize

2 June 2021, PhD defense

No science without computing

Arithmomètre (1851)



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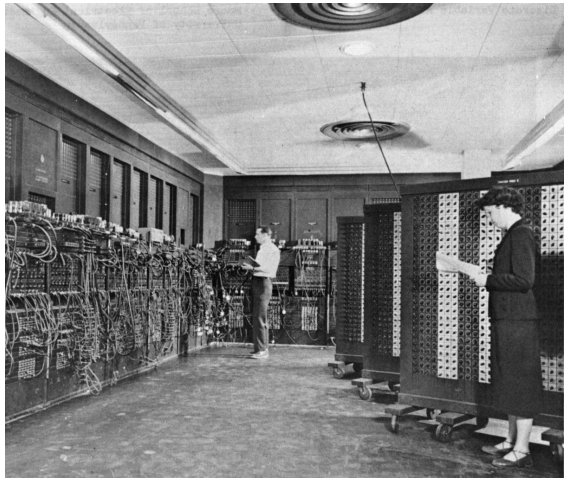

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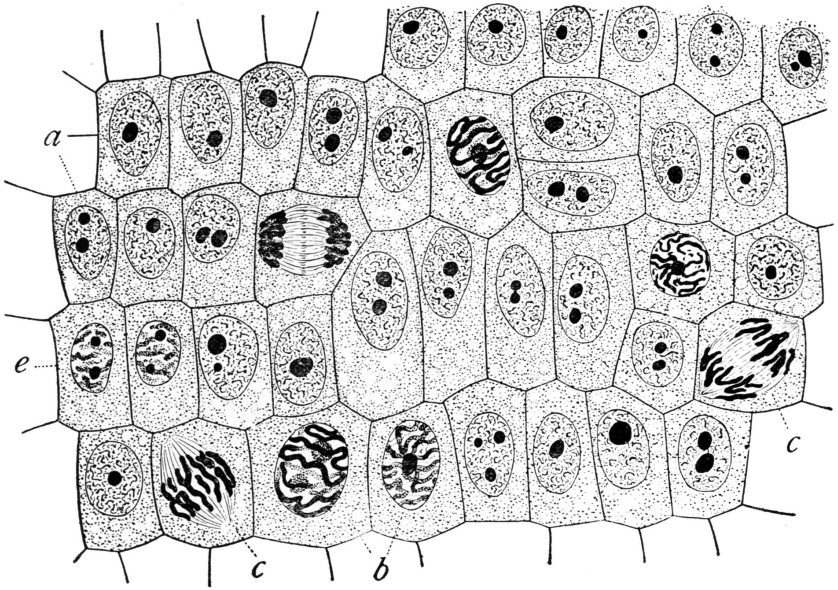
Last decades:

- 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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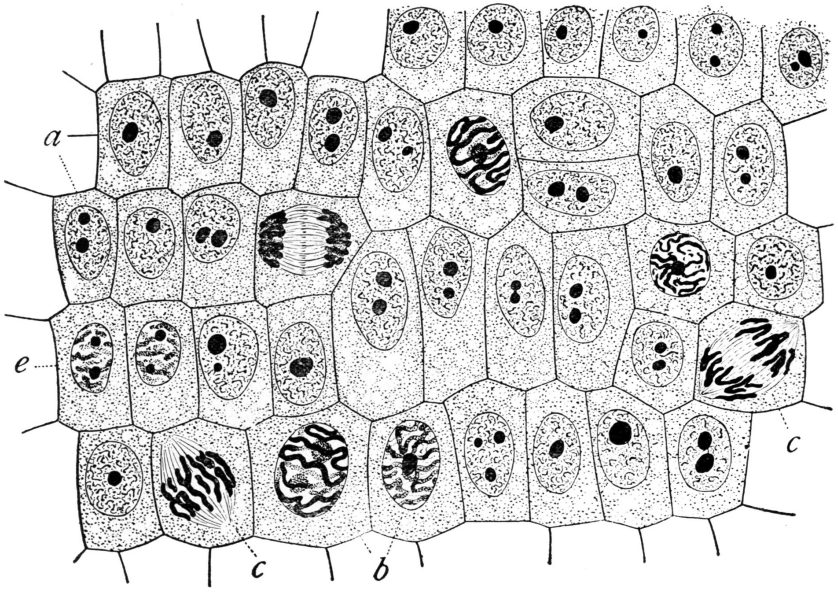

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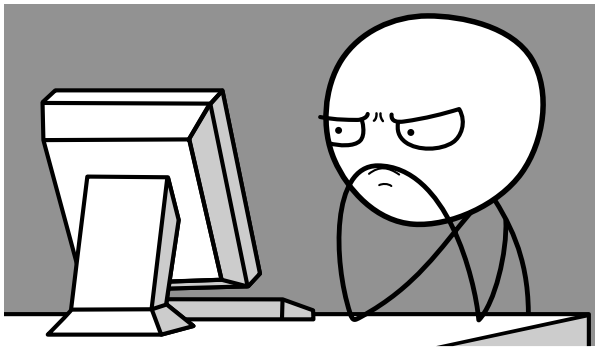
Experiments can be carried in reality or in simulation

Context

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



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  - How many nodes?
  - For how long?
  - Which parameters?

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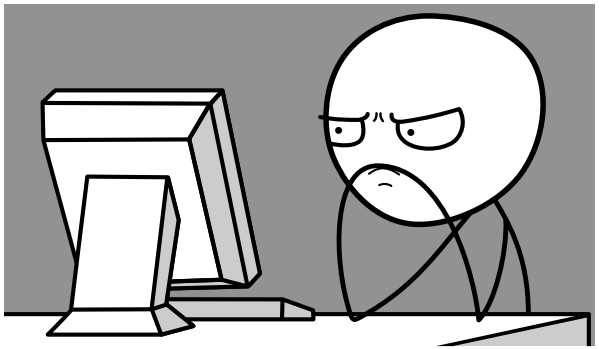

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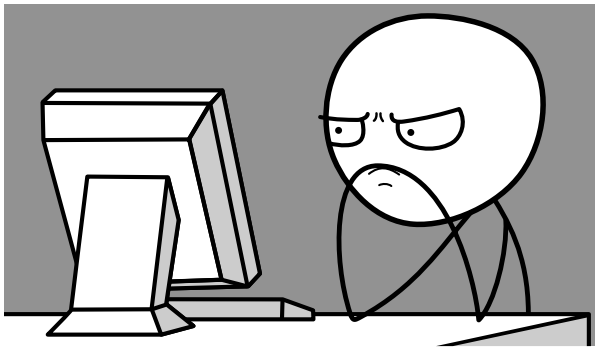

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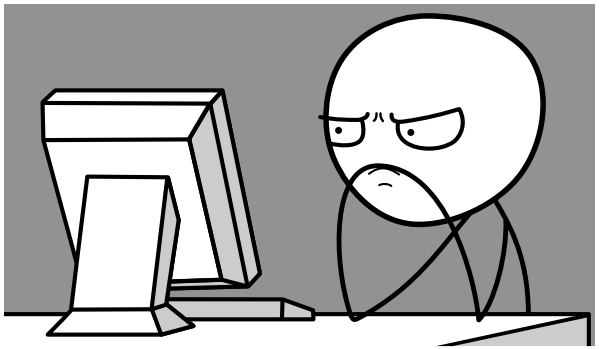

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Holy Grail: Predictive Simulation on a “Laptop”

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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- Experiment methodology, to bias or not to bias
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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?

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

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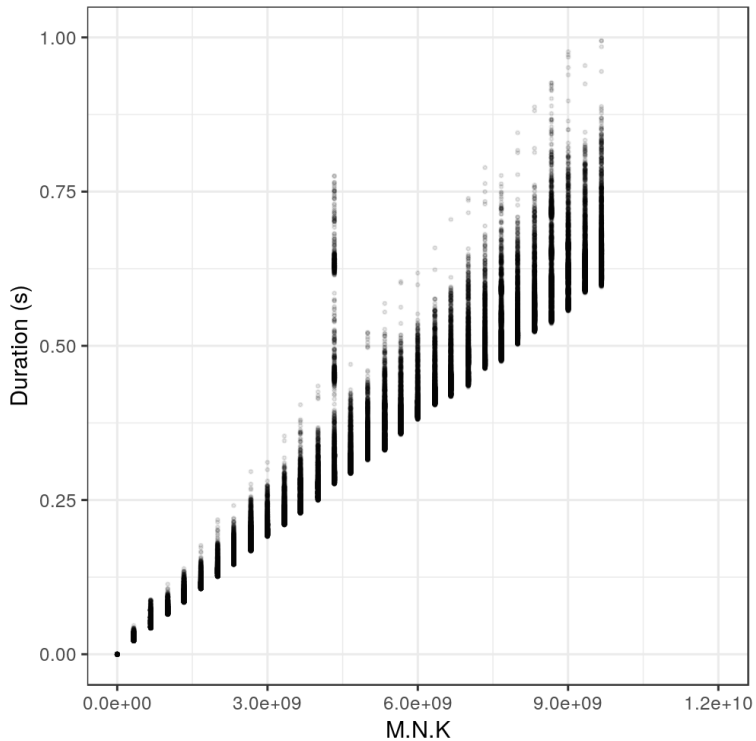
Contribution: Skip the expensive computations (mostly `dgemm`) and replace them by performance models

Modeling Commputations

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



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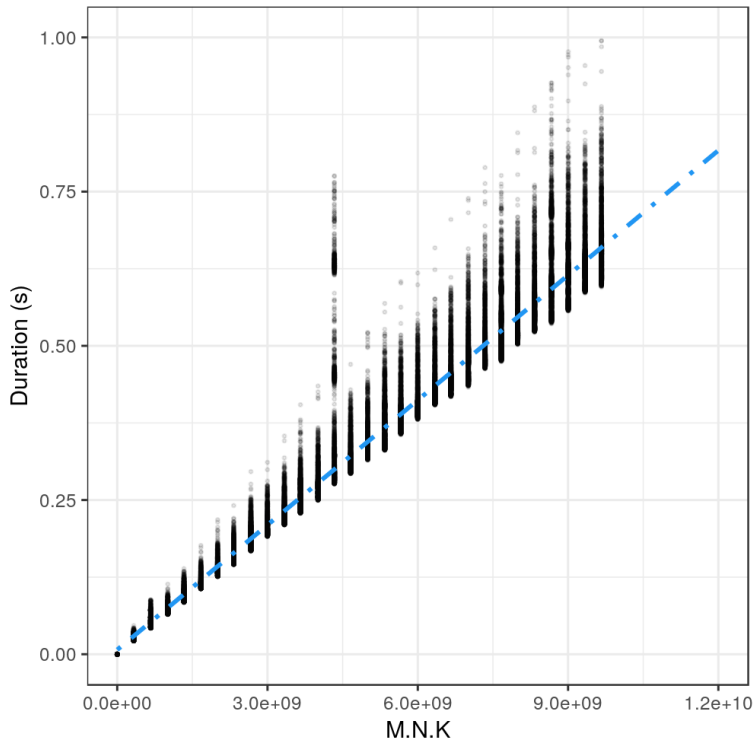
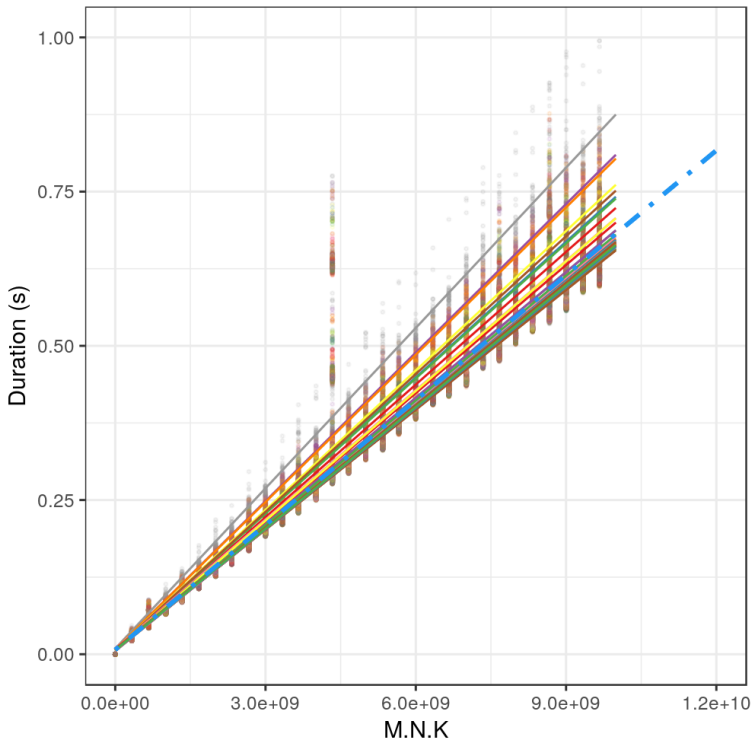


Modeling Commputations

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

Different color $\Rightarrow$ different host



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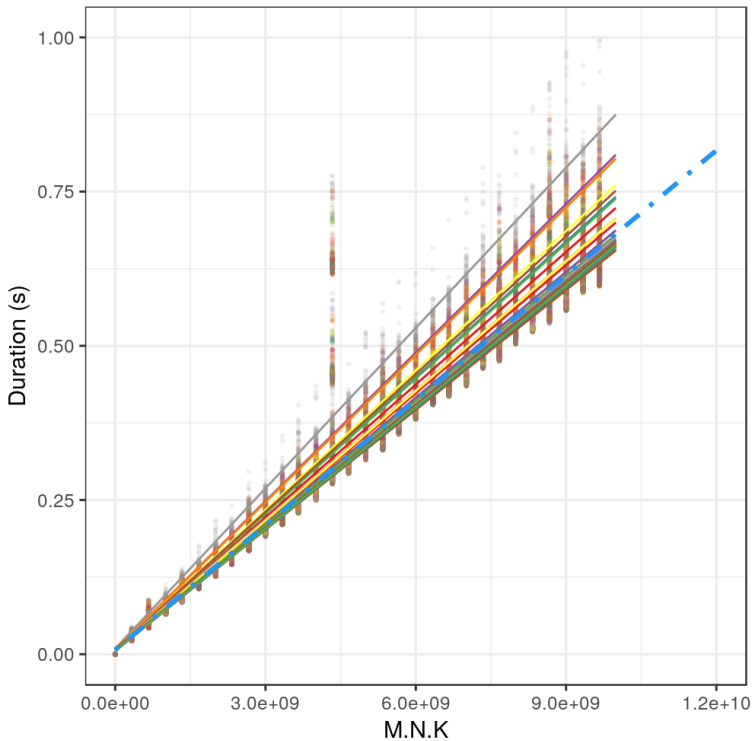
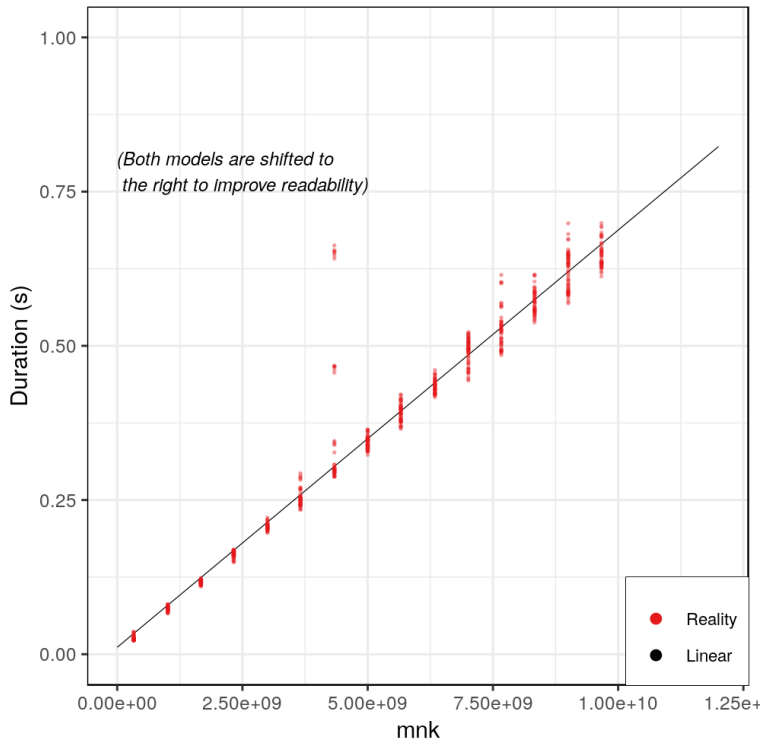


For a particular host



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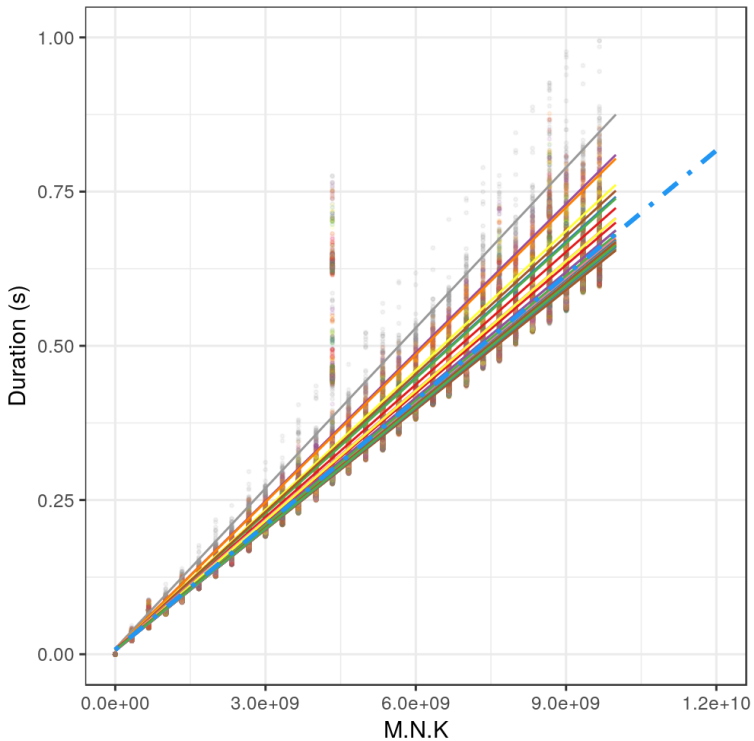

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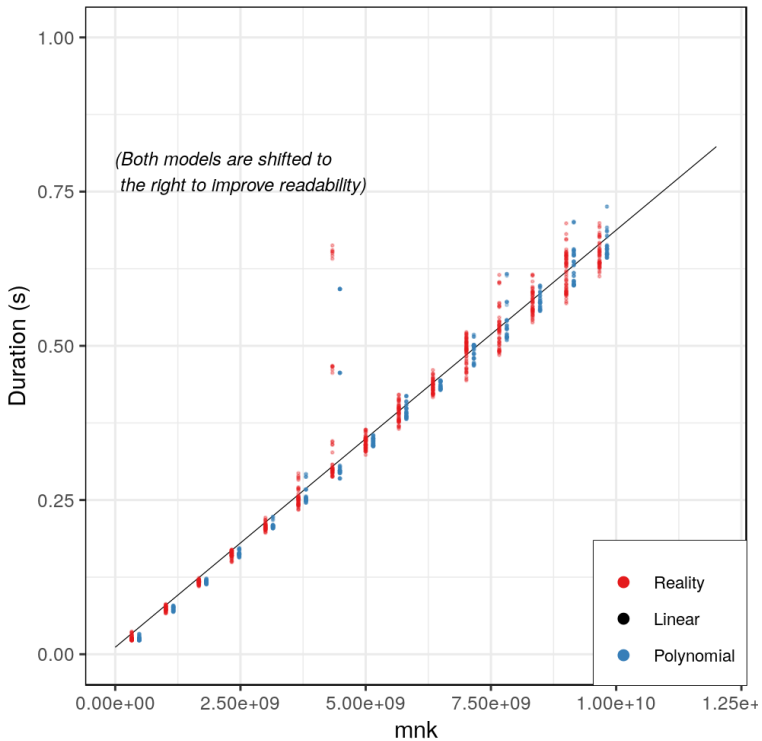

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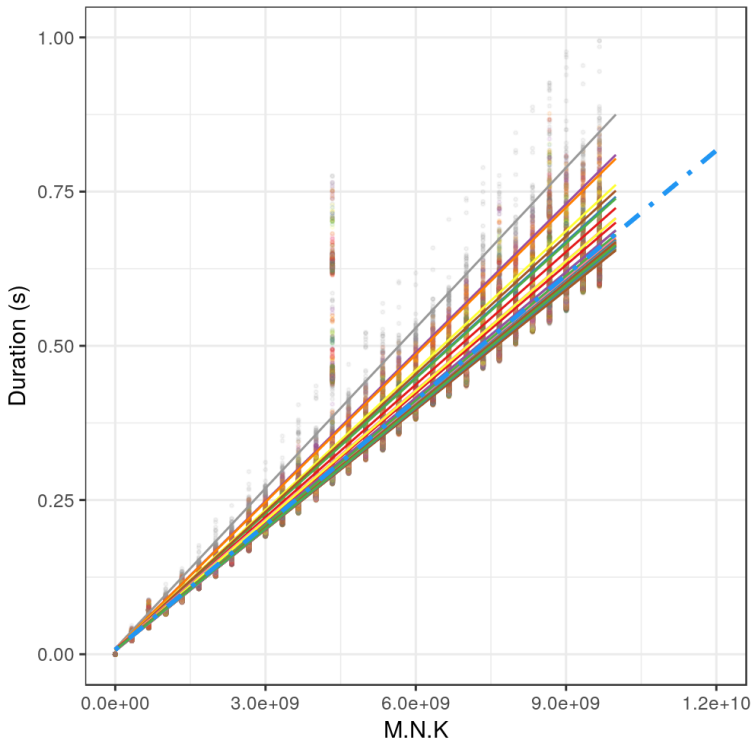

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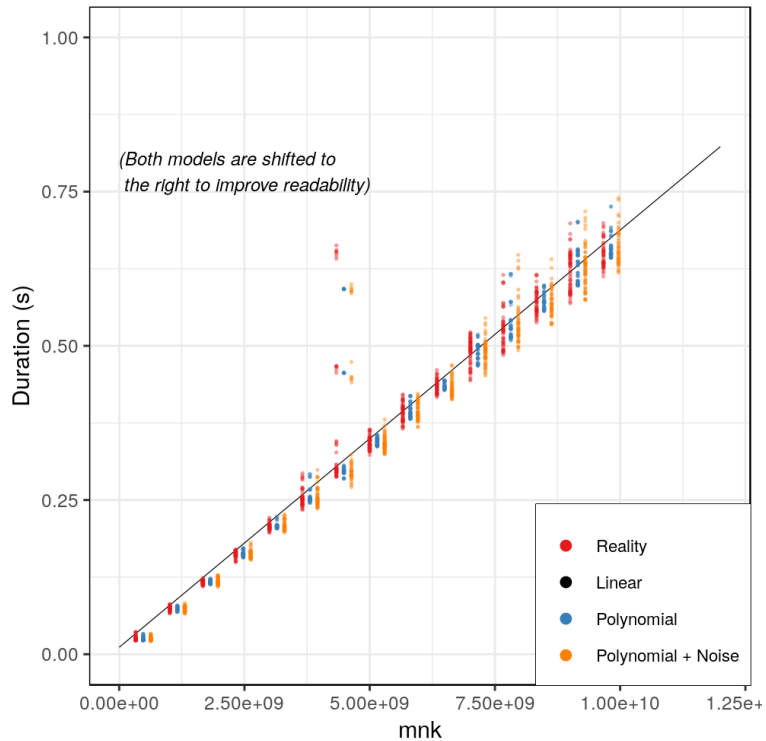

Modeling Communications

Hand-crafted non-blocking collective operations intertwinned with computations

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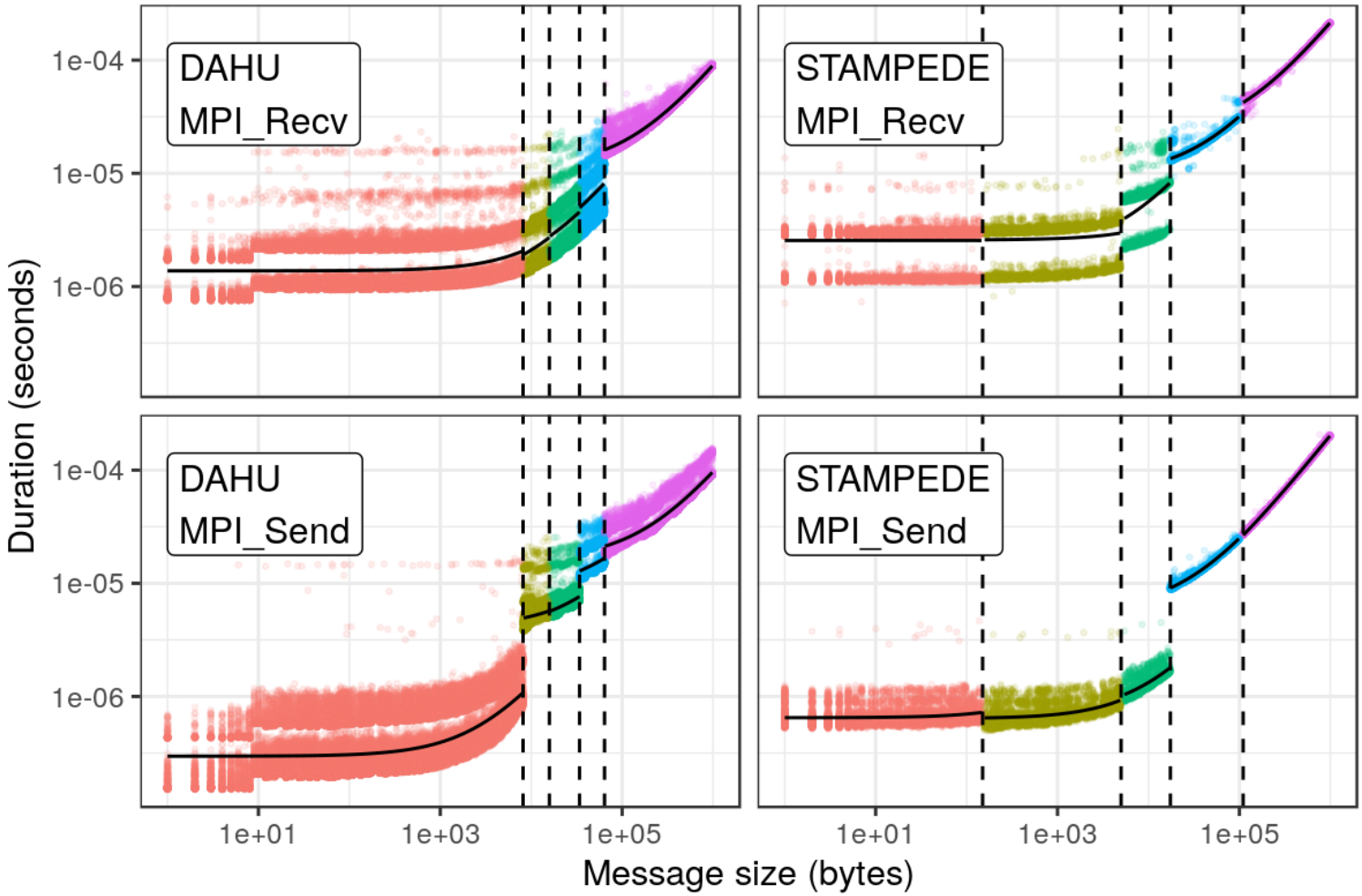

Parenthesis: on the difficulties of experimentation

Experimental biases when measuring `dgemm` or MPI durations

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

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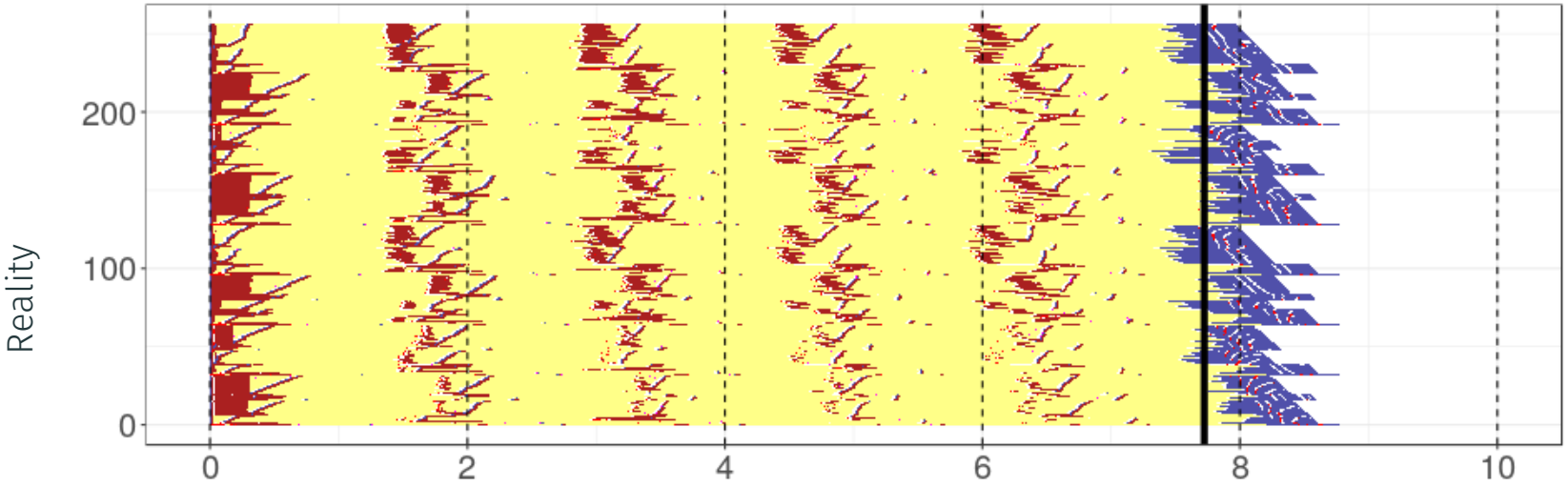
Bias may be desirable in some situations

Validating the predictions

Internal behavior of the application

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



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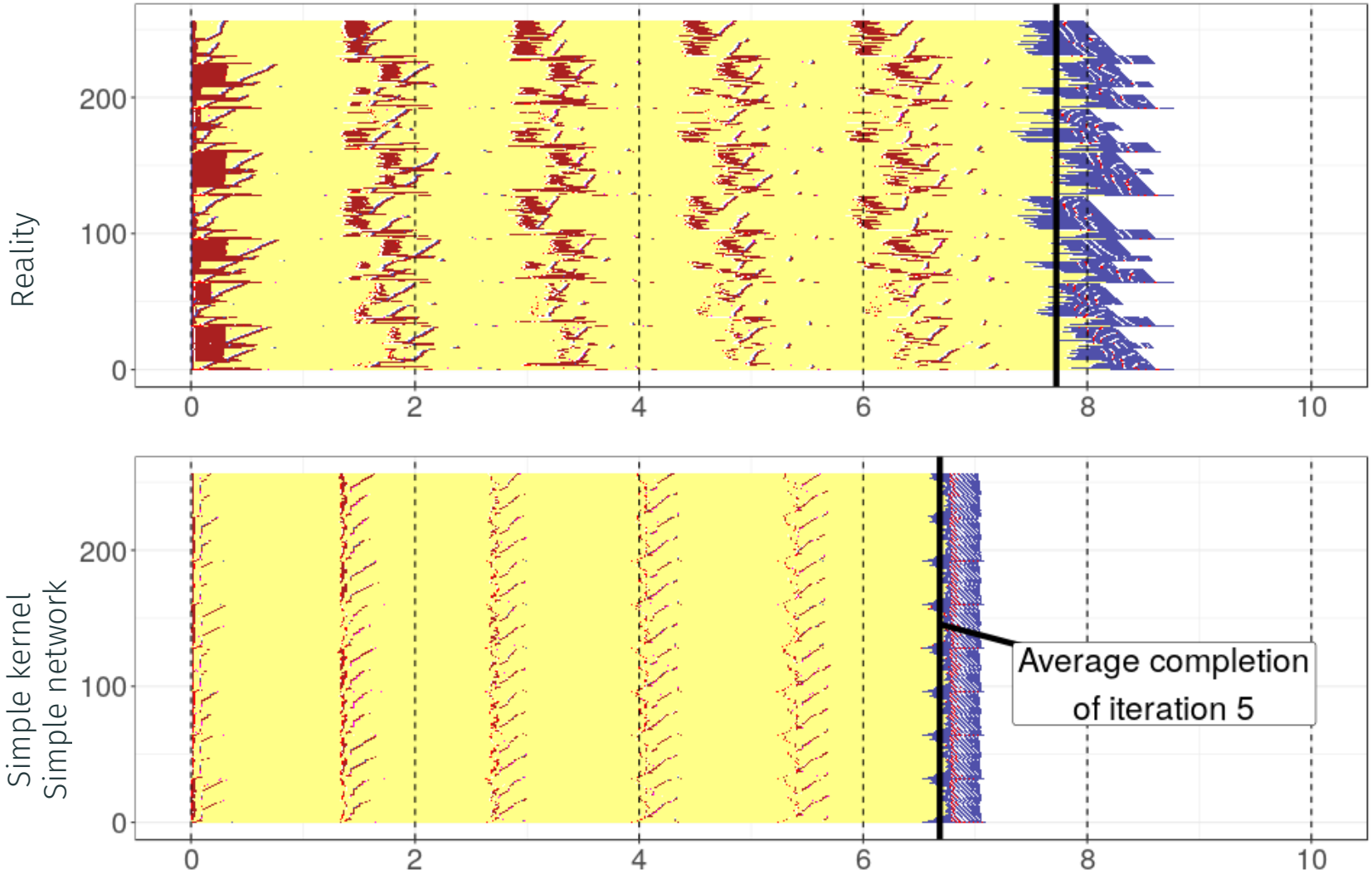

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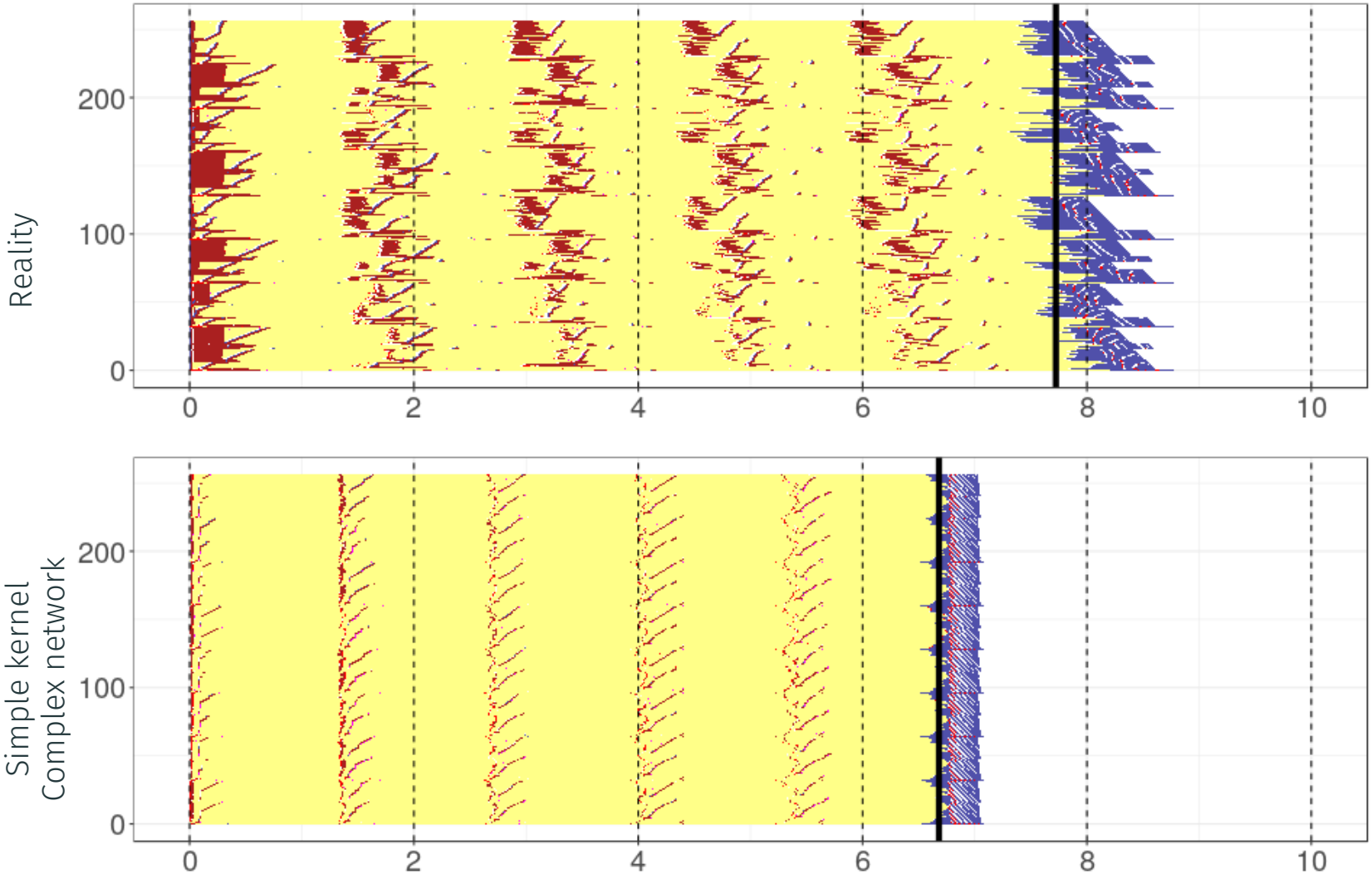

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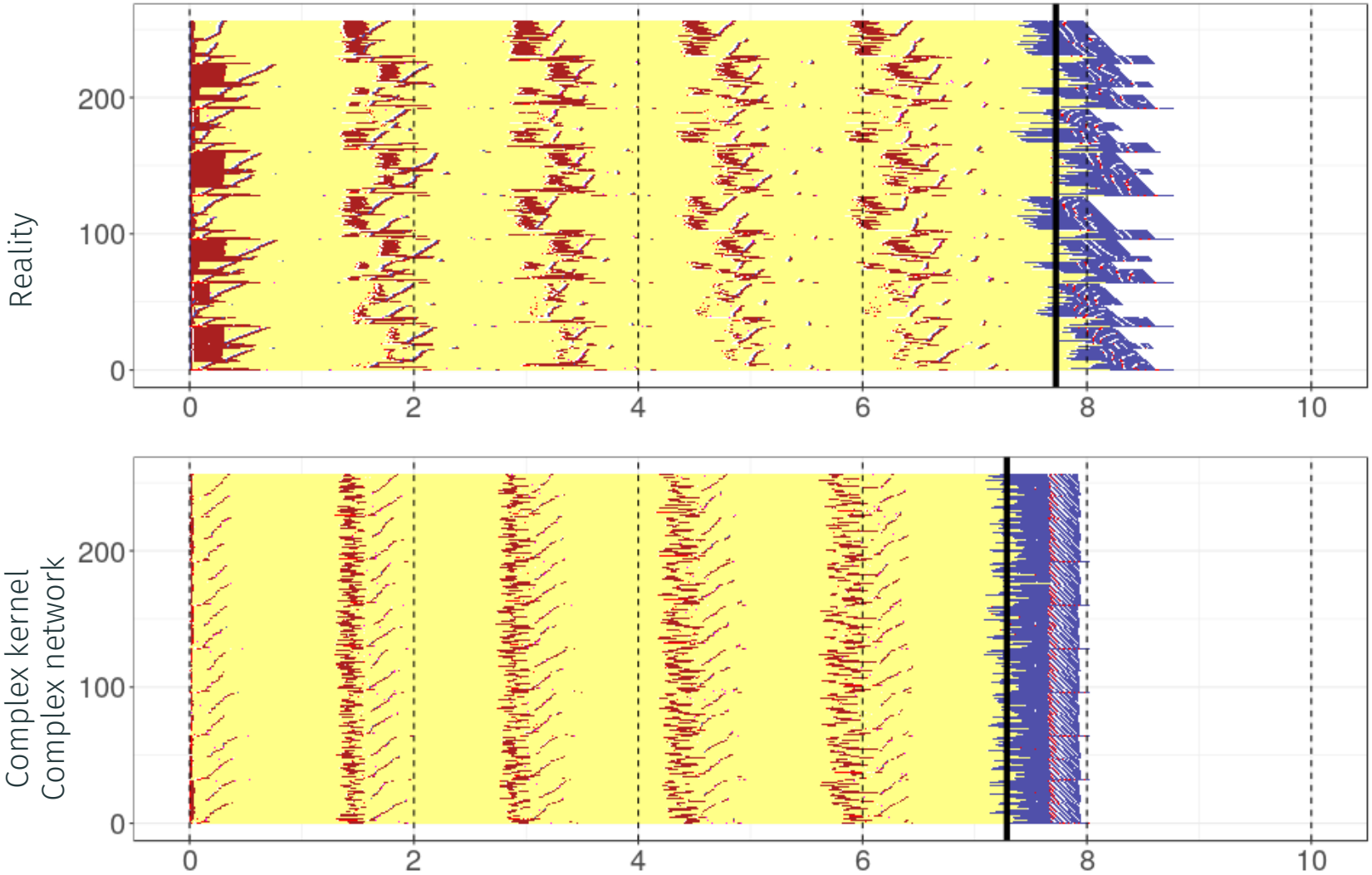
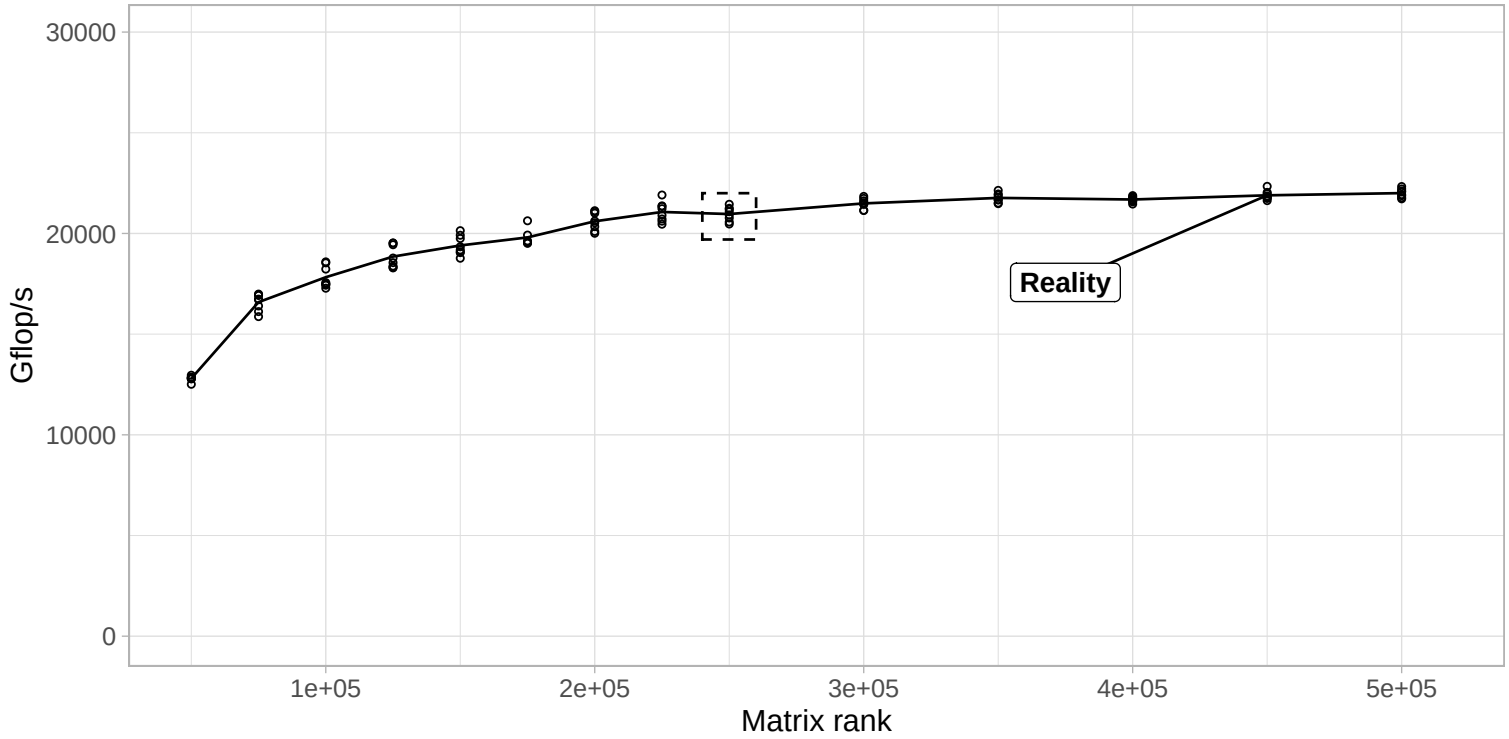


Influence of the problem size

Now the complete run, with 1024 MPI ranks



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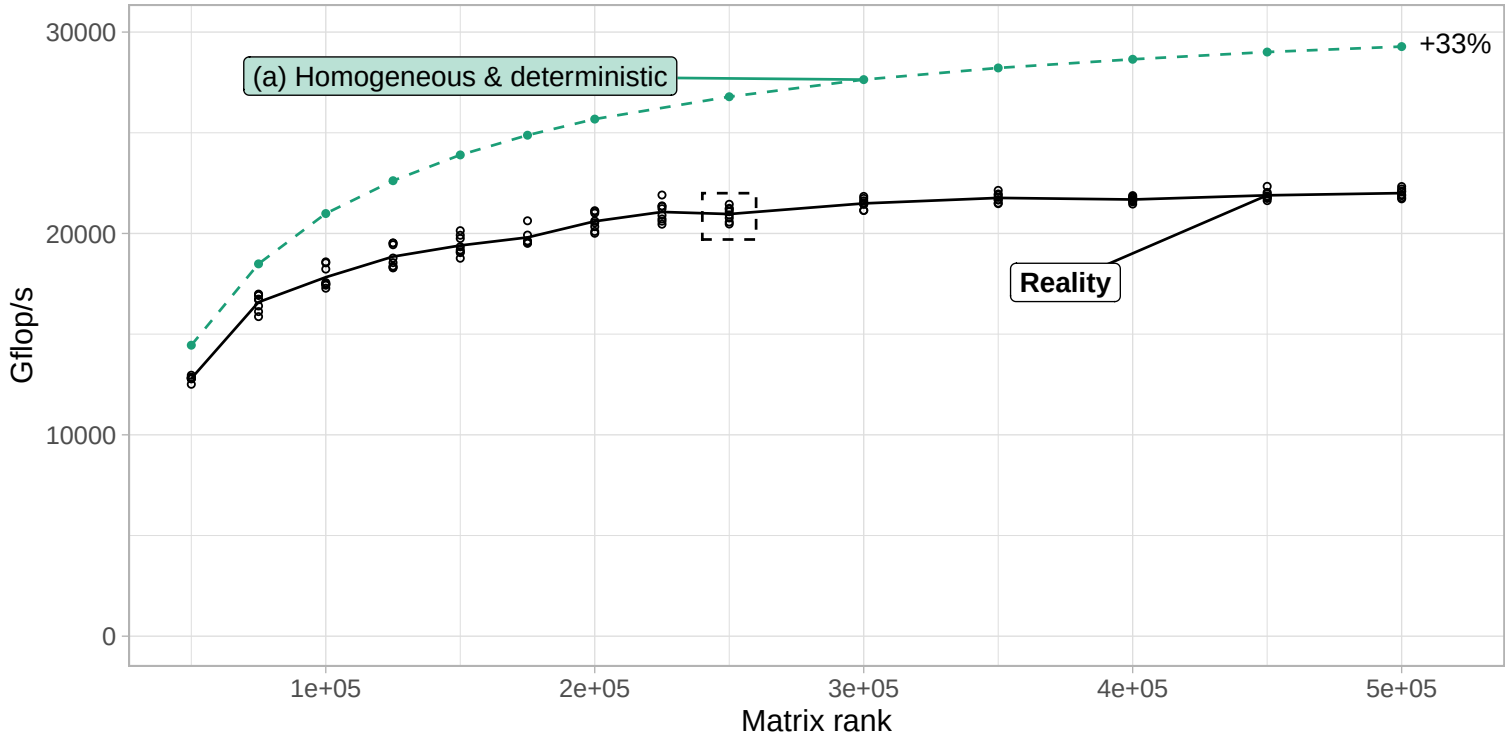

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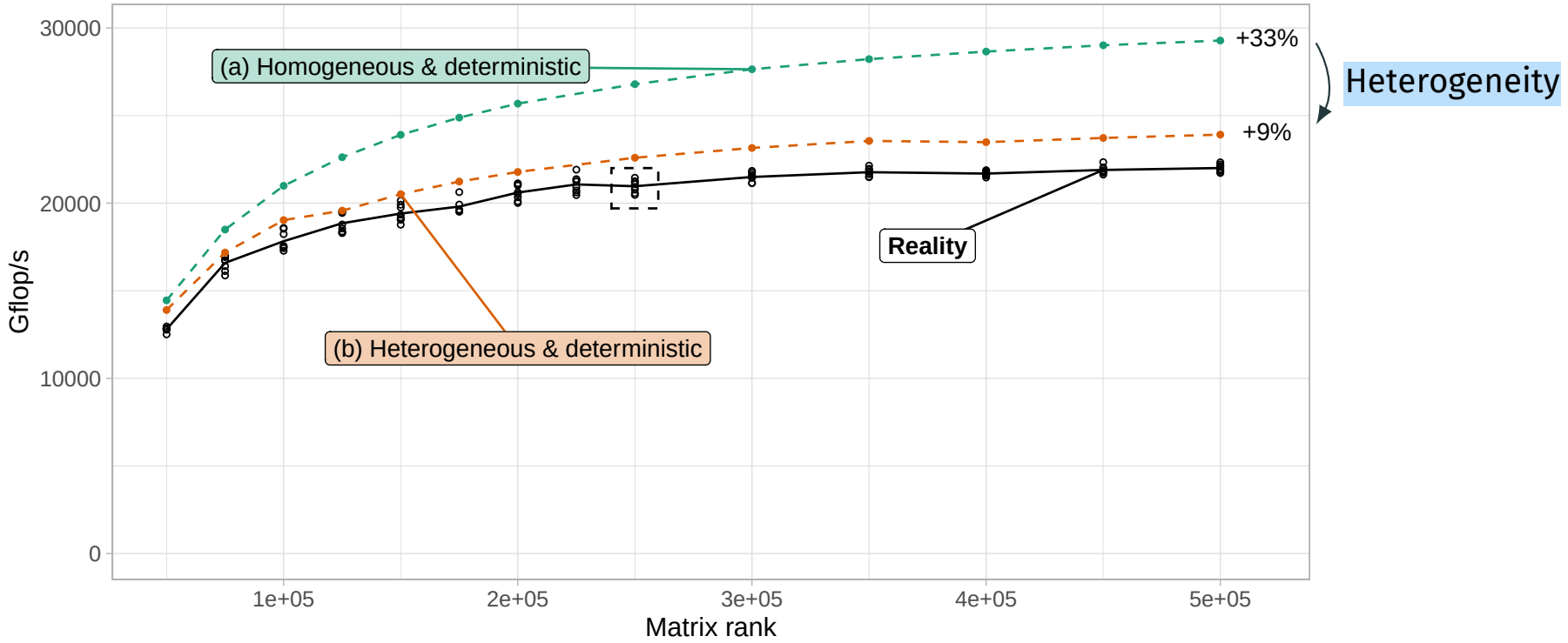

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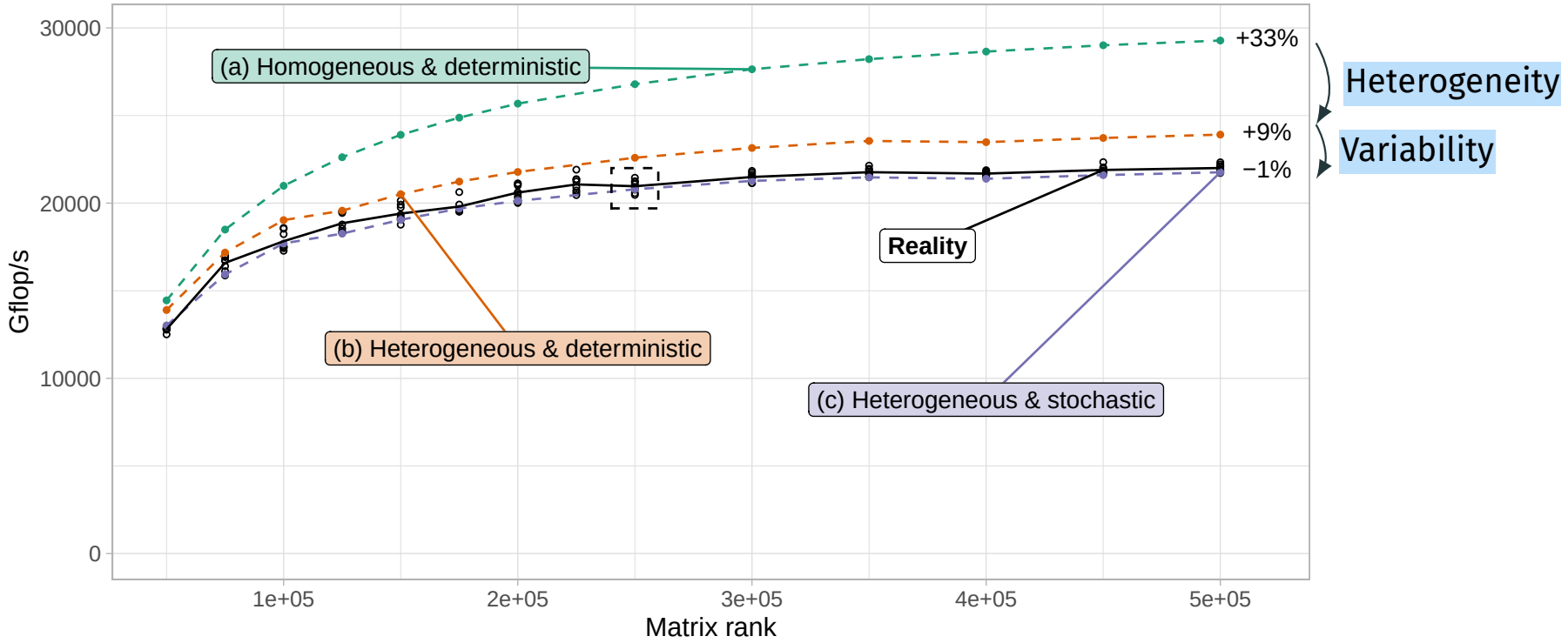

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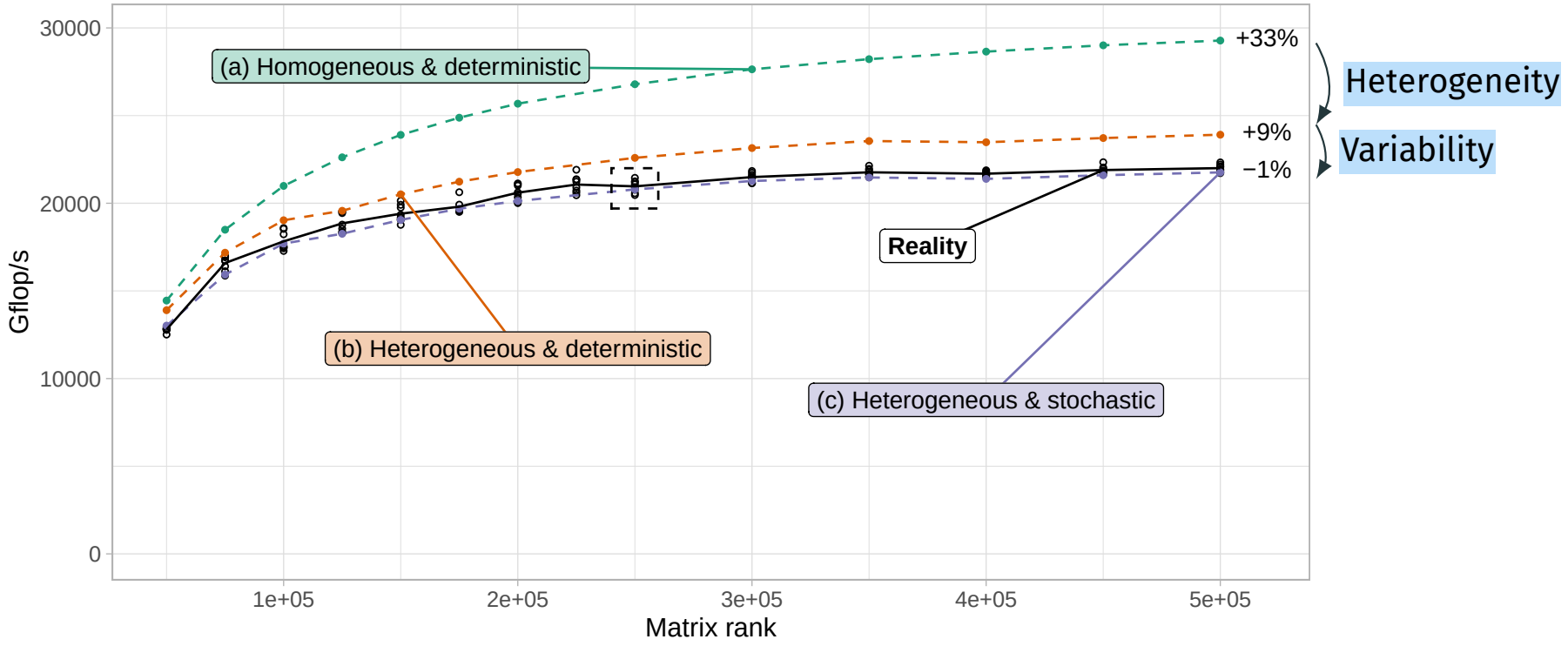
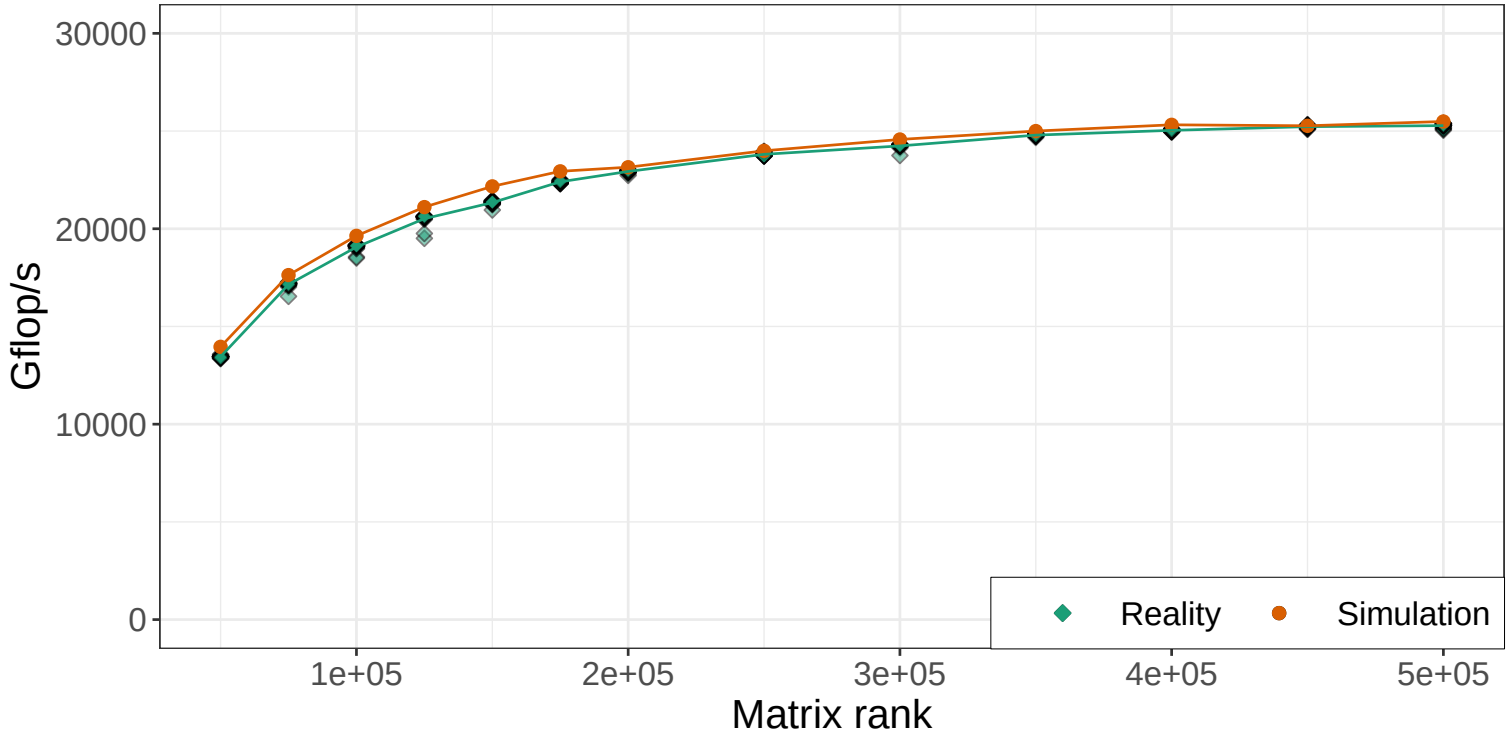


Take-Away Message: accurate prediction

Modeling both **spatial** and **temporal** computation variability is essential

Influence of a platform change



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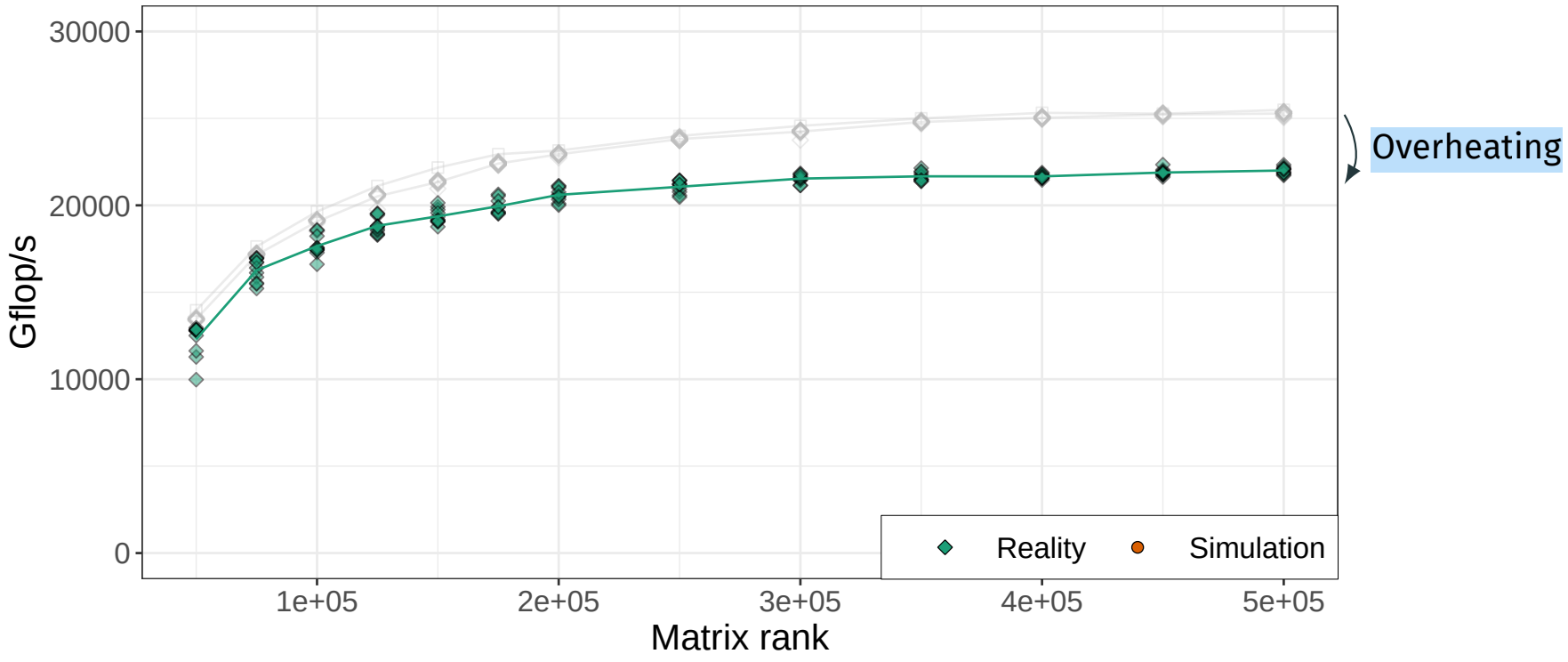

On four nodes, the cooling system malfunctionned for several weeks

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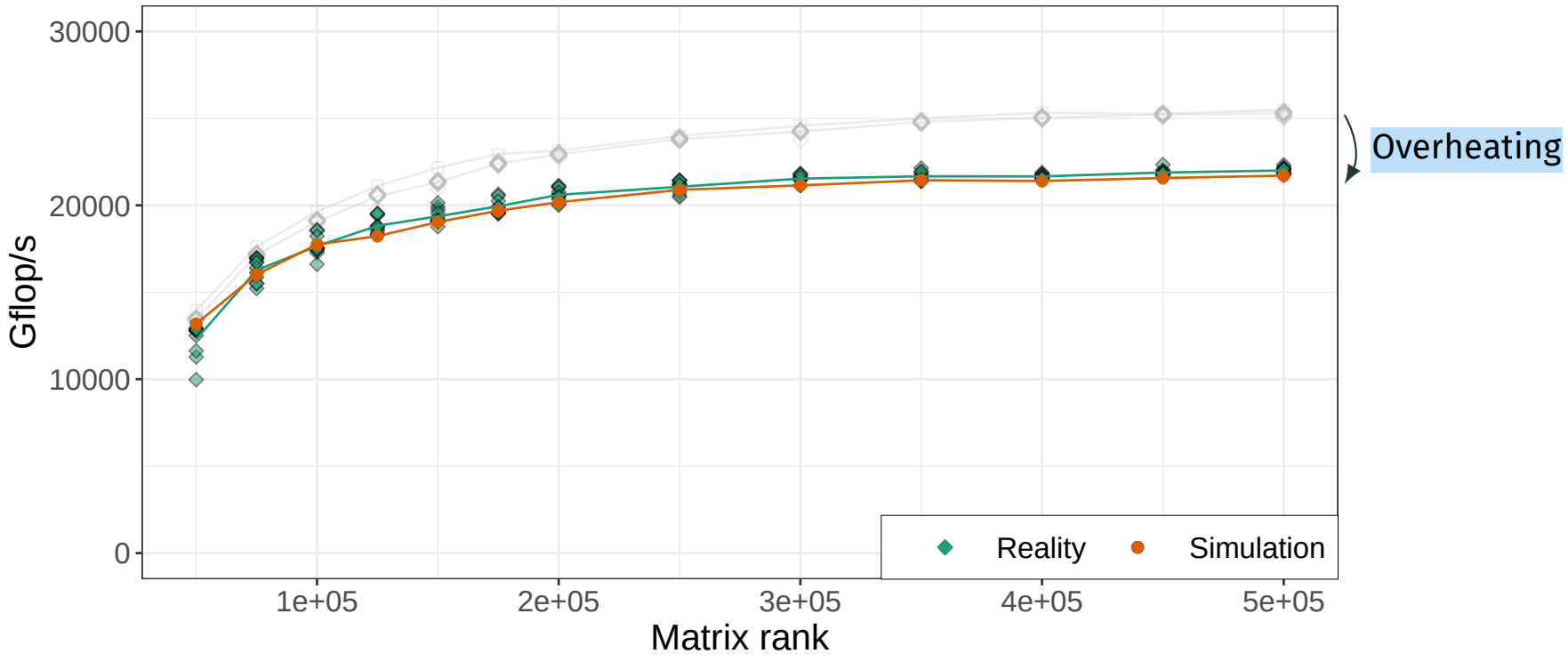

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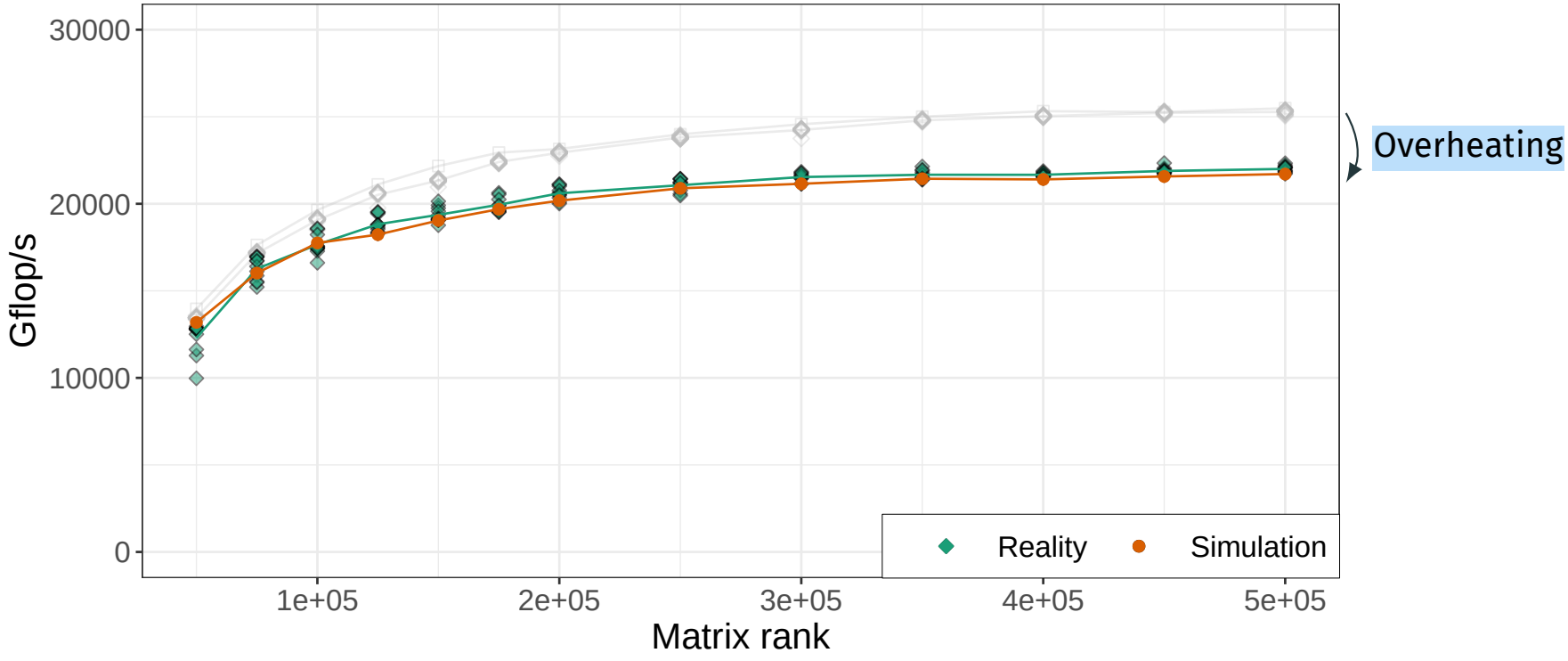

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Take-Away Message: Re-measuring `dgemm` durations to generate a new model was enough to account for the platform change

Performance tests

Regular measures

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

454 nodes (792 CPU) from 12 clusters

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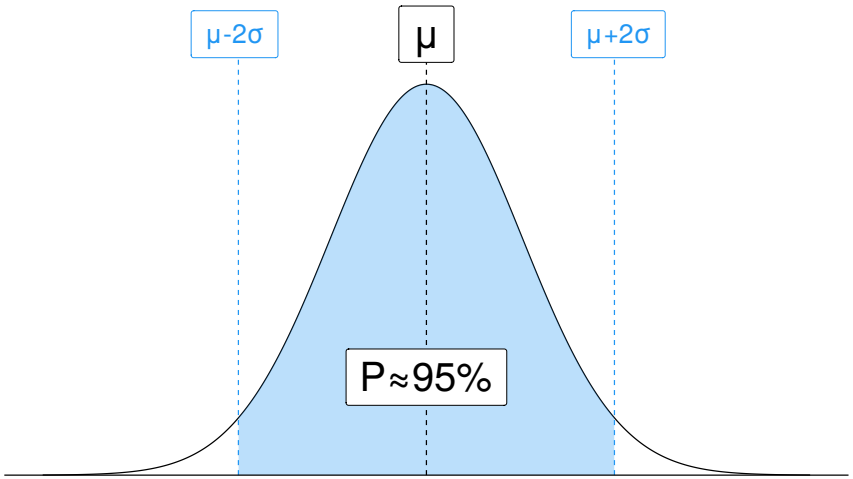
Each parameter is normally distributed (thanks to CLT)

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}?



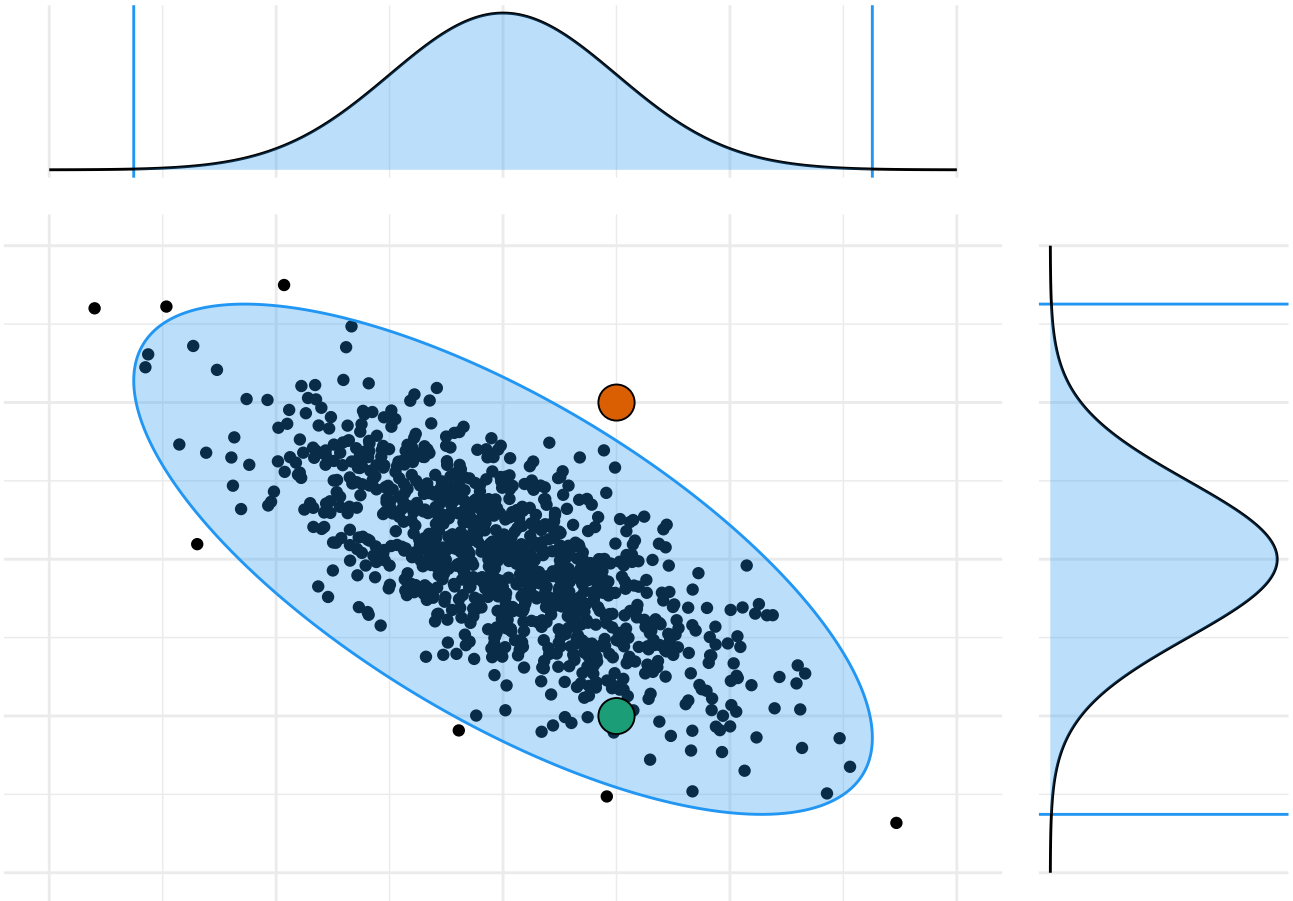
Take the sample mean μ and standard deviation σ of the old observations

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

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)