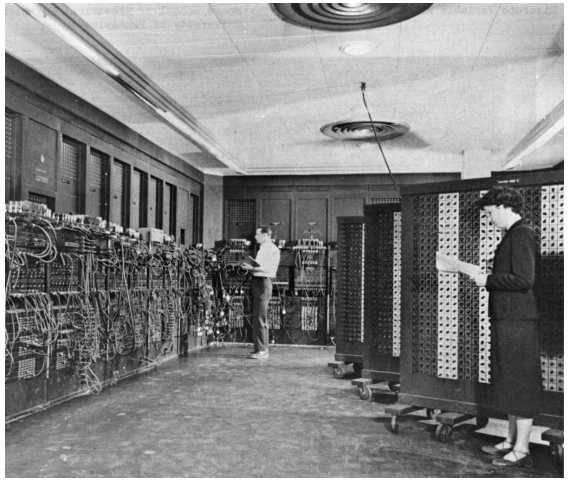
High Performance Computing: Towards Better Performance Predictions and Experiments

Tom Cornebize

2 June 2021, PhD defense

No science without computing

Arithmomètre (1851)

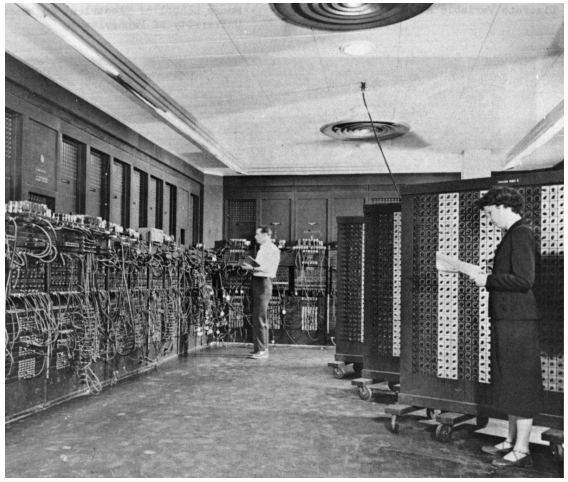


ENIAC (1945)

Fugaku (2021)

No science without computing

Arithmomètre (1851)



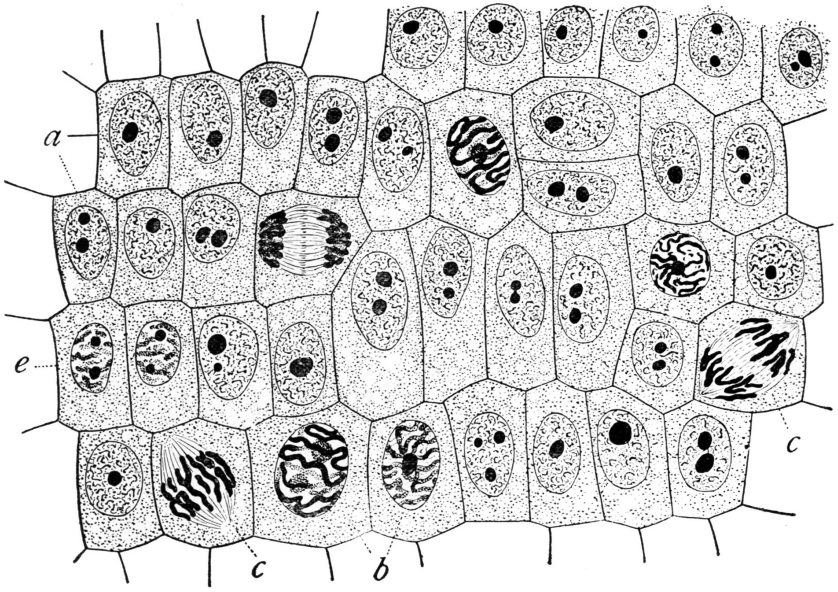
ENIAC (1945)

Fugaku (2021)

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



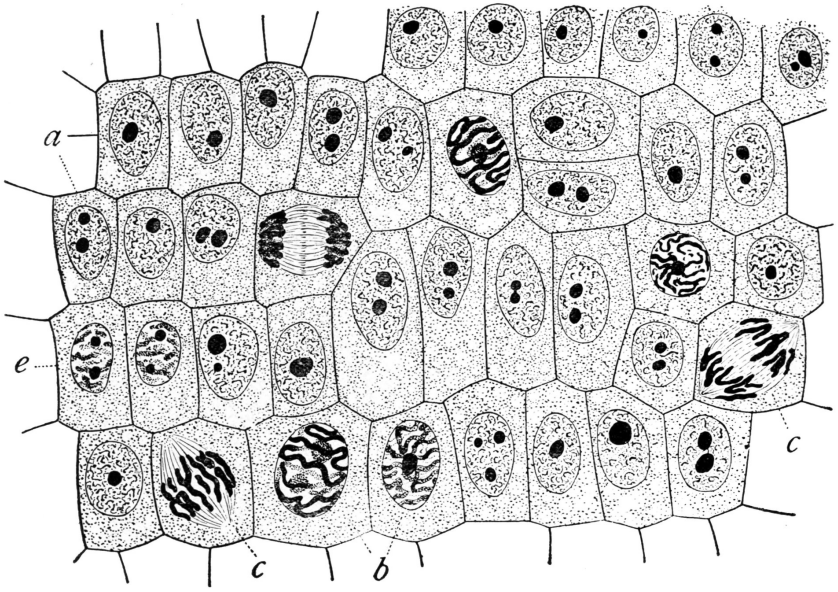
Similar to natural sciences

Complexity $\Rightarrow$ Variability and Opacity

$\Rightarrow$ No perfect model

$\Rightarrow$ Need for experiments

Experimental study of computer performance



Similar to natural sciences

Complexity $\Rightarrow$ Variability and Opacity

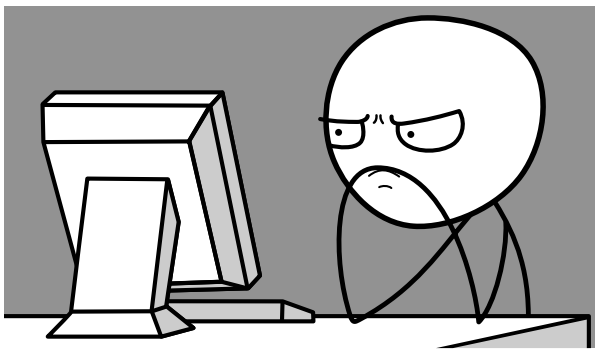
$\Rightarrow$ No perfect model

$\Rightarrow$ Need for experiments

Experiments can be carried in reality or in simulation

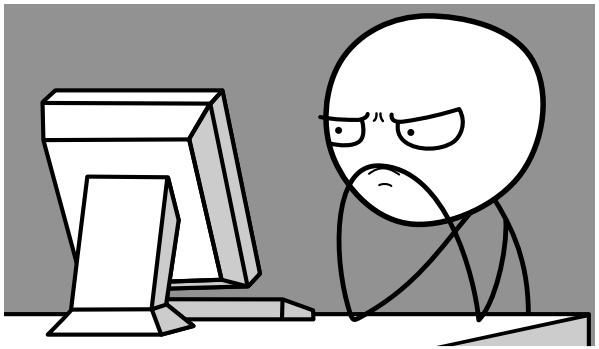
Context

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



- **Before** running
  - How many nodes?
  - For how long?
  - Which parameters?

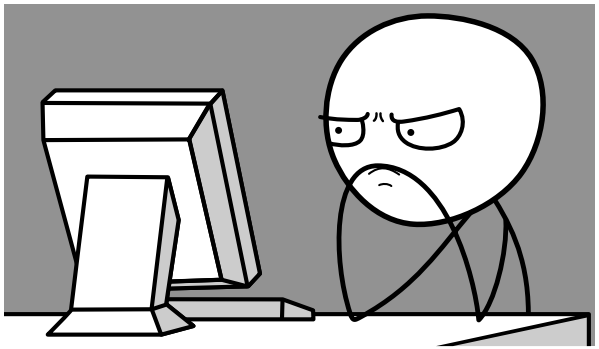
Typical Performance Evaluation Questions (Given my application and a supercomputer)



- **Before** running
  - How many nodes?
  - For how long?
  - Which parameters?
- **After** running
  - Performance as “expected”?
  - Problem in the app or the platform?

Context

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

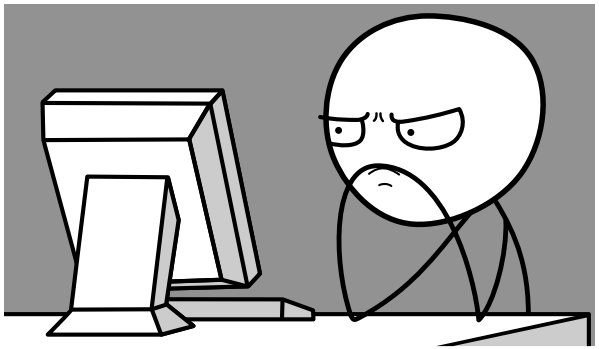


- **Before** running
  - How many nodes?
  - For how long?
  - Which parameters?
- **After** running
  - Performance as “expected”?
  - Problem in the app or the platform?

So many large-scale runs, solely to tune performance?!?

Context

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



- **Before** running
  - How many nodes?
  - For how long?
  - Which parameters?
- **After** running
  - Performance as “expected”?
  - Problem in the app or the platform?

So many large-scale runs, solely to tune performance?!?

Holy Grail: Predictive Simulation on a “Laptop”

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

Initial goal: predict the performance of a parallel application

Initial goal: predict the performance of a parallel application

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

Initial goal: predict the performance of a parallel application

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

Thesis contributions (made on the way)

- Automation (of experiments, statistical analyzes, etc.)
- Experiment methodology, to bias or not to bias
- Performance tests, to detect eventual platform changes

Initial goal: predict the performance of a parallel application

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

Thesis contributions (made on the way)

- Automation (of experiments, statistical analyzes, etc.)
- Experiment methodology, to bias or not to bias
- Performance tests, to detect eventual platform changes

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

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

Emulation: how?

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

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

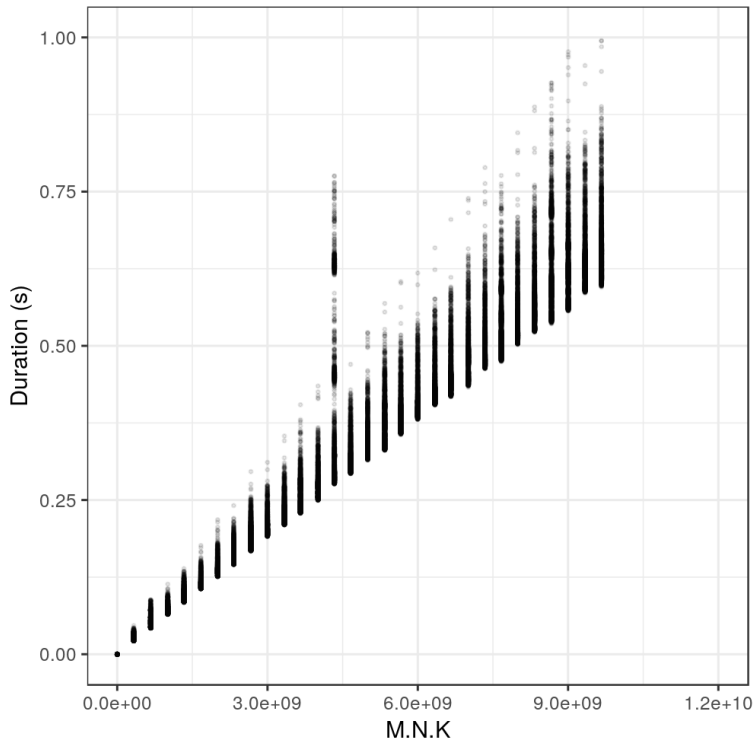
Emulation: how?

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

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

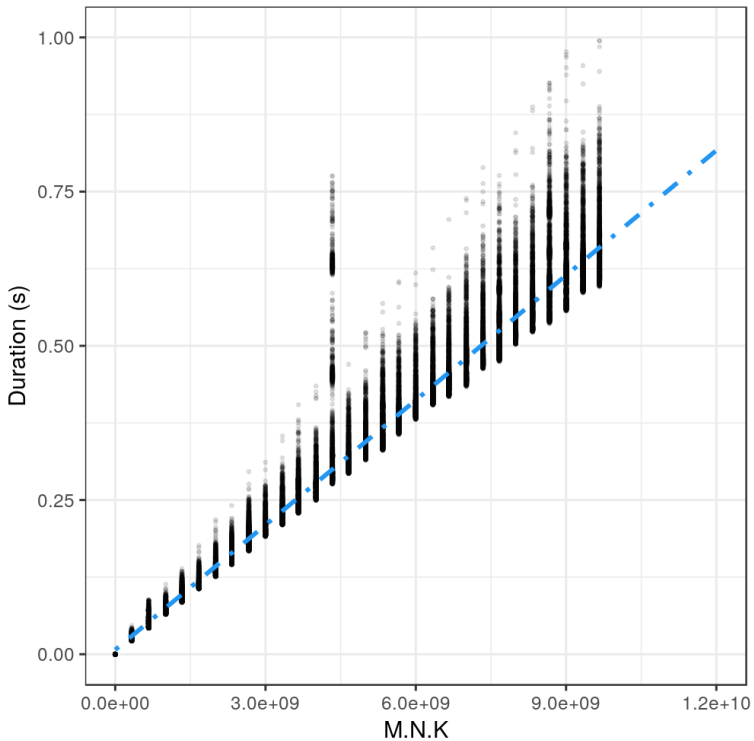
Modeling Commputations

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



Modeling Commputations

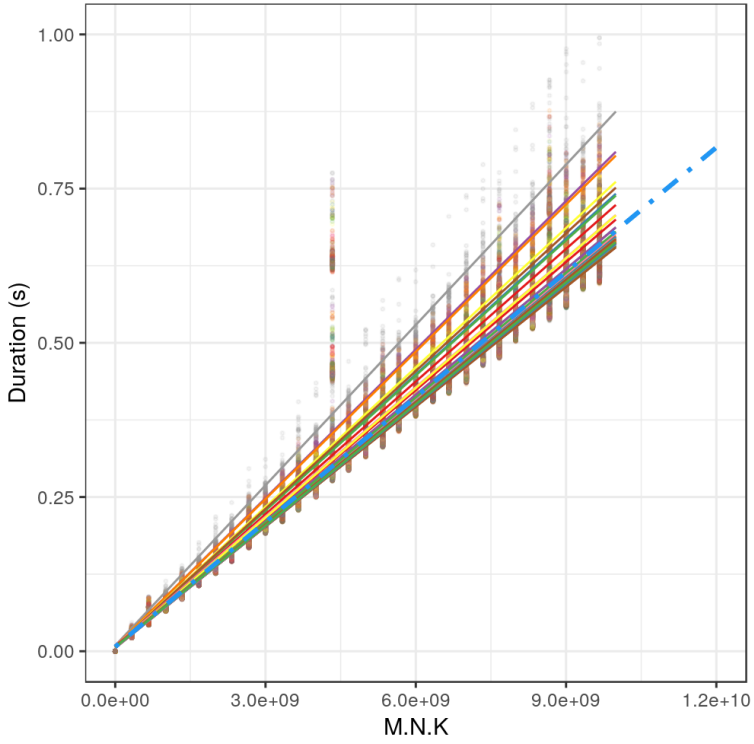
$$\texttt{dgemm}\,(M, N, K) = \alpha.M.N.K$$



Modeling Commputations

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

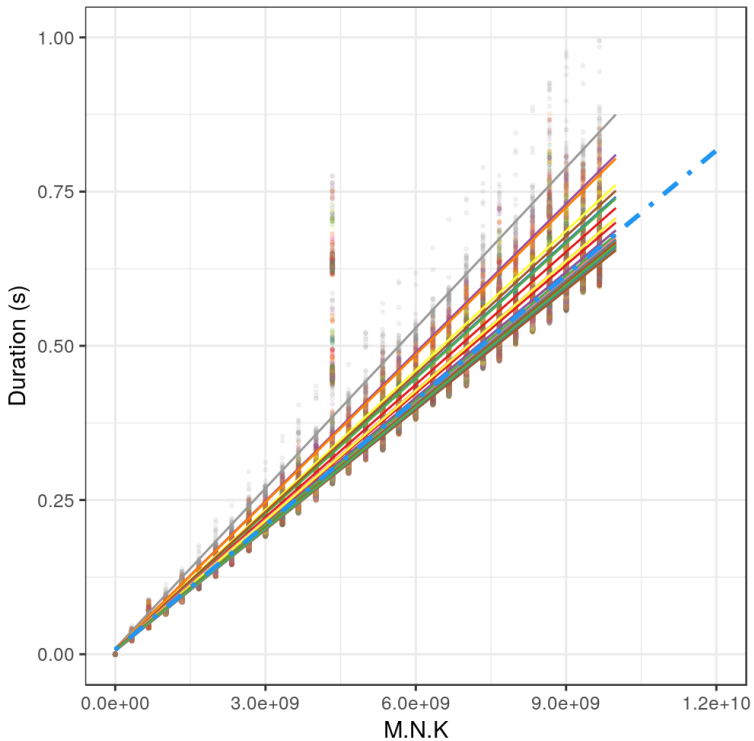
Different color $\Rightarrow$ different host



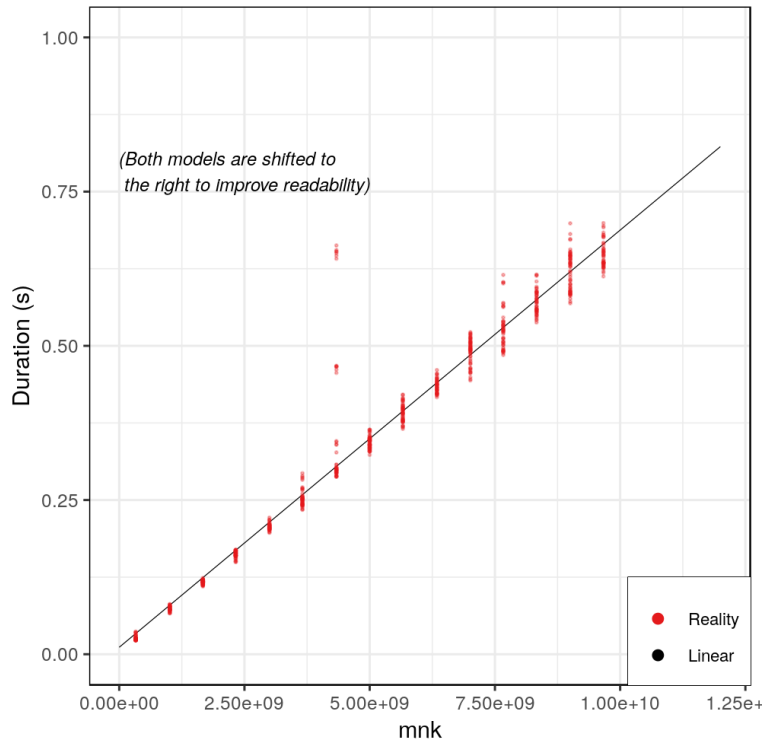
Modeling Commputations

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

Different color $\Rightarrow$ different host



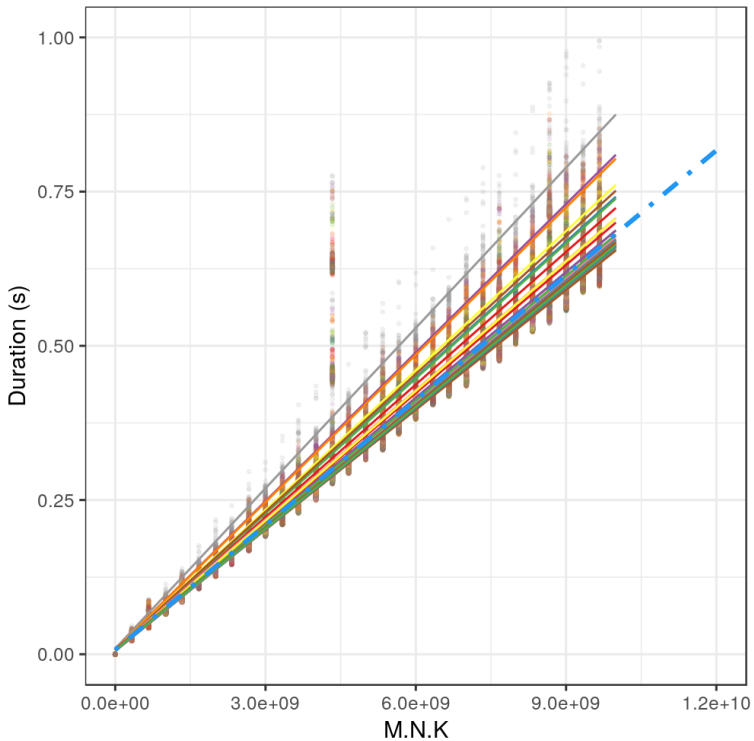
For a particular host



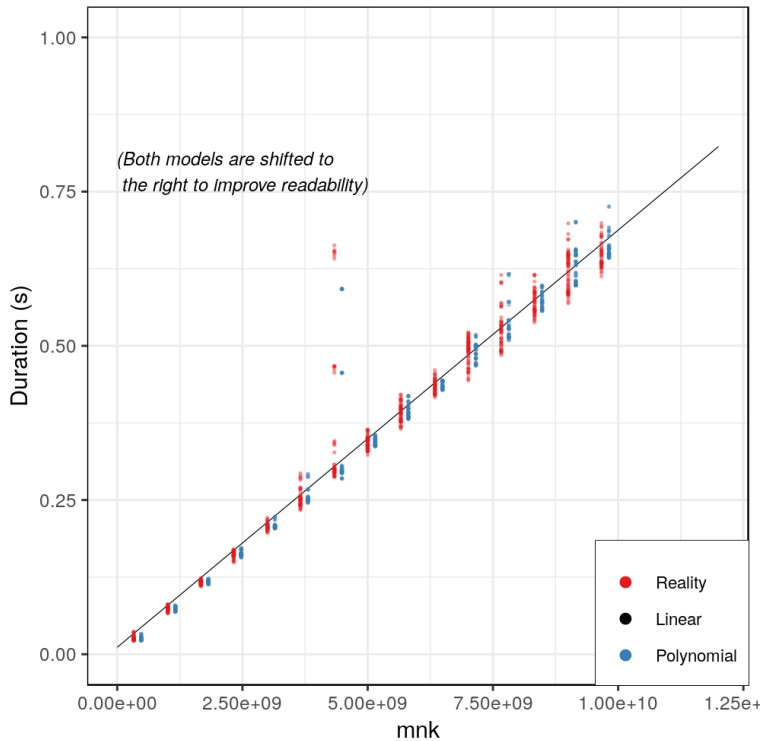
Modeling Commputations

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

Different color $\Rightarrow$ different host



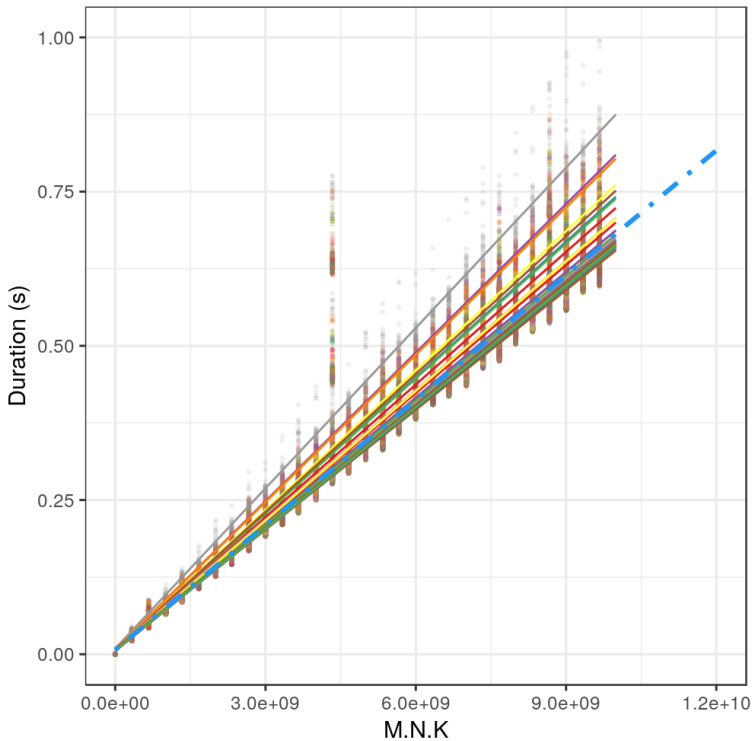
For a particular host



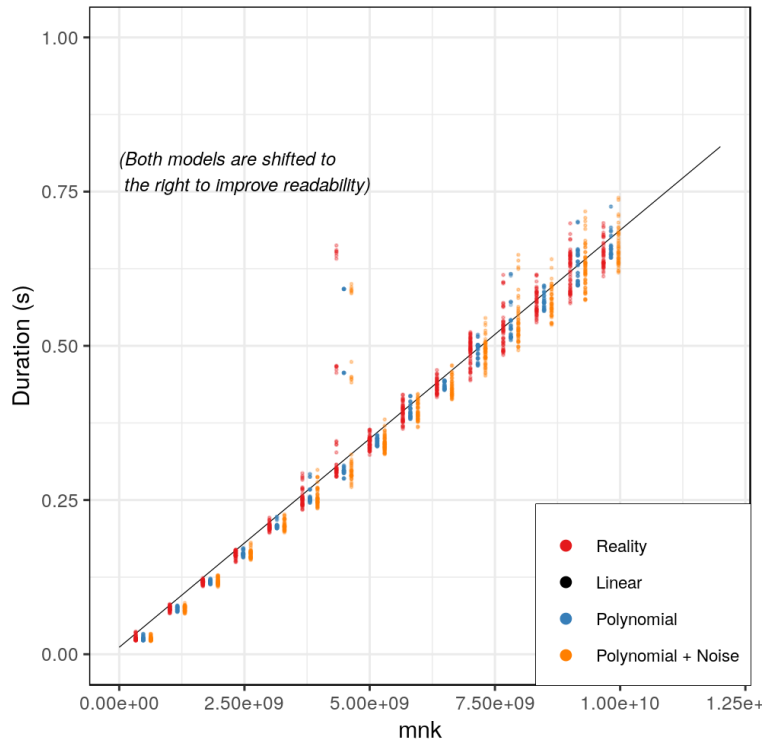
Modeling Commputations

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

Different color $\Rightarrow$ different host



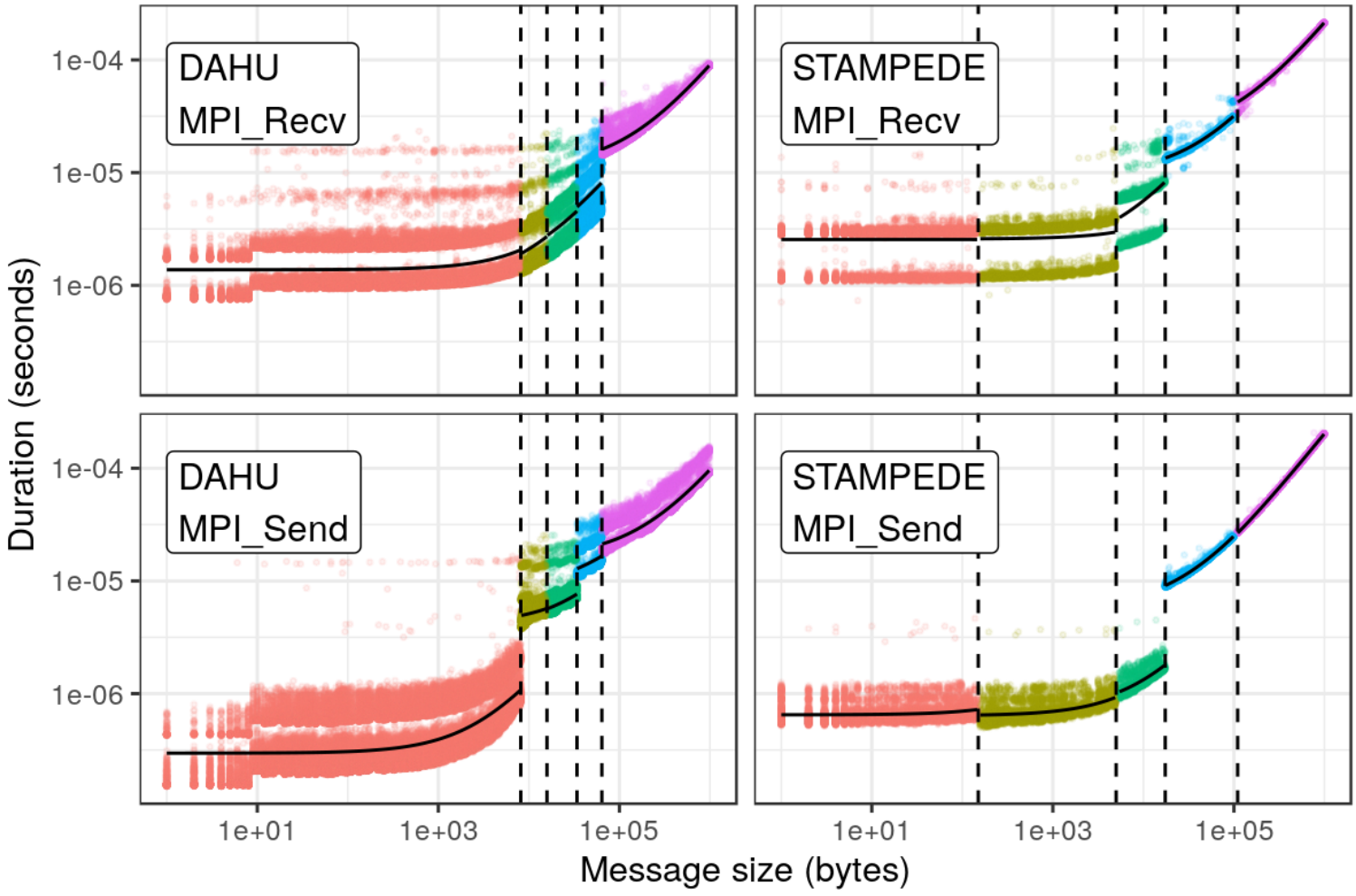
For a particular host



Modeling Communications

Hand-crafted non-blocking collective operations intertwinned with computations

Hand-crafted non-blocking collective operations intertwinned with computations



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

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

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)

- Sampling method for generating the sequence of calls
- Sample itself (for a given sampling method)

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)

- Sampling method for generating the sequence of calls
- Sample itself (for a given sampling method)
- Interferences between computations and communications

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)

- Sampling method for generating the sequence of calls
- Sample itself (for a given sampling method)
- Interferences between computations and communications
- Content of the matrices used by `dgemm`

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)

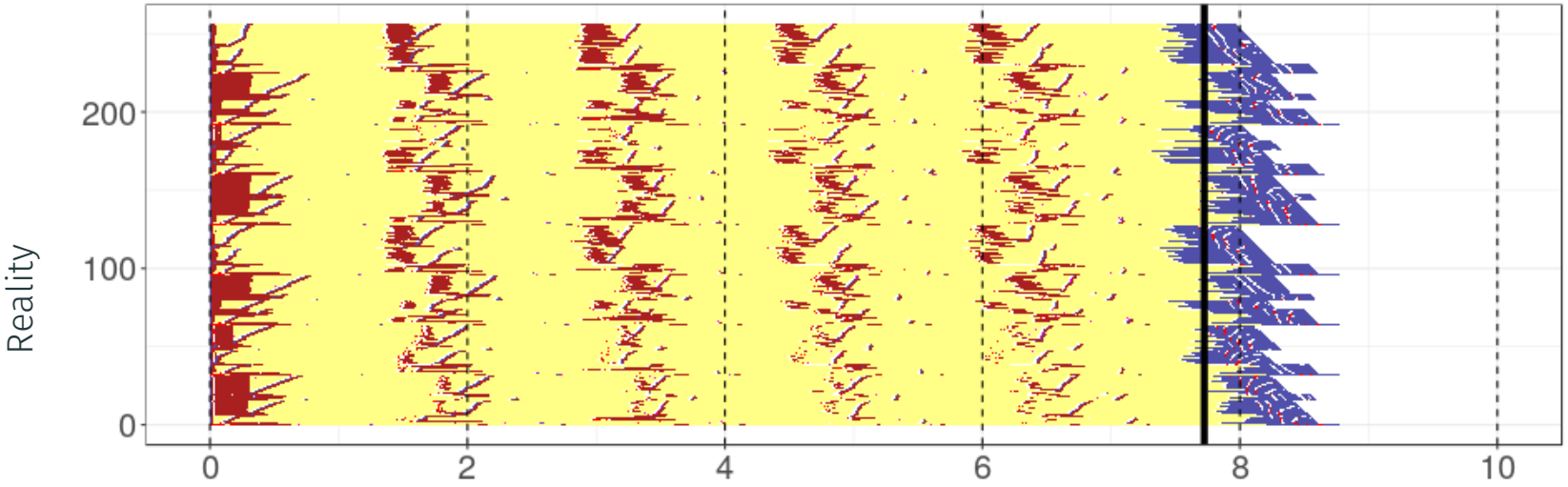
- Sampling method for generating the sequence of calls
- Sample itself (for a given sampling method)
- Interferences between computations and communications
- Content of the matrices used by `dgemm`

Bias may be desirable in some situations

Validating the predictions

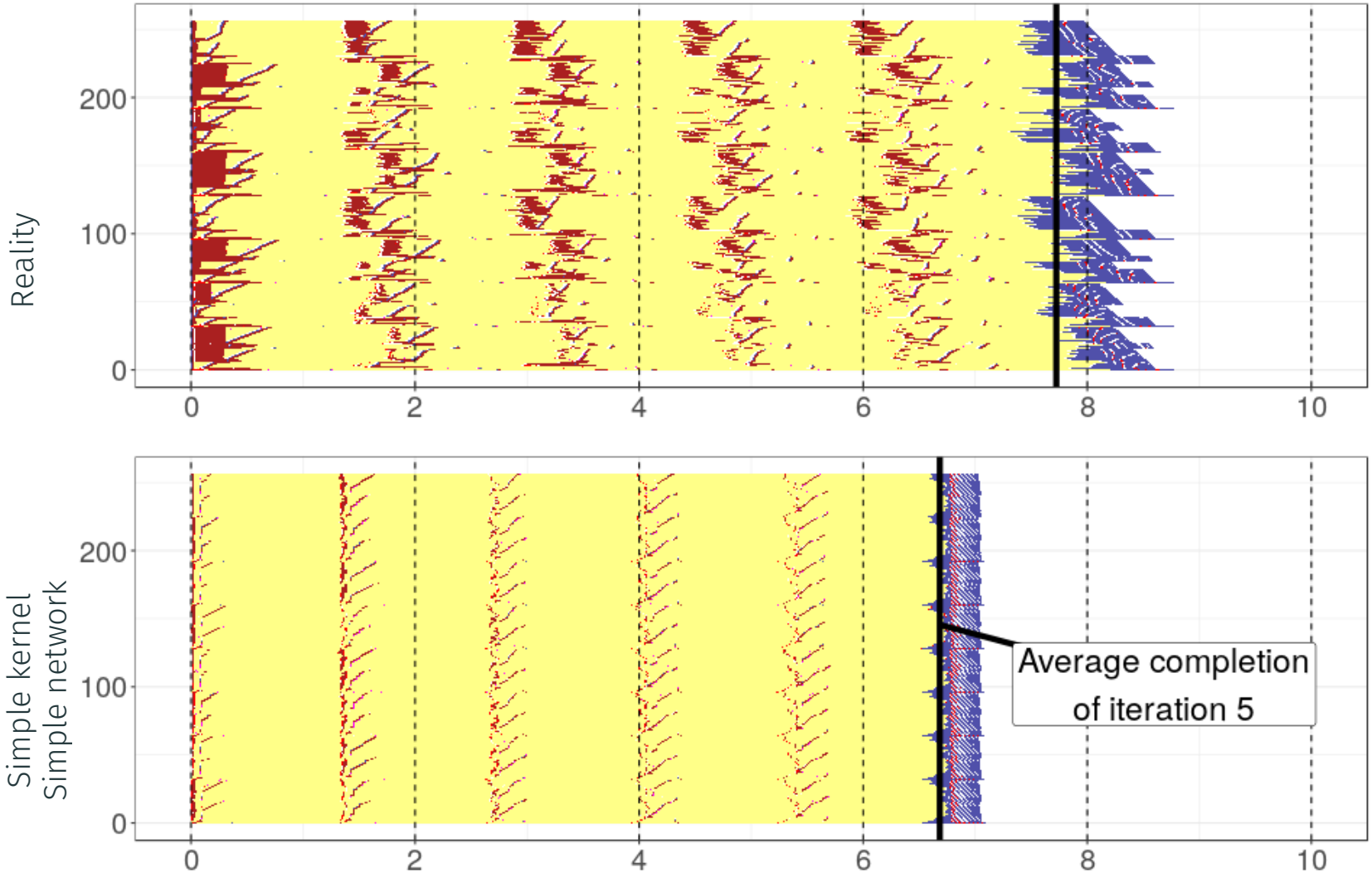
Internal behavior of the application

256 MPI ranks, interrupted after the 5th iteration



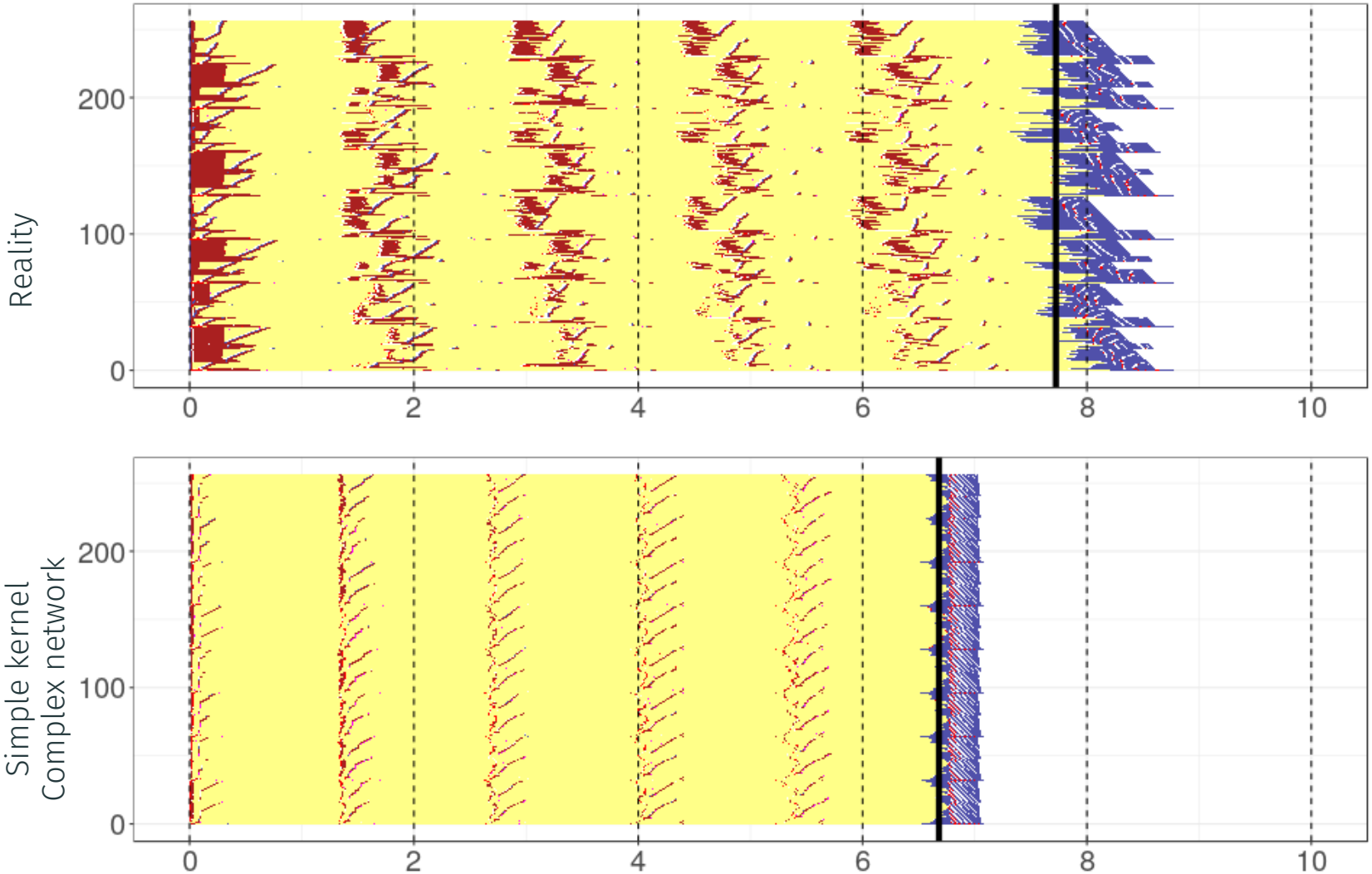
Internal behavior of the application

256 MPI ranks, interrupted after the 5th iteration



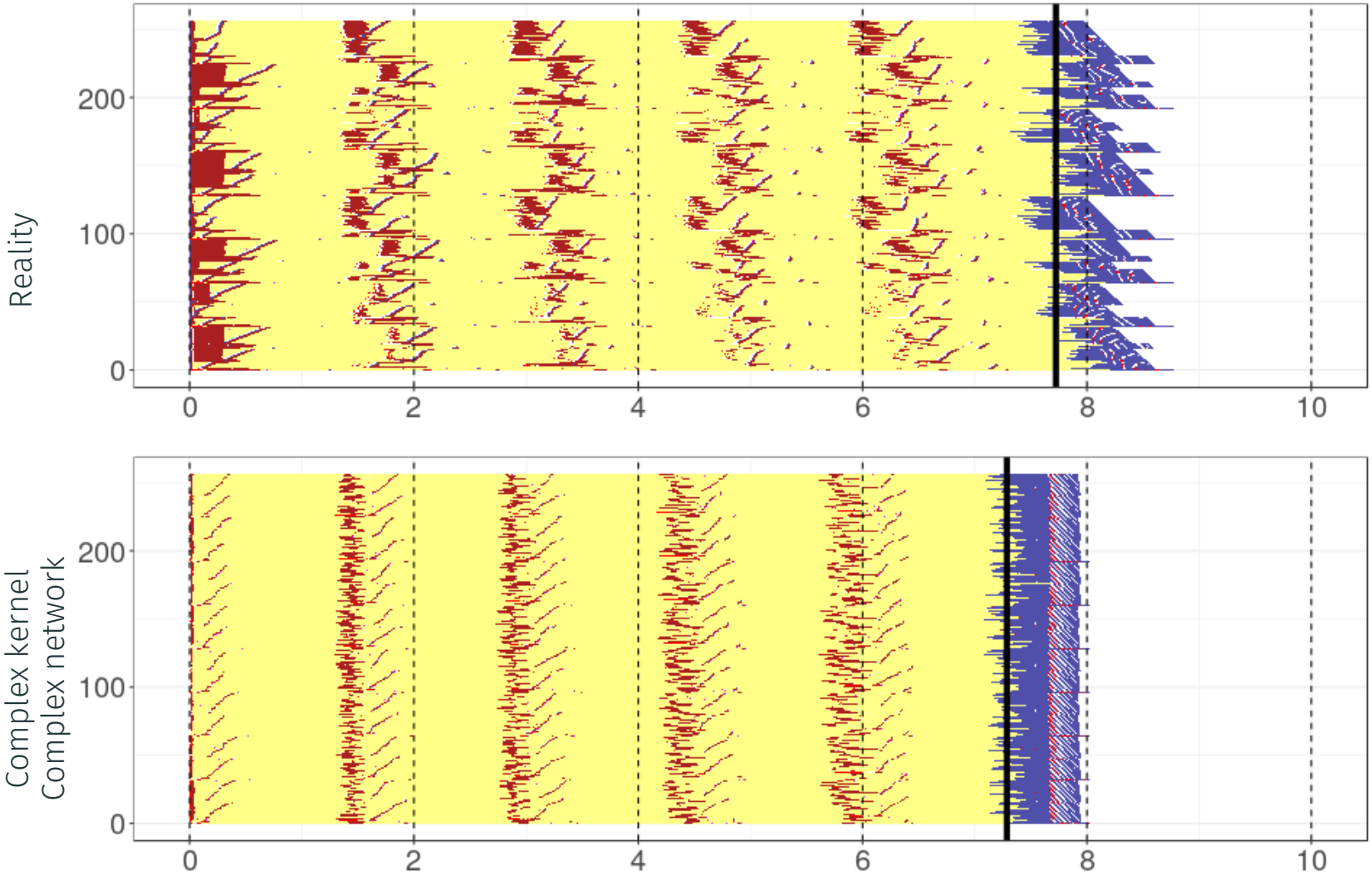
Internal behavior of the application

256 MPI ranks, interrupted after the 5th iteration



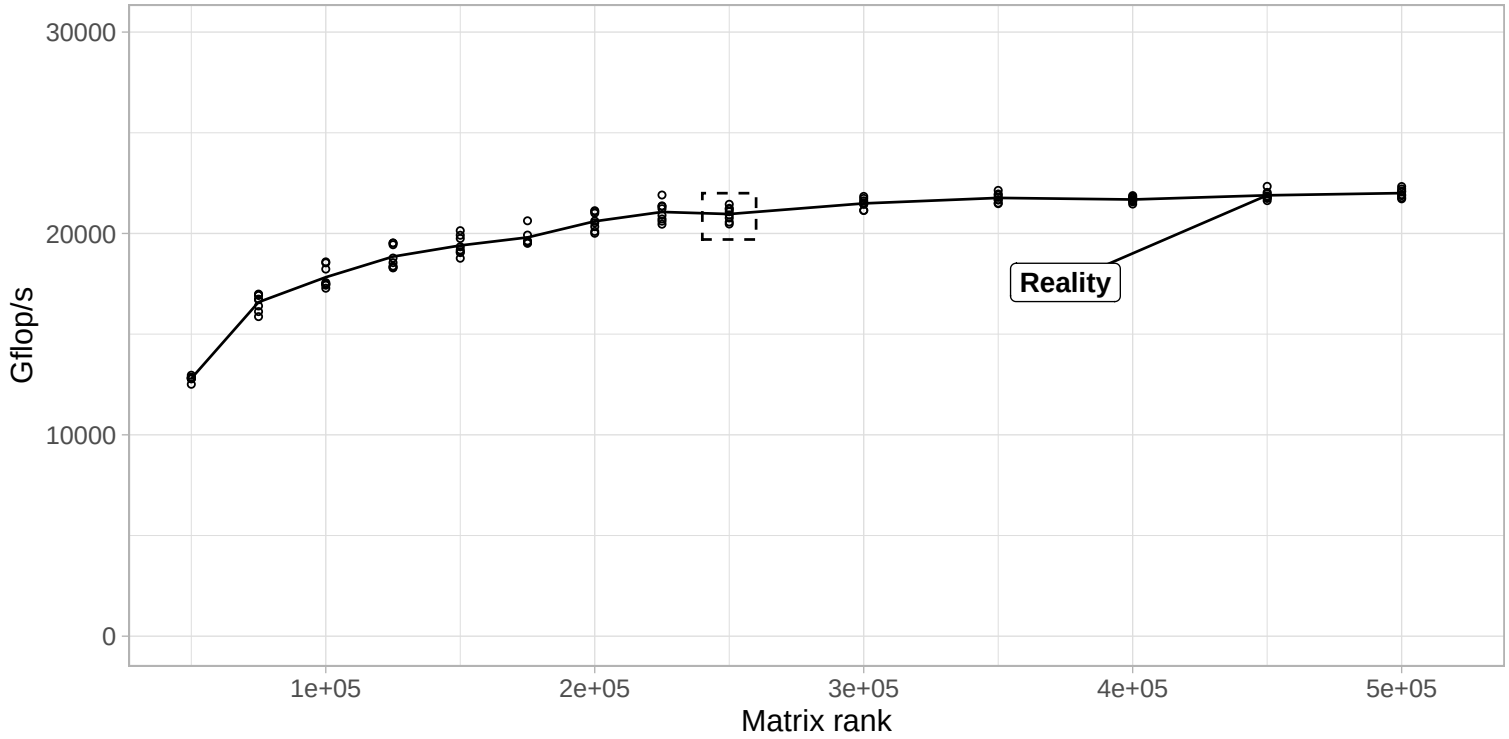
Internal behavior of the application

256 MPI ranks, interrupted after the 5th iteration



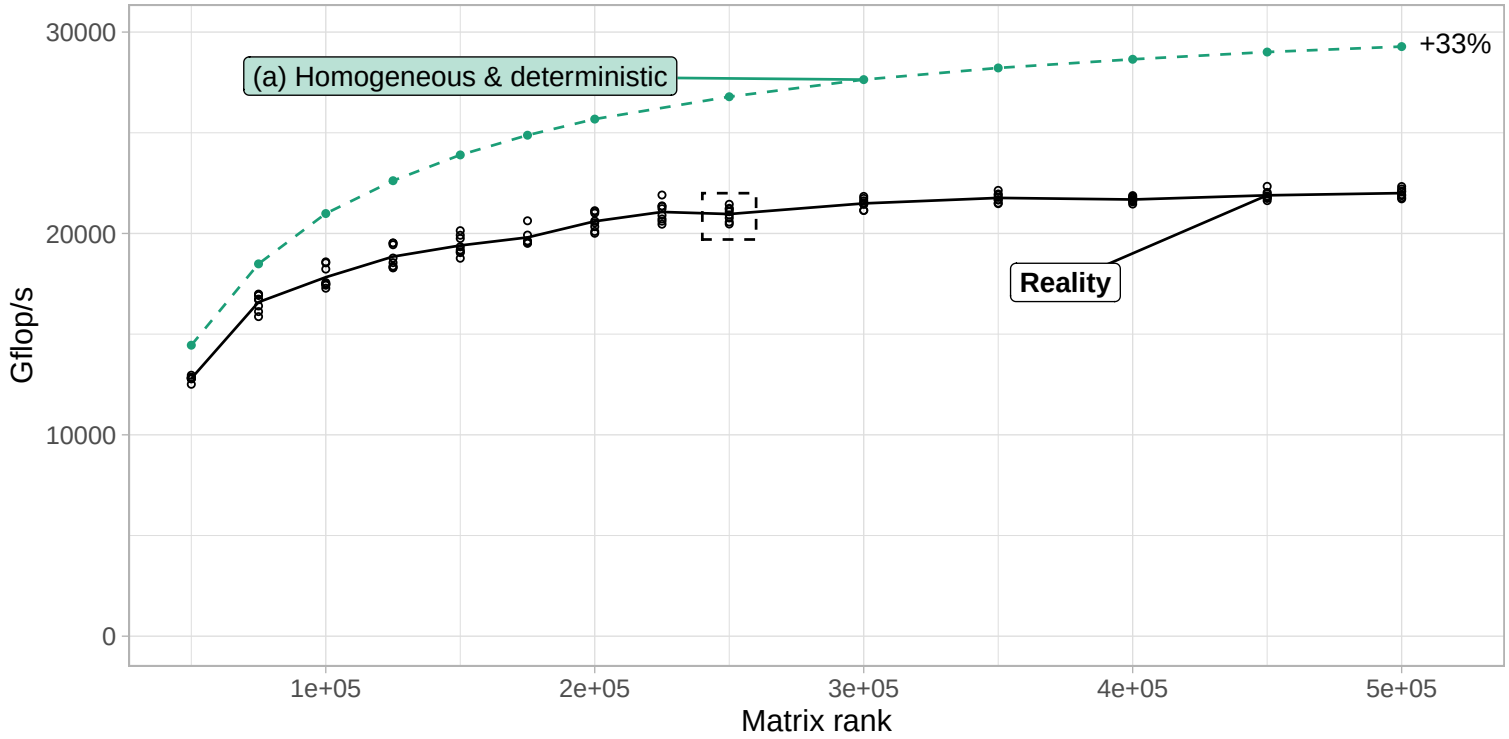
Influence of the problem size

Now the complete run, with 1024 MPI ranks



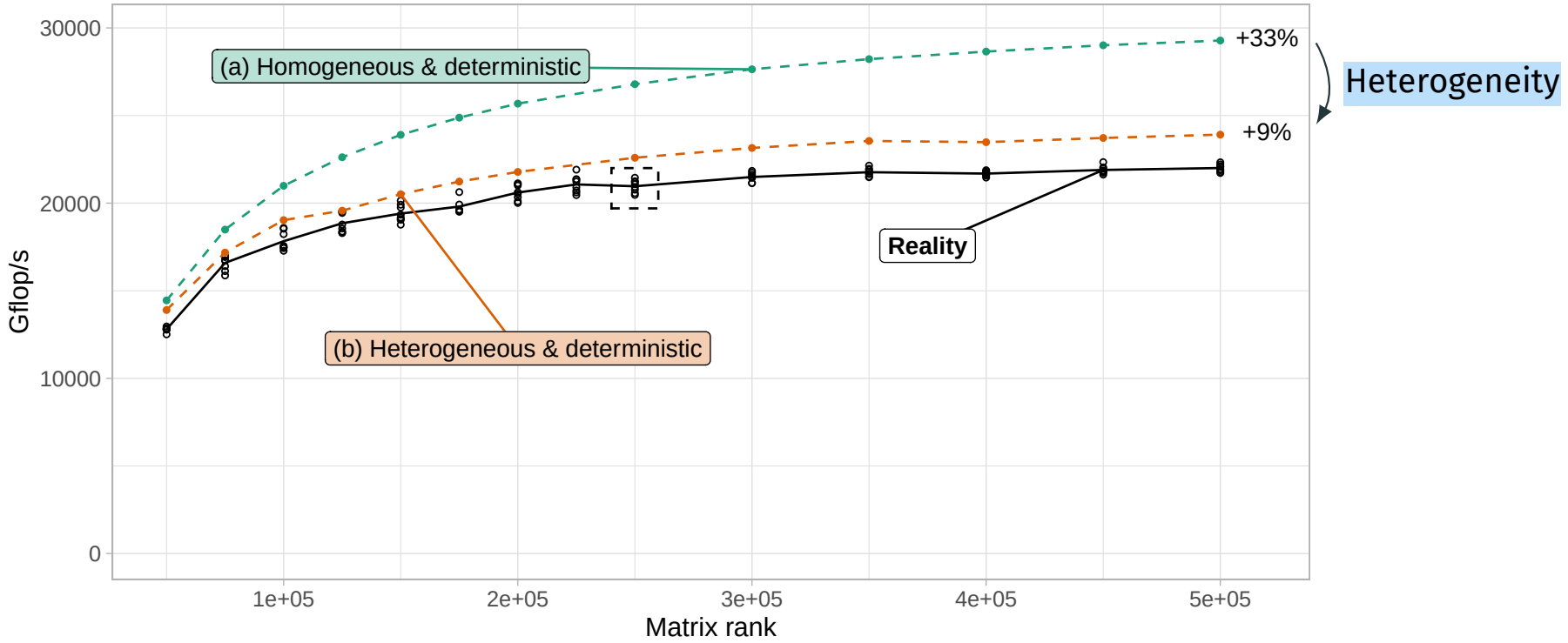
Influence of the problem size

Now the complete run, with 1024 MPI ranks



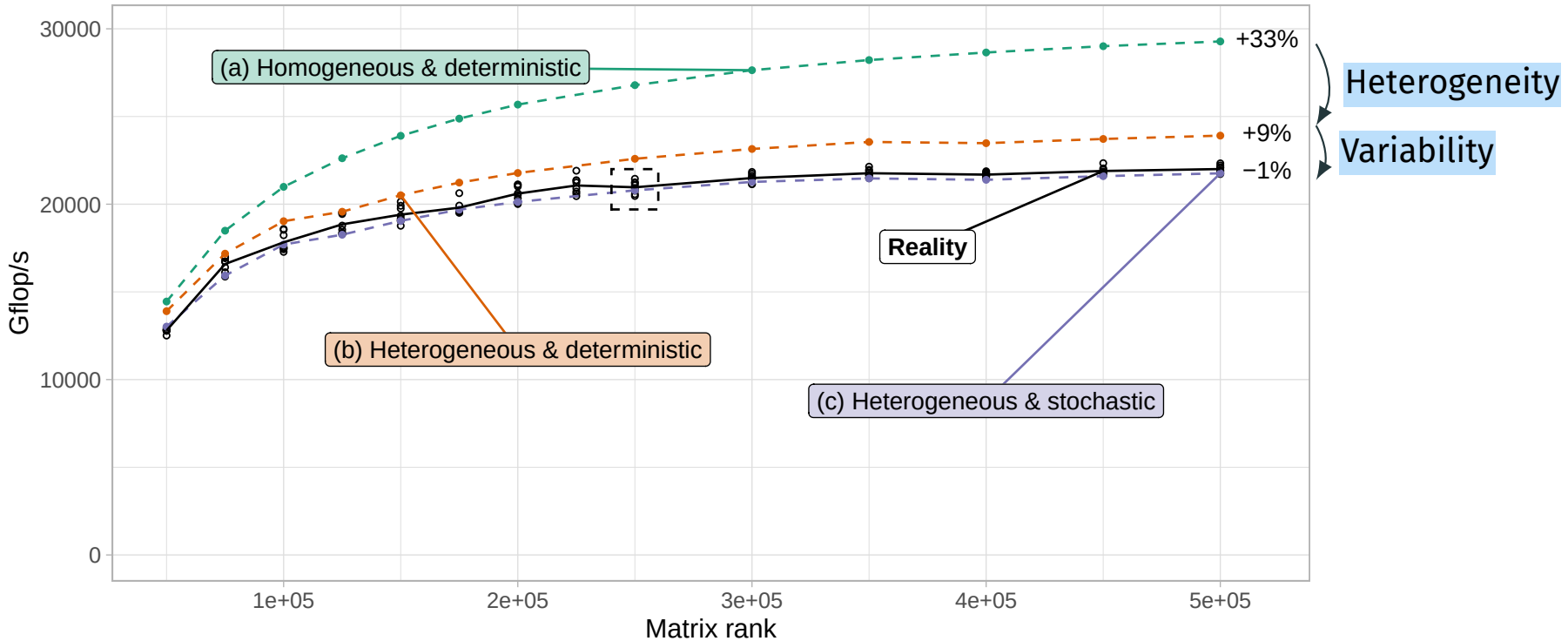
Influence of the problem size

Now the complete run, with 1024 MPI ranks



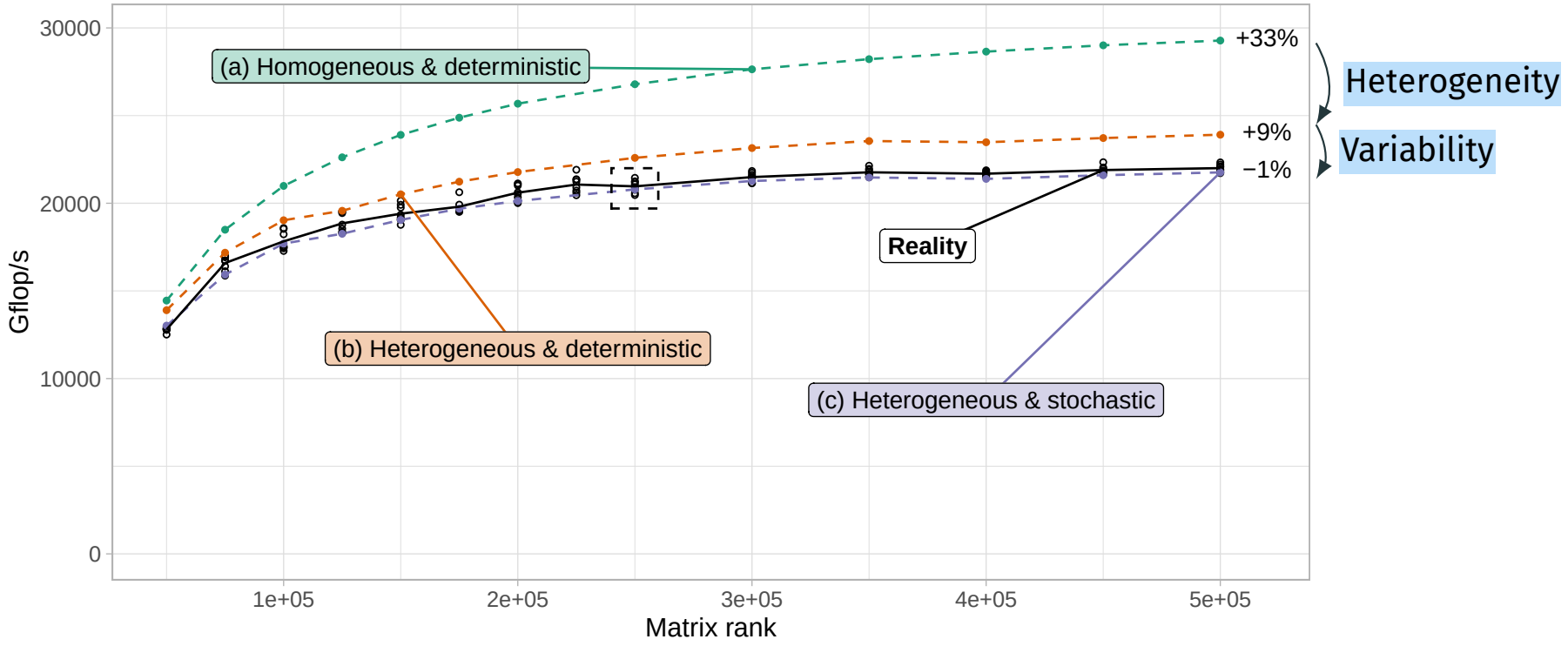
Influence of the problem size

Now the complete run, with 1024 MPI ranks



Influence of the problem size

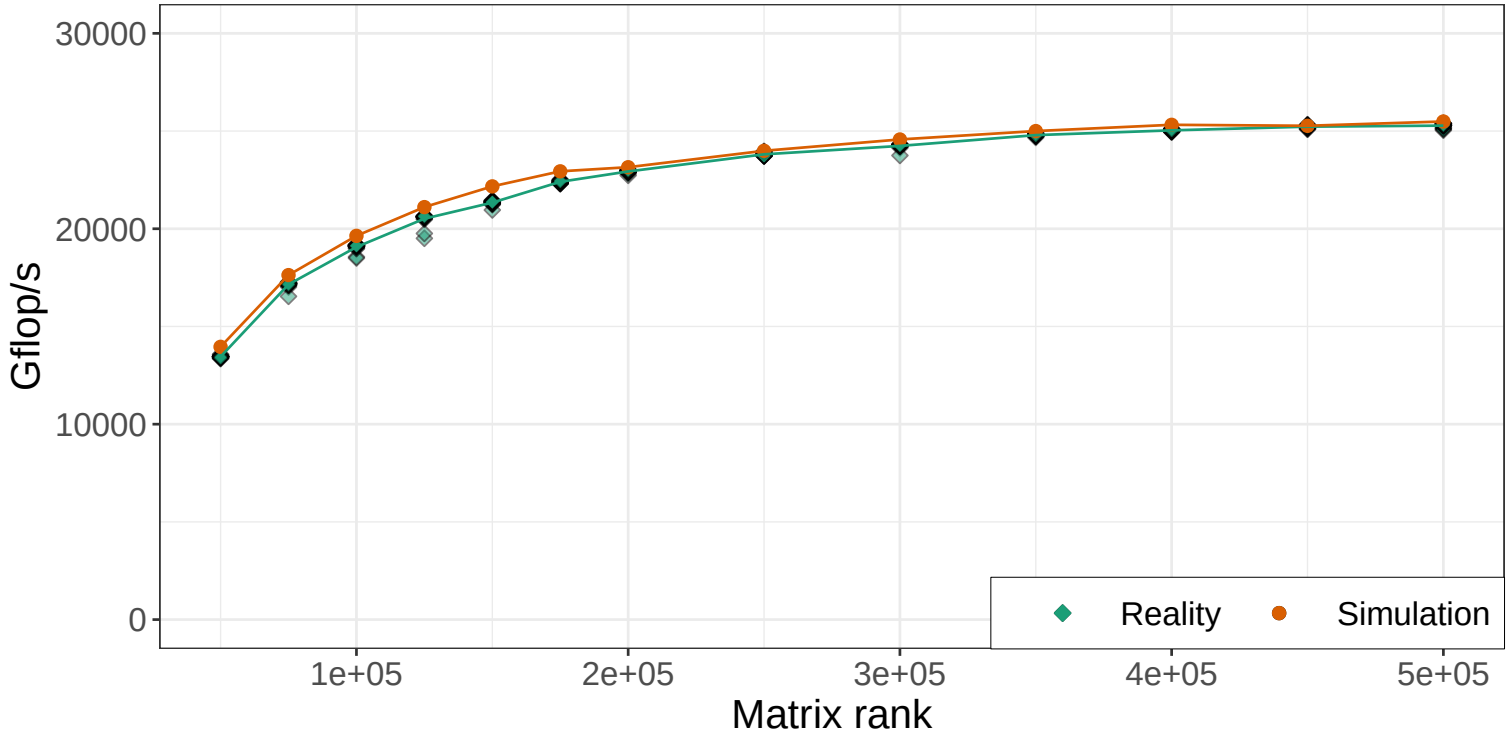
Now the complete run, with 1024 MPI ranks



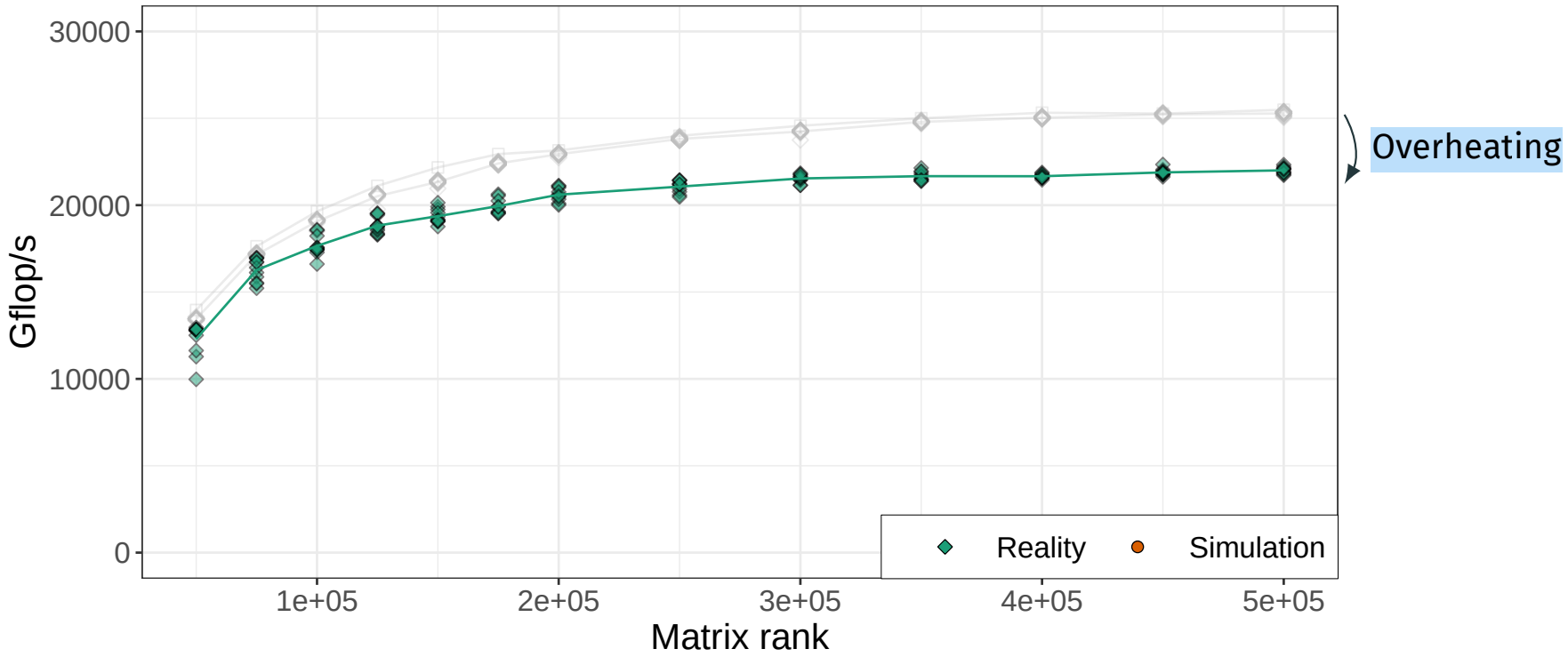
Take-Away Message: accurate prediction

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

Influence of a platform change

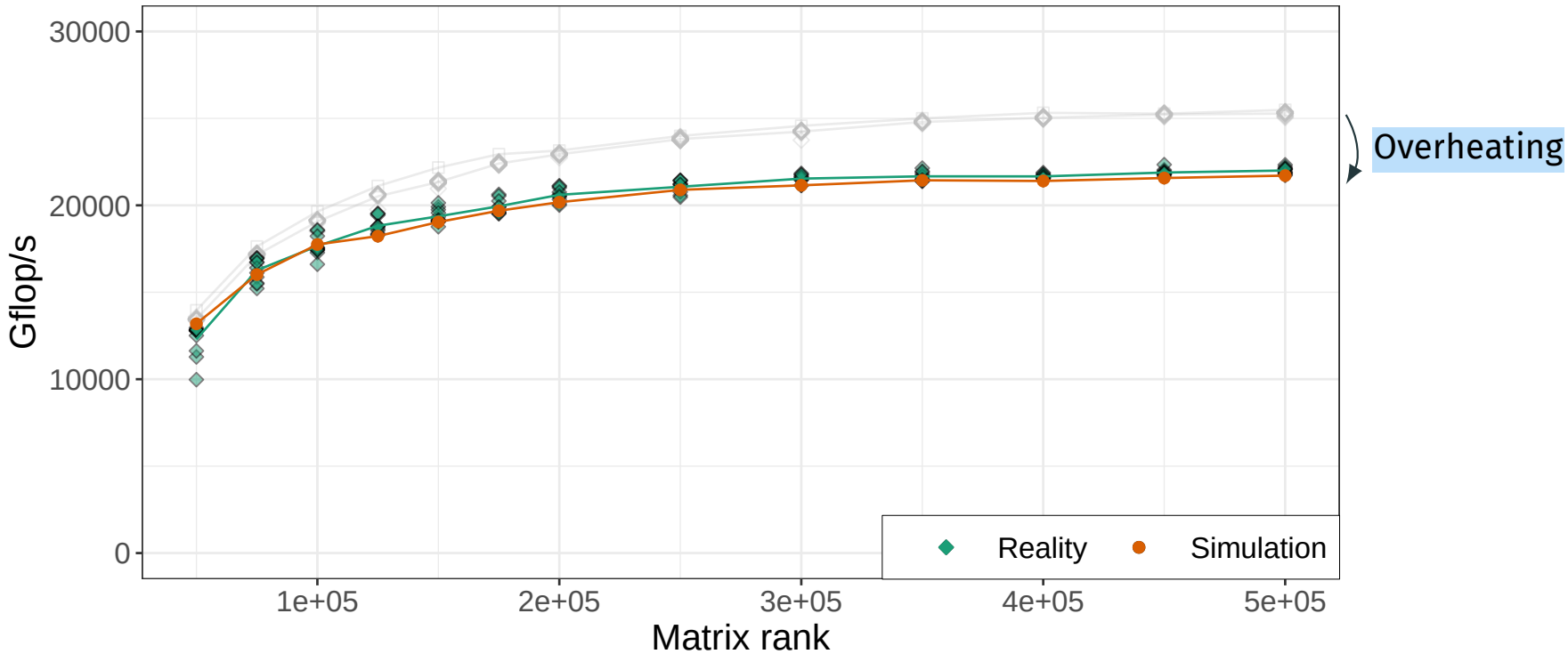


Influence of a platform change



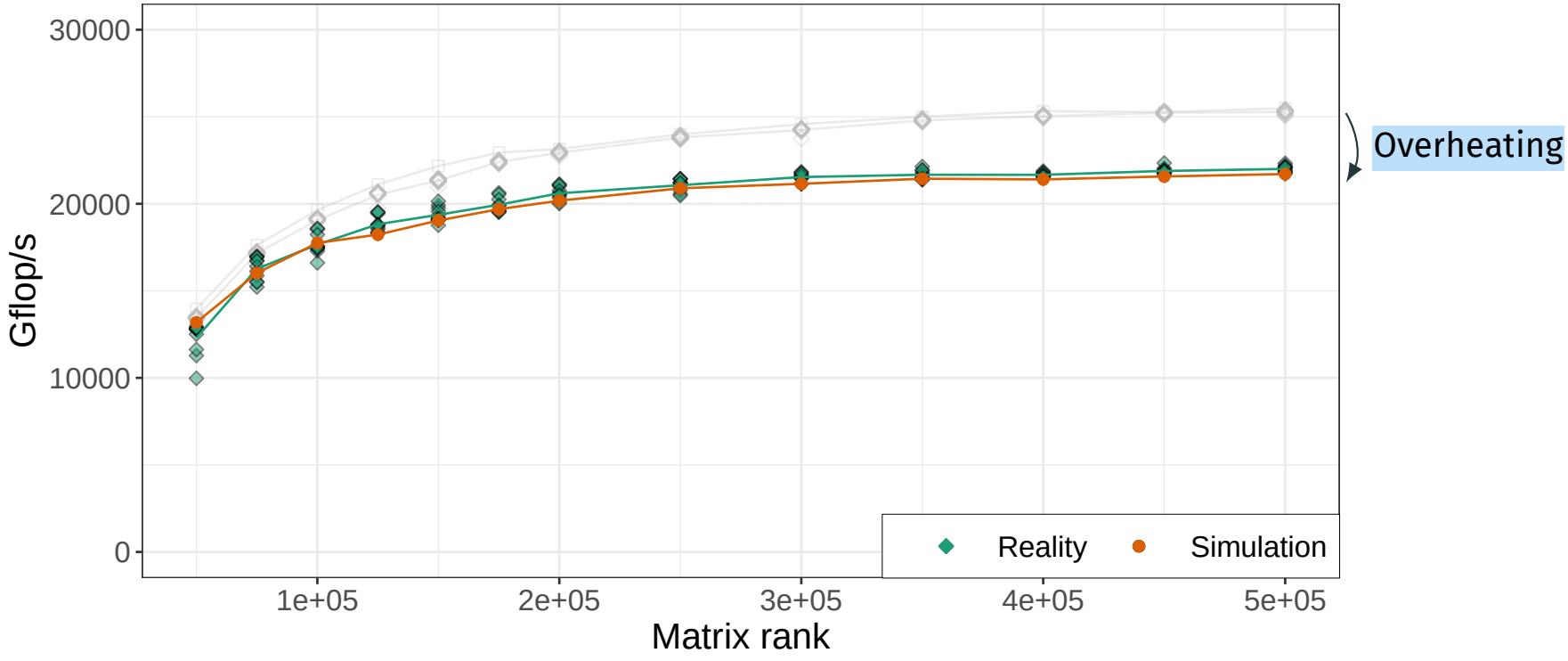
On four nodes, the cooling system malfunctionned for several weeks

Influence of a platform change



On four nodes, the cooling system malfunctionned for several weeks

Influence of a platform change



On four nodes, the cooling system malfunctionned for several weeks

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

Regular measures

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

454 nodes (792 CPU) from 12 clusters

For each CPU, collect:

- average `dgemm` performance
- `dgemm` coefficients of regression (i.e. the model for simulation)

Regular measures

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

454 nodes (792 CPU) from 12 clusters

For each CPU, collect:

- average `dgemm` performance
- `dgemm` coefficients of regression (i.e. the model for simulation)
- average CPU frequency
- average CPU power consumption
- average DRAM power consumption
- average temperature

Regular measures

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

454 nodes (792 CPU) from 12 clusters

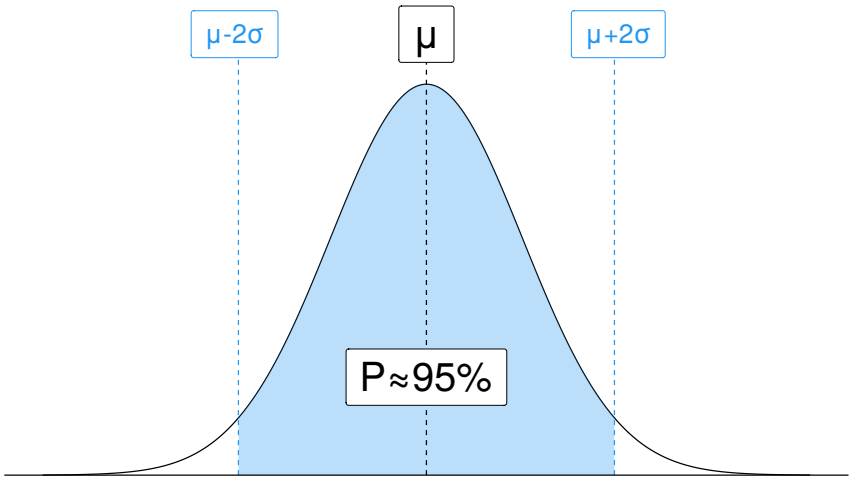
For each CPU, collect:

- average `dgemm` performance
- `dgemm` coefficients of regression (i.e. the model for simulation)
- average CPU frequency
- average CPU power consumption
- average DRAM power consumption
- average temperature

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}?



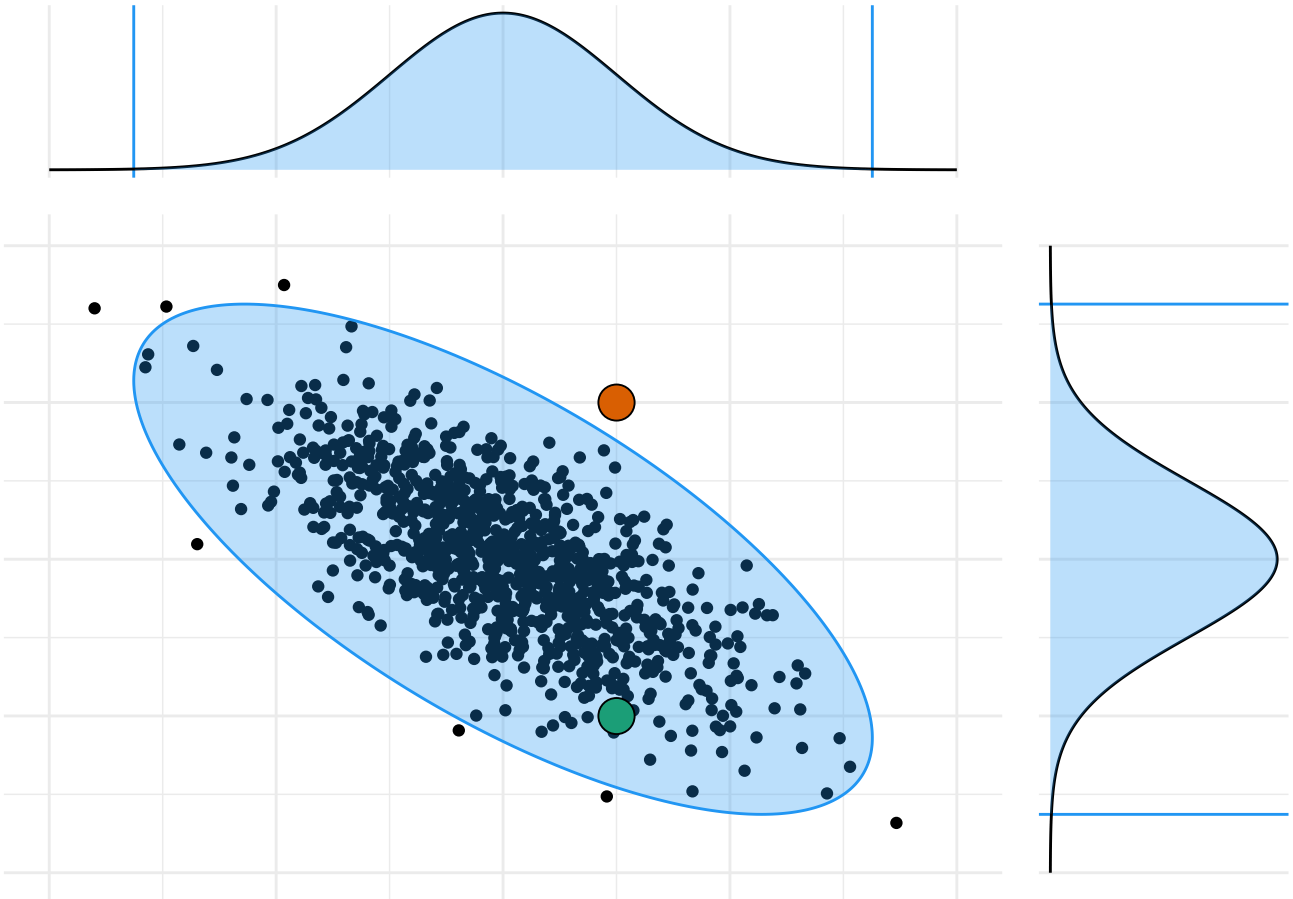
Take the sample mean μ and standard deviation σ of the old observations

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

Fluctuation interval for several variables

With several variables, using their covariance matrix

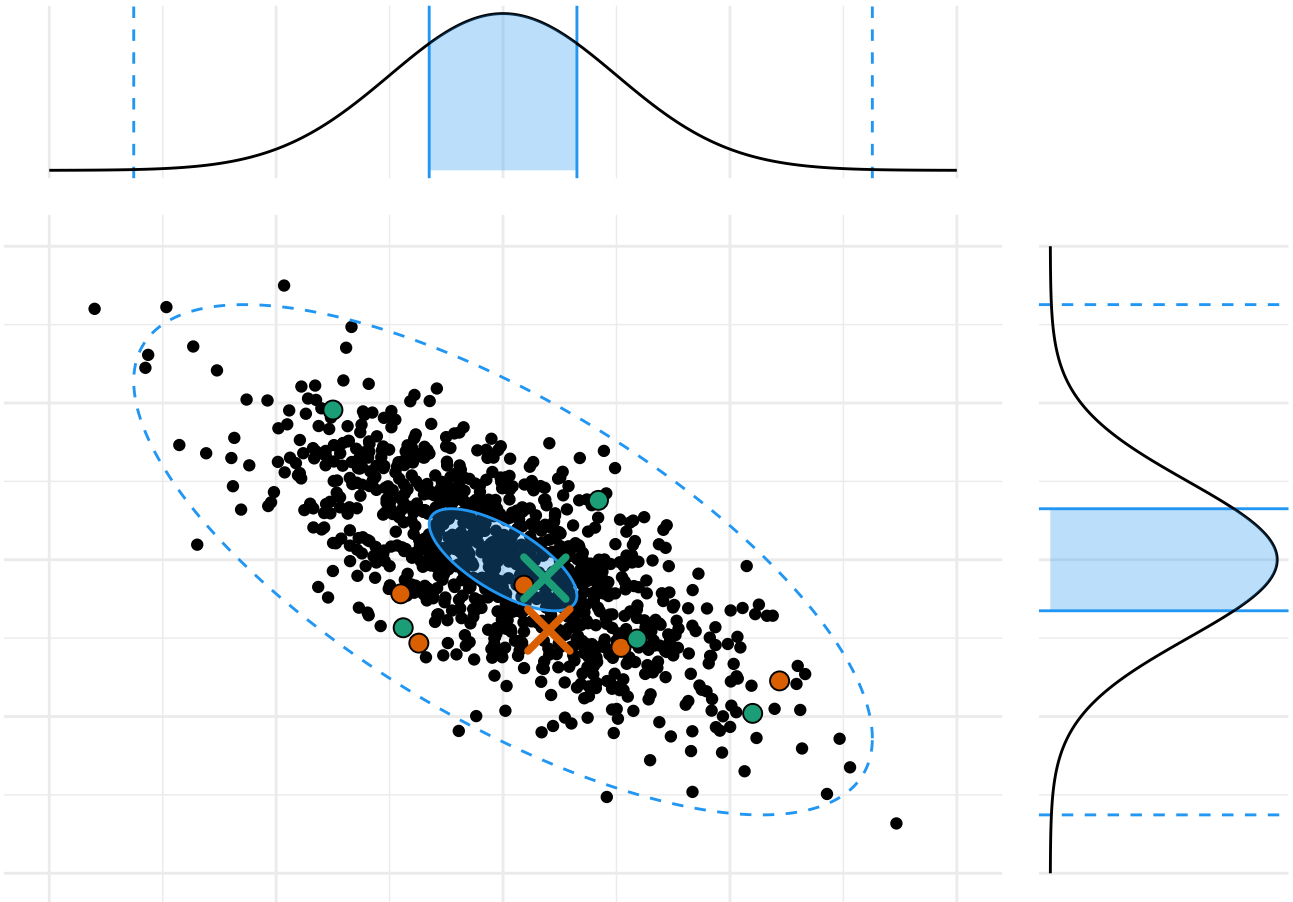
Example in dimension 2, with $\mathbb{P}(x_{n+1} \in \text{interval}) \approx 99.5\%$



Fluctuation interval for several measures

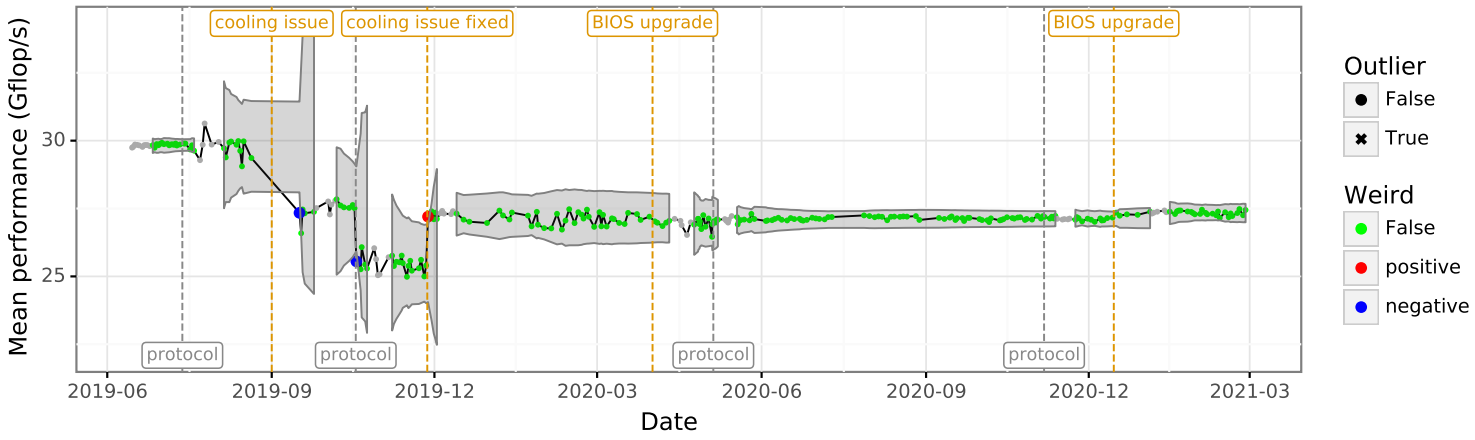
With several measures, using their average and shrinking the interval

Example with 5 measures (averages represented by crosses)



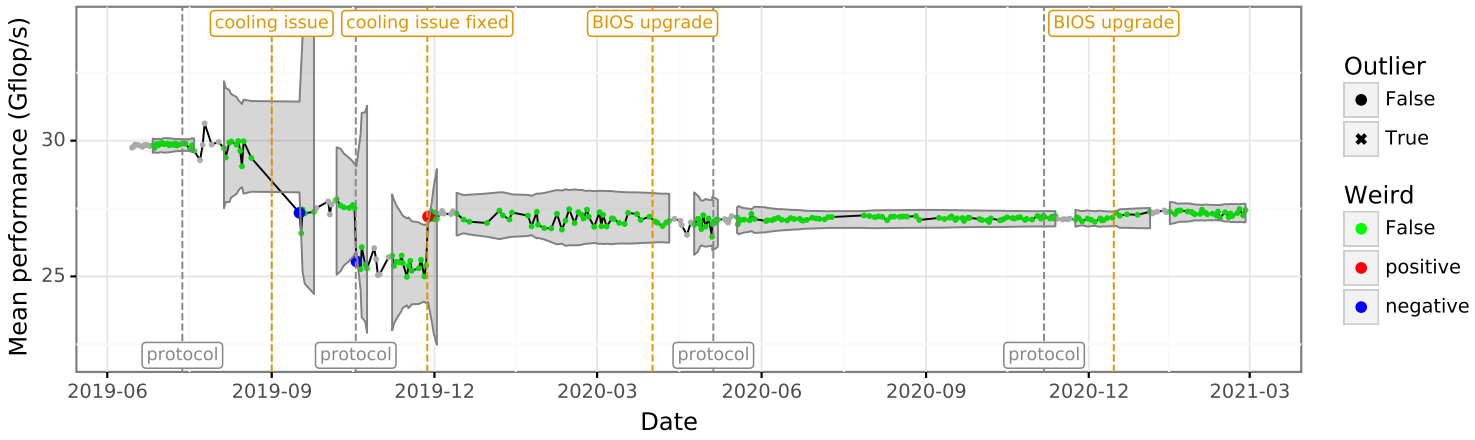
Result: performance fluctuation

Performance fluctuation of the node dahu-14

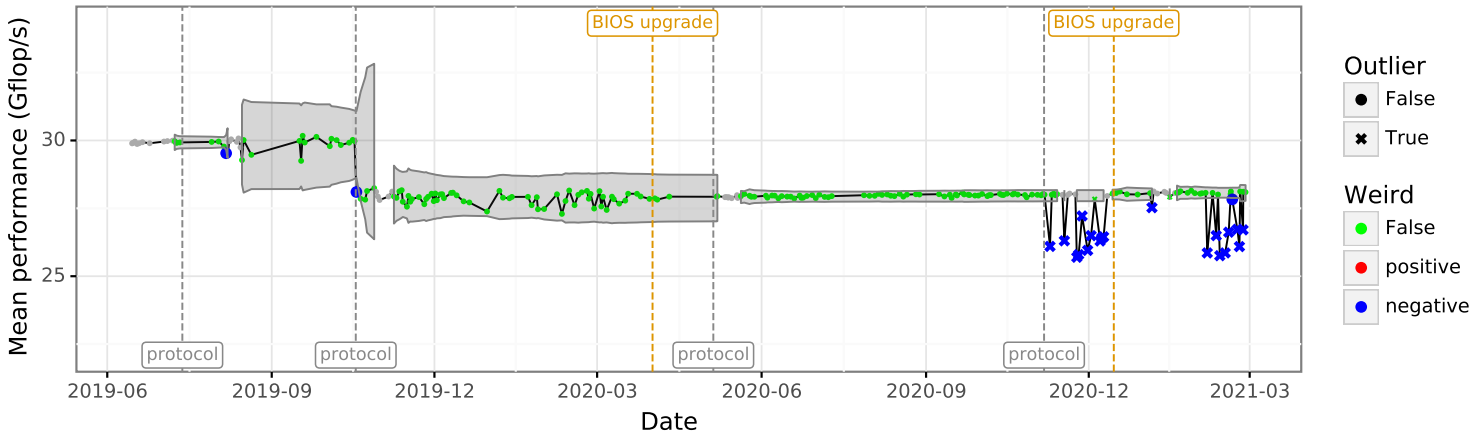


Result: performance fluctuation

Performance fluctuation of the node dahu-14

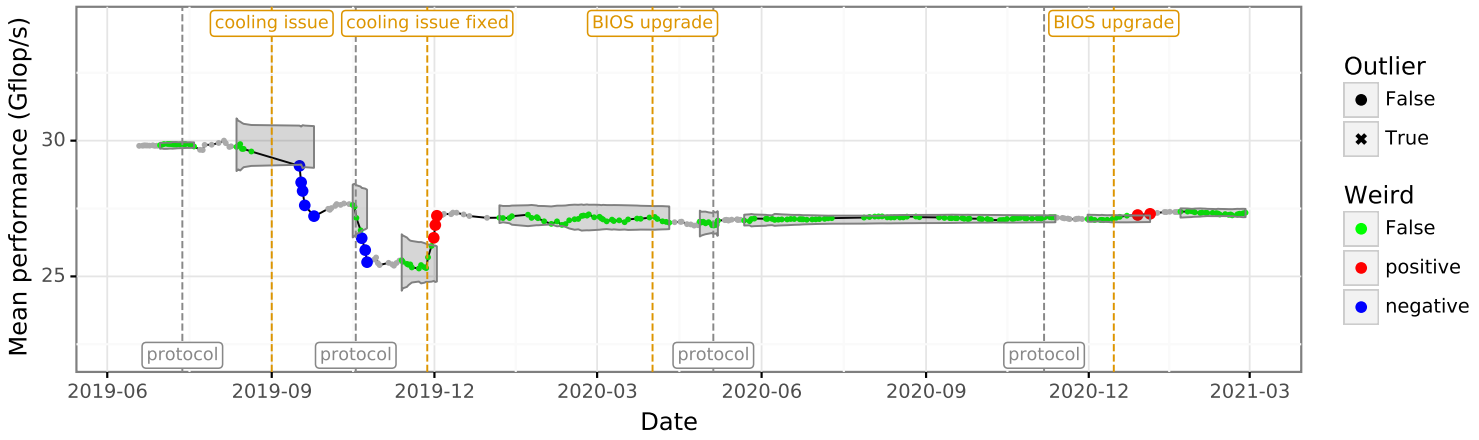


Performance fluctuation of the node dahu-32

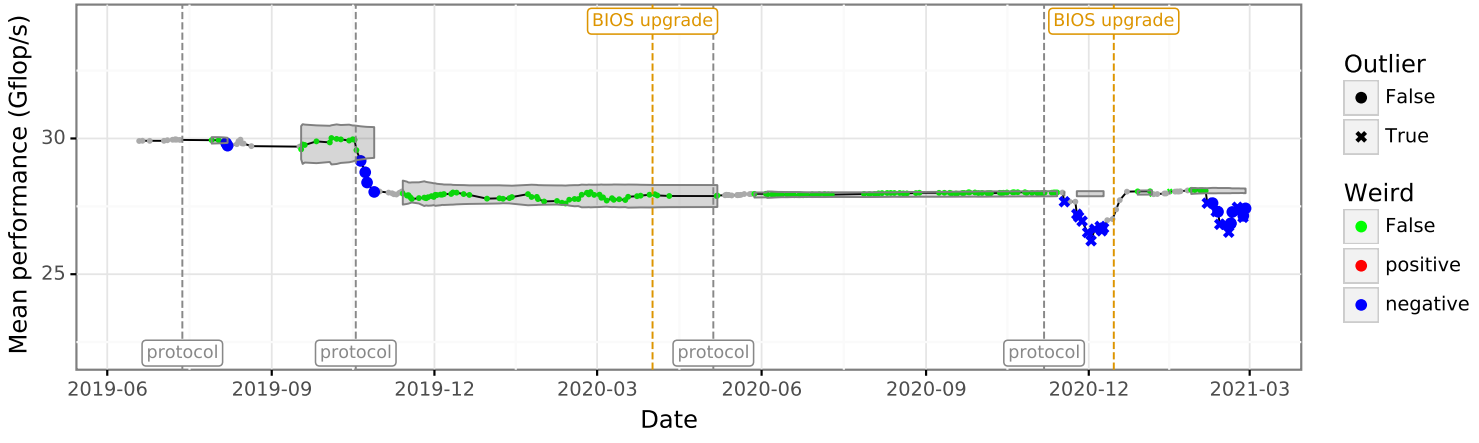


Result: performance fluctuation

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

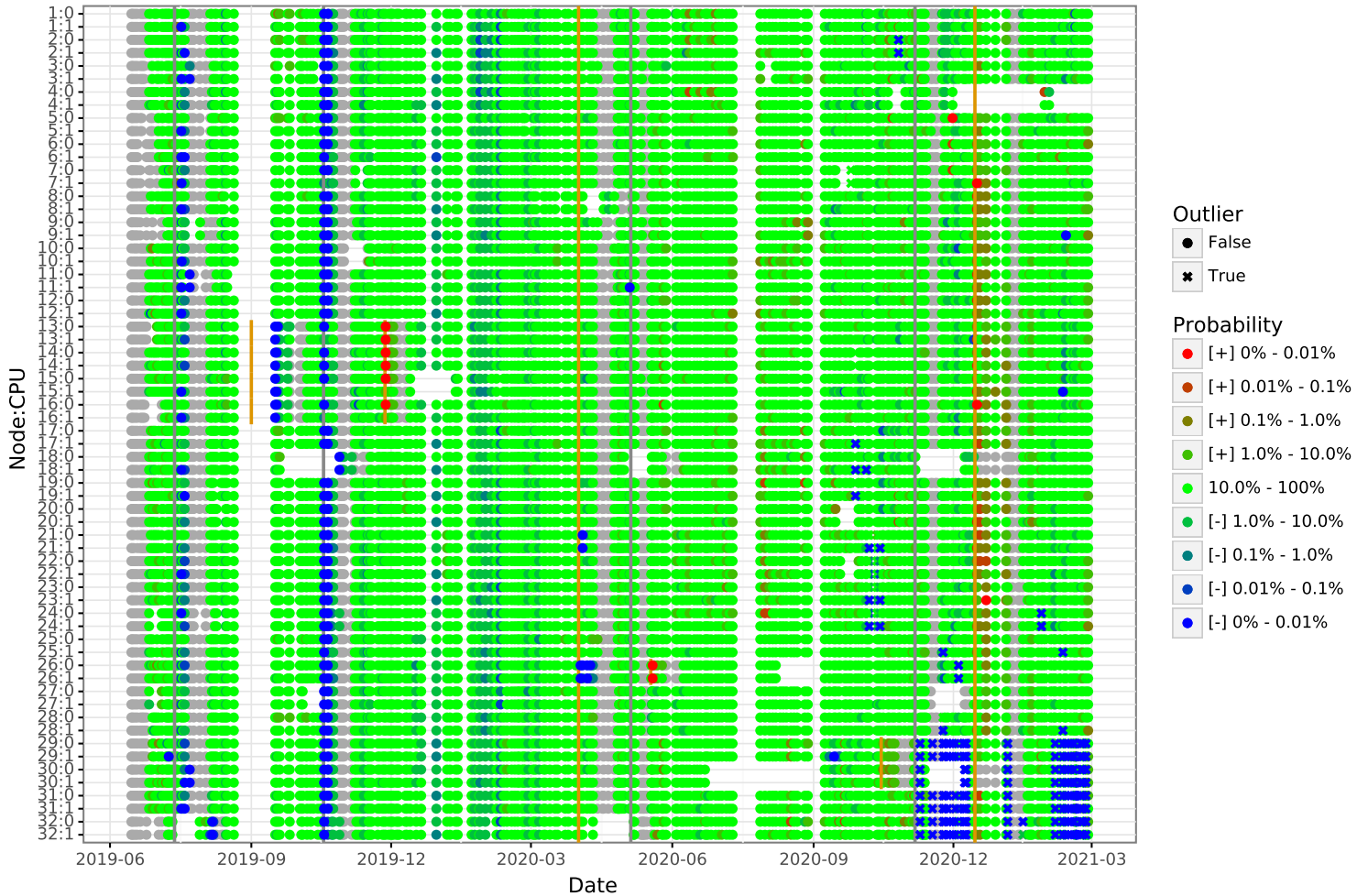


Performance fluctuation of the node dahu-32 (5-day window)



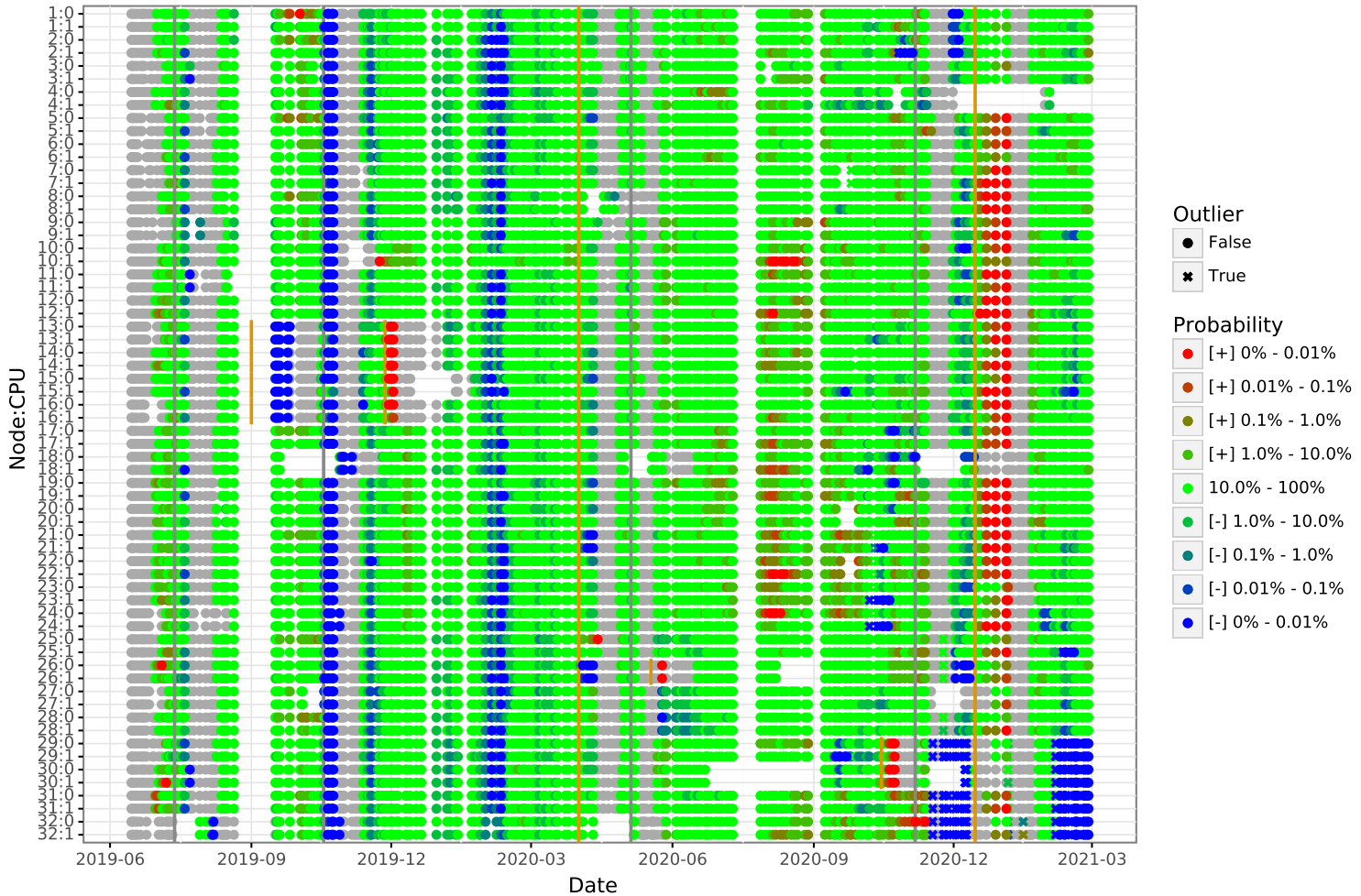
Result: performance overview

Overview of the performance on cluster dahu



Result: performance overview

Overview of the performance on cluster dahu (5-day window)



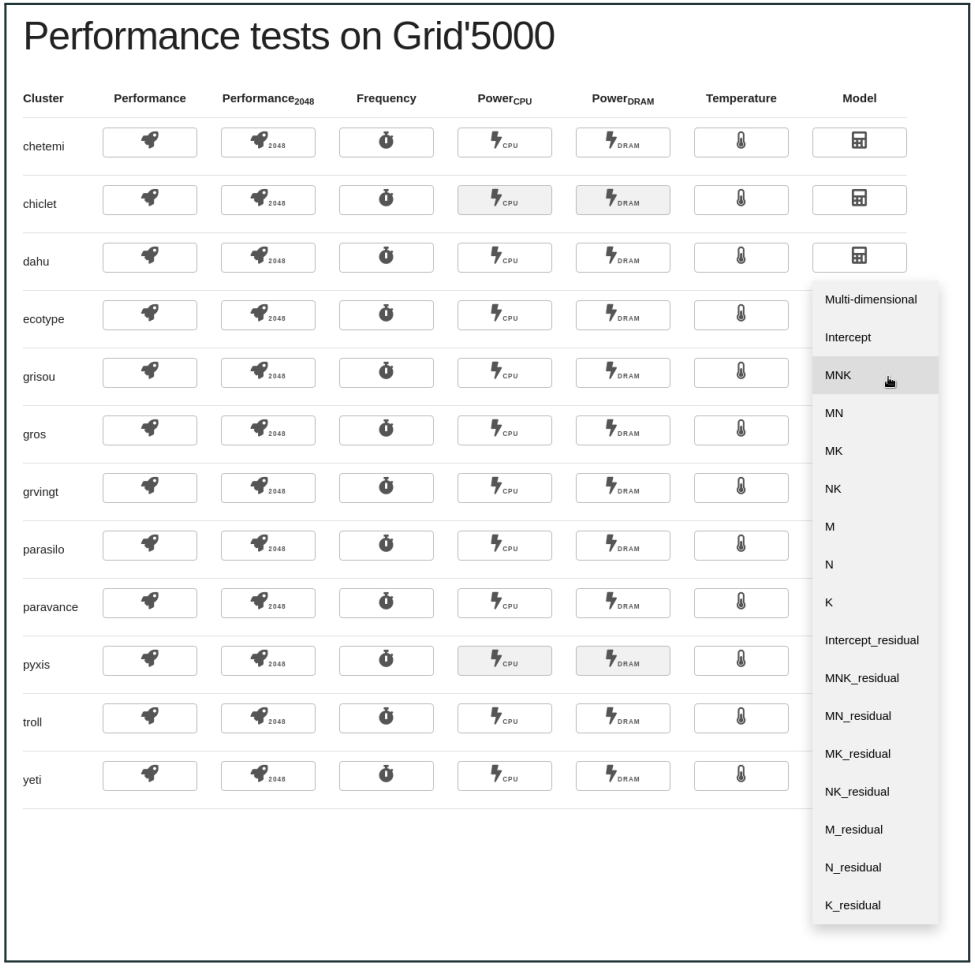
Performance tests: wraping up

Multi-variable test also implemented

Performance tests: wraping up

Multi-variable test also implemented

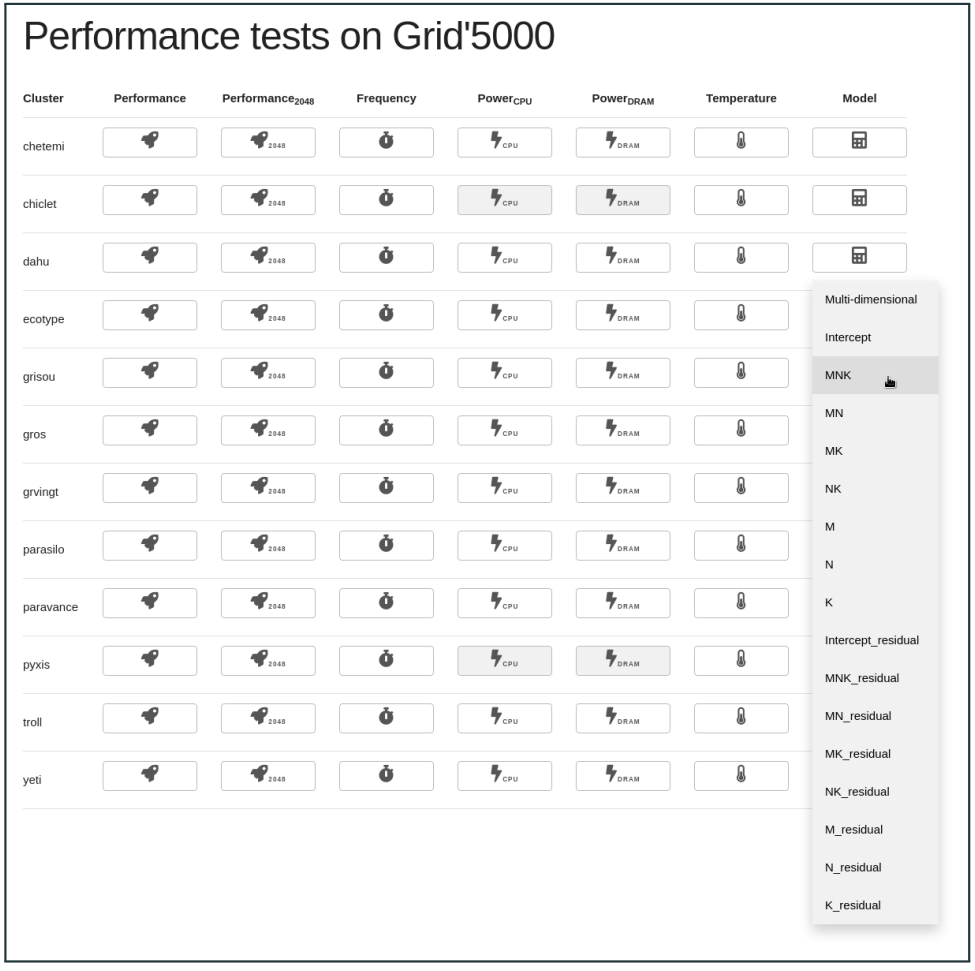
Results available on https://cornebize.net/g5k_test



Performance tests: wraping up

Multi-variable test also implemented

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



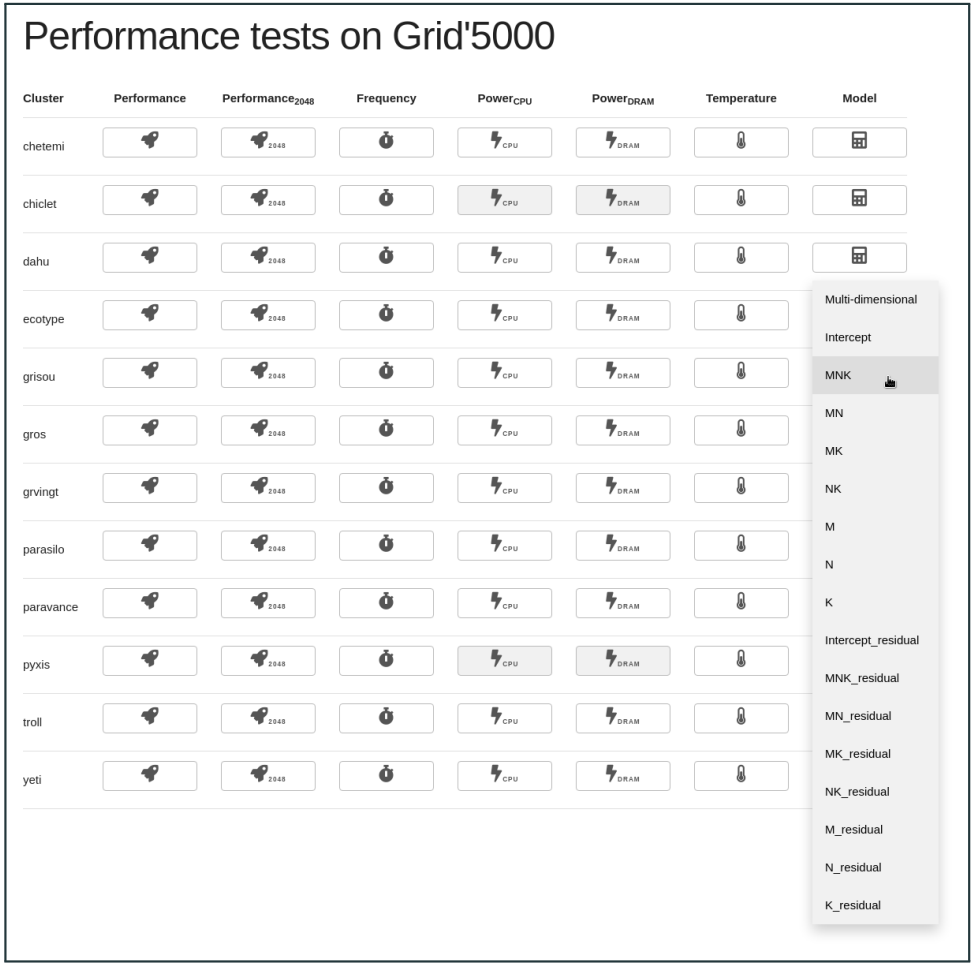
Detected events

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

Performance tests: wraping up

Multi-variable test also implemented

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



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