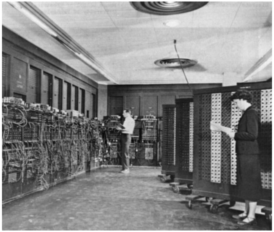
High Performance Computing: Towards Better Performance Predictions and Experiments

Tom Cornebize

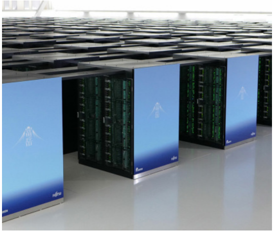
2 June 2021, PhD defense

No science without computing

Arithmomètre (1851)



ENIAC (1945)



Fugaku (2021)

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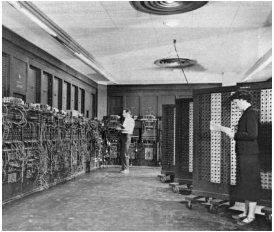
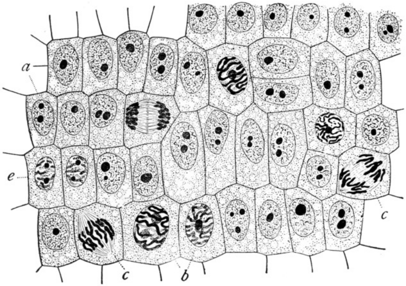


ENIAC (1945)

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)

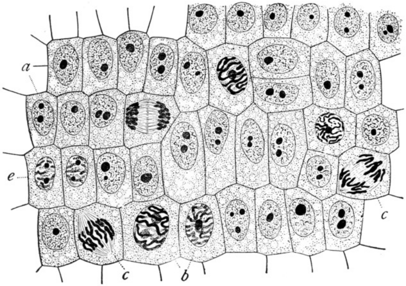


Similar to natural sciences

Complexity $\Rightarrow$ Variability and Opacity

$\Rightarrow$ No perfect model

$\Rightarrow$ Need for experiments



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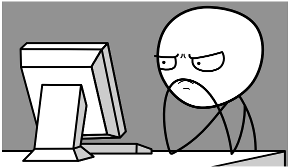
Empirical studies can be carried in reality or in simulation

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



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Context

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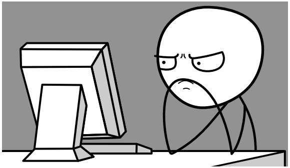

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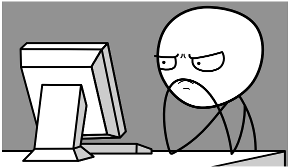

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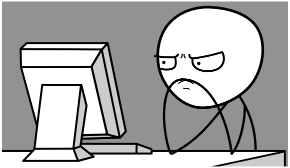

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Holy Grail: Predictive Simulation on a “Laptop”

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
- Performance tests, to detect eventual platform changes

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Performance prediction through simulation

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?

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- Communications are faked, good fluid network models
- Performance model for the target platform

Sim(Em)ulation: The SMPI Approach

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

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- Computations and communication overlap (custom collectives)
- More representative of some HPC applications
- Well established, used for the Top500

Quick word on HPL

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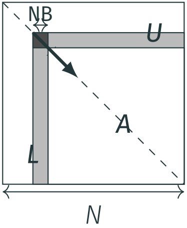

Allocate and initialize A
for $k = N$ ***to*** 0 ***step*** NB **do**
    Allocate the panel
    Factor the panel
    Broadcast the panel
    Update the sub-matrix

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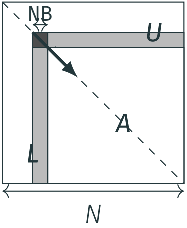

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- Block size
- Broadcast algorithm
- etc.

Hundreds of combinations

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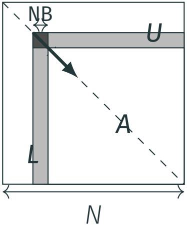

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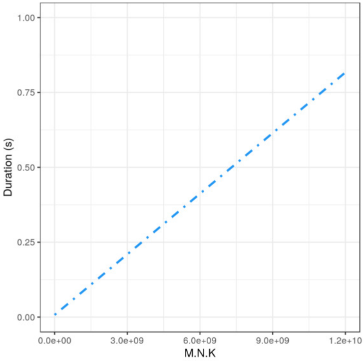
Contribution: Skip the expensive computations (mostly `dgemm`) and replace them by performance models

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



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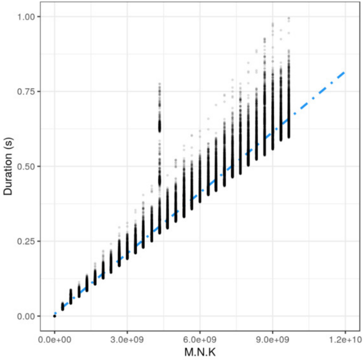
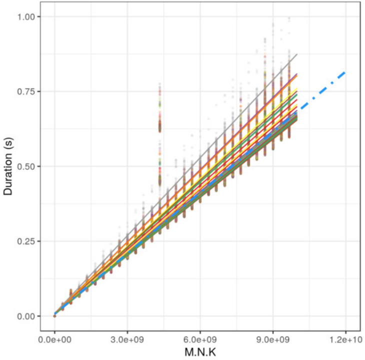


$$\texttt{dgemm}_i(M, N, K) = \underbrace{\alpha_i.M.N.K}_{\text{per host}}$$

Different color $\Rightarrow$ different host



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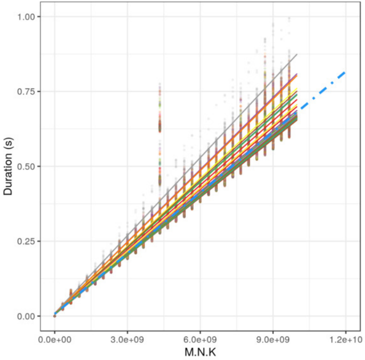
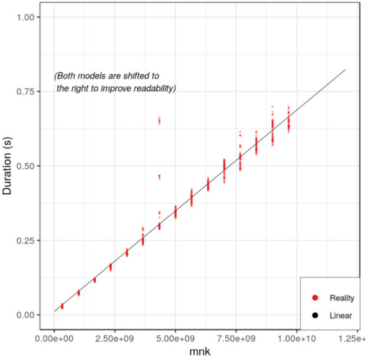


For a particular host



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

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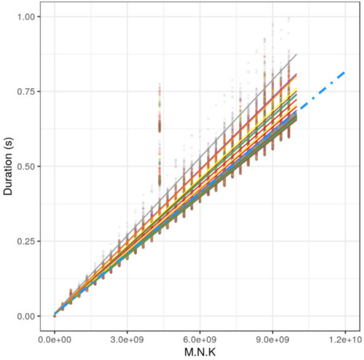

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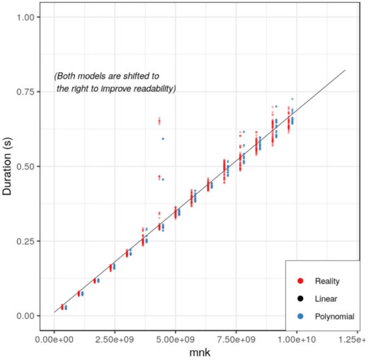

Modeling Commputations

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

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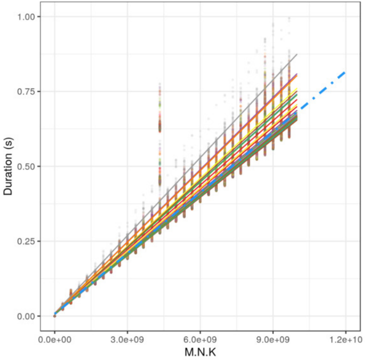

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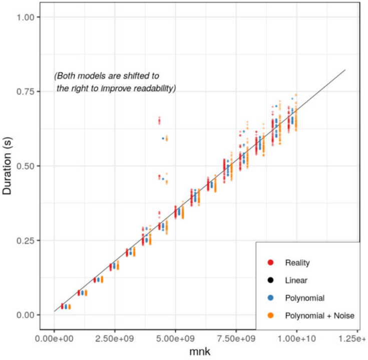

Hand-crafted non-blocking collective operations intertwinned with computations

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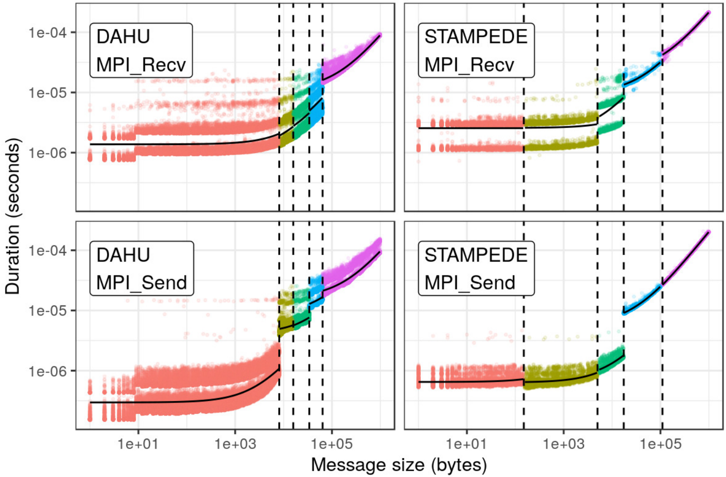
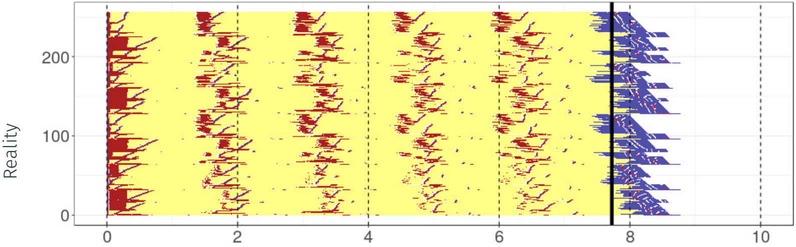


Validating the predictions

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



Internal behavior of the application

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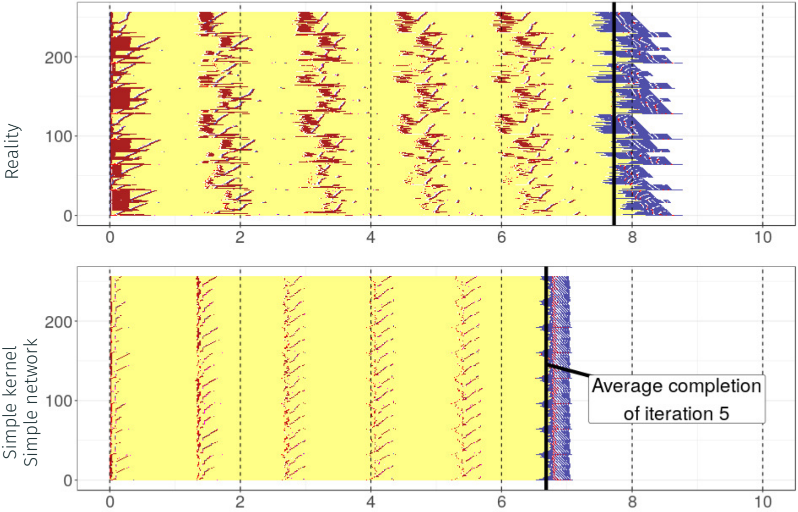

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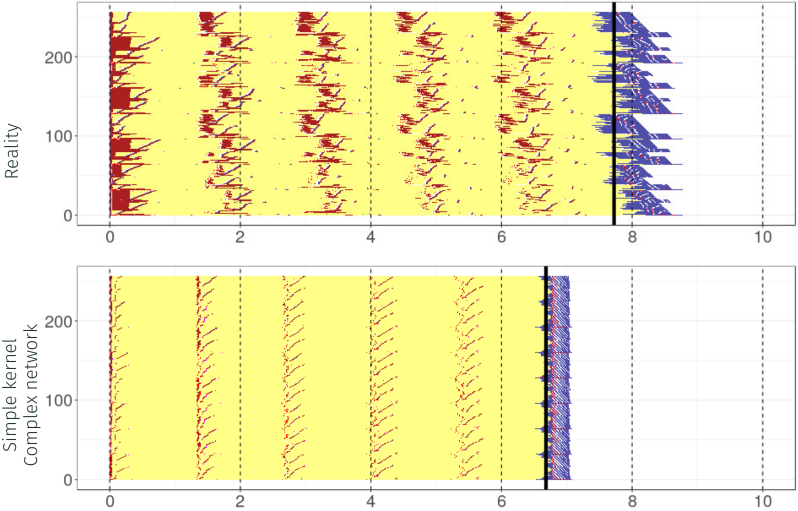

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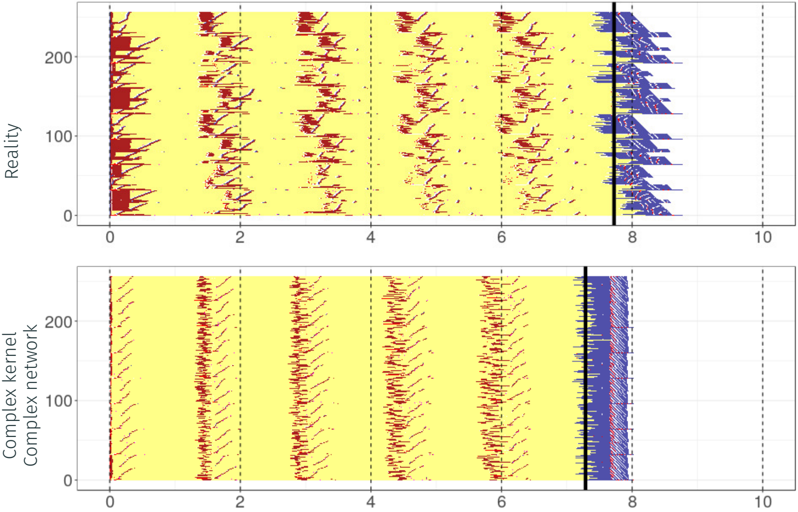
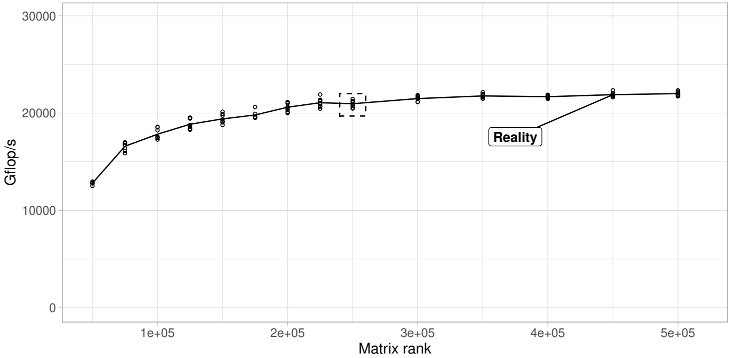


Now the complete run, with 1024 MPI ranks



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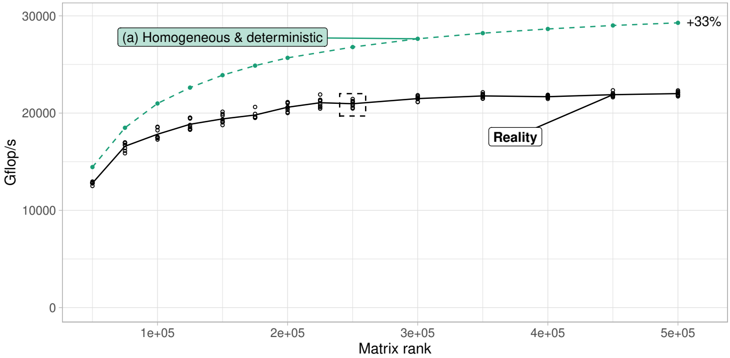

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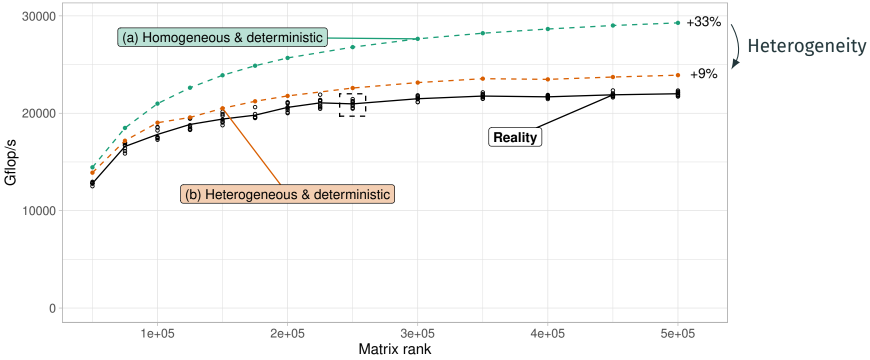

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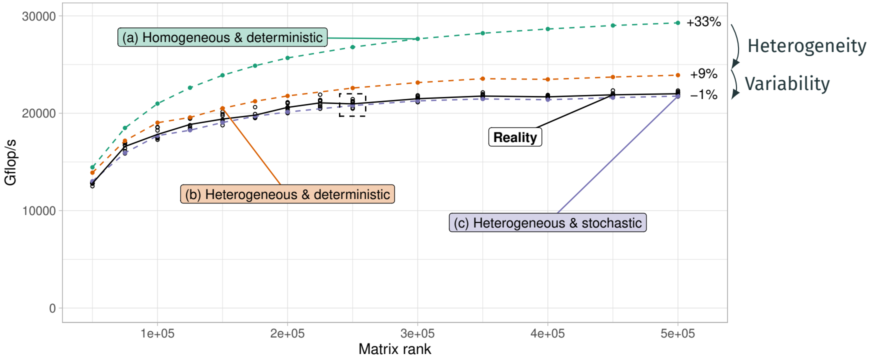

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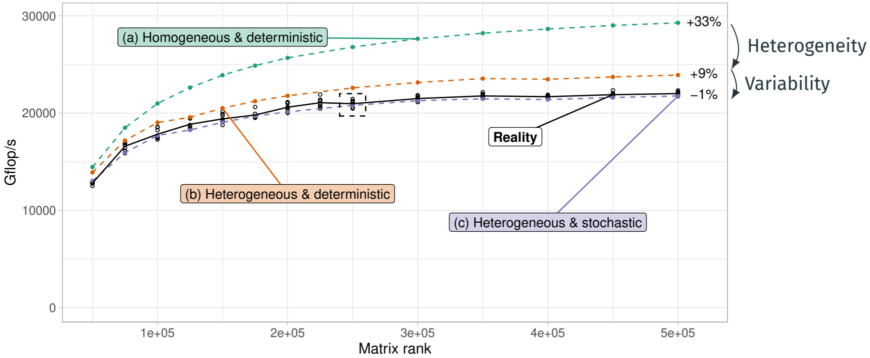
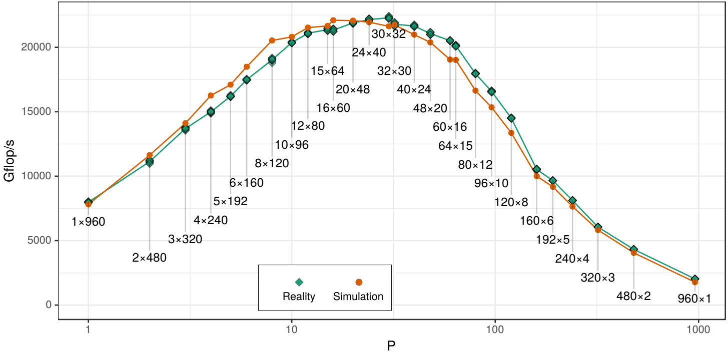


Take-Away Message: accurate prediction

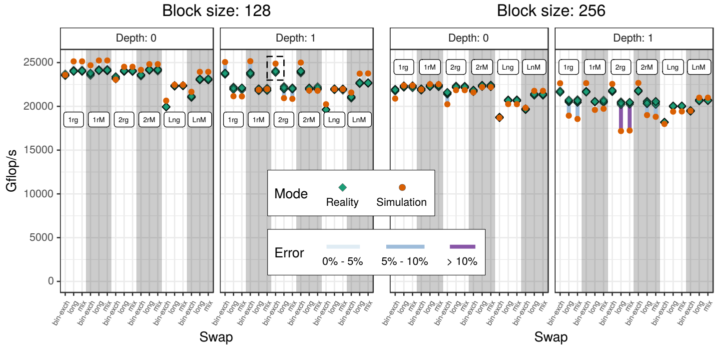
Modeling both spatial and temporal computation variability is essential

Influence of the geometry

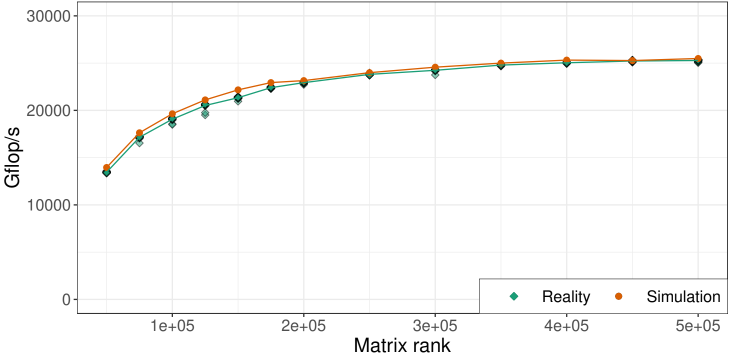
$P \times Q$ MPI processes, organized in a 2D grid



Tested the 72 combinations of the remaining parameters



Influence of a platform change



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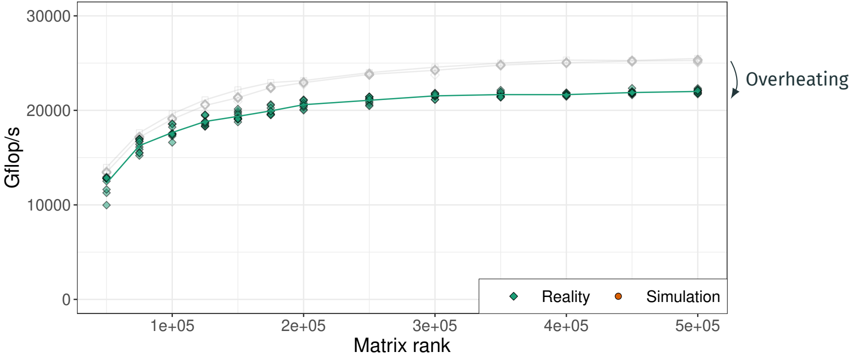
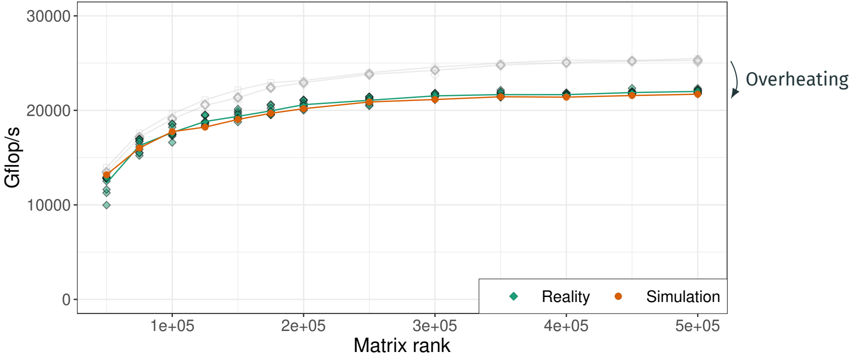


On four nodes, the cooling system malfunctionned for several weeks



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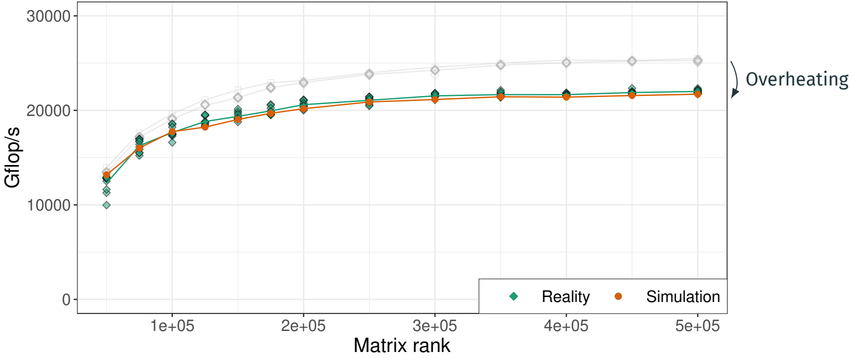

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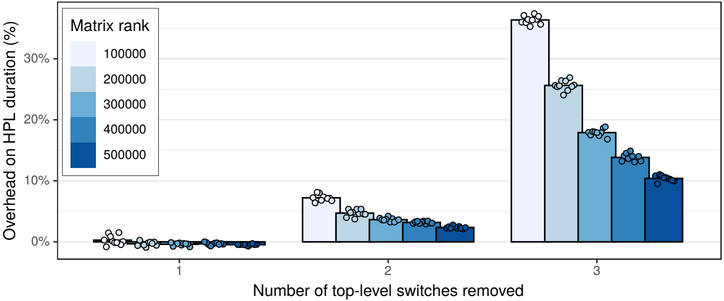
Take-Away Message: Re-measuring `dgemm` durations to generate a new model was enough to account for the platform change

What if the network topology of my cluster was different?



Use case: sensibility analysis

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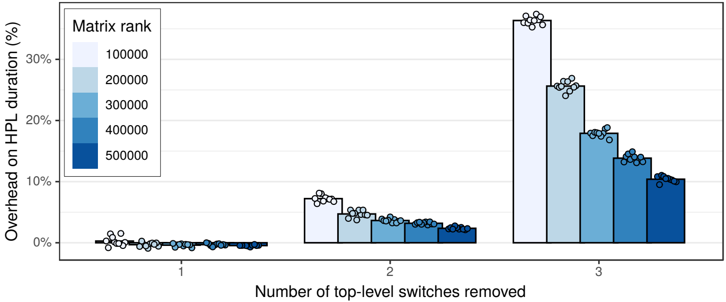

Faithful surrogate ⇒ Empirical studies of hypothetical platforms

⇒ Extrapolation of existing platforms

⇒ 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)

Experimental biases when measuring `dgemm` or MPI durations

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

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Parenthesis: on the difficulties of experimentation

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Bias may be desirable in some situations

Performance tests

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

454 nodes (792 CPU) from 12 clusters

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For each CPU, collect:

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

Regular measures

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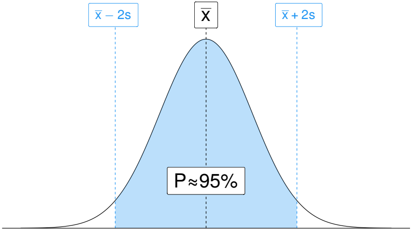
If the platform did not change, then each parameter is normally distributed (thanks to CLT)

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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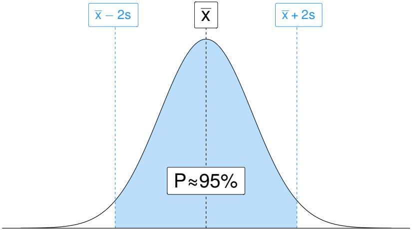

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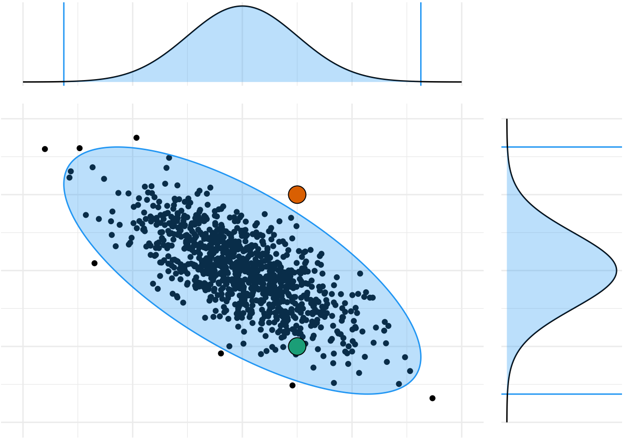
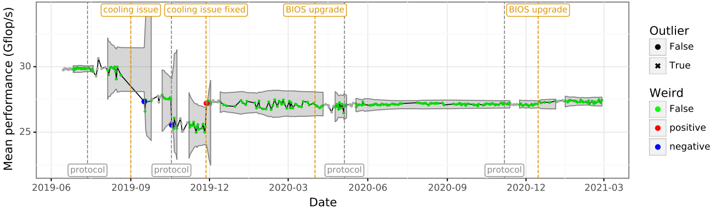
Note: using the F distribution instead of the normal distribution (the true mean and standard deviation are unknown)

With several variables, use their covariance matrix

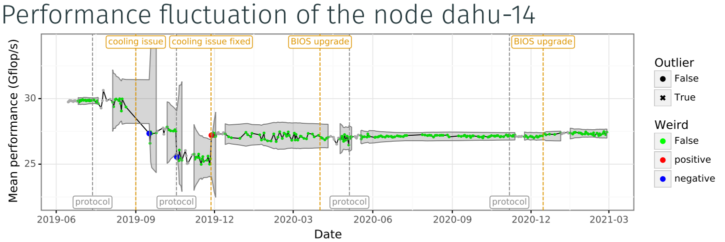
Example in dimension 2, with $\mathbb{P}(x_{n+1} \in \text{interval}) \approx 99.5\%$

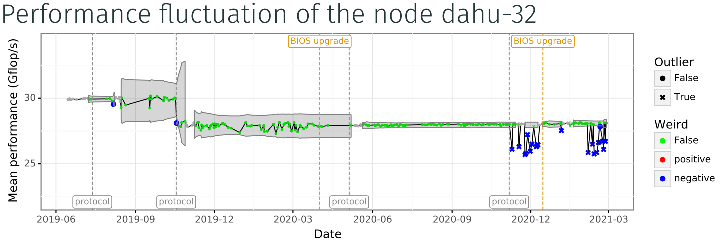


Performance fluctuation of the node dahu-14



Result: performance fluctuation





How to detect more subtle changes? Take several consecutive measures $x_{n+1}, \dots, x_{n+k}$, use their average and shrink the interval accordingly

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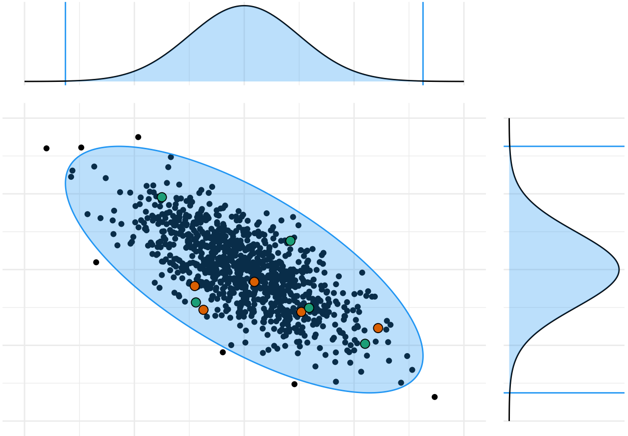
Example with 5 measures



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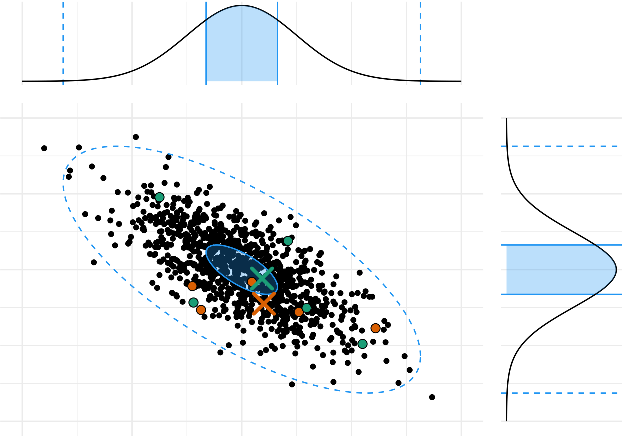
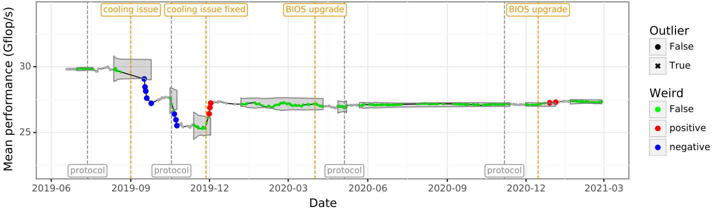
Example with 5 measures (averages represented by crosses)

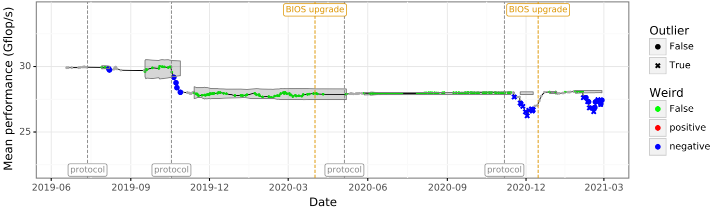


Result: performance fluctuation

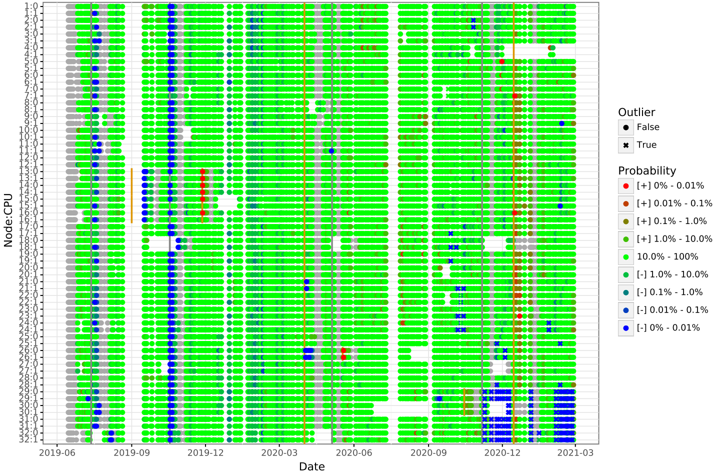
Performance fluctuation of the node dahu-14 (5-day window)



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



Overview of the performance on cluster dahu



Result: performance overview

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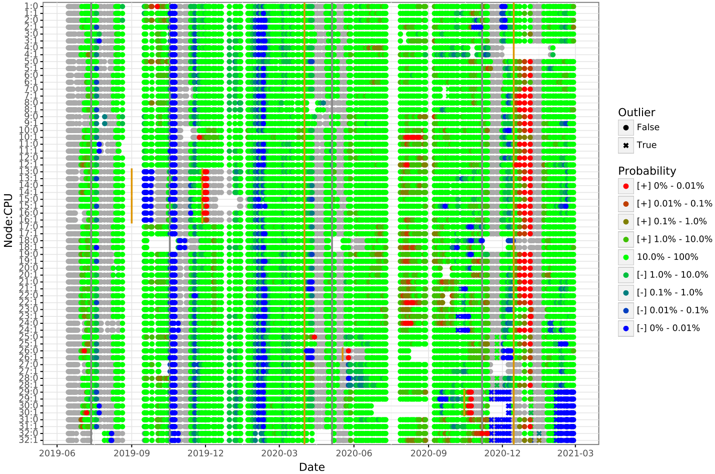
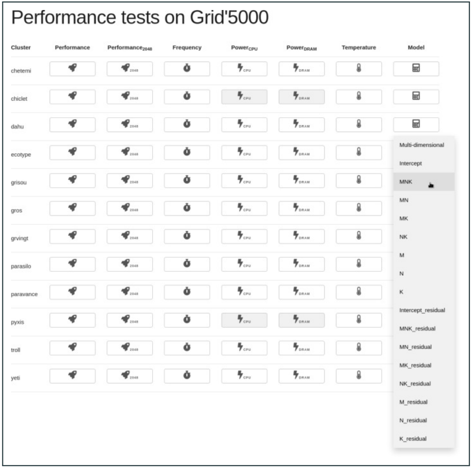


Multi-variable test also implemented, on all the model coefficients

Performance tests: wraping up

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

Results available at `https://cornebize.net/g5k_test`



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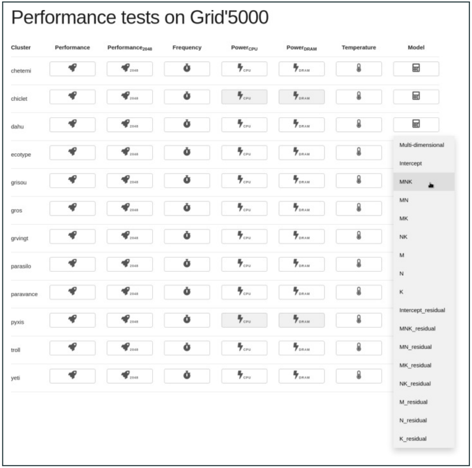

Detected events

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

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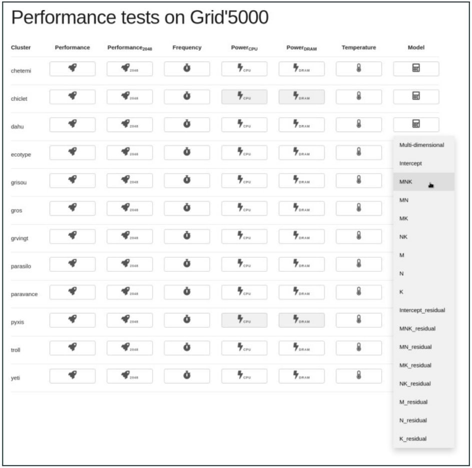

Detected events

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

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

$\Rightarrow$ Great help potential

Concluding thoughts

How to know if our predictions are faithful?

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

Can we trust our predictions?

How to know if our predictions are faithful?

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

How to know if our predictions are faithful?

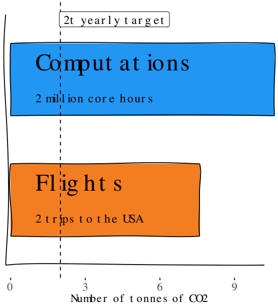
There is no *correctness proof*, a model can be validated only by trying to break it

$\Rightarrow$ 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?

About 18 t of CO2eq were emitted for this thesis



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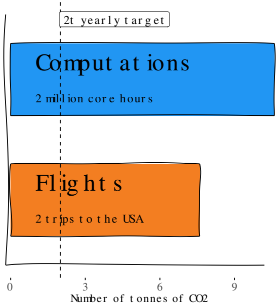

Do we really *need* to attend conferences in person?

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)
- Test less frequently (e.g. only once a week)
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Who should be responsible of tests?

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

Perspectives

Applying our approach on the whole life cycle of supercomputers:

Design Constructing the best machine for a given budget, using co-design

Scheduling Using predictions to improve the decisions of schedulers

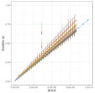
Development Debugging and improving software performance

Maintenance Ensuring that routine upgrades keep the performance as expected

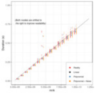
Modeling Commputations

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

Different color ⇒ different host

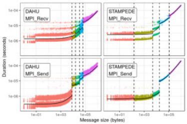


For a particular host



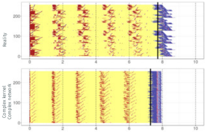
Modeling Communications

Hand-crafted non-blocking collective operations intertwinned with computations



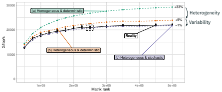
Internal behavior of the application

256 MPI ranks, interrupted after the 5th iteration



Influence of the problem size

Now the complete run, with 1024 MPI ranks

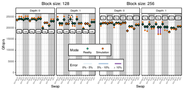


Take-Away Message: accurate prediction

Modeling both spatial and temporal computation variability is essential

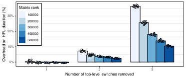
Influence of the other parameters

Tested the 72 combinations of the remaining parameters



Use case: sensibility analysis

What if the network topology of my cluster was different?

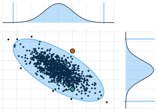


Faithful surrogate ⇒ Empirical studies of hypothetical platforms
⇒ Extrapolation of existing platforms
⇒ Accounting for spatial and temporal variability

Fluctuation interval for several variables

With several variables, use their covariance matrix

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



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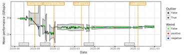

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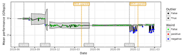

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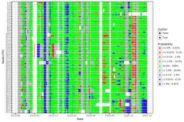

Thank you all!