

# HIGH PERFORMANCE COMPUTING: TOWARDS BETTER PERFORMANCE PREDICTIONS AND EXPERIMENTS

---

Tom Cornebize

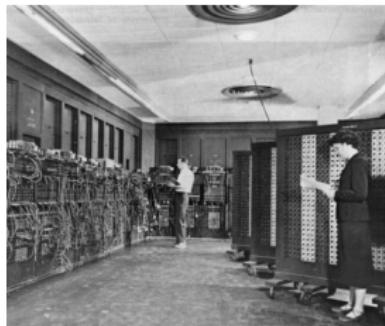
2 June 2021, PhD defense



# 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

- ⇒ Variability and Opacity
- ⇒ No perfect model
- ⇒ Need for [experiments](#)

# EXPERIMENTAL STUDY OF COMPUTER PERFORMANCE

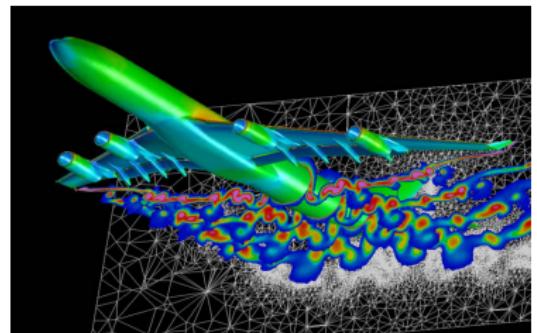


Similar to natural sciences

Complexity

- ⇒ Variability and Opacity
- ⇒ No perfect model
- ⇒ Need for experiments

Empirical studies can be carried in [reality](#) or in [simulation](#)



## 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?

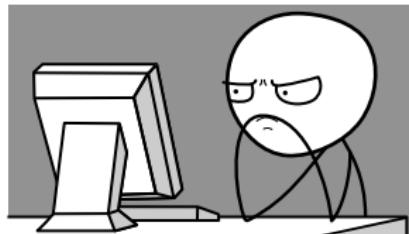
## Typical Performance Evaluation Questions (Given my application and a supercomputer)



- 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?!?

## 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
- Demonstrate it is possible to **predict faithfully** the behavior of complex parallel applications
- 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
- Demonstrate it is possible to **predict faithfully** the behavior of complex parallel applications
- 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
- Demonstrate it is possible to **predict faithfully** the behavior of complex parallel applications
- 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



- C/C++/F77/F90 codes run [unmodified out of the box](#)
- Simply replace mpicc/mpirun by smpicc/smpirun





Full reimplementation of MPI on top of 

- C/C++/F77/F90 codes run **unmodified out of the box**
- Simply replace mpicc/mpirun by smpicc/smpirun

Emulation: how?



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



Full reimplementation of MPI on top of 

- C/C++/F77/F90 codes run **unmodified out of the box**
- Simply replace mpicc/mpirun by smpicc/smpirun

Emulation: how?



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

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

## QUICK WORD ON HPL

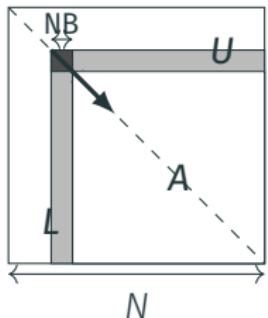


- Computations and communication overlap (custom collectives)
- More representative of some HPC applications
- Well established, used for the Top500

# QUICK WORD ON HPL



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

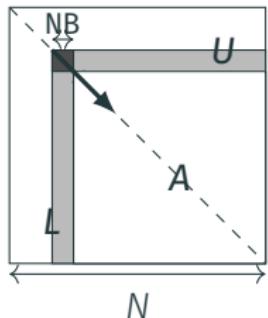


```
Allocate and initialize A  
for  $k = N$  to 0 step NB do  
    Allocate the panel  
    Factor the panel  
    Broadcast the panel  
    Update the sub-matrix
```

# QUICK WORD ON HPL



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



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

## Tuning parameters

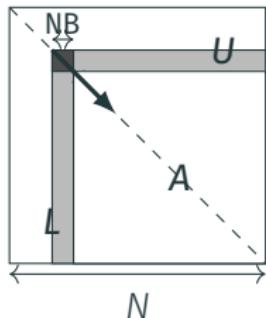
- Process grid
- Block size
- Broadcast algorithm
- etc.

Hundreds of combinations

# QUICK WORD ON HPL



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



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

## Tuning parameters

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

Hundreds of combinations

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

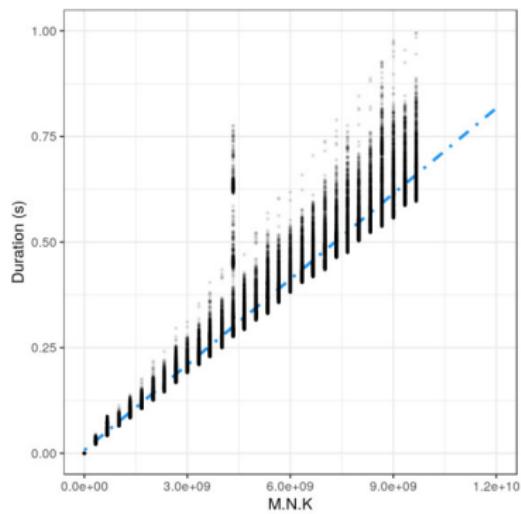
# MODELING COMPUTATIONS

$$\text{dgemm } (M, N, K) = \alpha \cdot M \cdot N \cdot K$$



# MODELING COMPUTATIONS

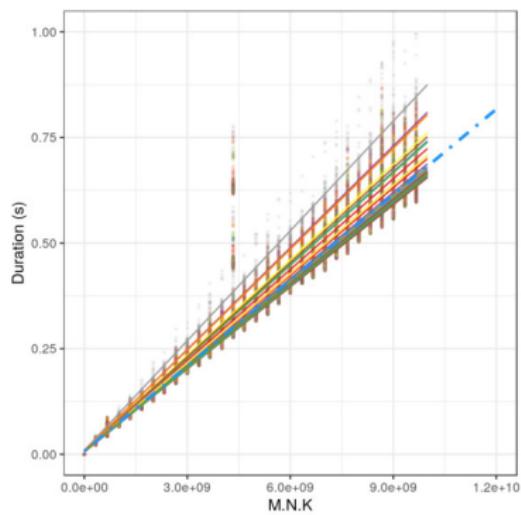
$$\text{dgemm } (M, N, K) = \alpha \cdot M \cdot N \cdot K$$



# MODELING COMPUTATIONS

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

Different color  $\Rightarrow$  different host



# MODELING COMPUTATIONS

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

Different color  $\Rightarrow$  different host



For a particular host



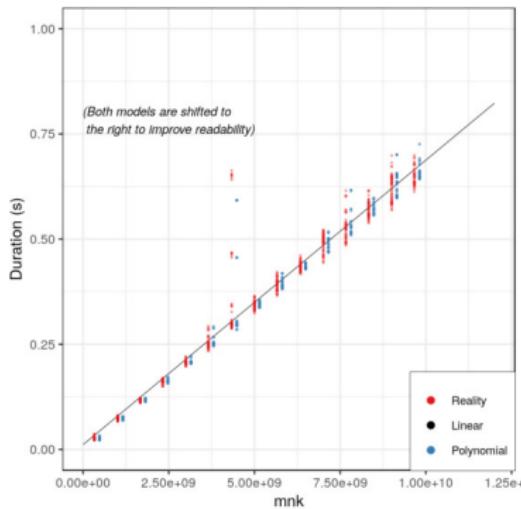
# MODELING COMPUTATIONS

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

Different color  $\Rightarrow$  different host



For a particular host



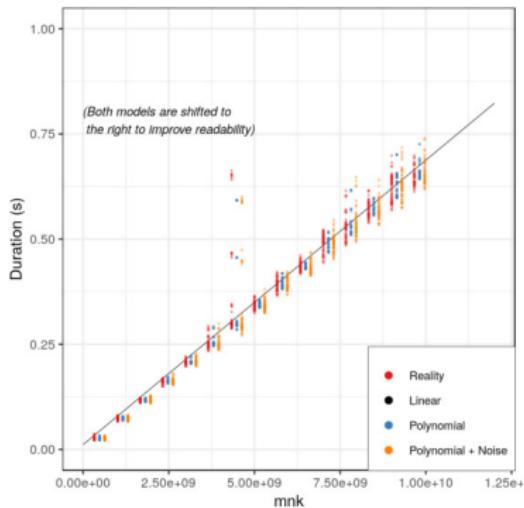
# MODELING COMPUTATIONS

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

Different color  $\Rightarrow$  different host



For a particular host



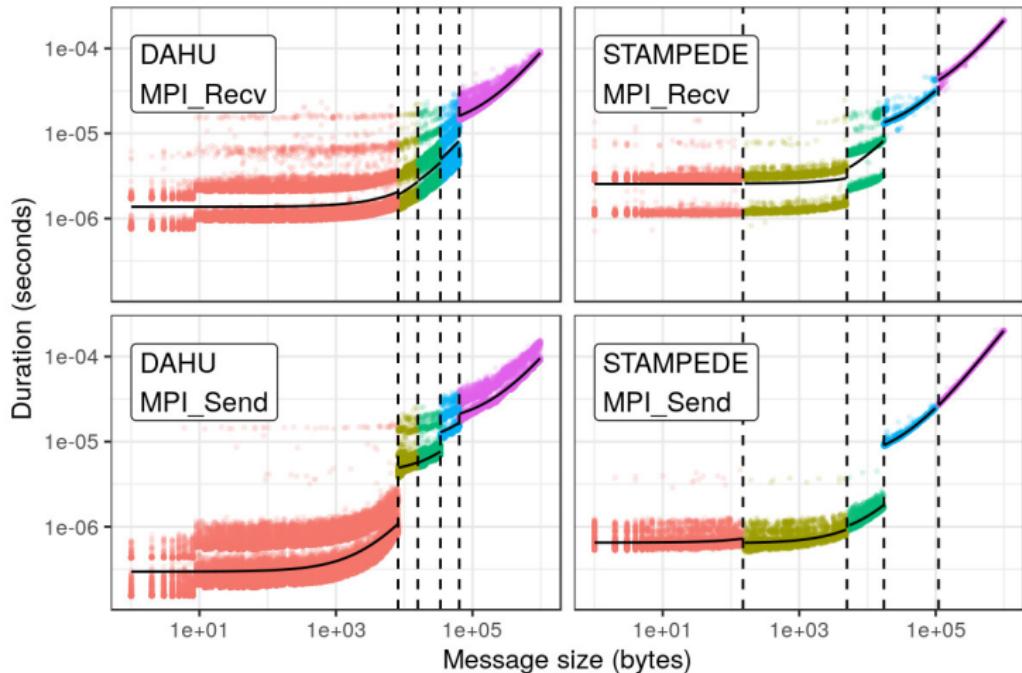
## MODELING COMMUNICATIONS

---

Hand-crafted non-blocking collective operations intertwined with computations

# MODELING COMMUNICATIONS

Hand-crafted non-blocking collective operations intertwined with computations



## VALIDATING THE PREDICTIONS

---

# INTERNAL BEHAVIOR OF THE APPLICATION

256 MPI processes, interrupted after the 5<sup>th</sup> iteration



# INTERNAL BEHAVIOR OF THE APPLICATION

256 MPI processes, interrupted after the 5<sup>th</sup> iteration



# INTERNAL BEHAVIOR OF THE APPLICATION

256 MPI processes, interrupted after the 5<sup>th</sup> iteration



# INTERNAL BEHAVIOR OF THE APPLICATION

256 MPI processes, interrupted after the 5<sup>th</sup> iteration



# INFLUENCE OF THE PROBLEM SIZE

Now the complete run, with 1024 MPI processes



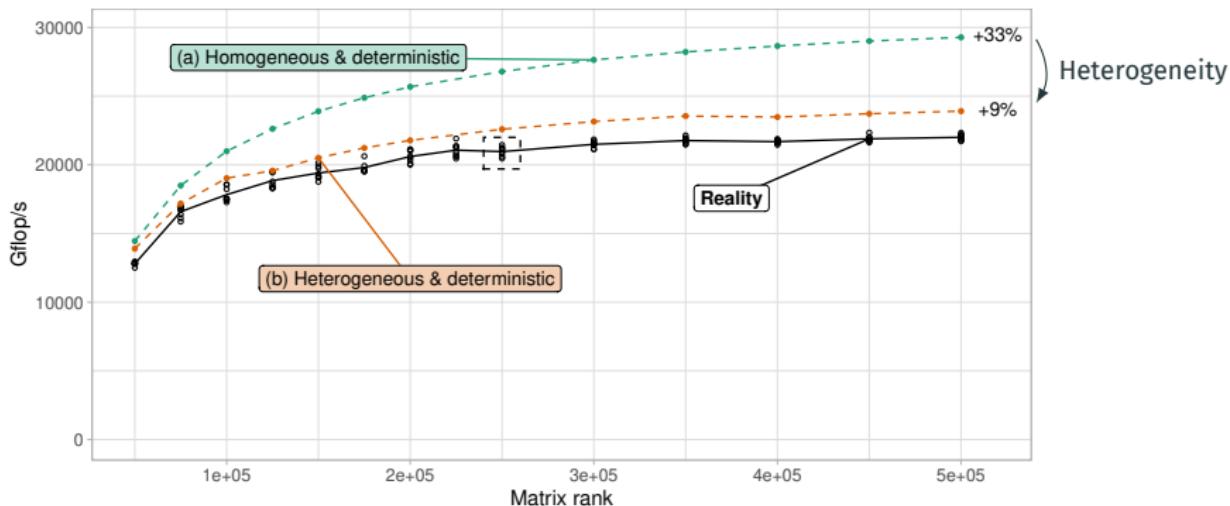
# INFLUENCE OF THE PROBLEM SIZE

Now the complete run, with 1024 MPI processes



# INFLUENCE OF THE PROBLEM SIZE

Now the complete run, with 1024 MPI processes



# INFLUENCE OF THE PROBLEM SIZE

Now the complete run, with 1024 MPI processes



# INFLUENCE OF THE PROBLEM SIZE

Now the complete run, with 1024 MPI processes



Take-Away Message: accurate prediction

Modeling both spatial and temporal computation variability is essential

# INFLUENCE OF THE GEOMETRY

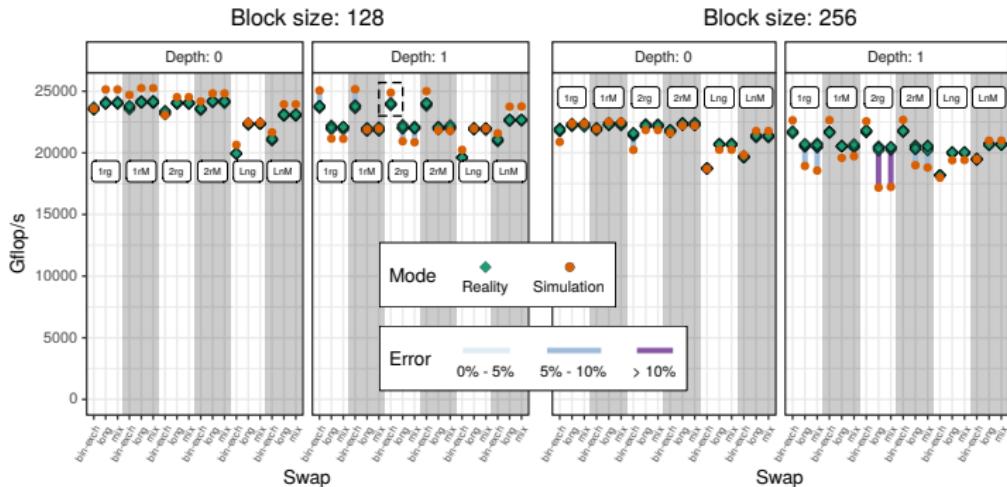
$P \times Q$  MPI processes, organized in a 2D grid



Perspective: geometry tuning in simulation

# INFLUENCE OF THE OTHER PARAMETERS

Tested the 72 combinations of the remaining parameters



Perspective: parameter tuning in simulation

# 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



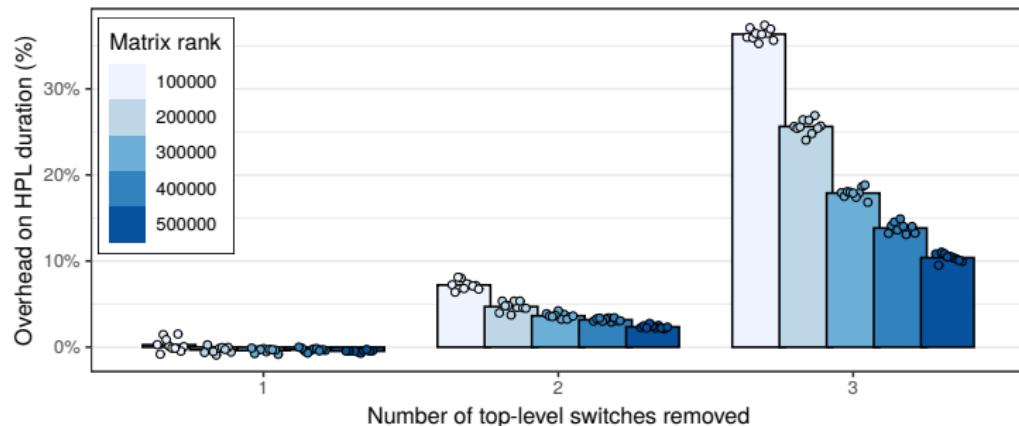
On four nodes, the cooling system malfunctionned for several weeks

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

## USE CASE: SENSIBILITY ANALYSIS

What if the network topology of my cluster was different?

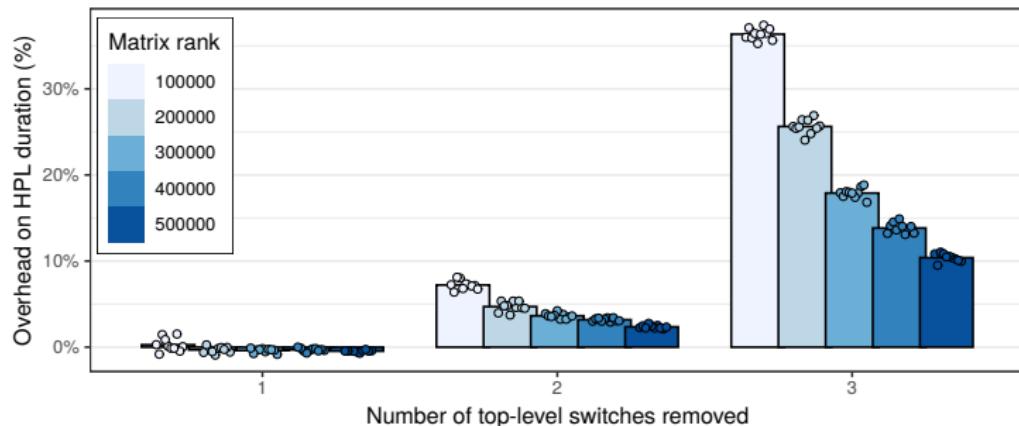
Study: take a 2-level fat tree with 4 top-level switches,  
remove them one by one



## USE CASE: SENSIBILITY ANALYSIS

What if the network topology of my cluster was different?

Study: take a 2-level fat tree with 4 top-level switches,  
remove them one by one



Faithful surrogate  $\Rightarrow$  Empirical studies of hypothetical platforms  
 $\Rightarrow$  Extrapolation of existing platforms

Goal: performance prediction ✓

Goal: performance prediction ✓

Main difficulties:

- Experimentation/calibration
- Platform changes (e.g., the cooling issue)

## ON THE DIFFICULTIES OF EXPERIMENTATION

---

Experimental biases when measuring `dgemm` or MPI durations

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

## 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  
~ 10% systematic performance change

# 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  
~ 10% systematic performance change
- Interferences between computations and communications  
~ 50% performance change in extreme configurations

# 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  
  ~ 10% systematic performance change
- Interferences between computations and communications  
  ~ 50% performance change in extreme configurations
- Content of the matrices used by `dgemm`  
  ~ 5% systematic performance change

# 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  
  ~ 10% systematic performance change
- Interferences between computations and communications  
  ~ 50% performance change in extreme configurations
- Content of the matrices used by `dgemm`  
  ~ 5% systematic performance change

## Take-Away Message:

- These biases could only be identified with a solid experimental methodology with heavy use of randomization
- Bias may be desirable, to increase prediction accuracy

## CONTINUOUS PLATFORM MODELING

---

## REGULAR MEASURES

---

On a near-daily basis, run the `dgemm` calibration code on  
454 nodes (792 CPU) from 12 clusters, ~ 30 min. jobs



## REGULAR MEASURES



On a near-daily basis, run the `dgemm` calibration code on  
454 nodes (792 CPU) from 12 clusters,  $\sim$  30 min. jobs

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,  $\sim$  30 min. jobs

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  
454 nodes (792 CPU) from 12 clusters,  $\sim$  30 min. jobs

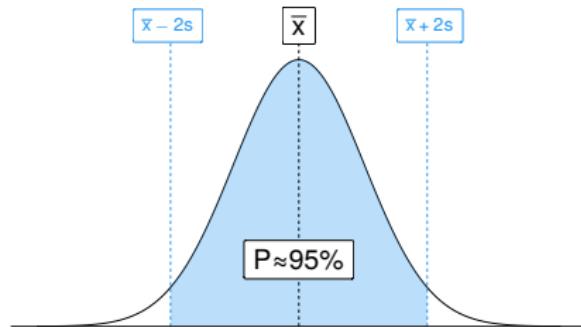
For each CPU, collect:

- 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

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

# FLUCTUATION INTERVAL

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



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

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

# FLUCTUATION INTERVAL

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



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

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

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, use their [covariance matrix](#)

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



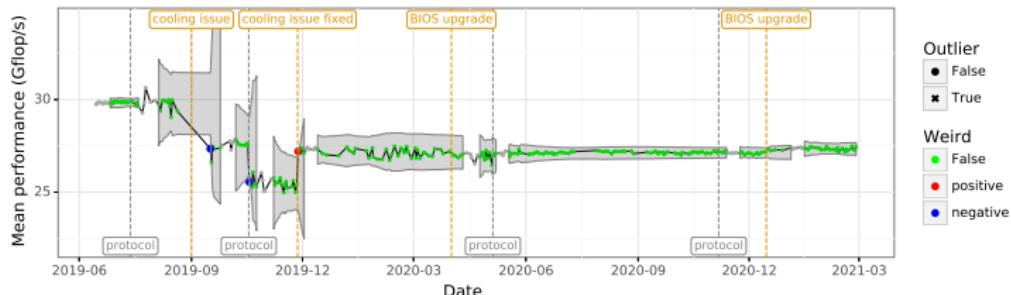
# RESULT: PERFORMANCE FLUCTUATION

## Performance fluctuation of the node dahu-14

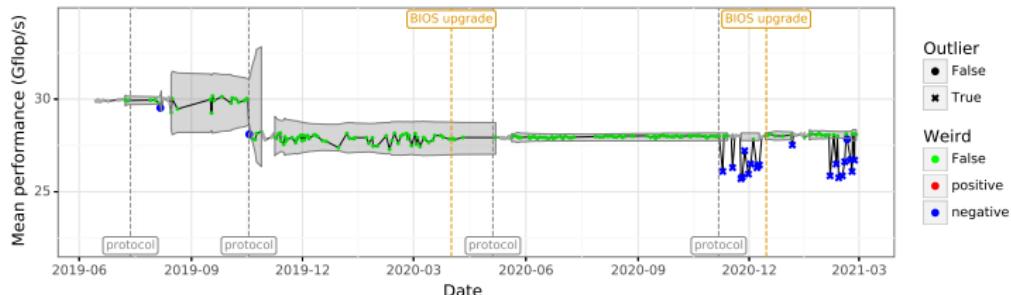


# RESULT: PERFORMANCE FLUCTUATION

## Performance fluctuation of the node dahu-14



## Performance fluctuation of the node dahu-32



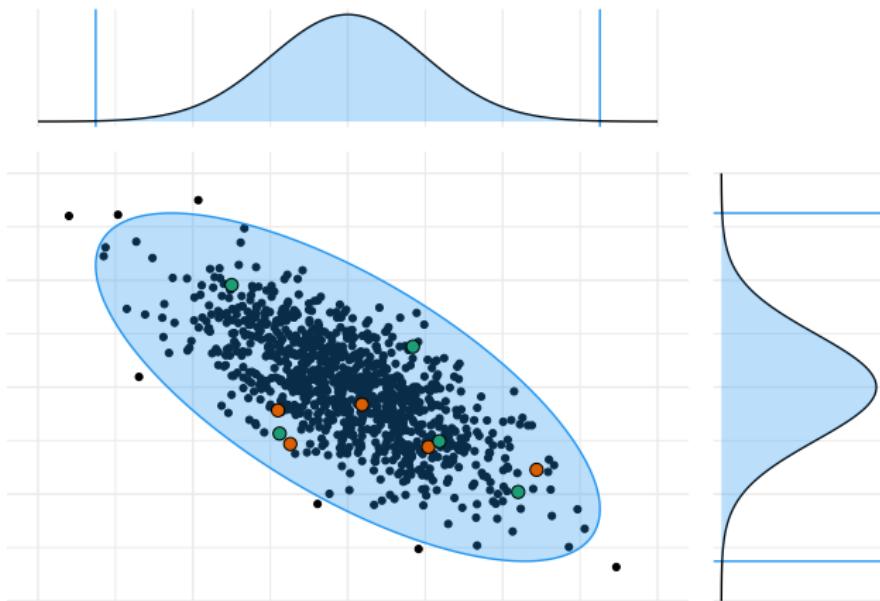
## FLUCTUATION INTERVAL FOR SEVERAL MEASURES

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

## FLUCTUATION INTERVAL FOR SEVERAL MEASURES

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

Example with 5 measures



## FLUCTUATION INTERVAL FOR SEVERAL MEASURES

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

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)



# 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, 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](https://cornebize.net/g5k_test)

Cluster	Performance	Performance <sub>2048</sub>	Frequency	Power <sub>CPU</sub>	Power <sub>DRAM</sub>	Temperature	Model
chetteri							
chiclet							
dehu							
ecotype							
grassu							
gras							
grvingt							
parasito							
panchine							
pynix							
troll							
yeti							

# PERFORMANCE TESTS: WRAPING UP

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

Results available at [https://cornebize.net/g5k\\_test](https://cornebize.net/g5k_test)

Cluster	Performance	Performance <sub>DMB</sub>	Frequency	Power <sub>CPU</sub>	Power <sub>DRAM</sub>	Temperature	Model
chetteri							
chiclet							
dehu							
ecotype							
grisou							
gross							
grivost							
parasito							
pantheon							
pynx							
troll							
yeti							

## Detected events

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

# PERFORMANCE TESTS: WRAPING UP

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

Results available at [https://cornebize.net/g5k\\_test](https://cornebize.net/g5k_test)

Cluster	Performance	Performance <sub>DMB</sub>	Frequency	Power <sub>CPU</sub>	Power <sub>DRAM</sub>	Temperature	Model
chetteri							
chiclet							
dehu							
ecotype							
grisou							
gross							
grivost							
parasilo							
pantheon							
pyxis							
troll							
yeti							

## 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

---

# CAN WE TRUST OUR PREDICTIONS?

---

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?

There is no *correctness proof*, a model can be validated only by  
[trying to break it](#)

⇒ Often broke the simulations during the last few years

# CAN WE TRUST OUR PREDICTIONS?

---

How to know if our predictions are faithful?

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

⇒ Often broke the simulations during the last few years

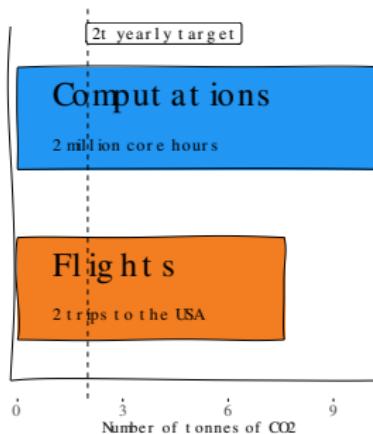
**Repeated** the whole study **from scratch** on a new cluster:



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

# THERE IS NO PLANET B

About 18t of CO<sub>2</sub>eq were emitted for this thesis



# THERE IS NO PLANET B

About 18t of CO<sub>2</sub>eq were emitted for this thesis



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

# WHY SO MANY COMPUTATIONS?

---

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

## How to reduce them?

- Change the experiment procedure (e.g. no full node reinstallation)
- Test less frequently (e.g. only once a week)
- Use a cheaper test (e.g. shorter warmup, less extensive coverage)

# WHY SO MANY COMPUTATIONS?

---

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

## How to reduce them?

- Change the experiment procedure (e.g. no full node reinstallation)
- Test less frequently (e.g. only once a week)
- Use a cheaper test (e.g. shorter warmup, less extensive coverage)

## Who should be responsible of tests?

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

Applying our approach on the whole life cycle of supercomputers:

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

**Development** Debugging and improving software performance

**Maintenance** Ensuring that routine upgrades keep the performance  
as expected



Thank you all!