

# HIGH PERFORMANCE COMPUTING: TOWARDS BETTER PERFORMANCE PREDICTIONS AND EXPERIMENTS

---

Tom Cornebize

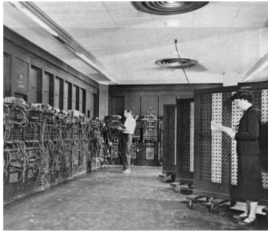
2 June 2021, PhD defense



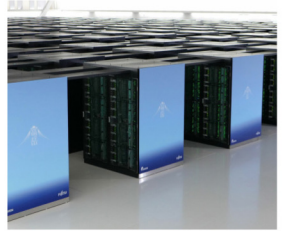
# NO SCIENCE WITHOUT COMPUTING



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

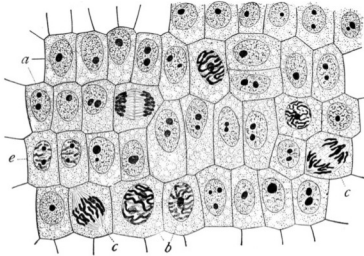
Complexity

⇒ Variability and Opacity

⇒ No perfect model

⇒ Need for **experiments**

# EXPERIMENTAL STUDY OF COMPUTER PERFORMANCE



Similar to natural sciences

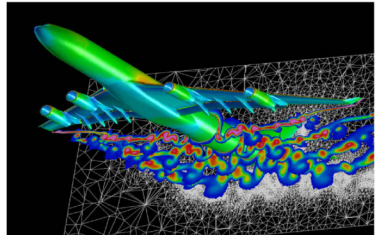
Complexity

⇒ 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)



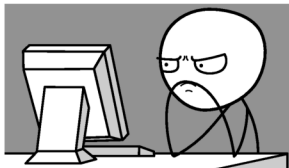
- **Before** running
  - How many nodes?
  - For how long?
  - Which parameters?

## 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)

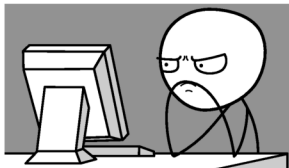


- **Before** running
  - How many nodes?
  - For how long?
  - Which parameters?
- **After** running
  - Performance as “expected”?
  - Problem in the app or the platform?

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  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?

- Application runs 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?**

- 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

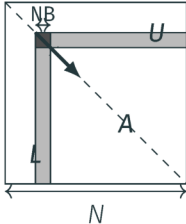


Allocate and initialize  $A$   
**for**  $k = N$  **to**  $0$  **step**  $NB$  **do**  
    Allocate the panel  
    Factor the panel  
    Broadcast the panel  
    Update the sub-matrix

# 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

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

