Capacity Planning of Supercomputers

Simulating MPI Applications at Scale

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Ensimag - Grenoble INP

Introduction

Top500

Sunway TaihuLight, China, #1
93 Pflops
Custom five level hierarchy
$40,950 \times 260$ cores

Tianhe-2, China, #2
34 Pflops
Fat tree
$32,000 \times 12$ cores $+ 48,000$ Xeon Phi

Piz Daint, Switzerland, #3
20 Pflops
Dragonfly
$5,272 \times (8$ cores $+ 1$ GPU$)$

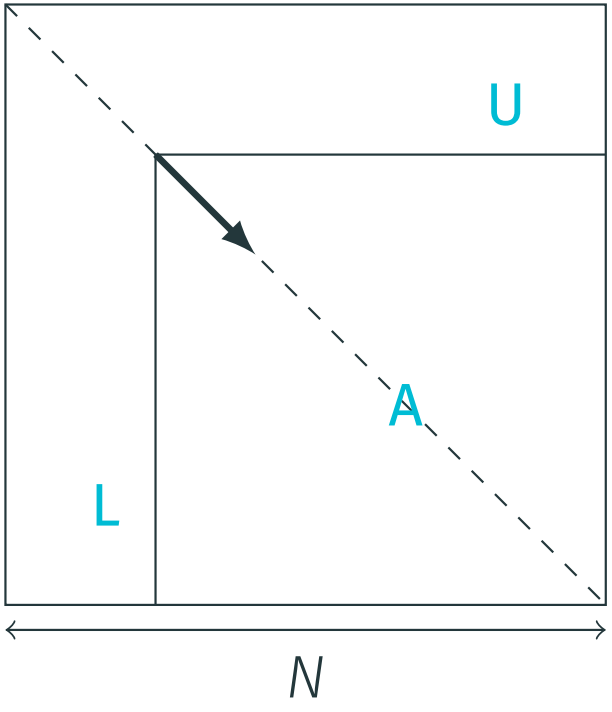
Stampede, United States, #20
5 Pflops
Fat tree
$6,400 \times (8$ cores $+ 1$ Xeon Phi$)$

High Performance LINPACK (HPL)

Benchmark used to establish the Top500

LU factorization, $A = L \times U$

Complexity: $\mathrm{flop}(N) = \frac{2}{3}N^3 + 2N^2 + O(N)$



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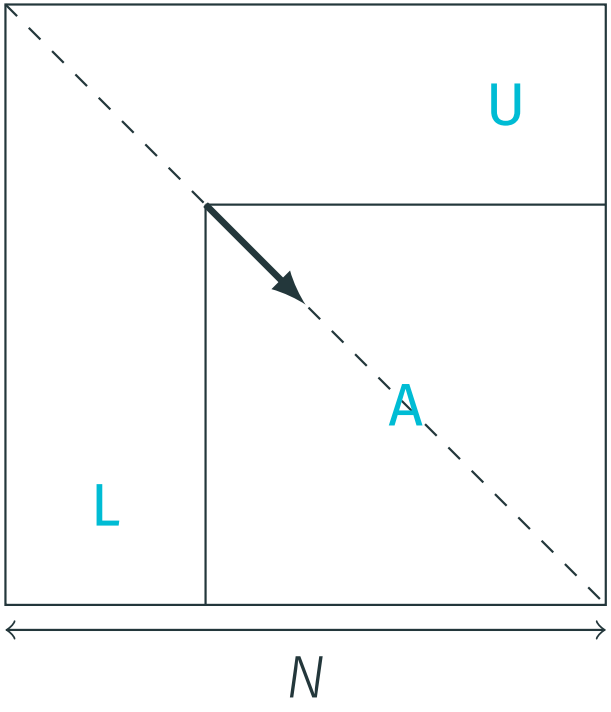

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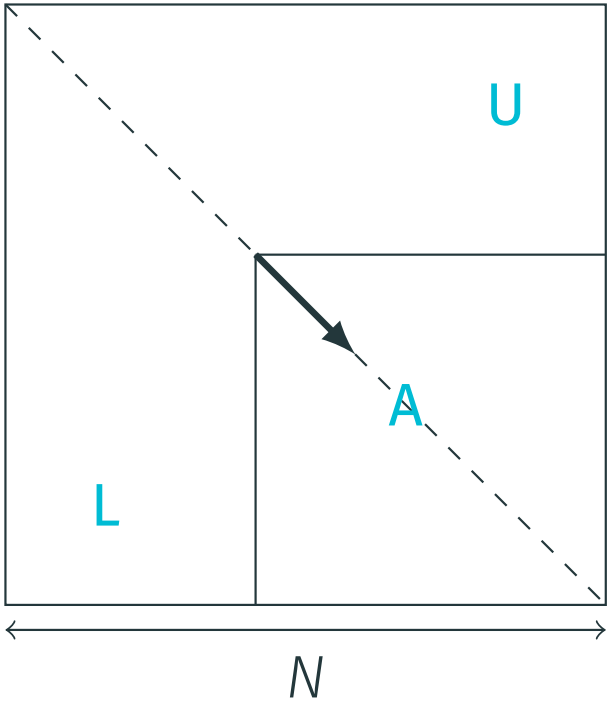

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Open questions in HPC

- Topology (torus, fat tree, dragonfly, etc.)
- Routing algorithm
- Scheduling (when? where?)
- Workload (job size, behavior)

Keywords: capacity planning, co-design

Simulation may help

Off-line

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- P5: MPI_Recv at t=0.872s
- P3: MPI_Wait at t=0.881s
- P7: MPI_Send at t=1.287s
- P5: MPI_Recv at t=1.568s
- P7: MPI_Send at t=2.221s
- P0: MPI_Recv at t=2.559s
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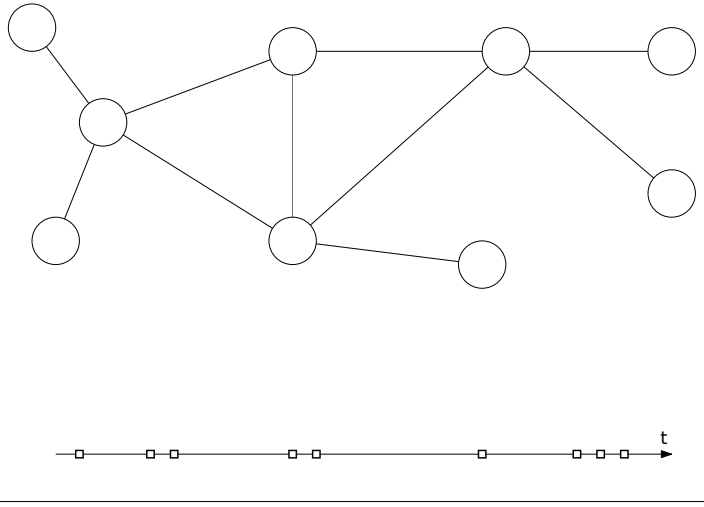

Simulation of HPC applications

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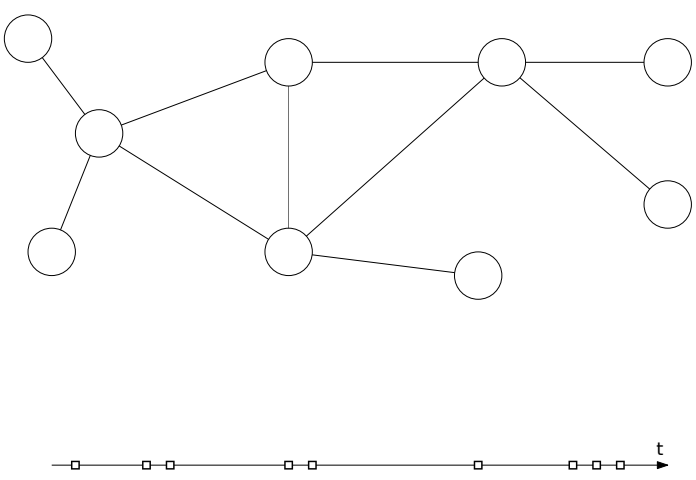

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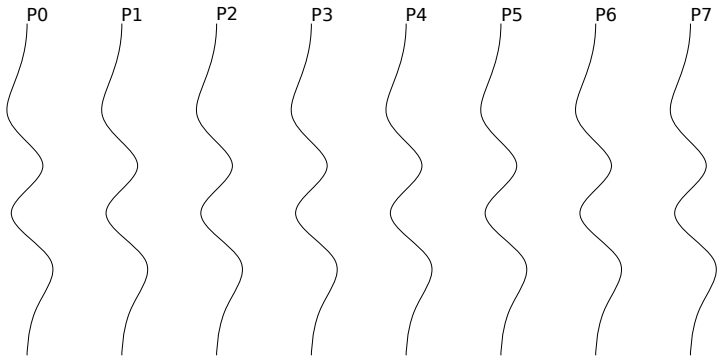

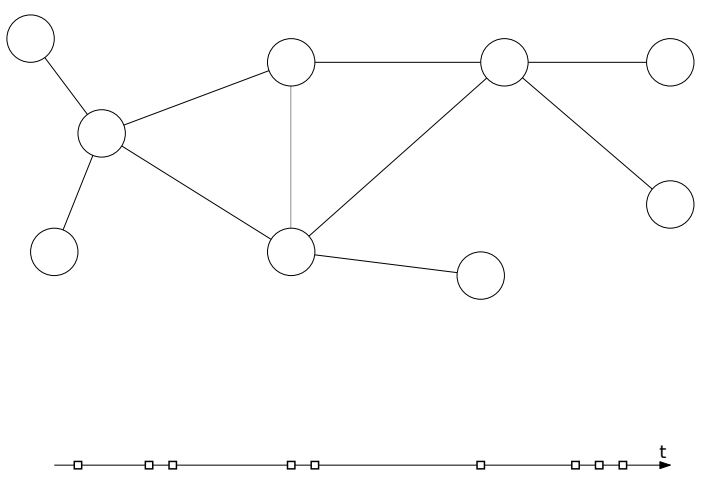

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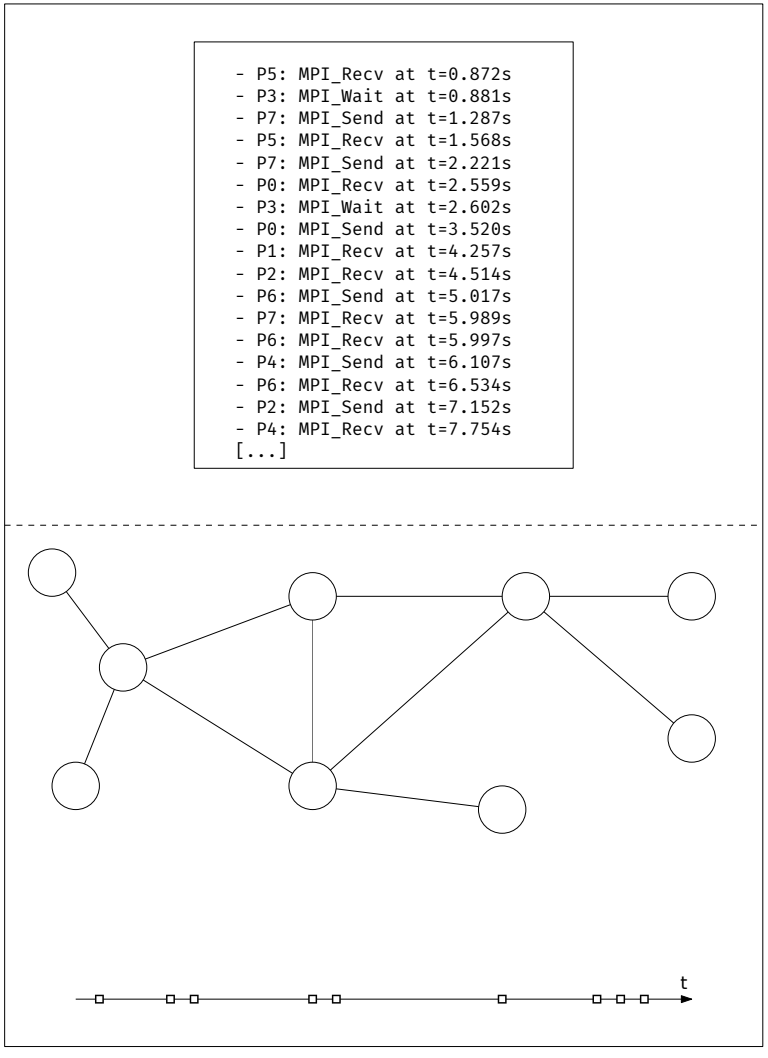

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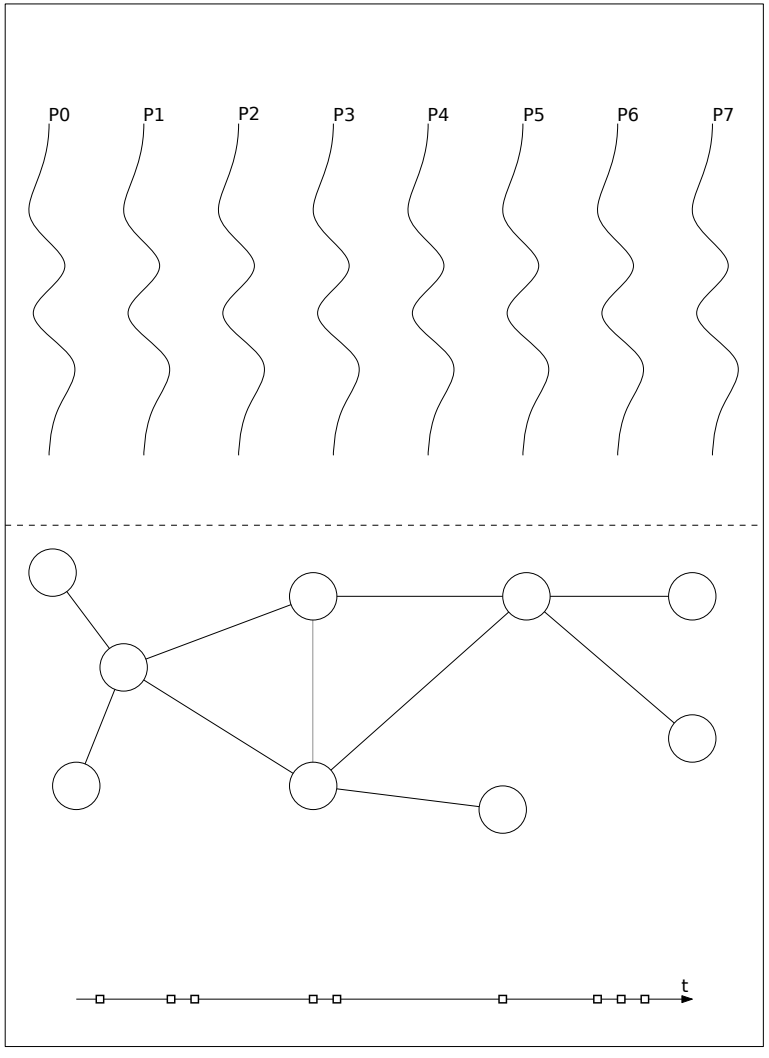

Simgrid: both approaches

Objective: simulation of Stampede's execution of HPL

Real execution:

- Matrix of size 3,875,000
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Requirement for the emulation of Stampede's execution:

- $\geq 3,875,000^2 \times 8$ bytes $\approx$ 120 terabytes of memory
- $\geq 6,006 \times 2$ hours $\approx$ 500 days

Very optimistic

Scalable HPL simulation

Methodology

Several optimizations. For each of them:

- Evaluate the (possible) loss of prediction accuracy
- Evaluate the (possible) gain of performance

Publicly available:

- Laboratory notebook
- Modified HPL
- Scripts
- Modifications to Simgrid (integrated in the main project)

Computation kernel sampling

`dgemm` and `dtrsm`

$\geq 90\%$ of the simulation time

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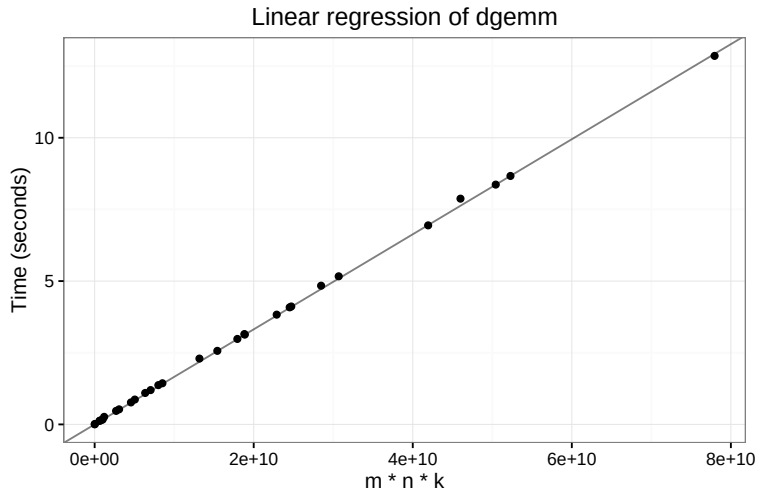

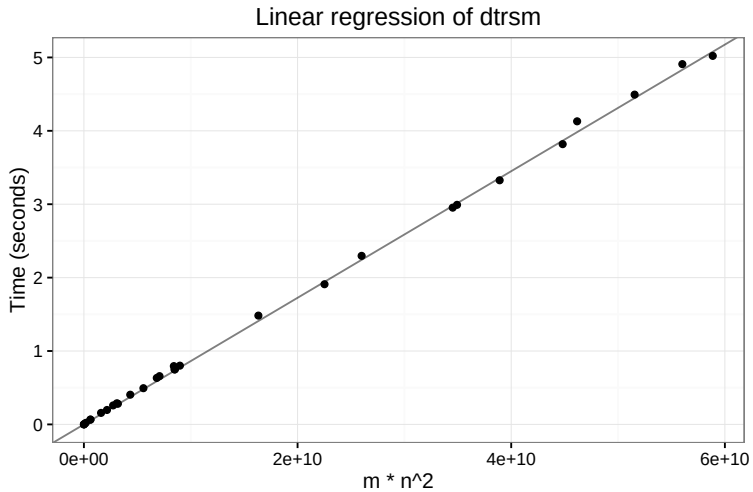

$$T_{dgemm}(M, N, K) = M \times N \times K \times 1.706348 \times 10^{-10}$$

$$T_{dtrsm}(M, N) = M \times N^2 \times 8.624970 \times 10^{-11}$$

Computation pruning

68% of the simulation time spent in HPL

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Culprits:

- Initialization and verification functions
- Other BLAS and HPL functions

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Solution: just skip them

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Reducing the memory consumption

Memory consumption still too large

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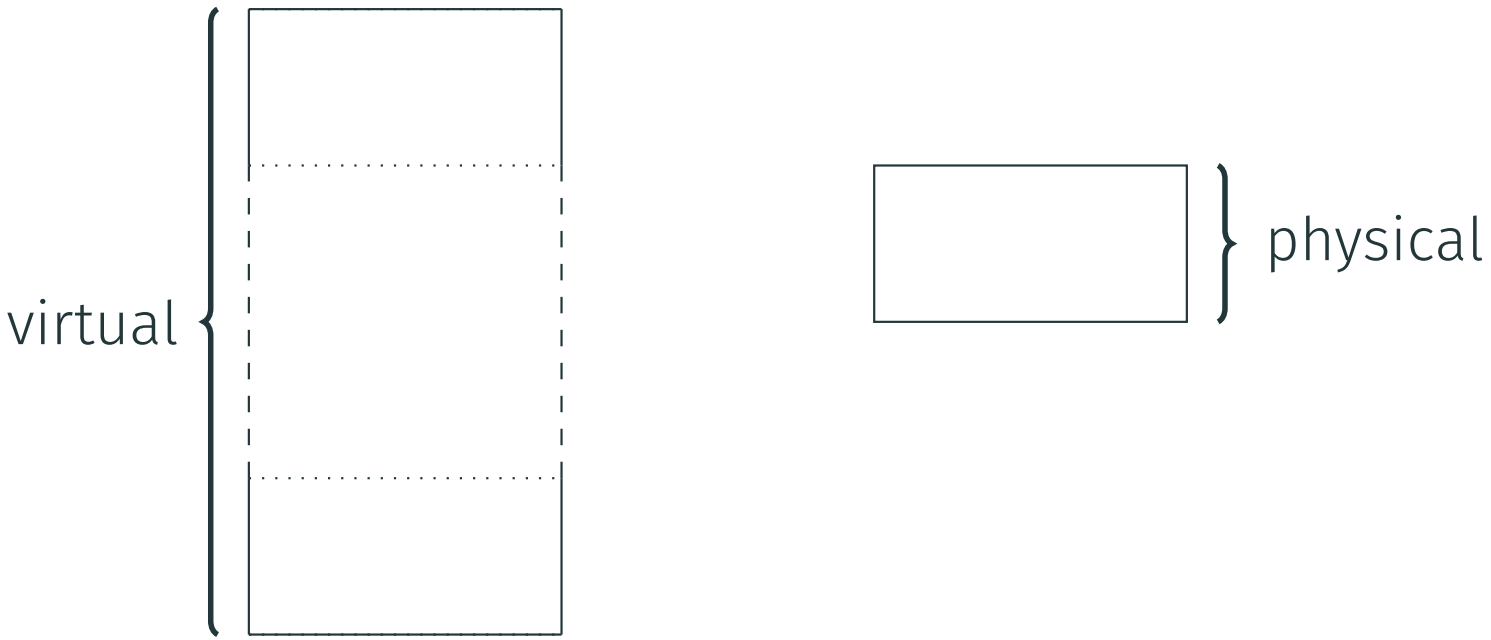

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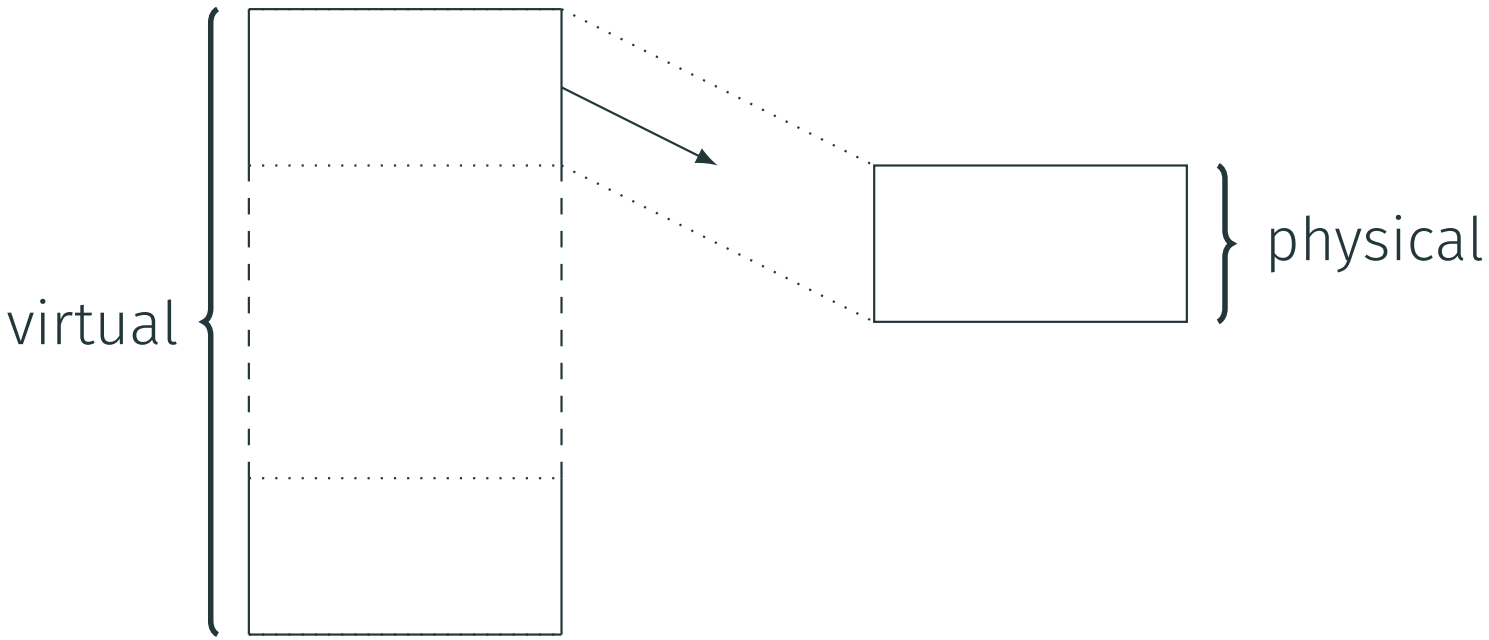

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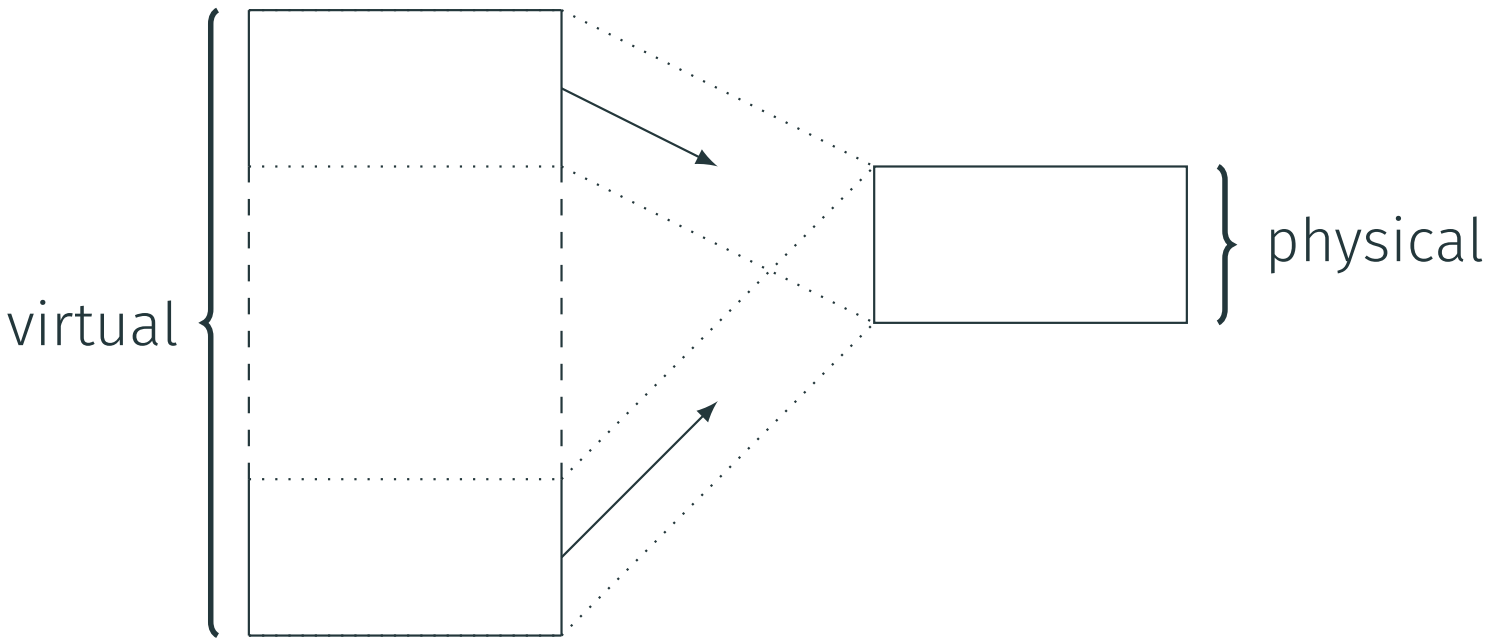

Problem: panel buffers

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Must remain contiguous

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#154

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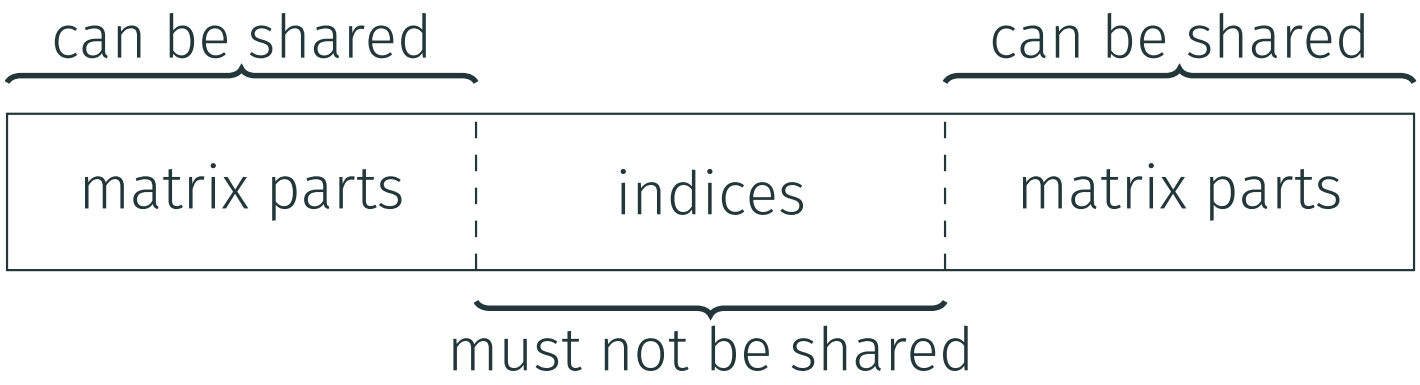

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Solution: `SMPI_PARTIAL_SHARED_MALLOC`

Arbitrary number of shared and private blocks.

Reusing the panel buffers

At each iteration, new allocation and deallocation by all processes

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Solution: reuse the buffers (sizes strictly decreasing)

Needs to be done carefully

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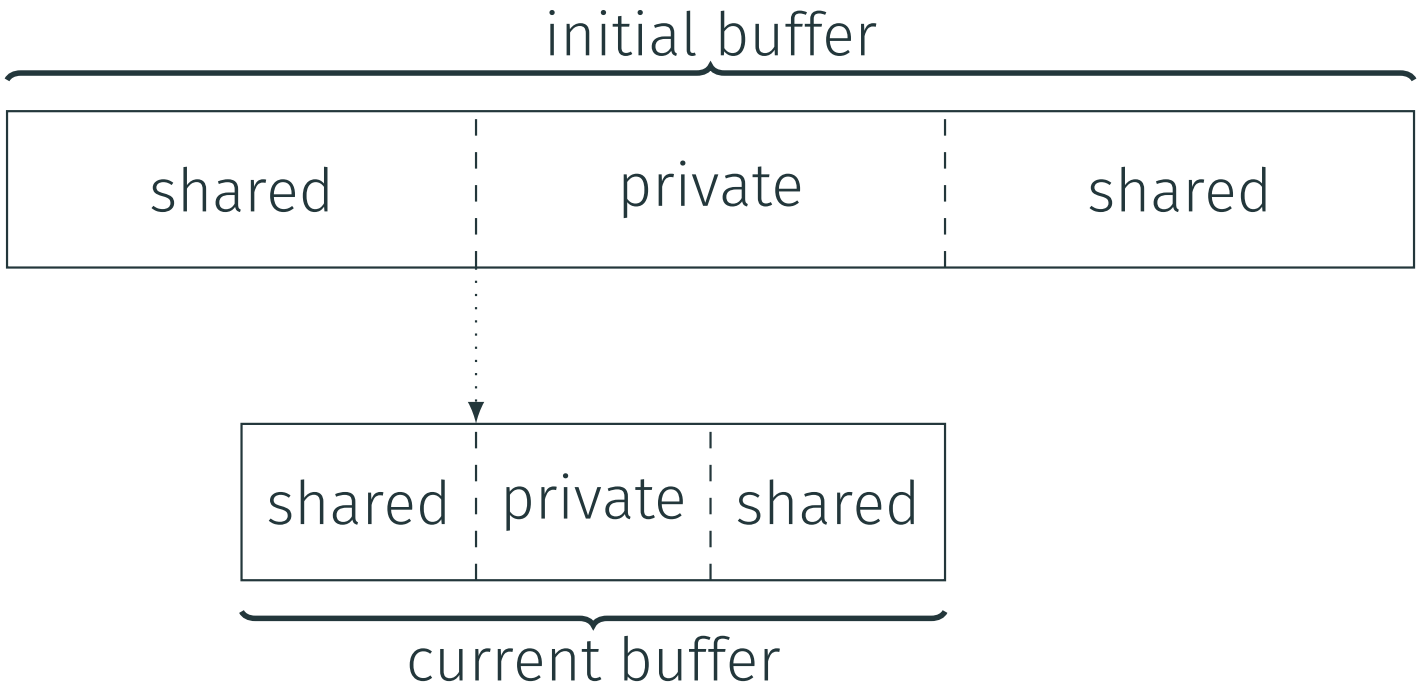
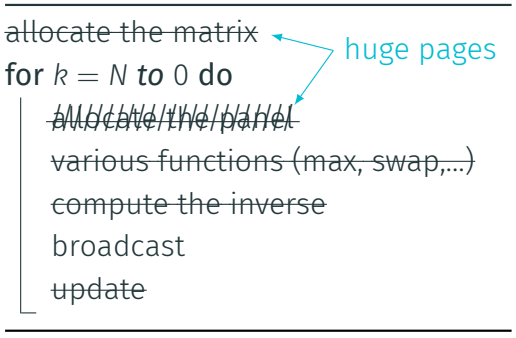


Using huge pages

#168

Problem: at large scales, CPU utilization drops and simulation time explodes



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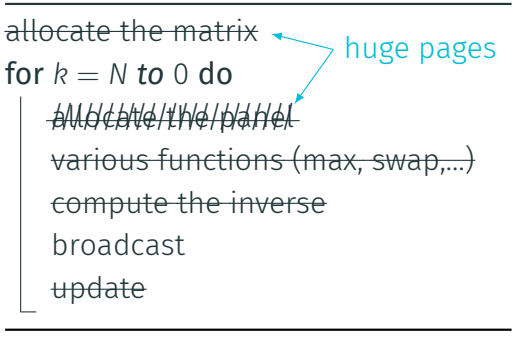
Reason: the page table becomes very large



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huge pages

Matrix of size $N \Rightarrow$ page table of size:

allocated virtual memory

$$PT_{size}(N) = \frac{N^2 \times 8}{4,096} \times 8$$

entry size

page size

$PT_{size}(600,000) \approx 5\text{GB}$

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Scalability

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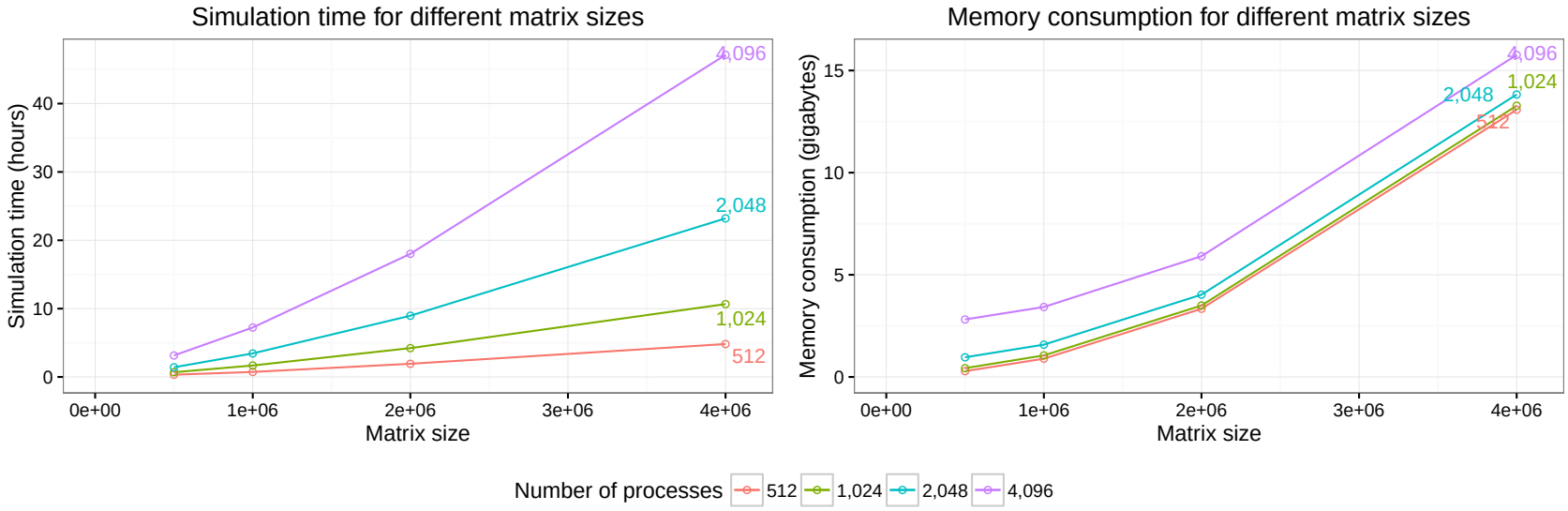
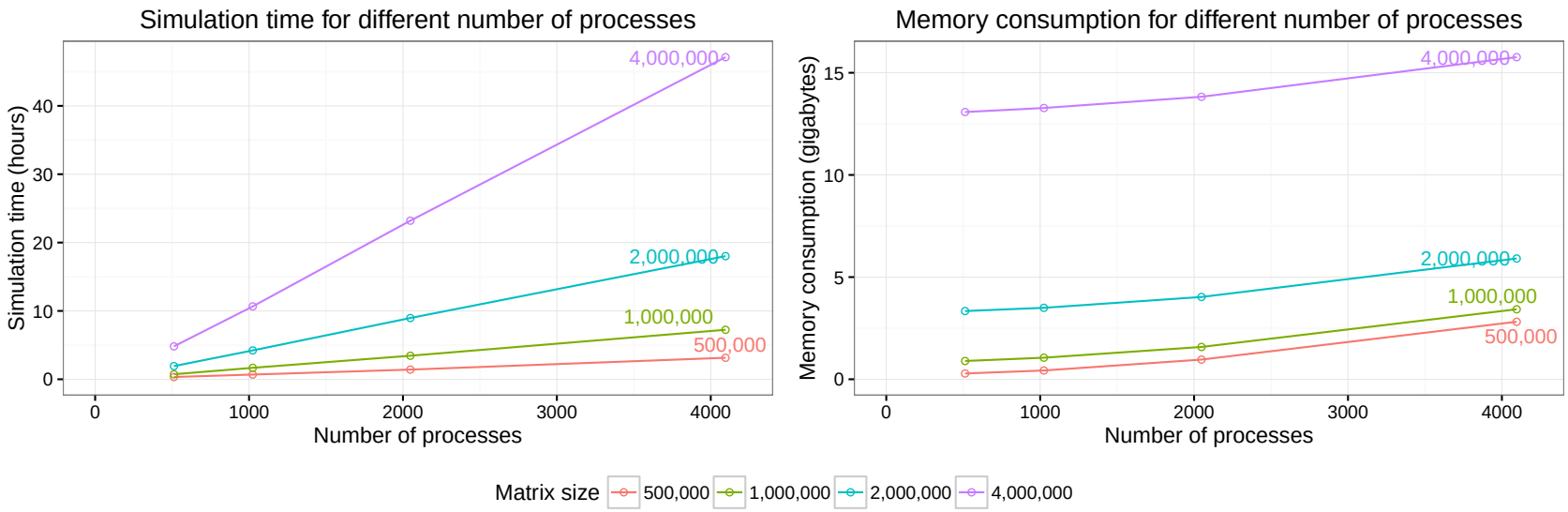




Validation

What?

Let's compare:

- a real experiment
- a vanilla simulation
- an optimized simulation

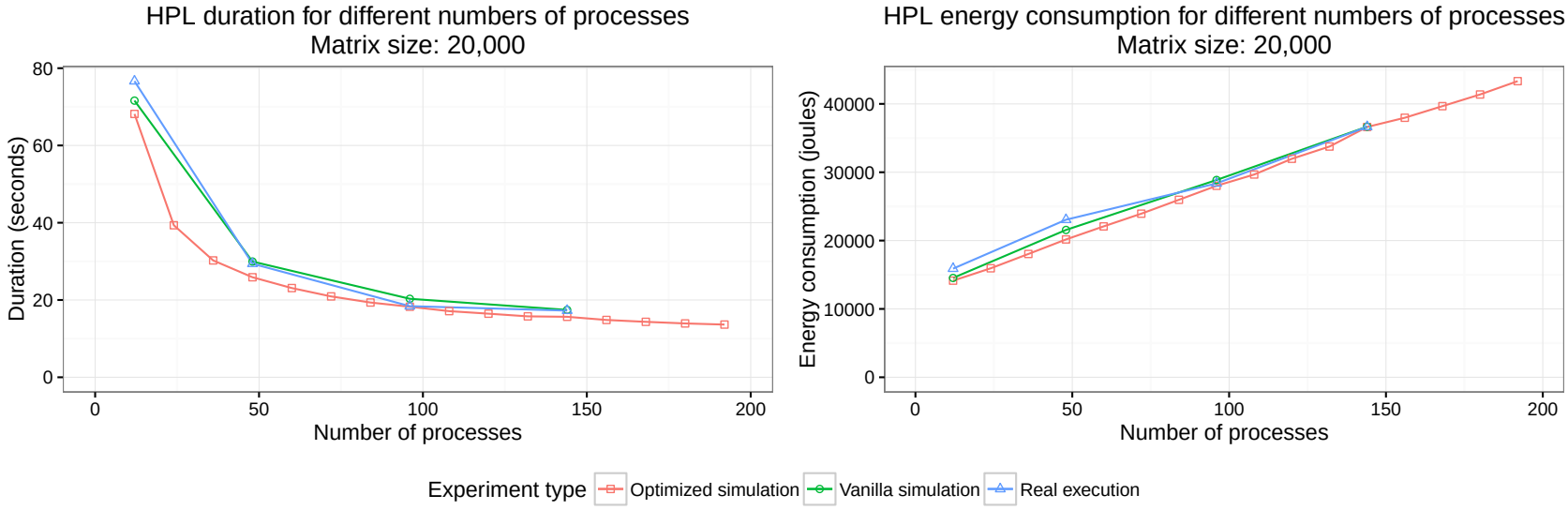
Measuring the duration of HPL and its energy consumption

How?

Using Grid'5000:

- Cluster Taurus, in Lyon
- 16 nodes
- 2 Intel Xeon E5-2630, 6 cores/CPU, 2.3GHz
- 32GB RAM
- 1 switch, 10Gbps links
- Hyperthreading and turbo-mode disabled

Result



Prediction error: $\leq 12\%$

Simulation systematically too optimistic

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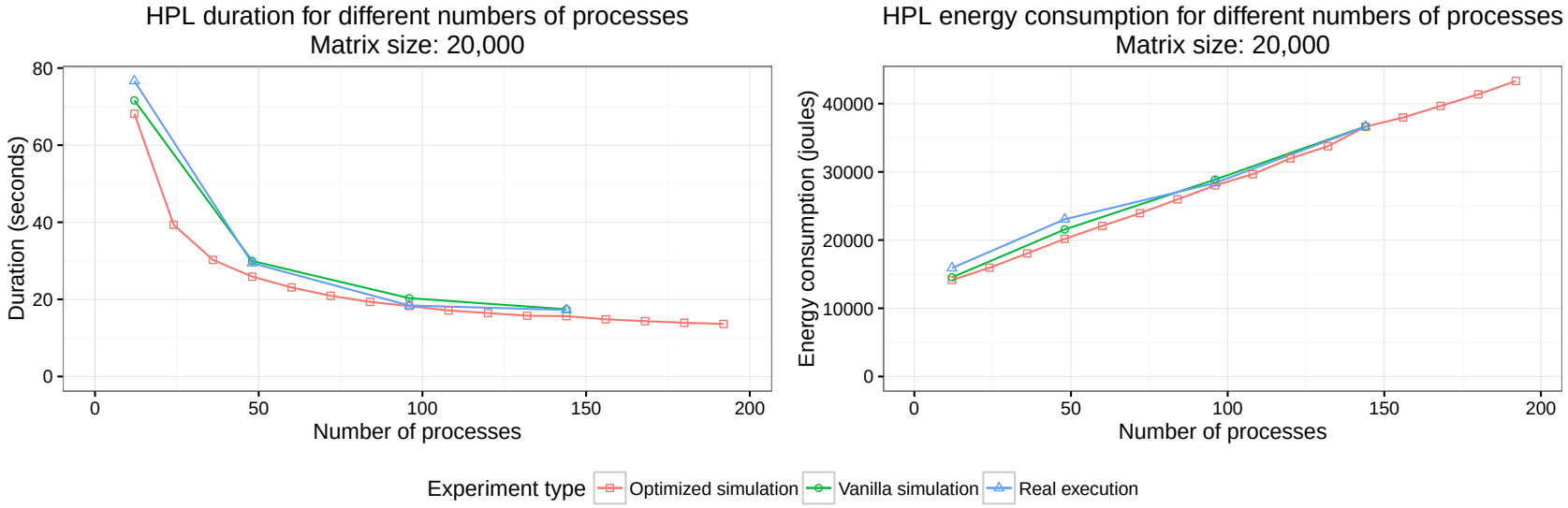

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- No outliers in `dgemm` and `dtrsm` duration
- Functions skipped
- Optimistic network model

Conclusion

To sum up

Simulation of HPL, accurate and efficient

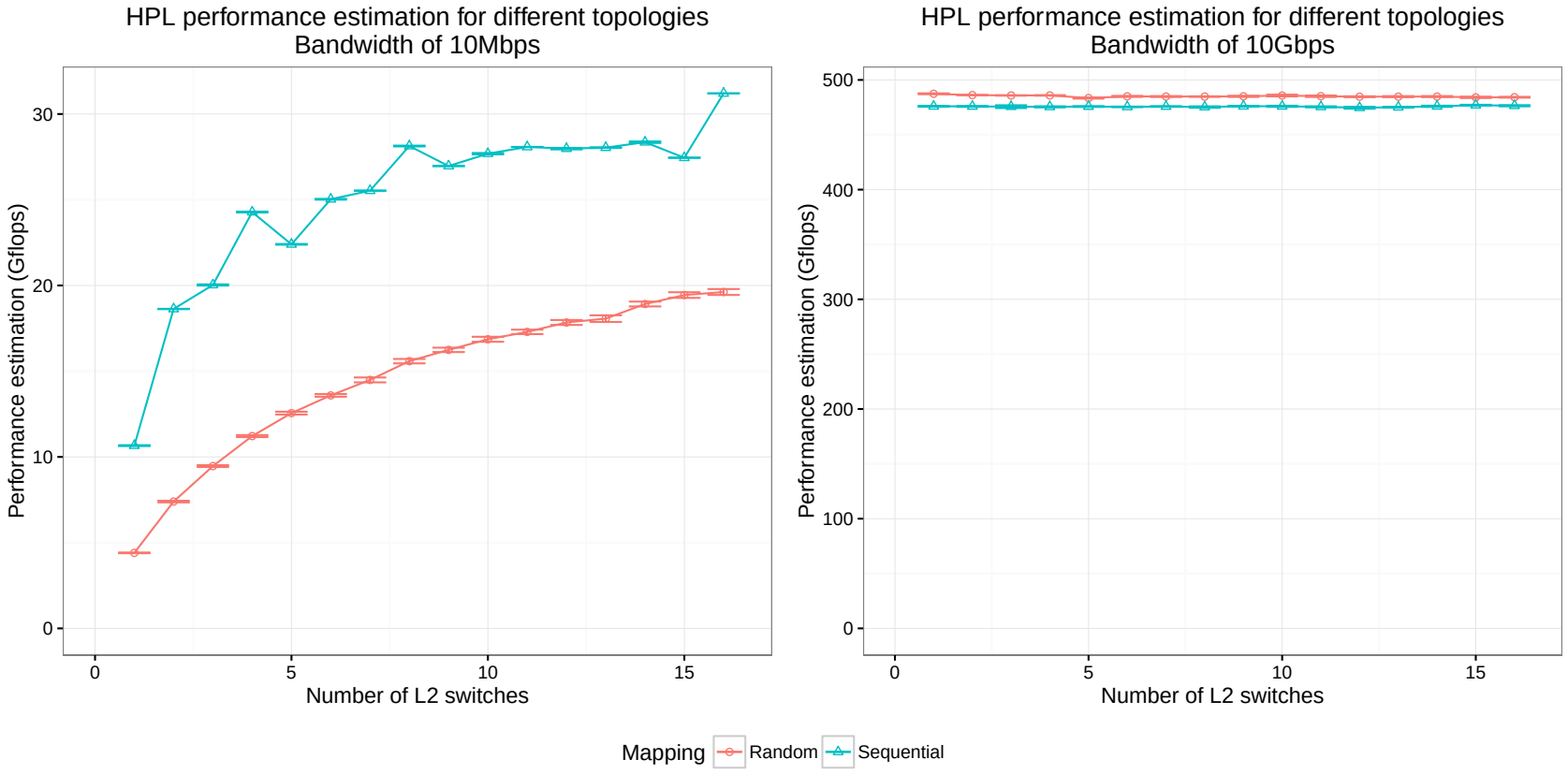
Can reach the scales of the largest supercomputers

Small modifications to HPL (300/34k lines)

Several improvements to Simgrid

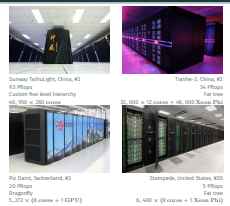
Coming soon...

Capacity planning of supercomputers



Failures, energy consumption

Top500



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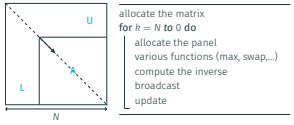

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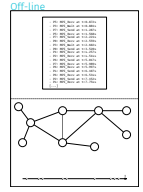

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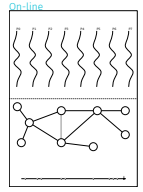

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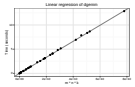
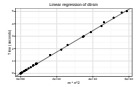
Solution: modeling these functions to inject their duration





$T_{dgemm}(M, N, K) = M \times N \times K \times 1.706348 \times 10^{-10}$

$T_{dtrsm}(M, N) = M \times N^2 \times 8.624970 \times 10^{-11}$

Computation pruning

68% of the simulation time spent in HPL

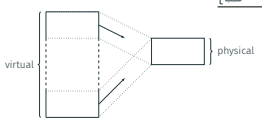
Culprits:

- Initialization and verification functions
- Other BLAS and HPL functions

Solution: just skip them

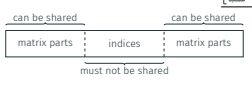
Reducing the memory consumption

Memory consumption still too large
Solution: use `SMPI_SHARED_MALLOC`



Reducing the memory consumption #154

Problem: panel buffers
Must remain contiguous

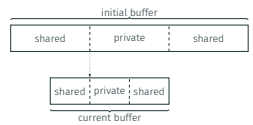


Solution: `SMPI_PARTIAL_SHARED_MALLOC`

Arbitrary number of shared and private blocks.

Reusing the panel buffers

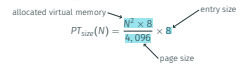
At each iteration, new allocation and deallocation by all processes
Solution: reuse the buffers (sizes strictly decreasing)
Needs to be done carefully



Using huge pages #168

Problem: at large scales, CPU utilization drops and simulation time explodes
Reason: the page table becomes very large

Matrix of size $N \Rightarrow$ page table of size:

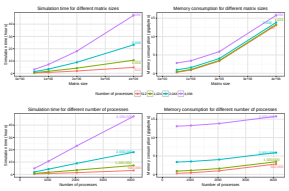


$PT_{size}(N) = \frac{N^2 \times 8}{4,096} \times 8$

$PT_{size}(600,000) \approx 5\text{GB}$

Solution: using huge pages

Scalability



What?

Let's compare:

- a real experiment
- a vanilla simulation
- an optimized simulation

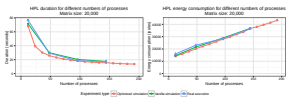
Measuring the duration of HPL and its energy consumption

How?

Using Grid'5000:

- Cluster Taurus, in Lyon
- 16 nodes
- 2 Intel Xeon E5-2630, 6 cores/CPU, 2.3GHz
- 32GB RAM
- 1 switch, 10Gbps links
- Hyperthreading and turbo-mode disabled

Result



Prediction error: $\leq$ 12%

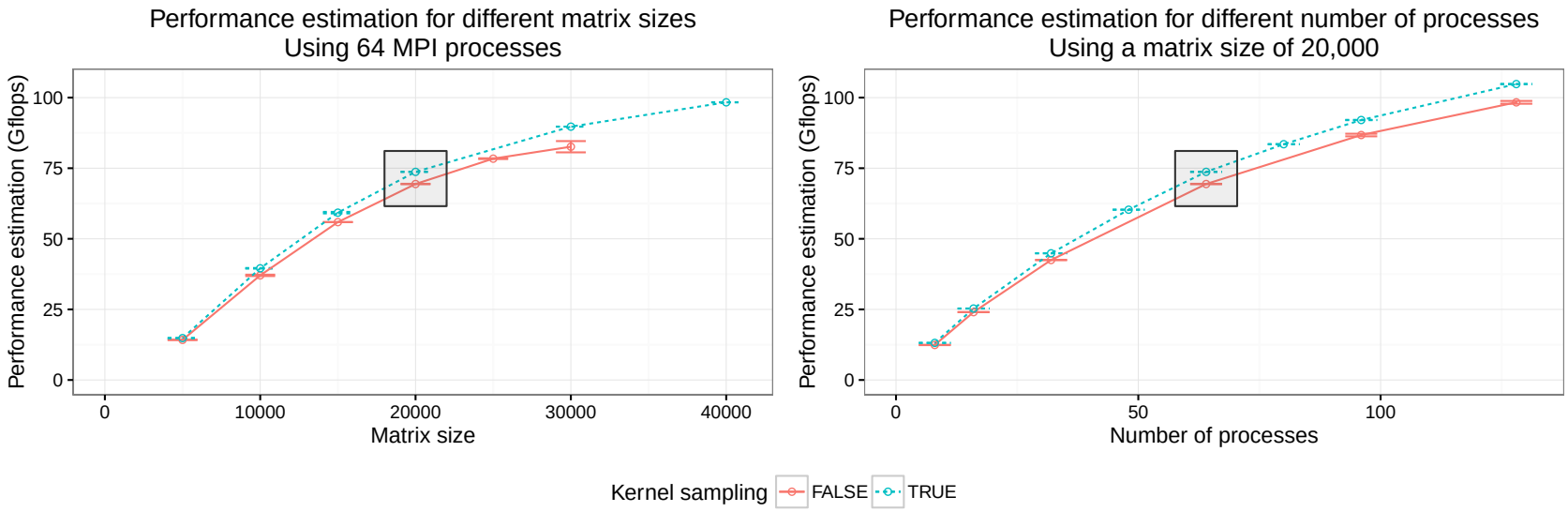
Simulation systematically too optimistic

- No outliers in `dgemm` and `dtrsm` duration
- Functions skipped
- Optimistic network model

Thanks for your attention!

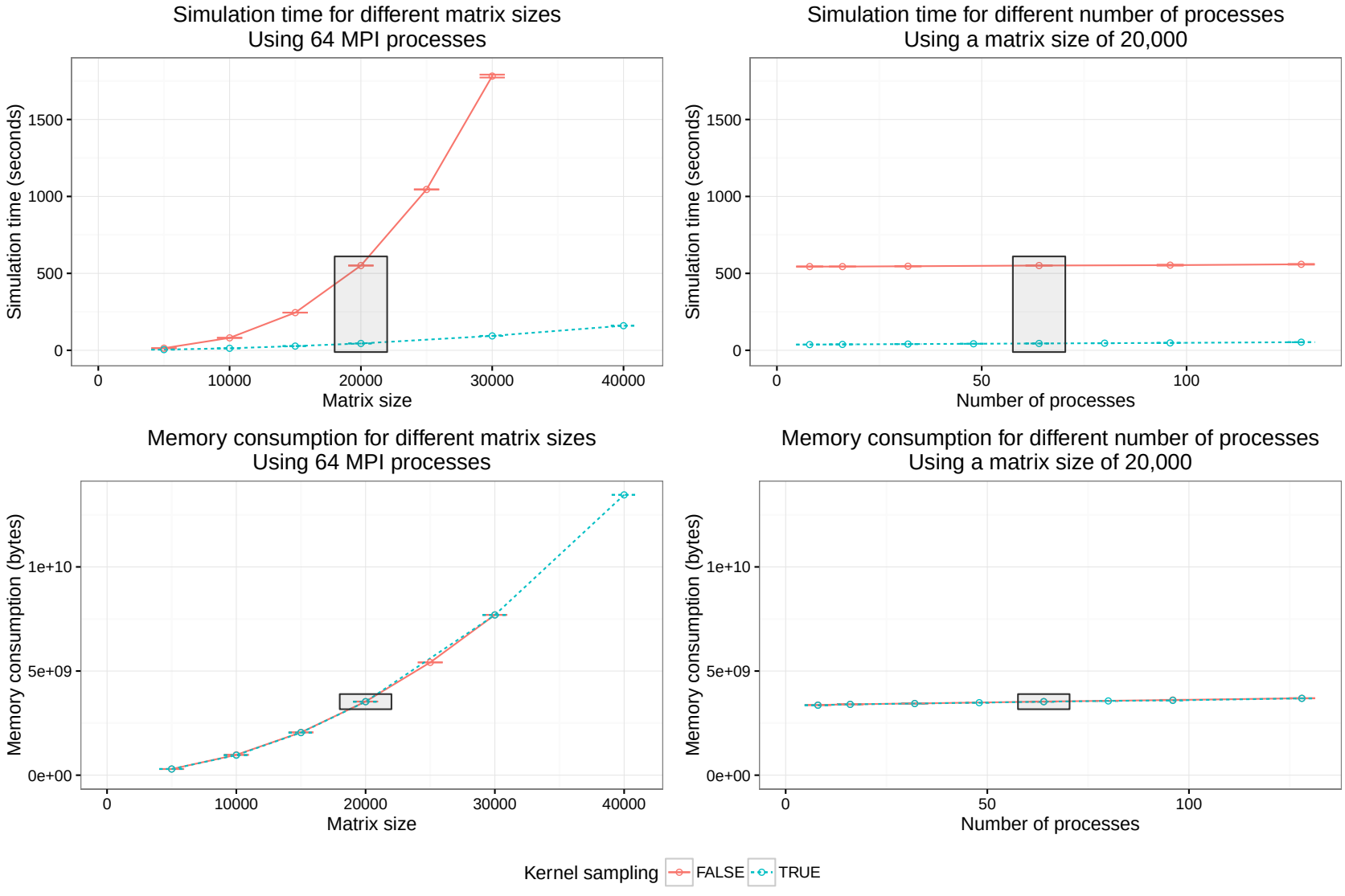
Any questions?

Computation kernel sampling

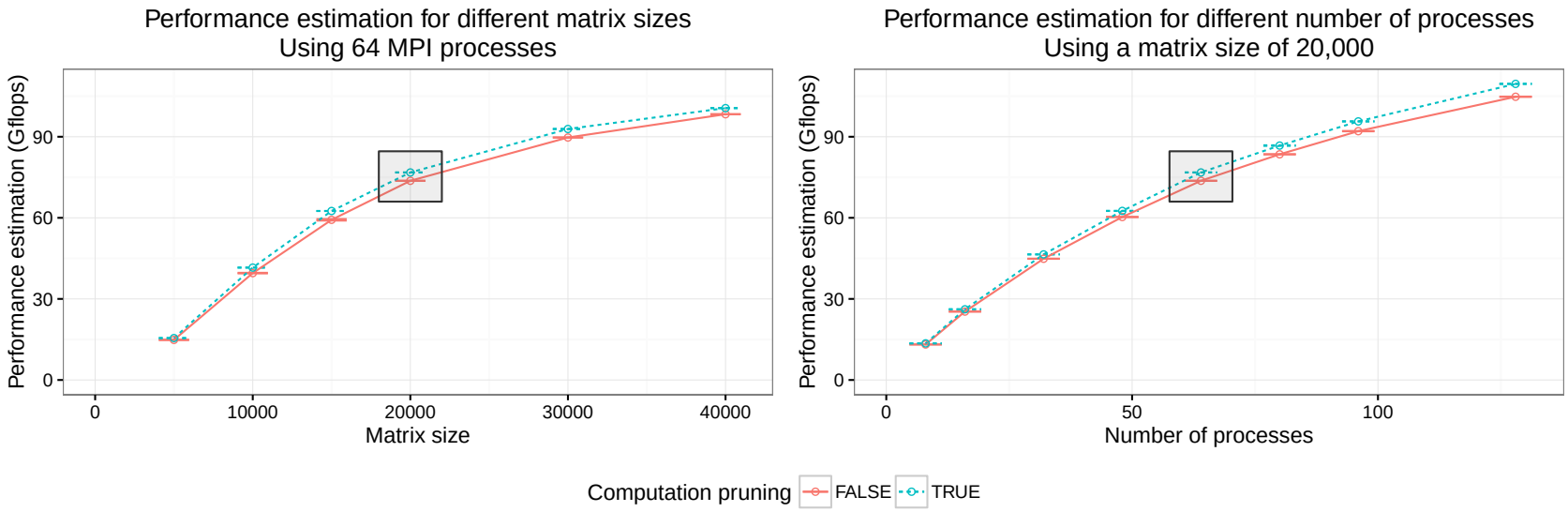


Prediction error: $\leq 10\%$

Computation kernel sampling

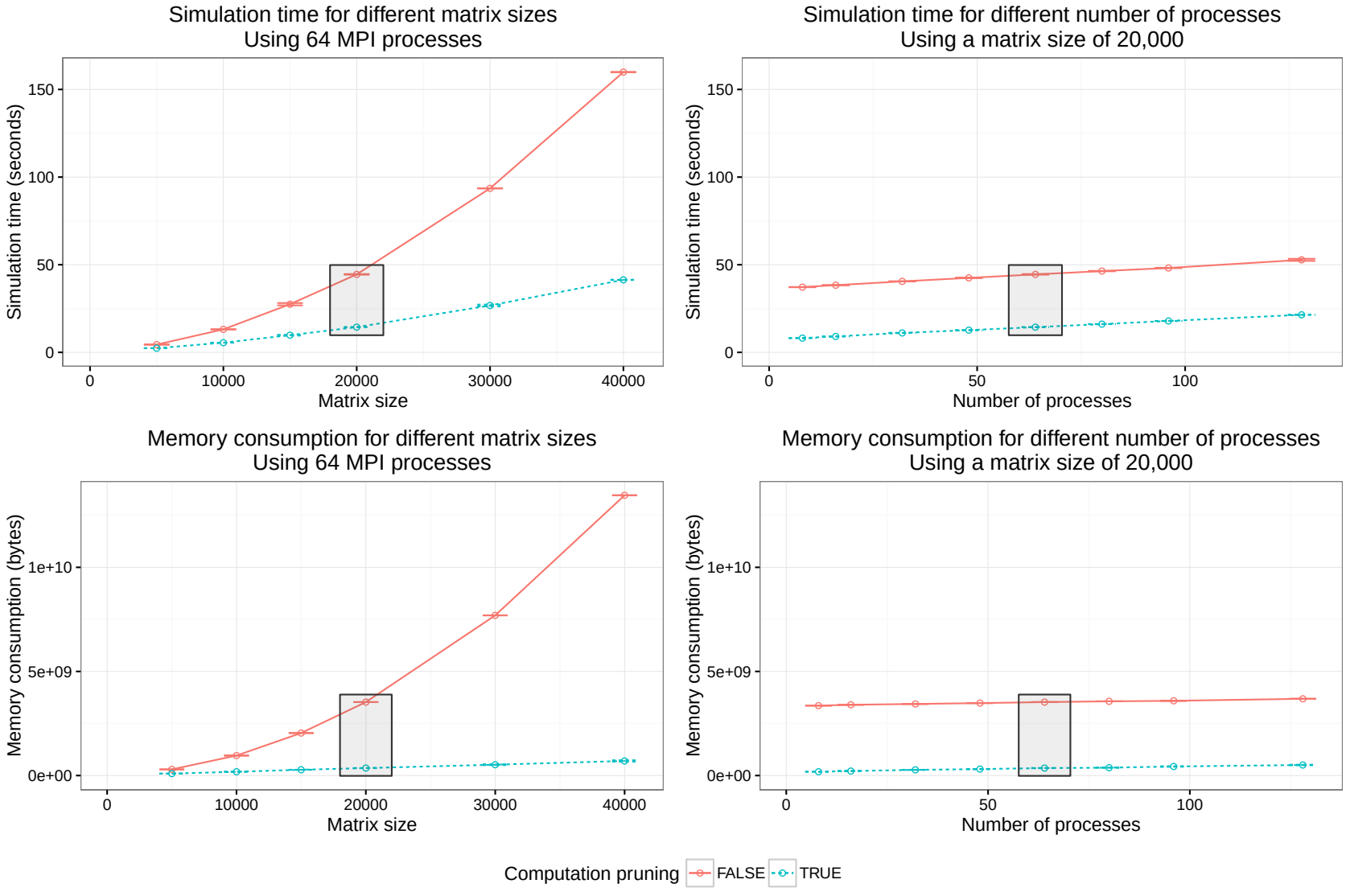


Computation pruning

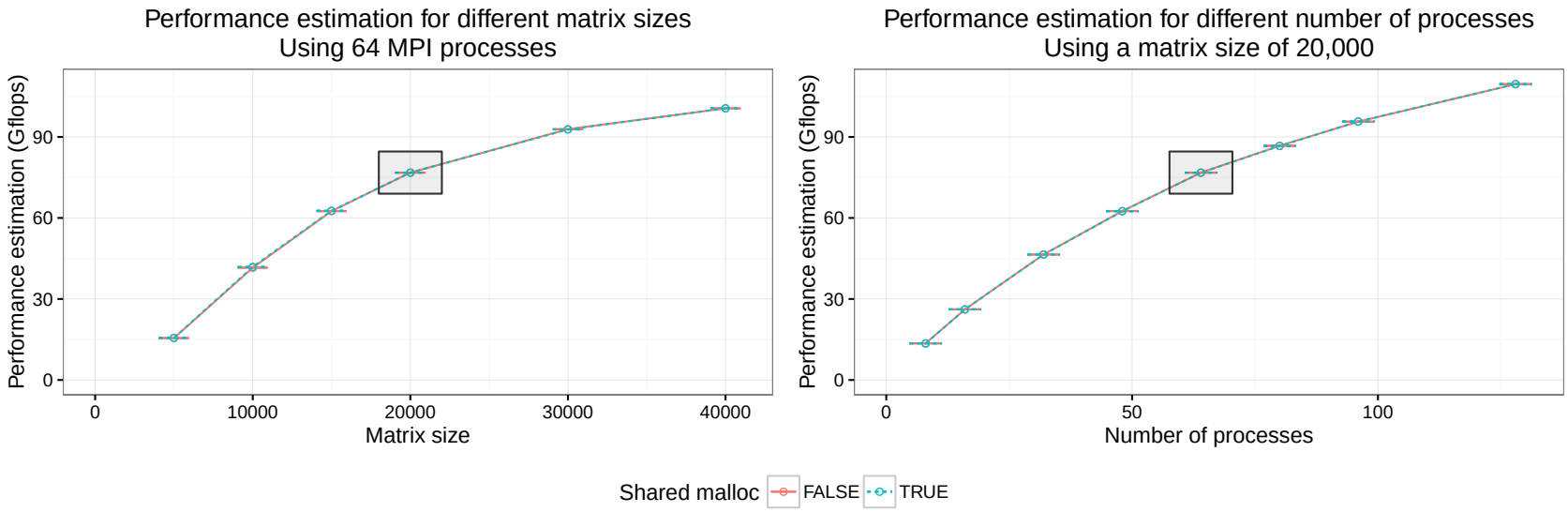


Prediction error: $\leq 5\%$

Computation pruning

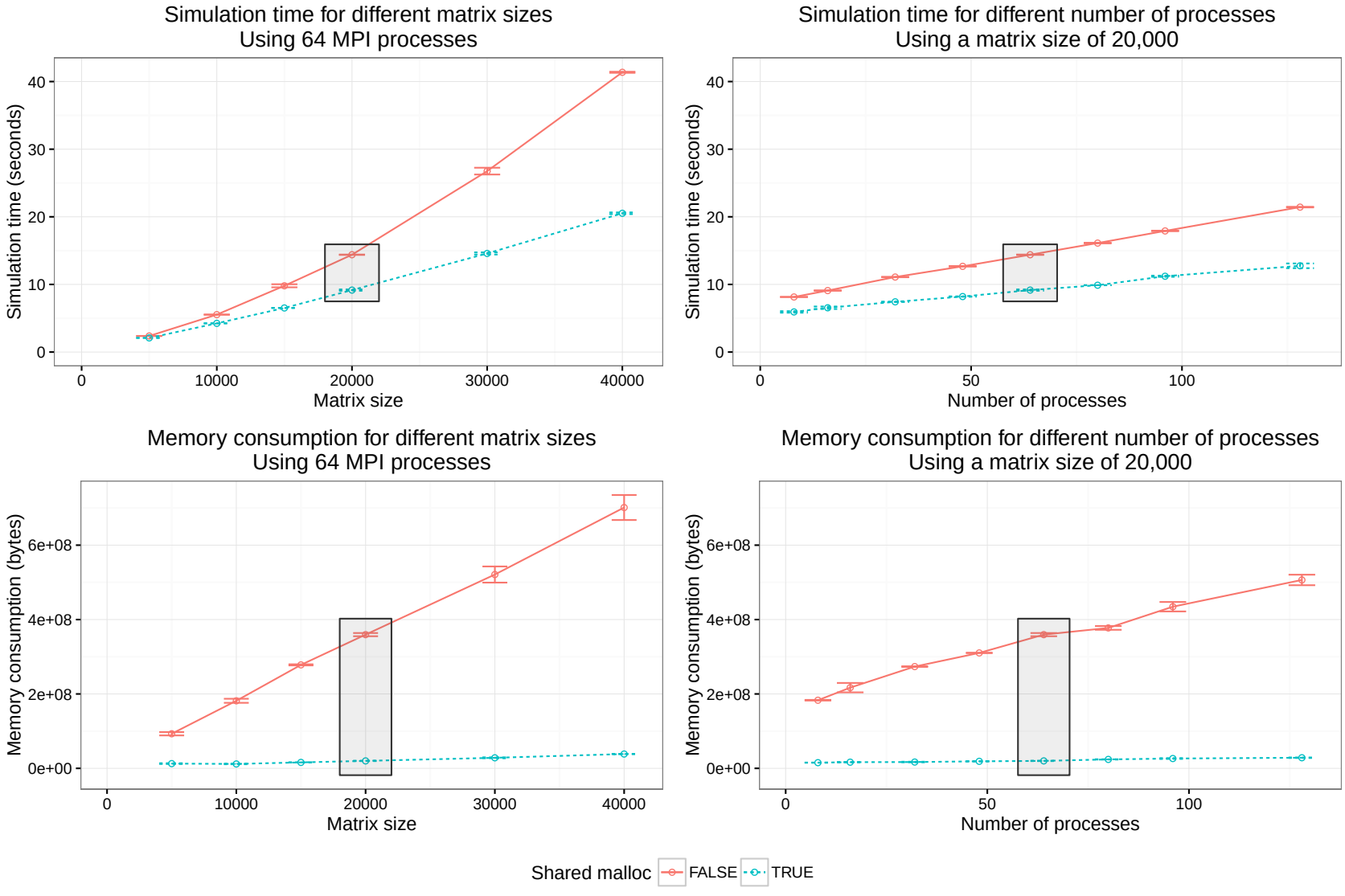


Reducing the memory consumption

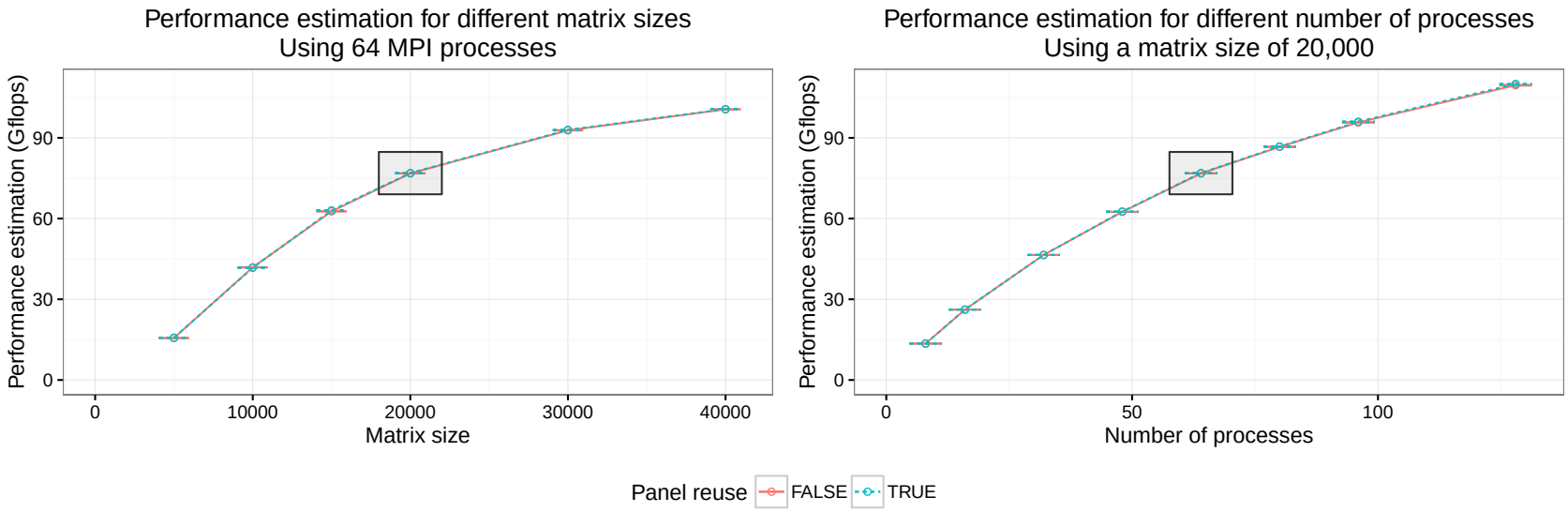


Prediction error: $\leq 1\%$

Reducing the memory consumption

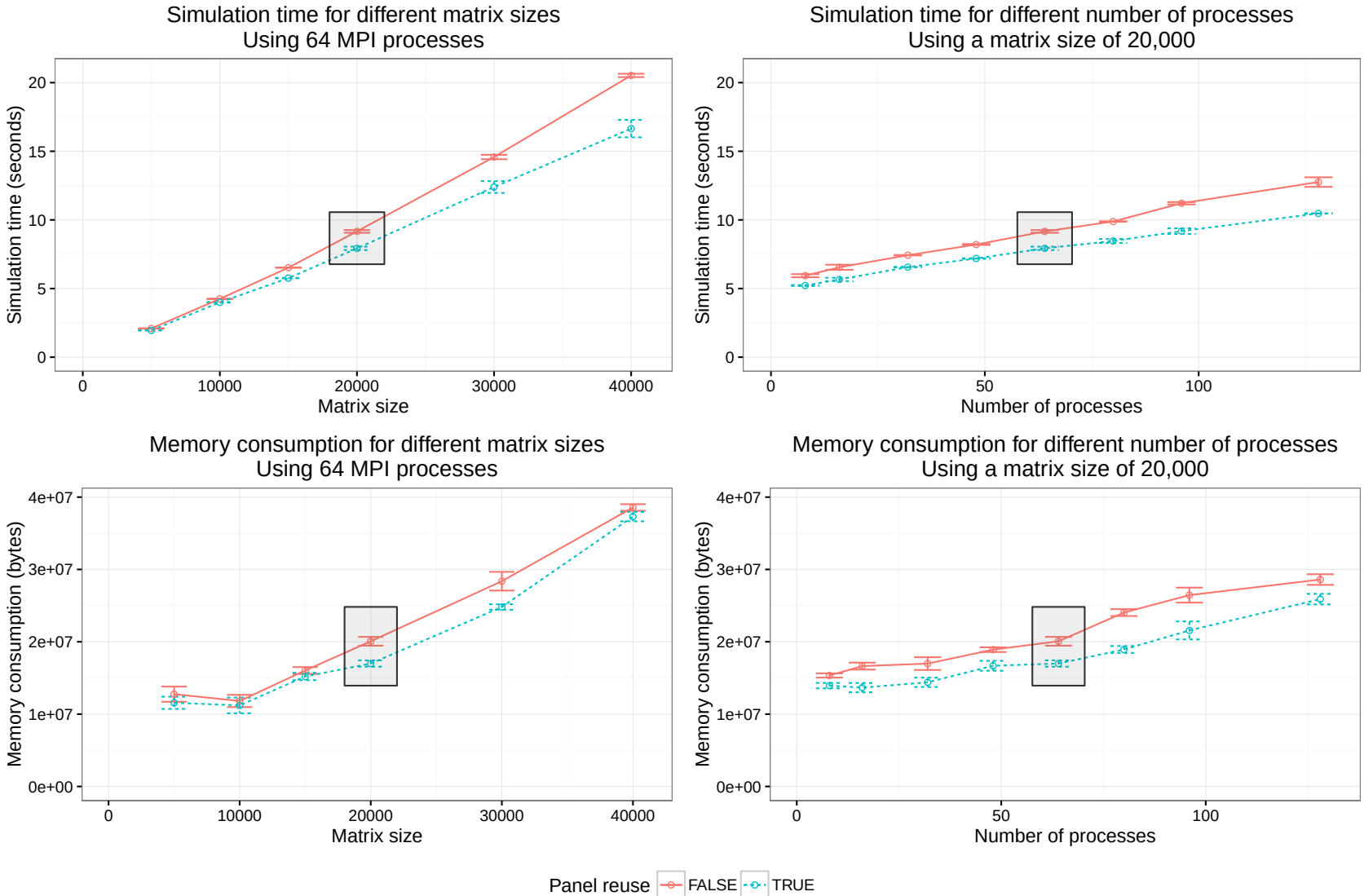


Reusing the panel buffers

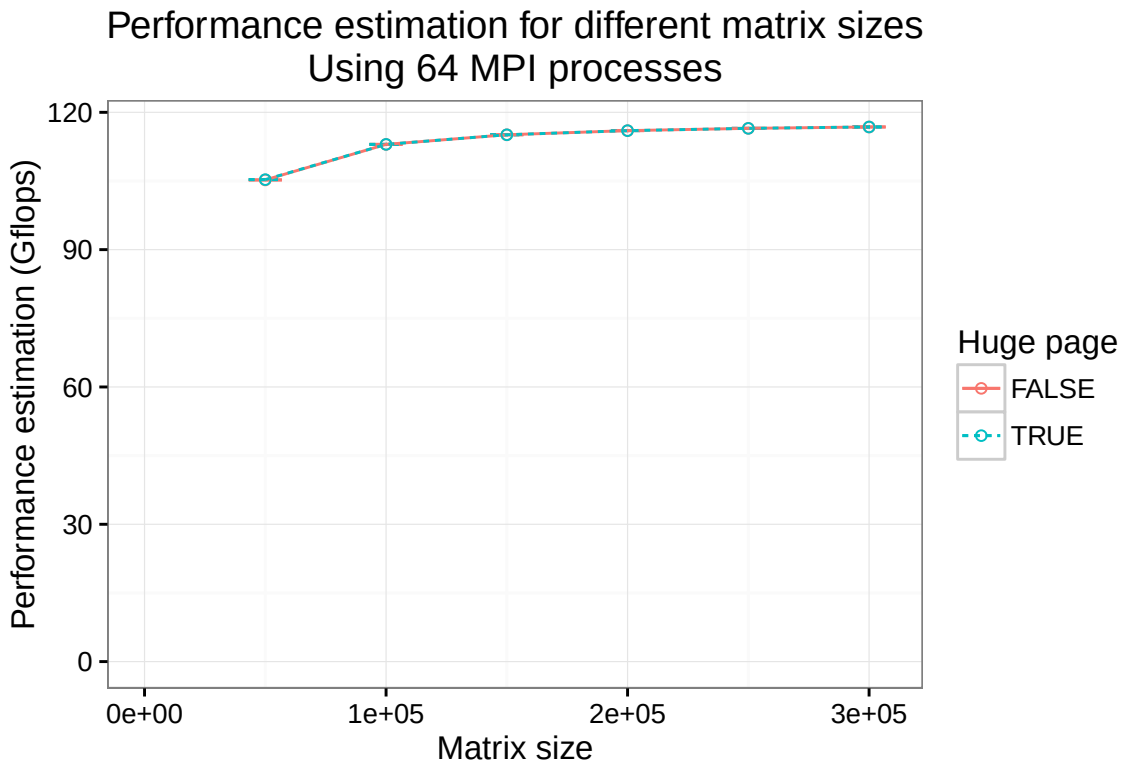


Prediction error: $\leq 1\%$

Reusing the panel buffers



Using huge pages



Prediction error: $\leq 0.1\%$

Using huge pages