L4: Experimental Design, Profiling, and Performance/Energy Optimization

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1. Experimental Design, Profiling, and Performance/Energy Optimization

2. Experimental Methodology

3. Plotting Tools

4. Profiling

5. Live Demo

Experimental Design, Profiling, and Performance/Energy Optimization

Plot Example - Intro

In the following slides, you will be shown a series of plots; mainly taken from the PPN course reports of previous students.

For each plot:

- Try to understand what is represented
- Explain what you observe
- Give a **definitive** conclusion from the data shown

Raise your hands when ready to propose an explanation.

Plot Example (1)

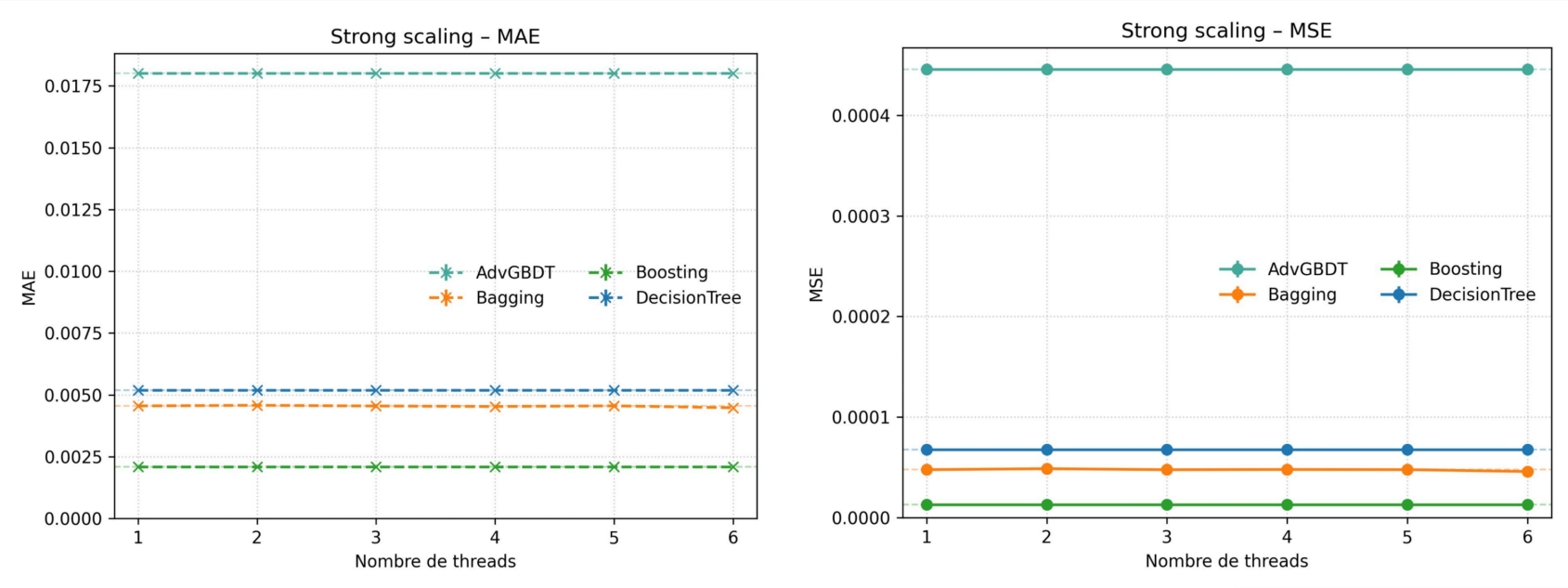


Figure 1: PPN Example - (No Caption)

Plot Example (2)

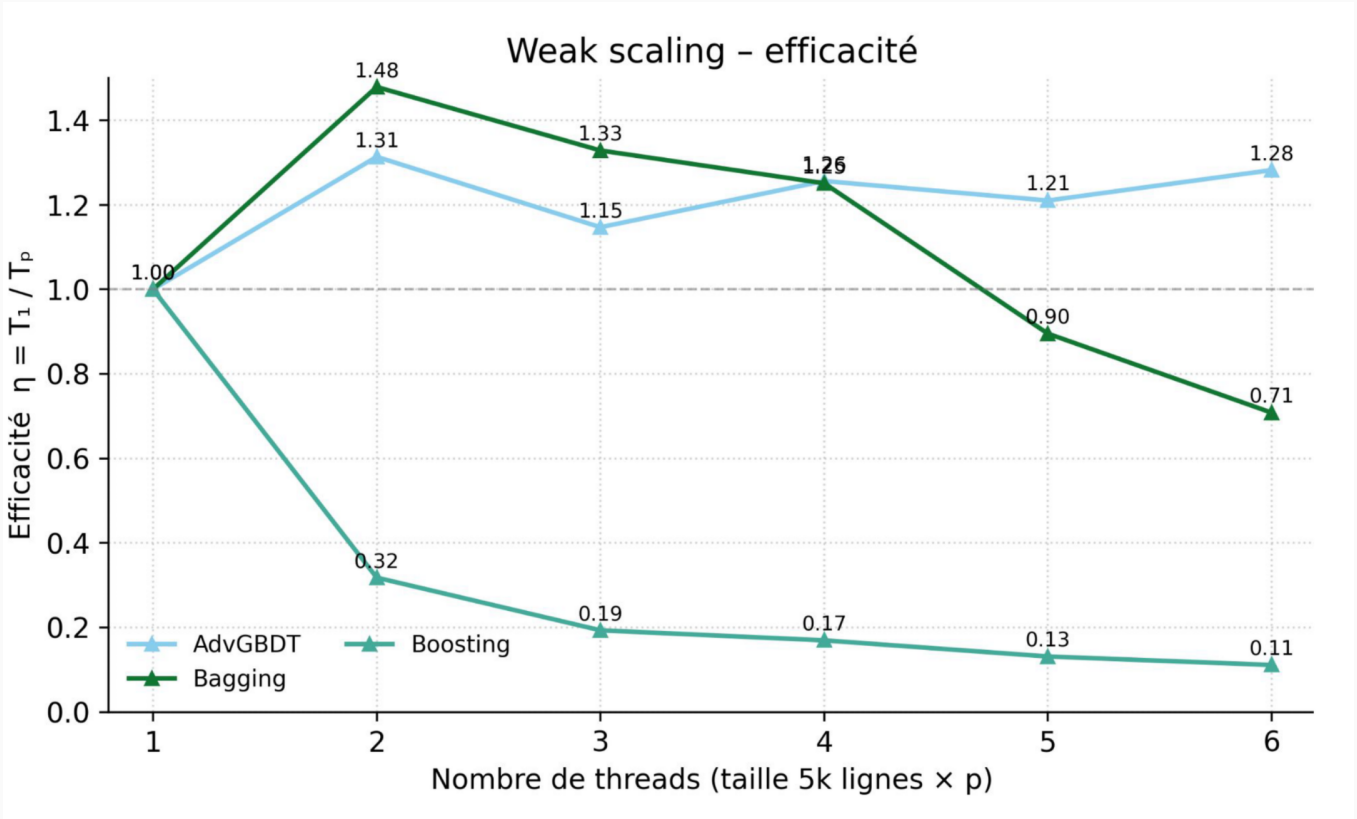


Figure 2: PPN Example - (No Caption)

Plot Example (3)

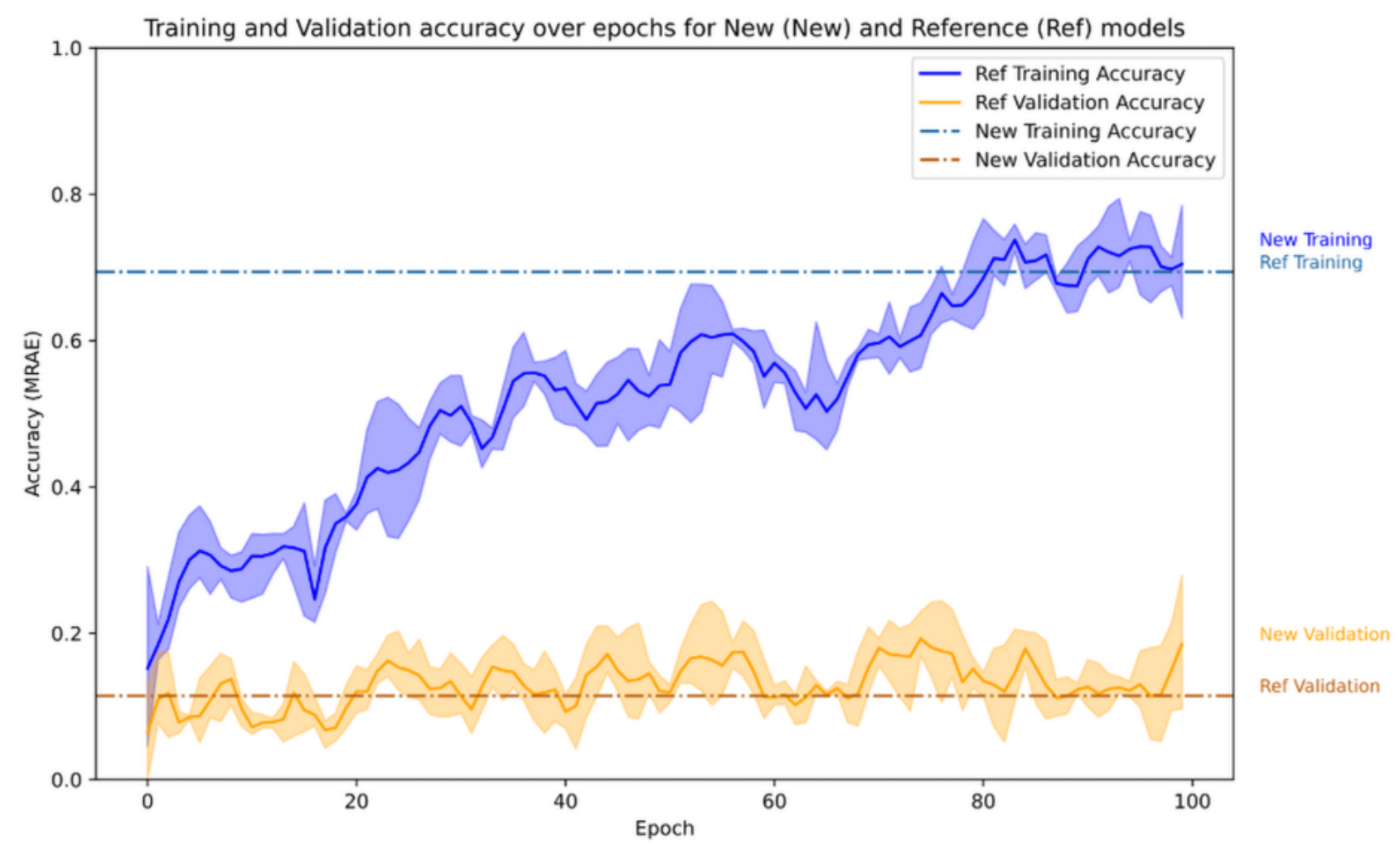


Figure 3: PPN Example - (No Caption)

Plot Example (4)

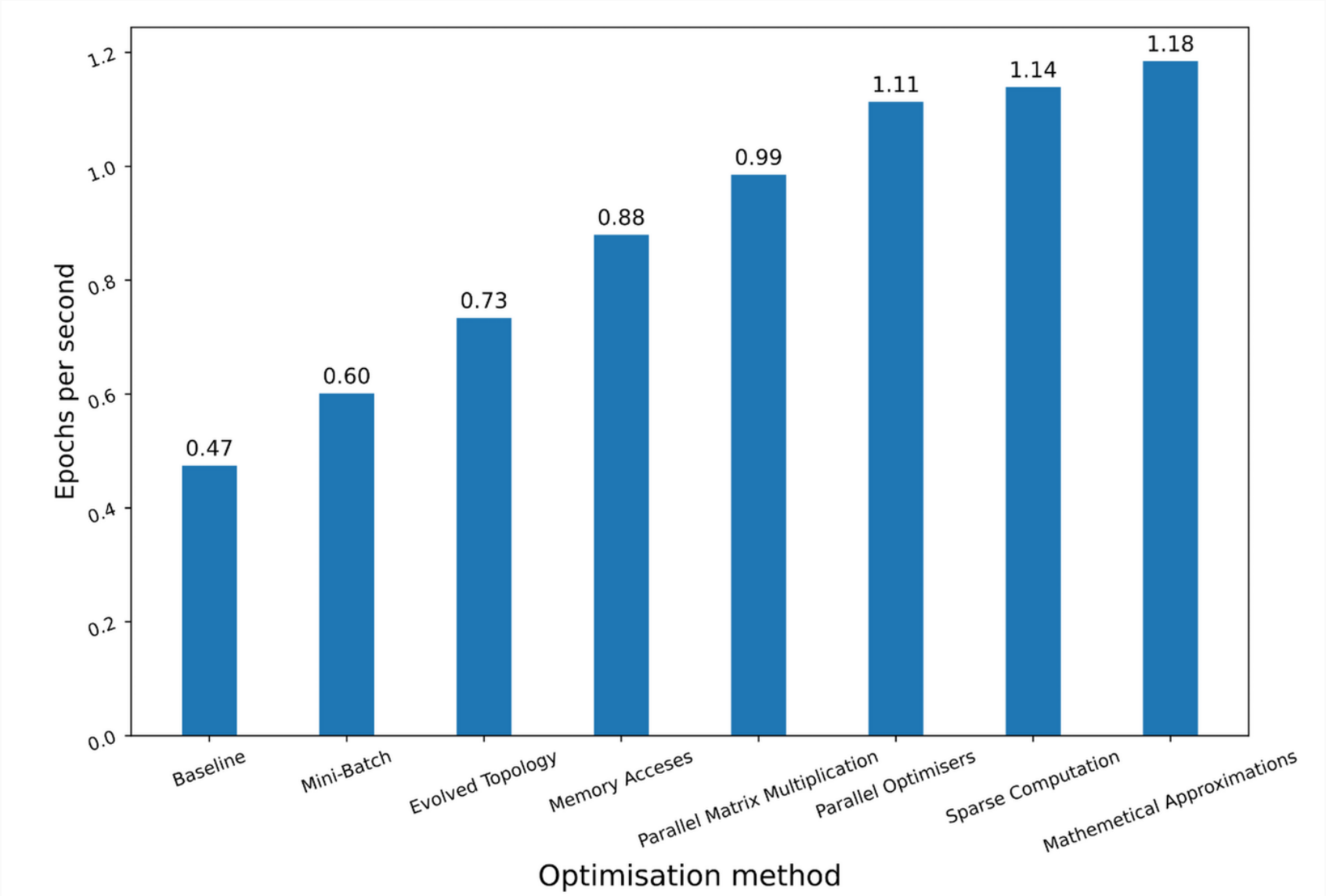


Figure 4: PPN Example - "Récapitulatif des optimisations faites"

Plot Example (5)

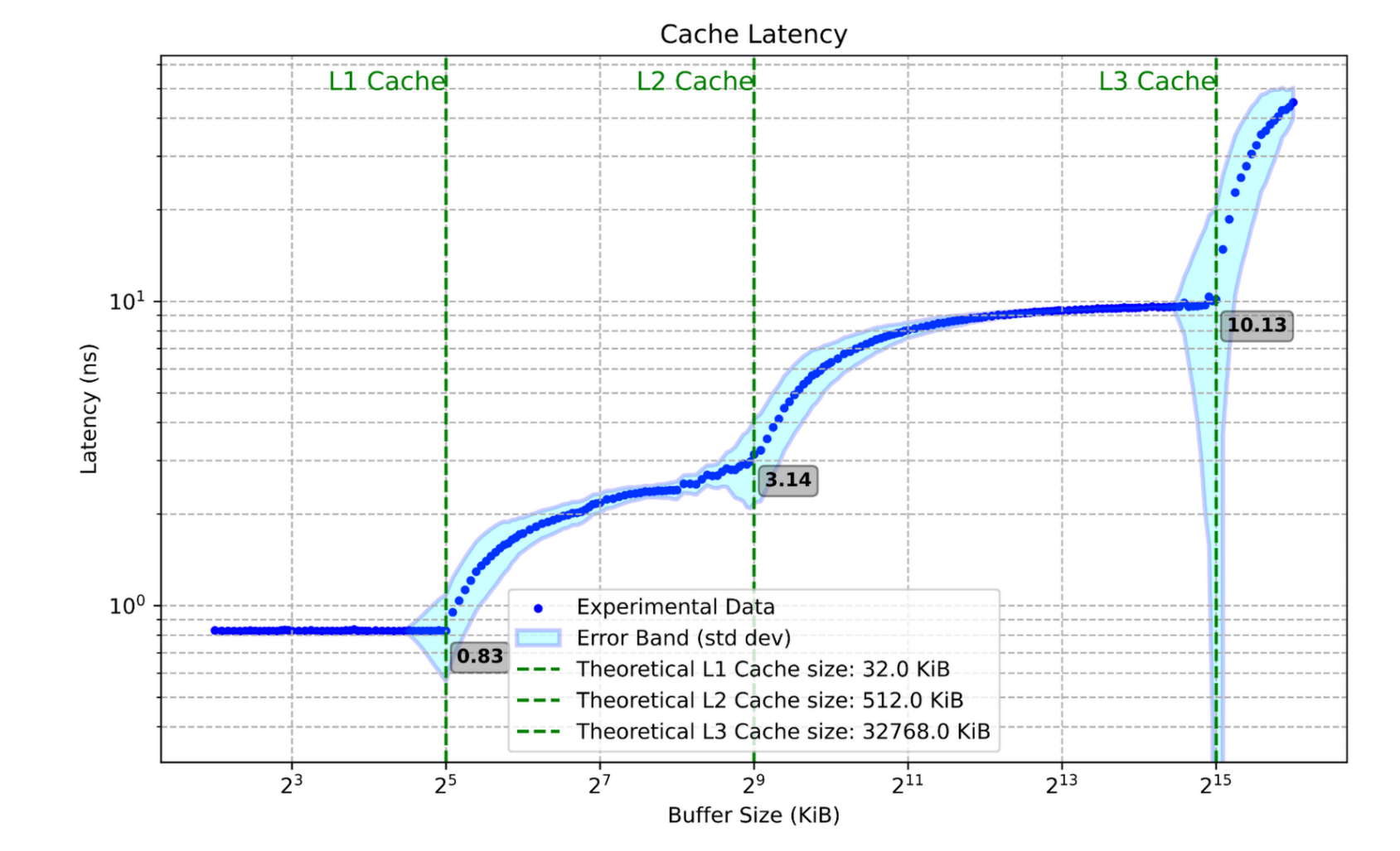


Figure 5: PPN Example - "Nouveau tracé de la latence cache"

Plot Example (6)

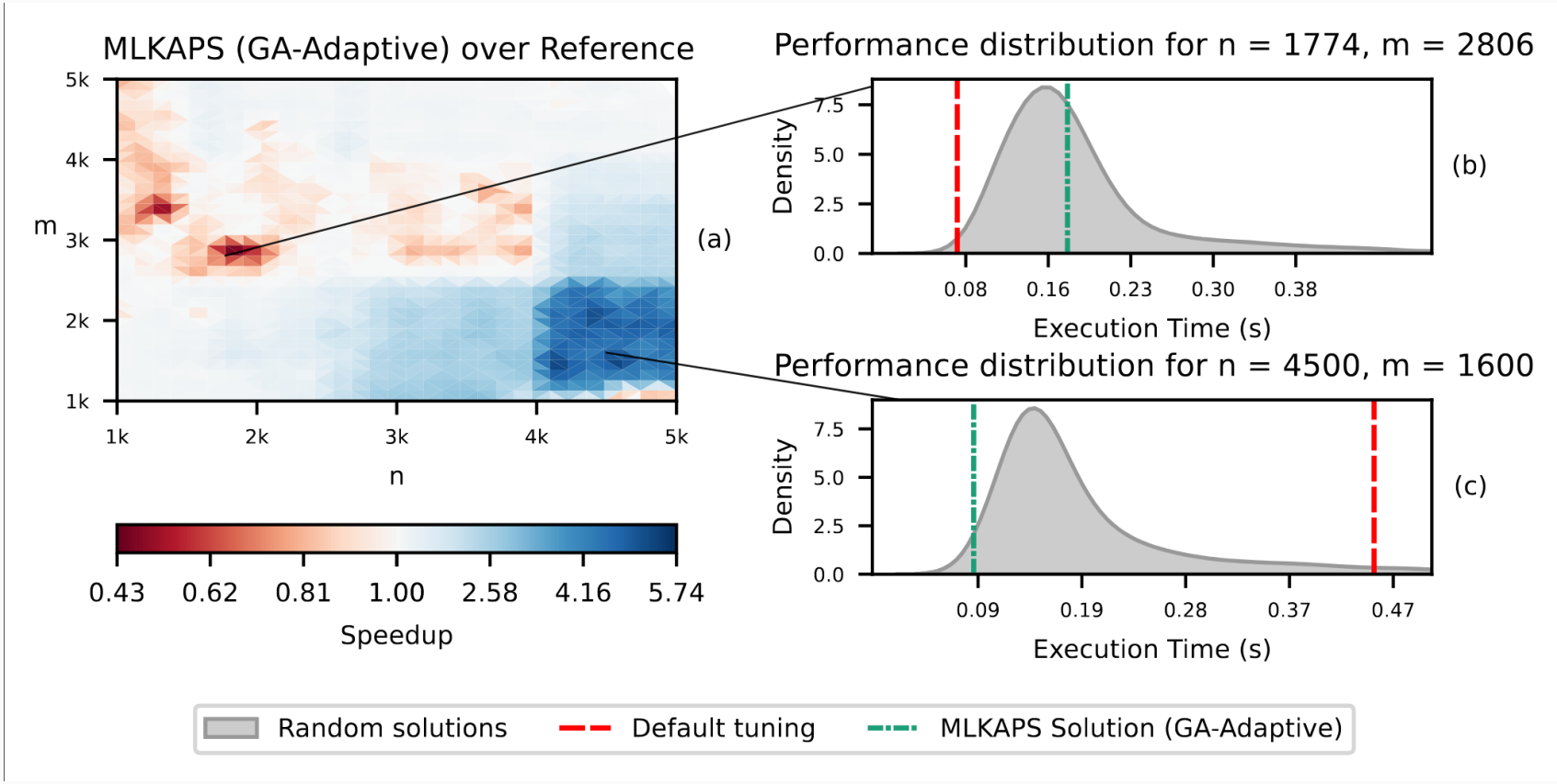


Figure 6: Prof Example - (KNM): (a) Speedup map of GA-Adaptive (7k samples) over the Intel MKL hand-tuning for `dgetrf` (LU), higher is better. (b) Analysis of the slowdown region (performance regression). (c) Analysis of the high speedup region. $3,000$ random solutions were evaluated for each distribution.

Plot Example (7)

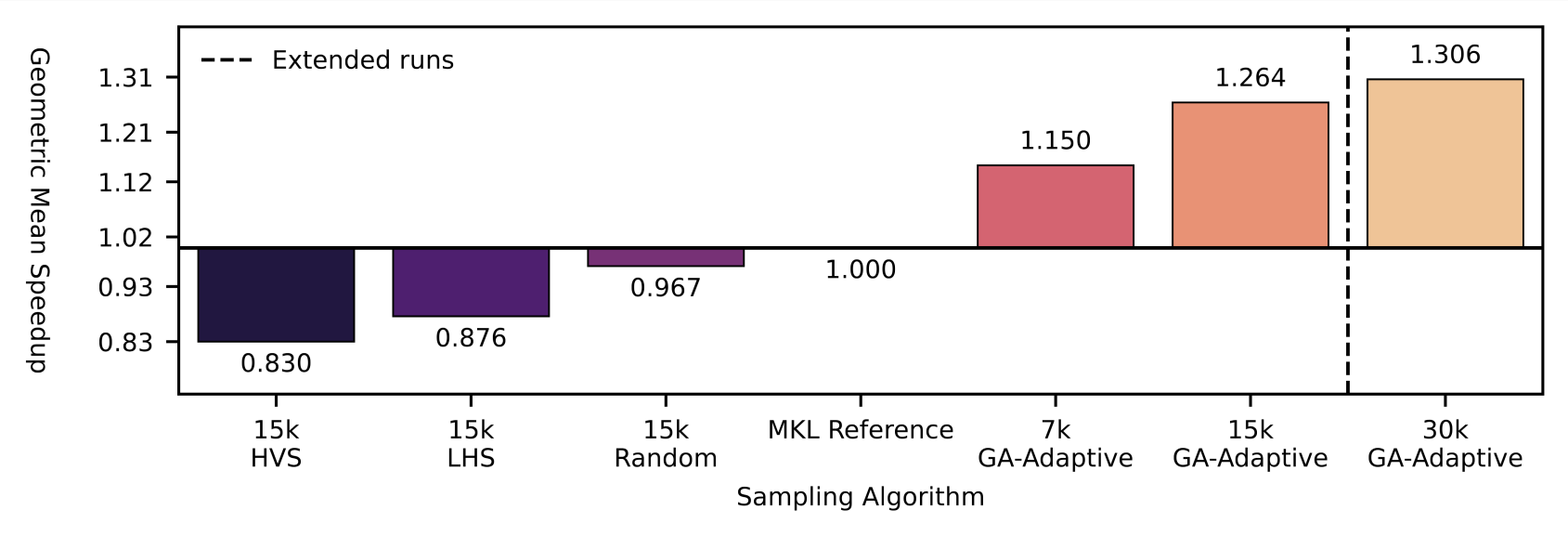


Figure 7: Prof Example - (SPR): Geometric mean Speedup (higher is better) against the MKL reference configuration on `dgetrf` (LU), depending on the sampling algorithm. 46x46 validation grid. 7k/15k/30k denotes the samples count. GA-Adaptive outperforms all other sampling strategies for auto-tuning. With 30k samples it achieves a mean speedup of $\times 1.3$ of the MKL dgetrf kernel.

Plot Example - What makes a good plot

Ask yourself:

- What do I want to communicate ?
- What data do I need ?
- **Is my plot understandable in ~10 seconds ?**
- Is my plot self-contained ?
- Is the context, environment, and methodology clear ?

Plot Example - Summary

HPC is a scientific endeavour; data analysis and plotting are essential.

- Plots drive decisions
- Plots make results trustworthy
- Plots explain complex behaviors

Datasets are large, multi-disciplinary, and often hard to reproduce.

Experimental Methodology

Experimental Methodology - Workflow

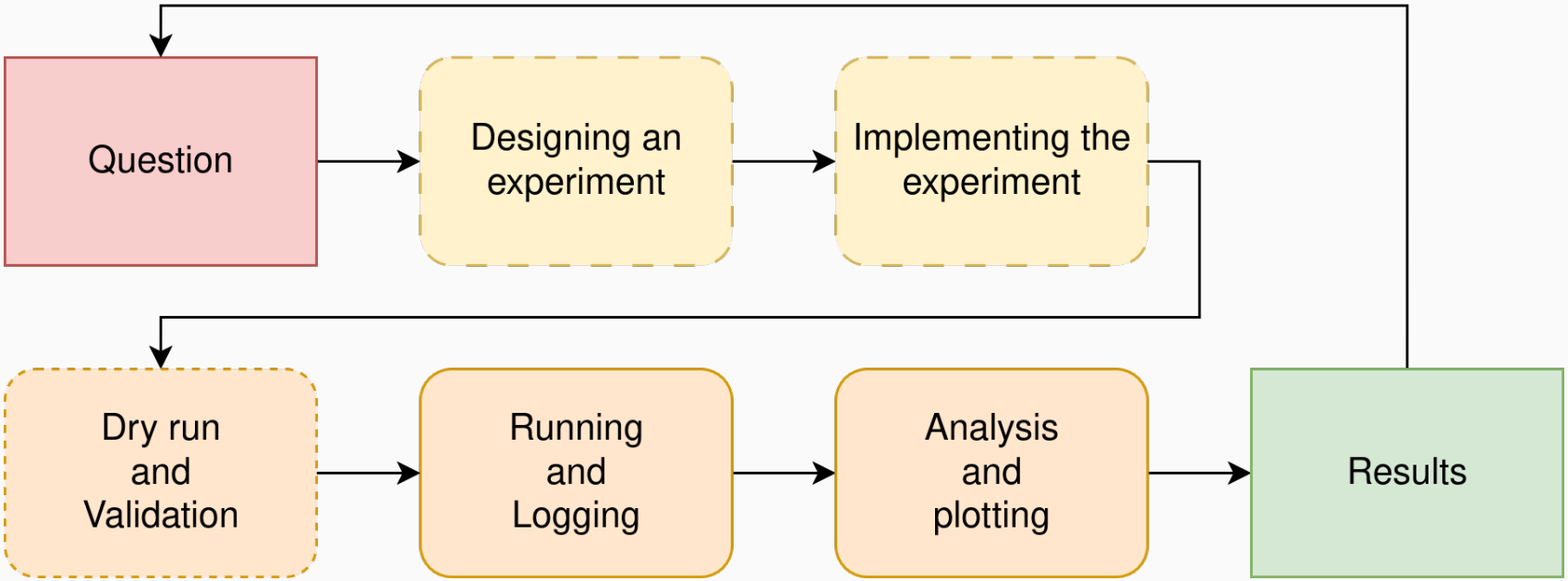


Figure 8: Typical experimental workflow

Statistical significance - Introduction

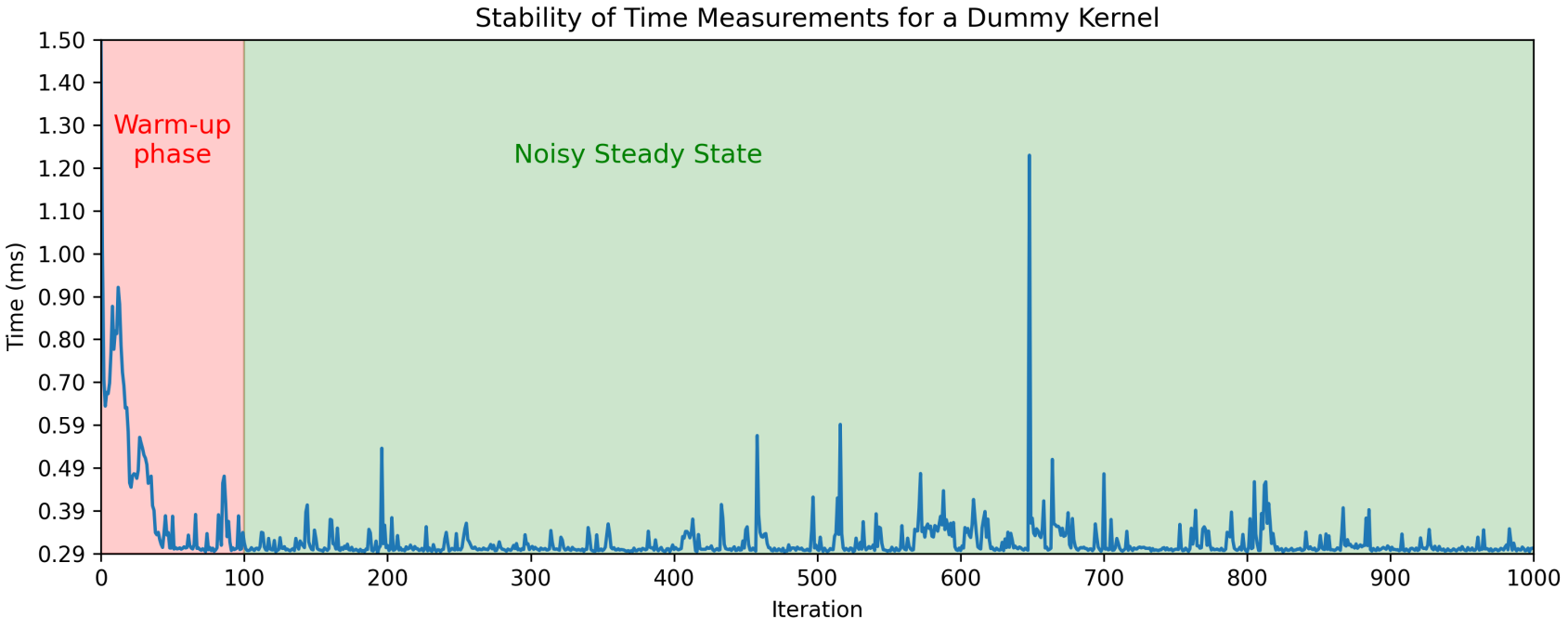
Computers are noisy, complex systems:

- Thread scheduling is non deterministic -> runtime varies between runs.
- Dynamic CPU frequency (Turbo/Boost)
- Systems are heterogeneous (CPU/GPU, dual socket, numa effects, E/P cores)
- Temperature/thermal throttling can alter runtime

How can we make sure our experimental measurements are reliable and conclusive?

Statistical significance - Warm-up effects

Systems need time to reach steady-state:



On a laptop: $\text{Mean} = 0.315\,\text{ms},\ \text{CV} = 13.55\%$

We need "warm-up" iterations to measure stable performance and skip cold caches, page faults, frequency scaling.

Statistical significance - Noise mitigation

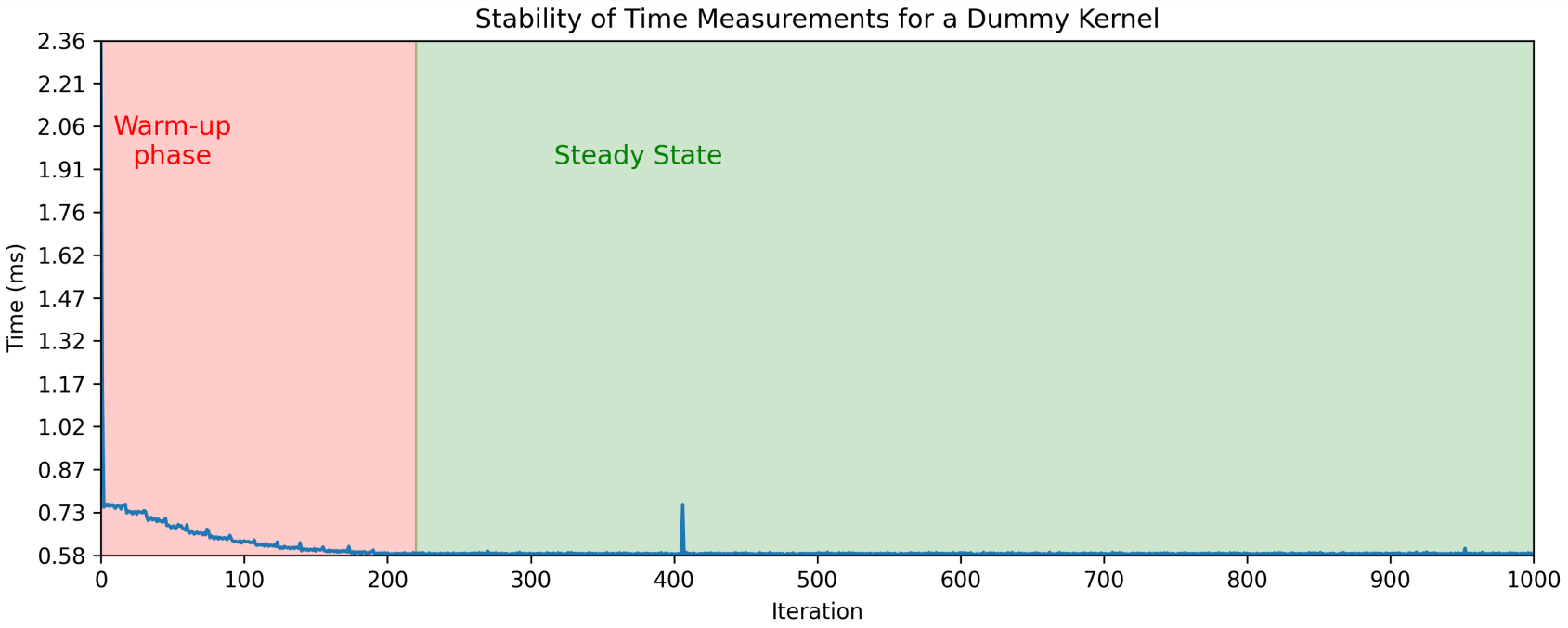
Noise can only be mitigated:

- Stop all other background processes (other users)
- Stabilize CPU Frequency (`sudo cpupower -g performance`)
  - Make sure laptops are plugged to avoid powersaving policies
- Pin threads via `taskset`, `OMP_PLACES` and `OMP_PROC_BIND`
- Consider hyperthreading
- Use stable compute nodes

Meta-repetitions are essential to mitigate noisy measurements.

Statistical significance - Example

Same experiment on a stabilized benchmarking server:



On a laptop: $\text{Mean} = 0.315\,\text{ms},\ \text{CV} = 13.55\%$
Stabilized node: $\text{Mean} = 0.582\,\text{ms},\ \text{CV} = 1.14\%$

Note

Timing on a laptop is always subpar

Statistical significance - Mean, Median, Variance

Single-run measurements are misleading; we need statistics.

- Mean runtime $\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$
- Median: less sensitive to outliers than the mean
- Variance/standard deviation: Measure of uncertainty
- Relative metrics are useful: Coefficient of variation ($CV = \frac{\sigma}{\bar{x}} \times 100\%$)

We usually give both the mean and standard deviation when giving performance results. Plots usually show $\bar{x} \pm 1\sigma$ as a shaded region around the mean to represent uncertainty.

Note

Distribution plots can be useful: stable measurements are often close to Gaussian, even if systematic noise may lead to skewed or heavy-tailed distributions.

Statistical significance - Confidence Intervals

How to decide how many repetitions we should perform ?

- Usually, the costlier the kernels, the less meta-repetitions are expected
- Short or really short kernels should have more metas to reduce the influence of noise

Remember that:

$$CI_{0.95} \approx \bar{x} \pm 1.96 \cdot \frac{\sigma}{\sqrt{n}}$$

More repetitions increase confidence, but returns diminish:
CI width $\propto \frac{1}{\sqrt{n}}$

Note

Confidence intervals are a bit less common in plots than $\pm 1\sigma$ but can also be used !

Statistical significance - p-score & Hypothesis testing

In HPC, mean/median and variance often suffice, but hypothesis testing can become handy in some contexts.

- Null hypothesis (H_0): GPU and CPU have the same performance for small matrixes
  - Differences in measurements are **only** due to noise
- Alternative hypothesis: CPU is faster for small matrixes
- **p-value** is the probability that H_0 explains a phenomenon.
- If $p < 0.05$, we can safely reject H_0 (Statistically significant difference)

Example: $\bar{x}_{GPU} = 5.0\text{s}$, $\sigma_{GPU} = 0.20$, $\bar{x}_{CPU} = 4.8\text{s}$, $\sigma_{CPU} = 0.4$, Two-sample t-test with 10 samples $p = 0.02$.

The measured differences between CPU and GPU execution time are **statistically significant**.

Experimental Methodology – Reproducibility

Reproducibility is a very hot topic (Reproducibility crisis in science):

- **Data and protocols are first-class citizens**: as important as the plots themselves
- **Transparency** matters: make data, scripts, and parameters accessible
- Enables others to **verify, build on, and trust your results**

Note

Beware of your mindset: your results should be credible and honest before being "good".

"Our results are unstable, we have yet to understand why, this is what we tried" is a completely valid answer

Plotting Tools

Plotting tools - Cheetsheet

Name	Use
pandas	Storing and saving tabular data
numpy	Numerical arrays, manipulating data
matplotlib	Basic 2D plots, full control
seaborn	Statistical plots, higher-level API
logging	Logging experiment progress/results
OpenCV	Image processing, animations/videos
ffmpeg	Generating and encoding videos

Lookup the quick reference plotting gallery in the annex!
Both `matplotlib` and `seaborn` provide extensive online galleries.

[Live Example of the matplotlib gallery
https://matplotlib.org/stable/gallery/index.html]

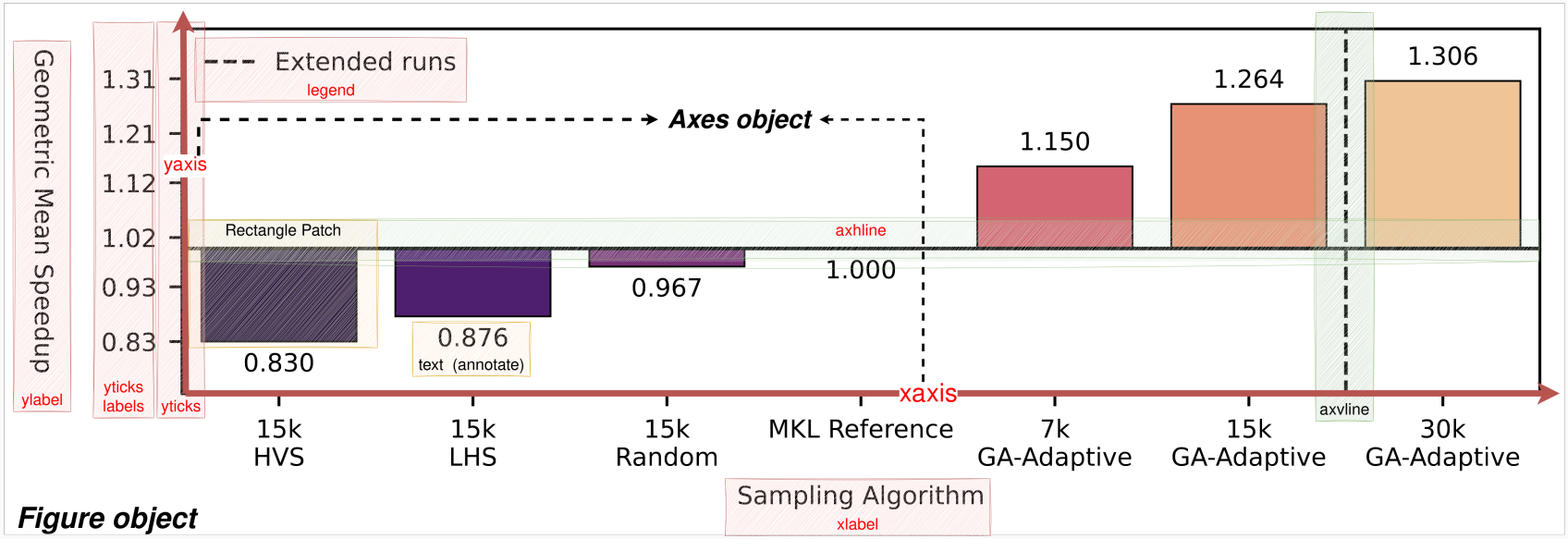
Plotting tools - Matplotlib

Matplotlib is one of the most widely used plotting libraries.
A figure is built hierarchically from nested elements:

```
- Figure (The canvas)
  - (Subfigures)
    - Axes (One or more subplots)
      - Axis (x/y/z scales, ticks, labels)
      - Artists (Lines, markers, text, patches, etc.)
```

- Data is plotted using axis-level functions like `ax.plot`, `ax.histogram`
- Customization occurs at both the Figure and Axes levels
- Complex multi plots layout occur at the Figure level

Plotting tools - Matplotlib



Plotting tools - Matplotlib

```python
import matplotlib.pyplot as plt

x = [0, 1, 2, 3]
y = [2.8, 5.7, 12.5, 14]

# Create a new figure, single axis
# Size is 8 inches by 8 inches, and constrained layout
fig, ax = plt.subplots(figsize=(8, 8), layout="constrained")

# Plot a simple line
ax.plot(x, y, color="red", label="My Algorithm")

# Customize the axes
ax.set_xlabel("Iteration") # Name of the X axis
ax.set_ylabel("Time (s)") # Name of the y axis
# Title of the plot
ax.set_title("Evolution of Time with the number of iteration")

ax.margins(0, 0) # Remove white spaces around the figure
ax.legend(loc="upper right") # Draw the legend in the upper right
    corner

fig.savefig("my_plot.png", dpi=300) # Higher DPI -> bigger image
plt.close() # End the plot and release resources
```

Plotting tools - Matplotlib (Multi axis)

We can easily have multiple plots on the same figure:

```
nrows = 5, ncols = 1
fig, axs = plt.subplots(5, 1, figsize(8 * ncols, 3 * nrows))

ax = axs[0]
ax.plot()
...

ax = axs[1]
ax.plot()
...

fig.tight_layout() # Alternative to constrained layout
fig.savefig("my_multiplot.png", dpi=300)
```

Each axis is its own plot, with its own legend and artists.

Note

Use the reference (https://matplotlib.org/stable/api/index.html) and gallery (https://matplotlib.org/stable/gallery/index.html) extensively !

Plotting tools - Seaborn

Seaborn is an extension of Matplotlib dedicated to statistical visualization:

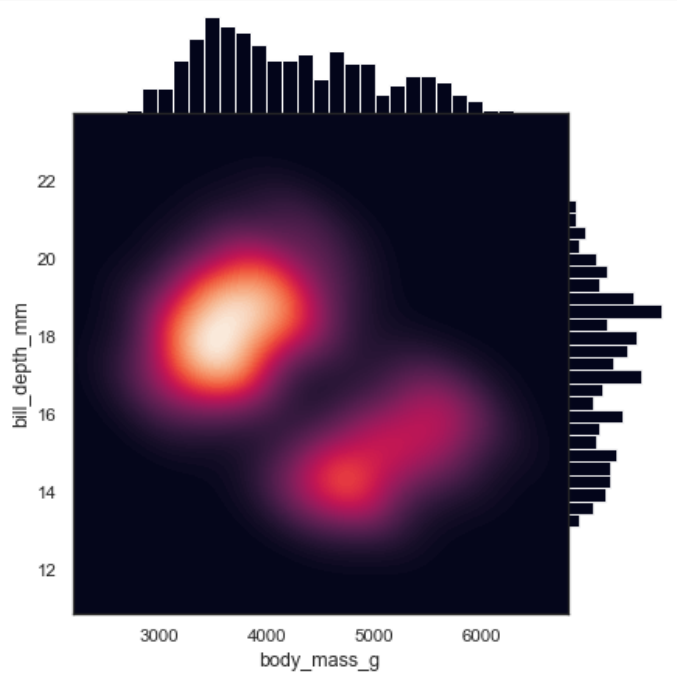


Figure 9: https://seaborn.pydata.org/examples/index.html

It's useful for histograms, bar charts, kdeplots, scatterplots, and is overall a very good companion library.

Plotting tools - Seaborn

```python
import matplotlib.pyplot as plt
import seaborn as sns
import pandas as pd
import numpy as np

df = pd.read_csv(...) # Read the dataframe from somewhere

fig, ax = plt.subplots(figsize=(8, 8), layout="constrained")

# We must pass the axis to plot on as an argument
sns.kdeplot(data=df, x="Time", label="Algorithm", color="red",
    fill=True, ax=ax)

ax.set_title("Distribution of Execution time for the algorithm")
ax.margins(0, 0)
ax.set_xlabel("Time (s)", fontweight="bold")
ax.set_ylabel("Density", fontweight="bold")

ax.set_xticks(np.linspace(df["Time"].min(), df["Time"].max(), 10)
# Format the x axis ticks: `3.25s`
ax.xaxis.set_major_formatter(StrMethodFormatter("{x:.2f}s"))

fig.savefig("my_distribution.png")
```

https://matplotlib.org/stable/gallery/ticks/tick-formatters.html

Profiling

Profiling - Motivation

- HPC codes are massive, complex and heterogeneous
- Humans are **bad** at predicting bottlenecks
- Don't blindly optimize everything
- Profiling guides optimization

Remember: **Always profile first**.

Profiling - Amdahl's law

$$\text{Speedup} = \frac{1}{1 - f + \frac{f}{S}}$$

Where f is the fraction of program improved, and S is the speedup on that fraction.

Example:

- I have optimized 80% of my application, with a speedup of x10
- In total, my application is now $\frac{1}{0.2+(0.8/10)} = 3.57\times$ faster

The 20% are a bottleneck !

Profiling - Steps

1. Where (Hotspots) ?

- What functions are we spending time/energy in ?
- What **call-tree** are we spending time/energy in ?

2. Why ?

- Arithmetic density, memory access patterns
- Cache misses, branch misspredictions, vectorization efficieny (Hardware counters)

3. What goal ?

- Should I optimize for speed ? For energy ? Memory footprint ?
  - What about cold storage size/compression ?
- Do I have constraints (i.e. limited memory) ?
- Should I optimize or switch algorithm ?

Profiling - Time

It's rather easy to benchmark a single function using a (high-resolution monotonic) clock:

```
begin = time.now()
my_function()
end = time.now()
elapsed = end - begin
```

Very simple way to evalute a function cost

Profiling - Time (Stability)

But we have to account for noise:

```
for _ in range(NWarmup):
  my_function()

times = []
for _ in range(NMeta):
  begin = time.perf_counter()
  my_function()
  times.append(time.perf_counter() - begin)

median = np.median(times)
std = np.std(times)
print(f"Time: {median} +/- {std}")
```

We must check that our measures are valid !

Profilers - Introduction

Full application -> Thousands of functions to measure !

- Profilers are tools to automate this
- Two main types:
  - Sampling: Pause the program and log where the program is (Costly functions -> More samples !)
  - Instrumentation: Modify the program to automatically add timers

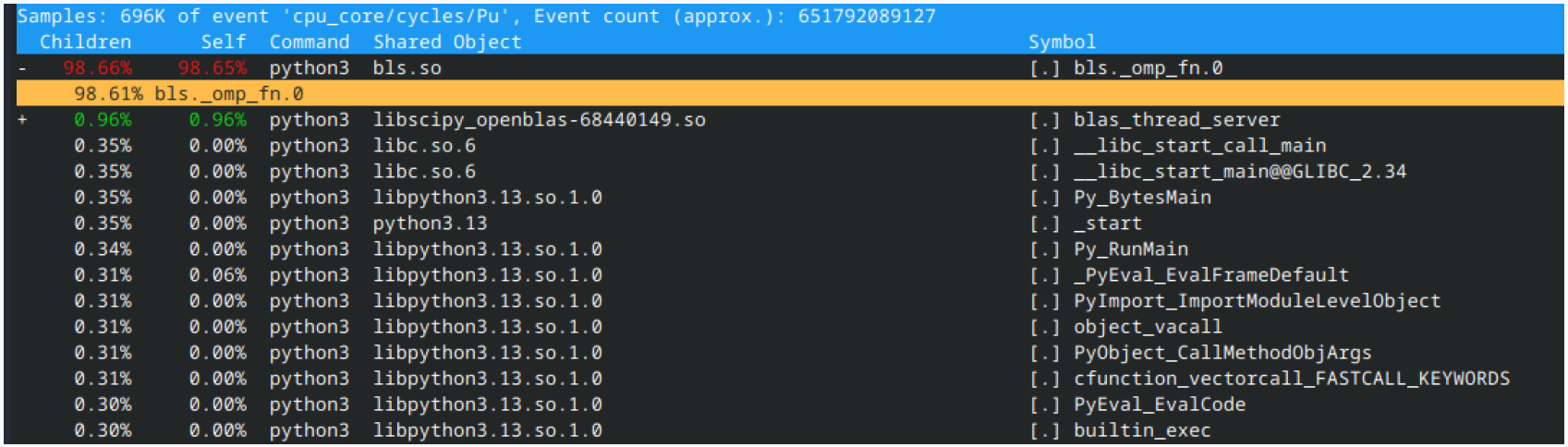
Profilers can also check for thread usage, vectorization, memory access, etc.

Perf - Record

Linux Perf is a powerful and versatile profiler:

```
perf record -g -- python3 ./scripts/run_bls.py kepler-8
[ perf record: Woken up 255 times to write data ]
[ perf record: Wrote 85.474 MB perf.data (1220354 samples) ]

pert report perf.out
```



```
Samples: 696K of event 'cpu_core/cycles/Pu', Event count (approx.): 651792089127
  Children      Self  Command  Shared Object                                  Symbol
-   98.66%    98.65%  python3  bls.so                                         [.] bls._omp_fn.0
     98.61% bls._omp_fn.0
+    0.96%     0.96%  python3  libscipy_openblas-68440149.so                  [.] blas_thread_server
     0.35%     0.00%  python3  libc.so.6                                      [.] __libc_start_call_main
     0.35%     0.00%  python3  libc.so.6                                      [.] __libc_start_main@@GLIBC_2.34
     0.35%     0.00%  python3  libpython3.13.so.1.0                          [.] Py_BytesMain
     0.35%     0.00%  python3  python3.13                                     [.] _start
     0.34%     0.00%  python3  libpython3.13.so.1.0                          [.] Py_RunMain
     0.31%     0.06%  python3  libpython3.13.so.1.0                          [.] _PyEval_EvalFrameDefault
     0.31%     0.00%  python3  libpython3.13.so.1.0                          [.] PyImport_ImportModuleLevelObject
     0.31%     0.00%  python3  libpython3.13.so.1.0                          [.] object_vacall
     0.31%     0.00%  python3  libpython3.13.so.1.0                          [.] PyObject_CallMethodObjArgs
     0.31%     0.00%  python3  libpython3.13.so.1.0                          [.] cfunction_vectorcall_FASTCALL_KEYWORDS
     0.30%     0.00%  python3  libpython3.13.so.1.0                          [.] PyEval_EvalCode
     0.30%     0.00%  python3  libpython3.13.so.1.0                          [.] builtin_exec
```

It's a great tool to quickly get a Tree stack without any dependencies.

Profiling - Hardware counters

In reality, perf is not realy a profiler !

- The Linux Perf API can be used to access many hardware counters
- Perf record is just one usage of perf

Most CPUs/GPUs have hardware counters that monitors different events:

- Number of cycles
- Number of instructions
- Number of memory access
- RAPL

Profiling - Perf for Hardware counters

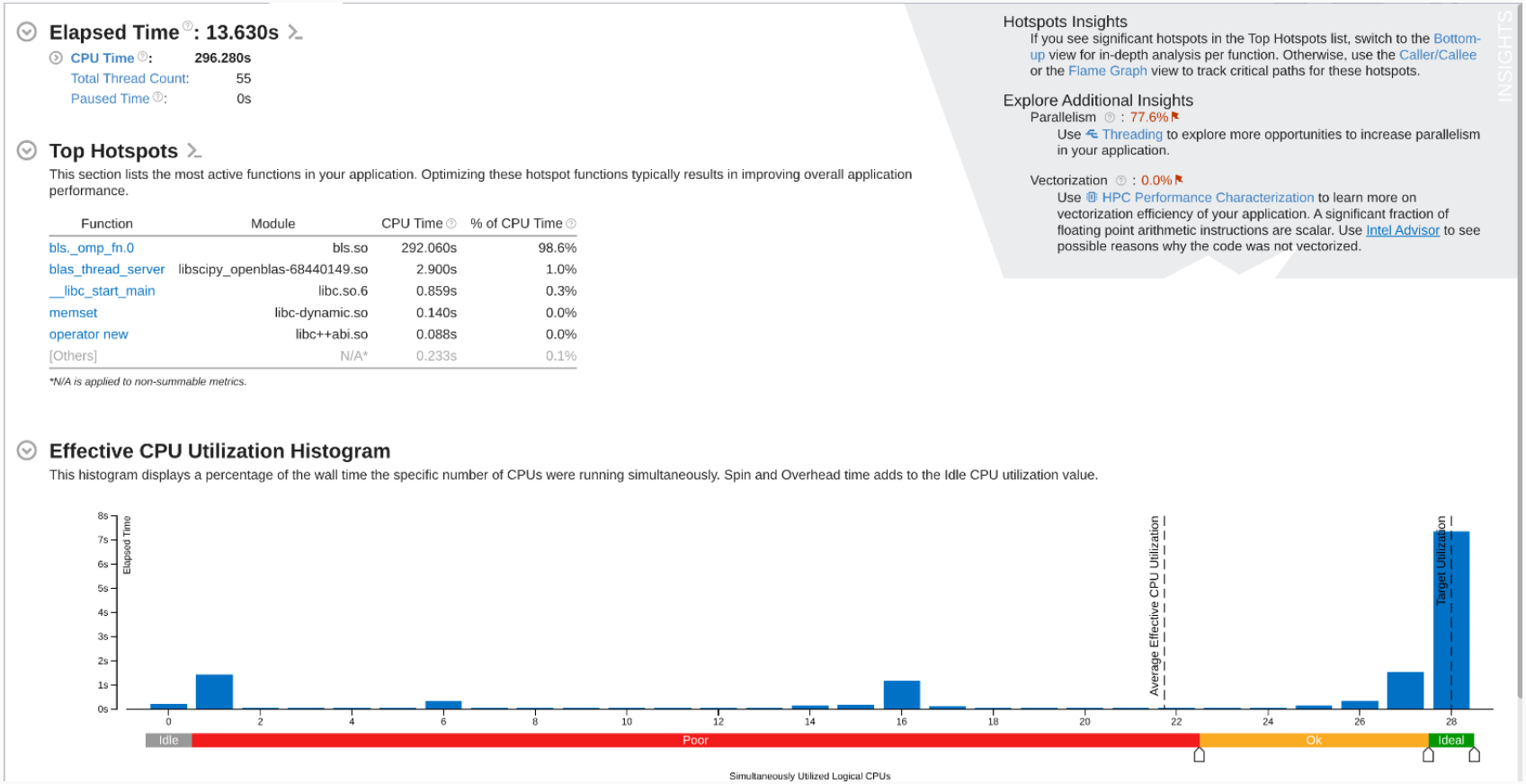
```
perf stat -e cycles,instructions python3 ./scripts/run_bls.py
    kepler-8
{'period': 3.520136229965055, 'duration': 0.1166267356998523 4, '
    phase': 0.43, 'depth': 0.004983530583444806, 'power':
    0.02886167865134445 2}

 Performance counter stats for 'python3 ./scripts/run_bls.py
    kepler-8':

   962,187,248,452      cpu_atom/cycles/
                                 (43.66%)
 1,119,319,677,606      cpu_core/cycles/
                                 (56.34%)
 3,547,146,665,075      cpu_atom/instructions/           #
    3.69  insn per cycle              (43.66%)
 2,837,633,772,530      cpu_core/instructions/           #
    2.54  insn per cycle              (56.34%)

      12.507192456 seconds time elapsed
```

The Intel VTune profiler is more complex but more self-contained than perf:



Elapsed Time: 13.630s

CPU Time: 296.280s
Total Thread Count: 55
Paused Time: 0s

Top Hotspots

This section lists the most active functions in your application. Optimizing these hotspot functions typically results in improving overall application performance.

Function	Module	CPU Time	% of CPU Time
bls._omp_fn.0	bls.so	292.060s	98.6%
blas_thread_server	libscipy_openblas-68440149.so	2.900s	1.0%
__libc_start_main	libc.so.6	0.859s	0.3%
memset	libc-dynamic.so	0.140s	0.0%
operator new	libc++abi.so	0.088s	0.0%
[Others]	N/A*	0.233s	0.1%

*N/A is applied to non-summable metrics.

Hotspots Insights

If you see significant hotspots in the Top Hotspots list, switch to the Bottom-up view for in-depth analysis per function. Otherwise, use the Caller/Callee or the Flame Graph view to track critical paths for these hotspots.

Explore Additional Insights

Parallelism : 77.6%

Use Threading to explore more opportunities to increase parallelism in your application.

Vectorization : 0.0%

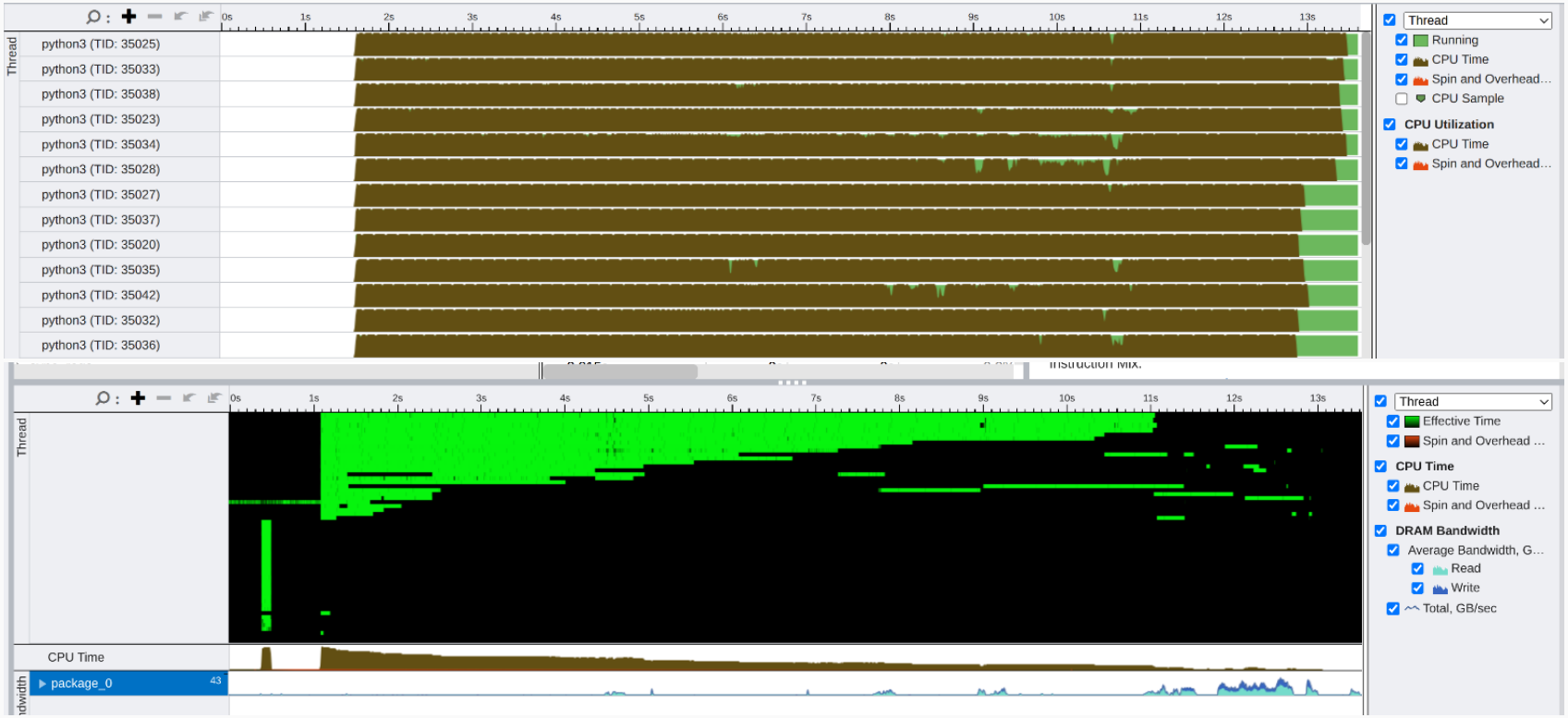
Use HPC Performance Characterization to learn more on vectorization efficiency of your application. A significant fraction of floating point arithmetic instructions are scalar. Use Intel Advisor to see possible reasons why the code was not vectorized.

INSIGHTS

Effective CPU Utilization Histogram

This histogram displays a percentage of the wall time the specific number of CPUs were running simultaneously. Spin and Overhead time adds to the Idle CPU utilization value.

VTune - CPU Usage



VTune - HPC Performance

VTune has multiple collection mode:

Memory Bound: 1.0% of Pipeline Slots

- **Performance-core (P-core):**
  - **Memory Bound:** 1.0% of Pipeline Slots
- **Efficient-core (E-core):**
  - **Memory Bound:** 0.3% of Clockticks

*N/A is applied to metrics with undefined value. There is no data to calculate the metric.

- **Bandwidth Utilization Histogram**

Vectorization: 0.0% of Packed FP Operations

- Instruction Mix:
  - SP FLOPs: 0.0% of uOps
    - Packed: 0.0% from SP FP
    - Scalar: 100.0% from SP FP
  - DP FLOPs: 16.1% of uOps
    - Packed: 0.0% from DP FP
    - Scalar: 100.0% from DP FP
  - x87 FLOPs: 0.0% of uOps
  - Non-FP: 83.9% of uOps

Metrics were collected from Big Cores only.

- **Top Loops/Functions with FPU Usage by CPU Time**

This section provides information for the most time consuming loops/functions with floating point operations.

Function	CPU Time	% of FP Ops	FP Ops: Packed	FP Ops: Scalar	Vector Instruction Set	Loop Type
[Loop@0x1940 in bls._omp_fn.0]	120.926s	16.3%	0.0%	100.0%	SSE2(128)	
[Loop@0x184f in bls._omp_fn.0]	0.106s	3.2%	0.0%	100.0%		
native_write_msr	0.040s	1.6%	0.0%	100.0%		
[Loop@0x1920 in bls._omp_fn.0]	0.029s	10.5%	0.0%	100.0%	SSE(128); SSE2(128)	

*N/A is applied to non-summable metrics.

Other profilers

- MAQAO is a profiler developped by the LIPARAD
- AMD, NVIDIA and ARM have their own profilers for their platforms
- And many, many others (likwid, gprof, etc.)

Usually, we combine a “quick” profiler like gprof/perf record with a more indepth one when needed.

Profiling - Energy

Energy is a growing concern:

- One HPC cluster consume millions of dollars in electricity **yearly**
- ChatGPT and other LLM are computationally intensive:
  - Nvidia GPUs consumes lots of energy

On the flip side, measuring energy is harder than measuring time.

Many actors still focus on execution time only -> Energy is perceived as “Second rank”

Profiling - RAPL

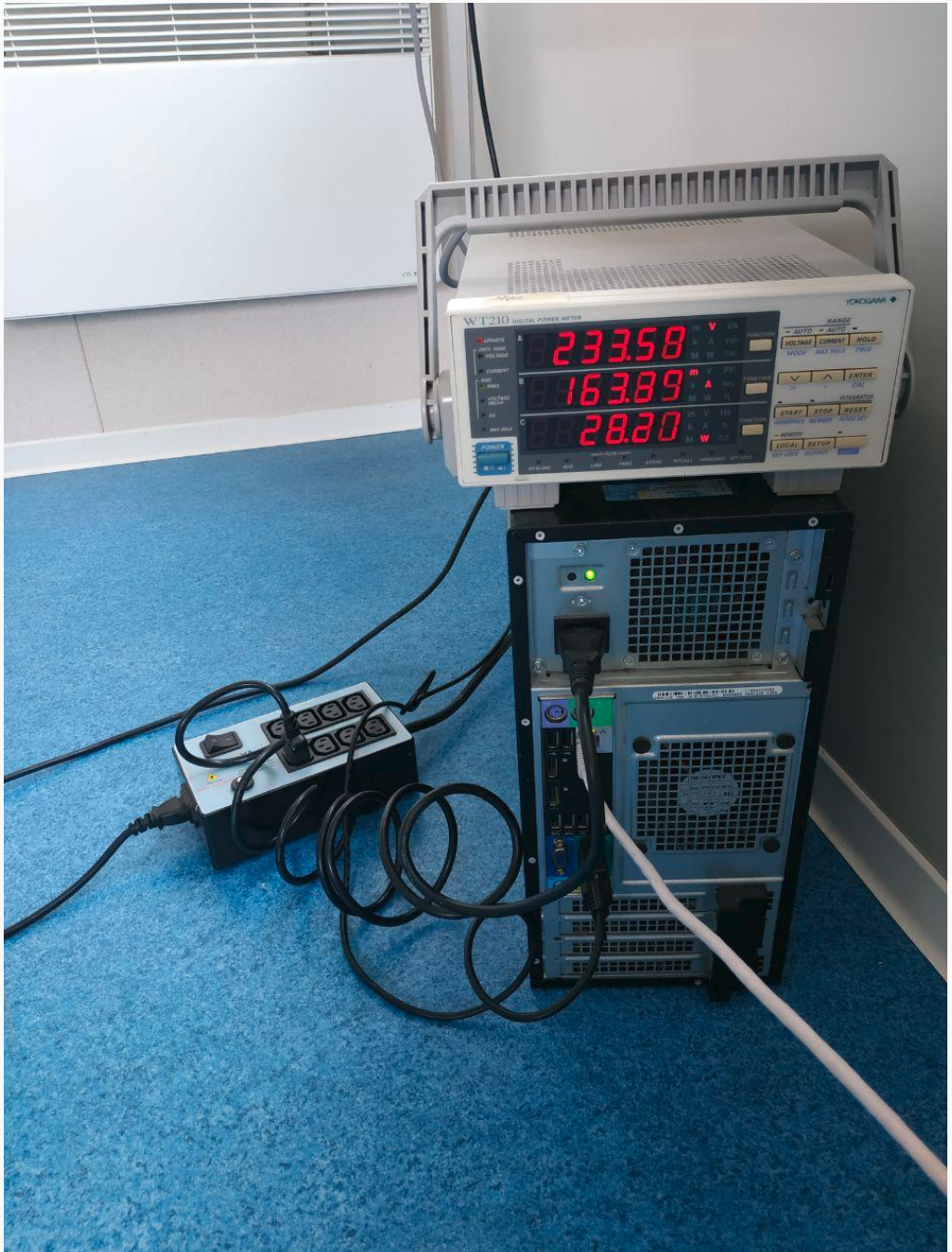
Running Average Power Limit (RAPL) is an x86 hardware counter that monitors energy consumption:

- Energy is tracked at different level
  - Core, Ram, Package, GPU, etc.
- It does not account for secondary power consummers (Fans, Water cooling, etc.)
- RAPL is not event based: The entire machine is measured ! (Background processes, etc.)

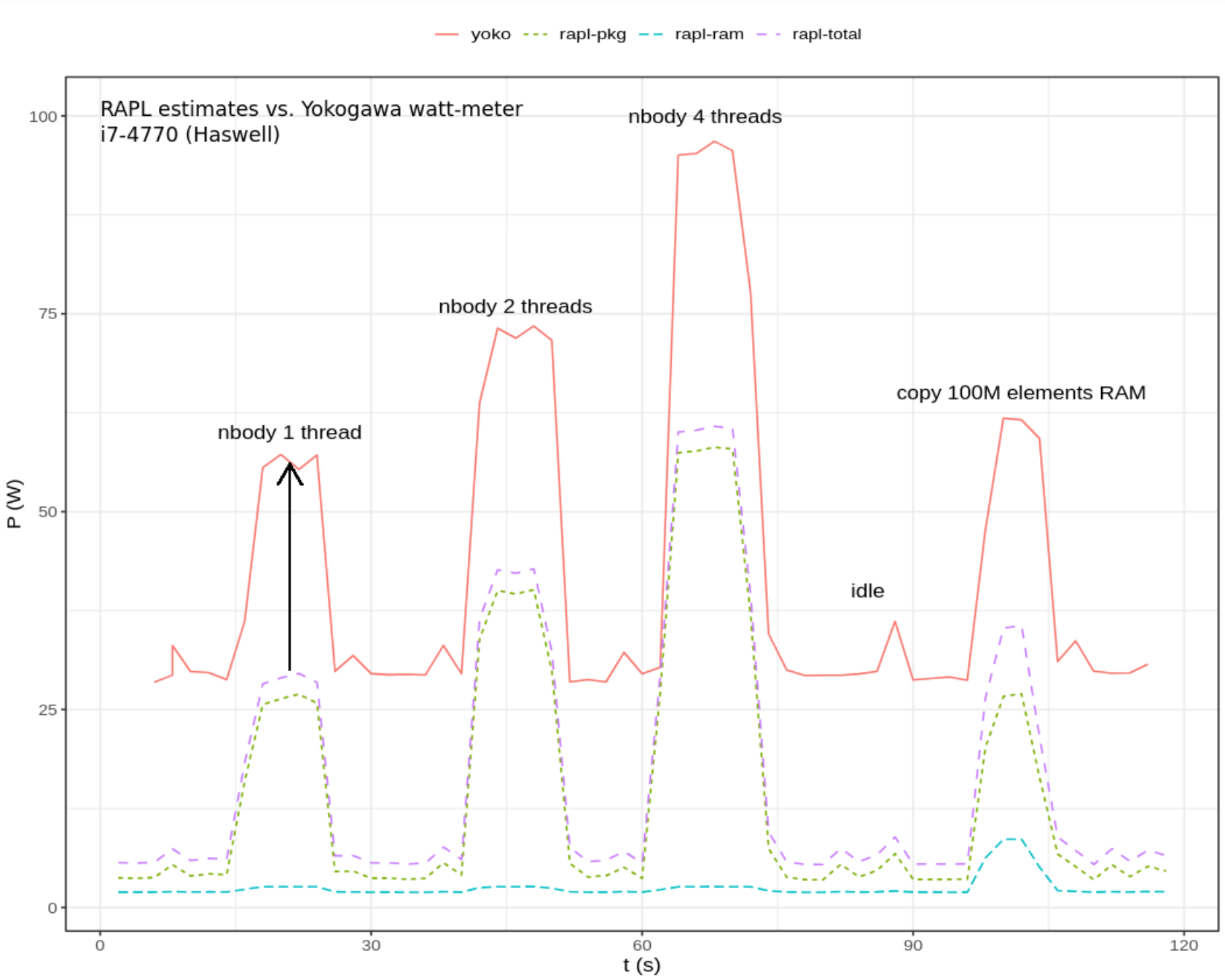
It requires sudo permissions to access (compared to a clock)

```
perf stat -a -j -e power/energy-pkg,power/energy-cores <app>
{"counter-value" : "88.445740", "unit" : "Joules", "event" : "
    power/energy-pkg/", "event-runtime" : 10002168423, "pcnt-
    running" : 100.00}
{"counter-value" : "10.848633", "unit" : "Joules", "event" : "
    power/energy-cores/", "event-runtime" : 10002166697, "pcnt-
    running" : 100.00}
```

Profiling - Watt-Meter



Profiling - RAPL accuracy



Live Demo

Experiment example

Annex/run_experiment.sh

Annex/model_convergence.py