

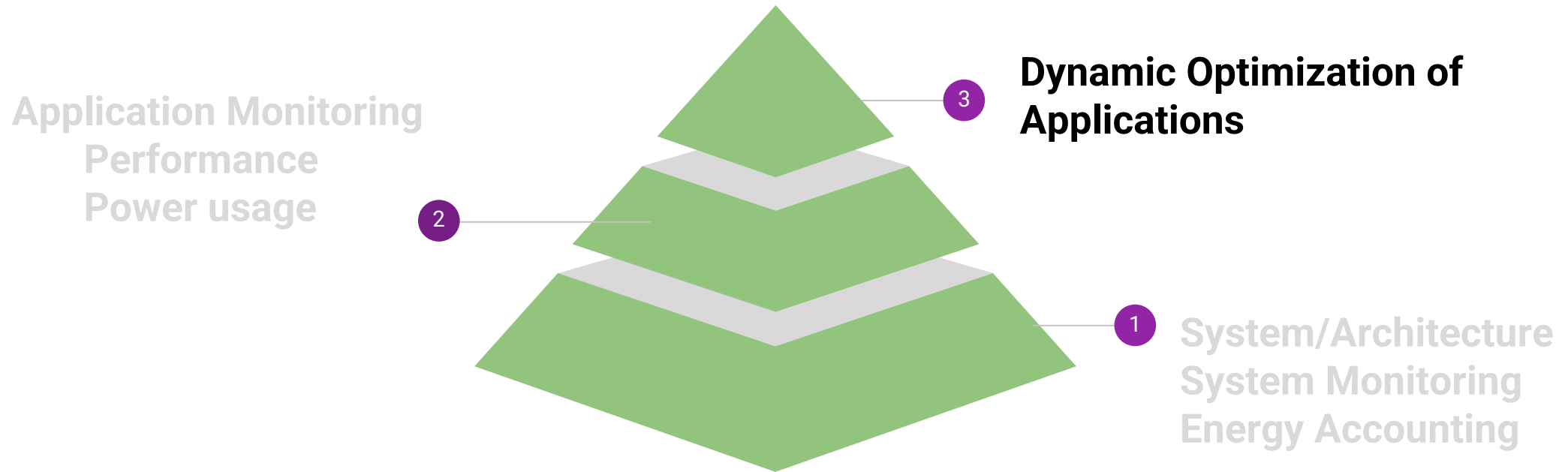
Energy Aware Simulations

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HPC Advisor SURF
April 2024

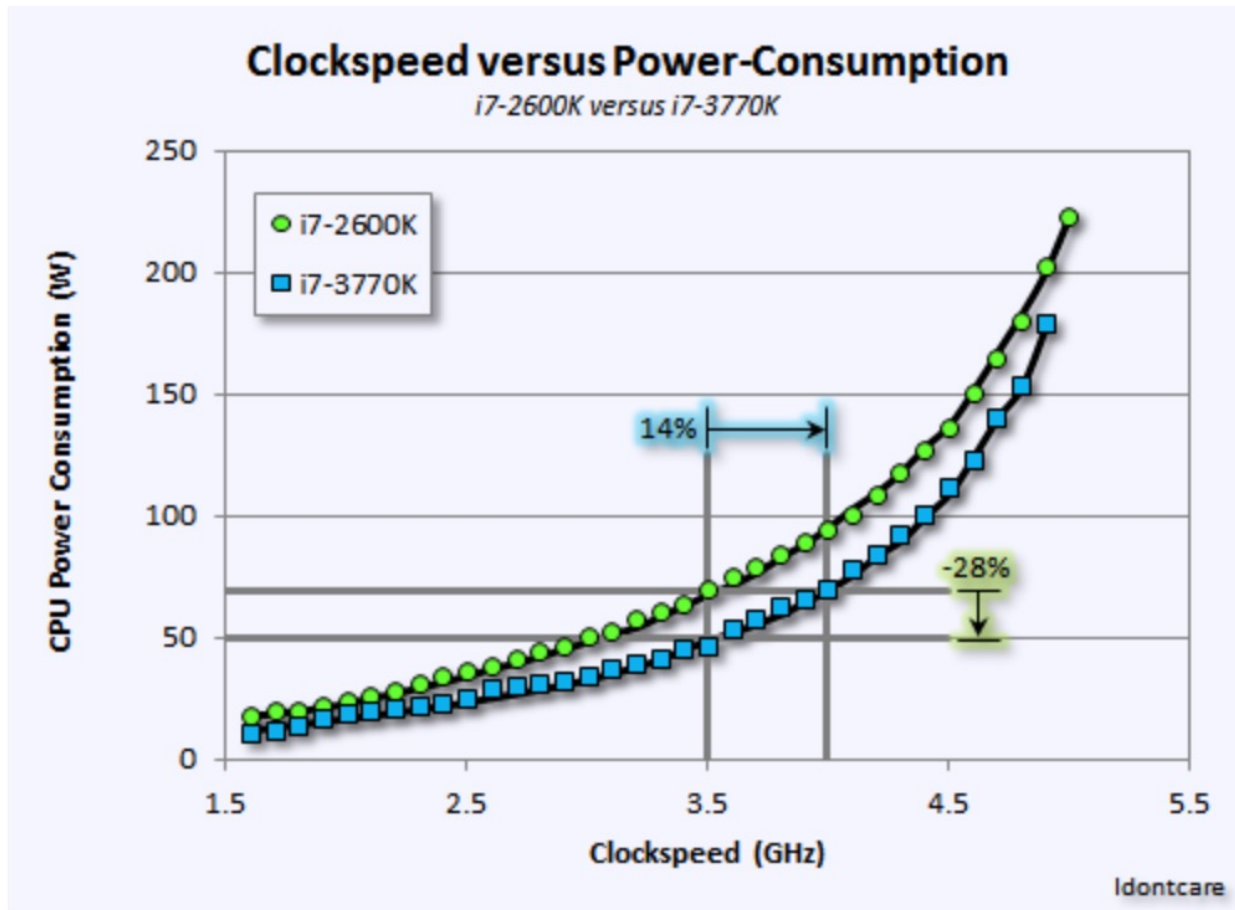
<https://ondemand.snellius.surf.nl/>

<https://github.com/sara-nl/energy-efficient-computing>

Energy-aware focus



Power scales with CPU Frequency

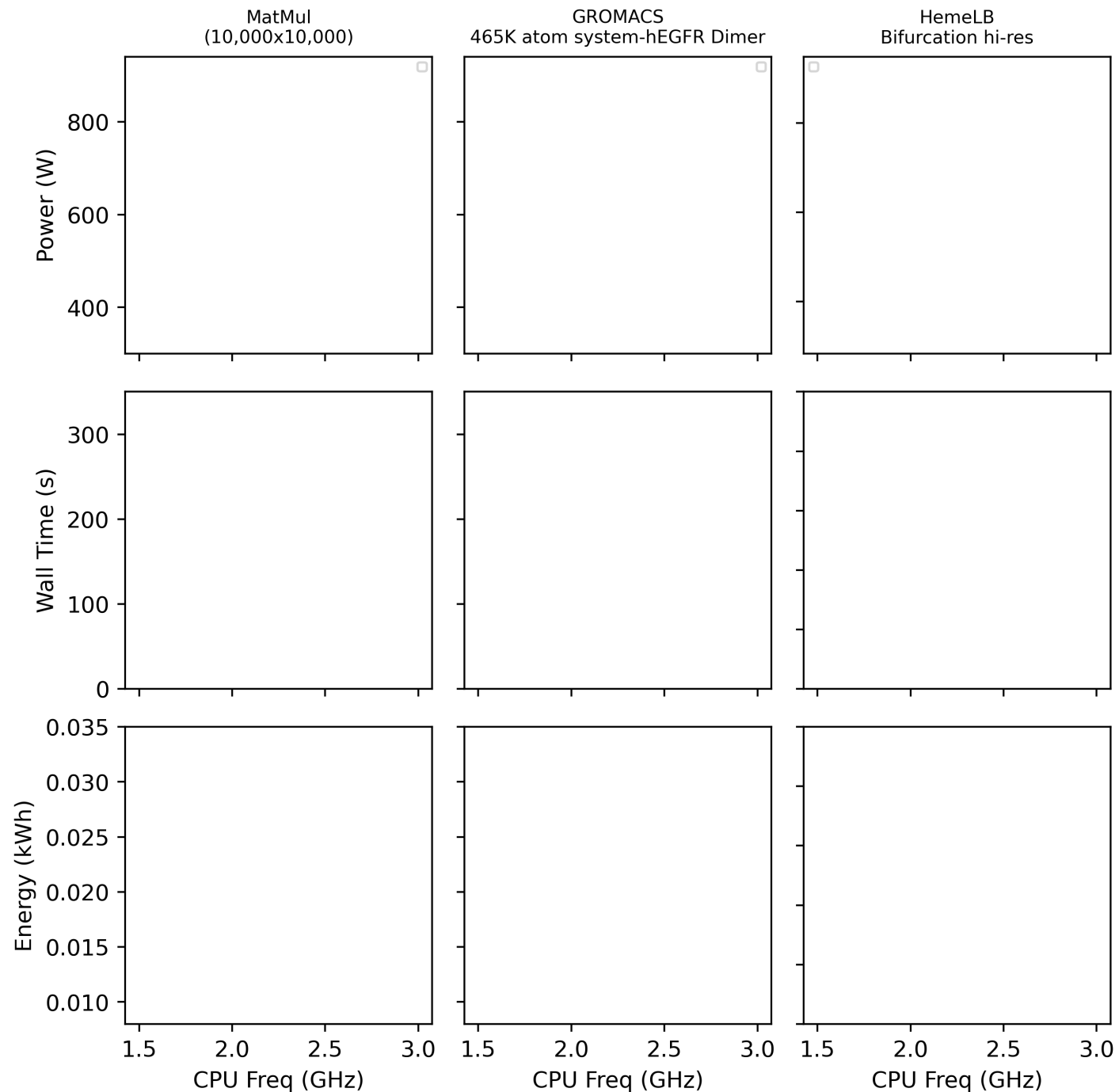


$$Power \propto Freq * Voltage^2$$

Dynamic Voltage Frequency Scaling on Snellius:

To boost, or not too boost, that is the question

- Rome “Zen2” Released 07 August 7 2019
 - Nominal Freq (2.6 Ghz)
- Genoa “Zen4” Released 10 November 2022
 - Nominal Freq (2.4 Ghz)



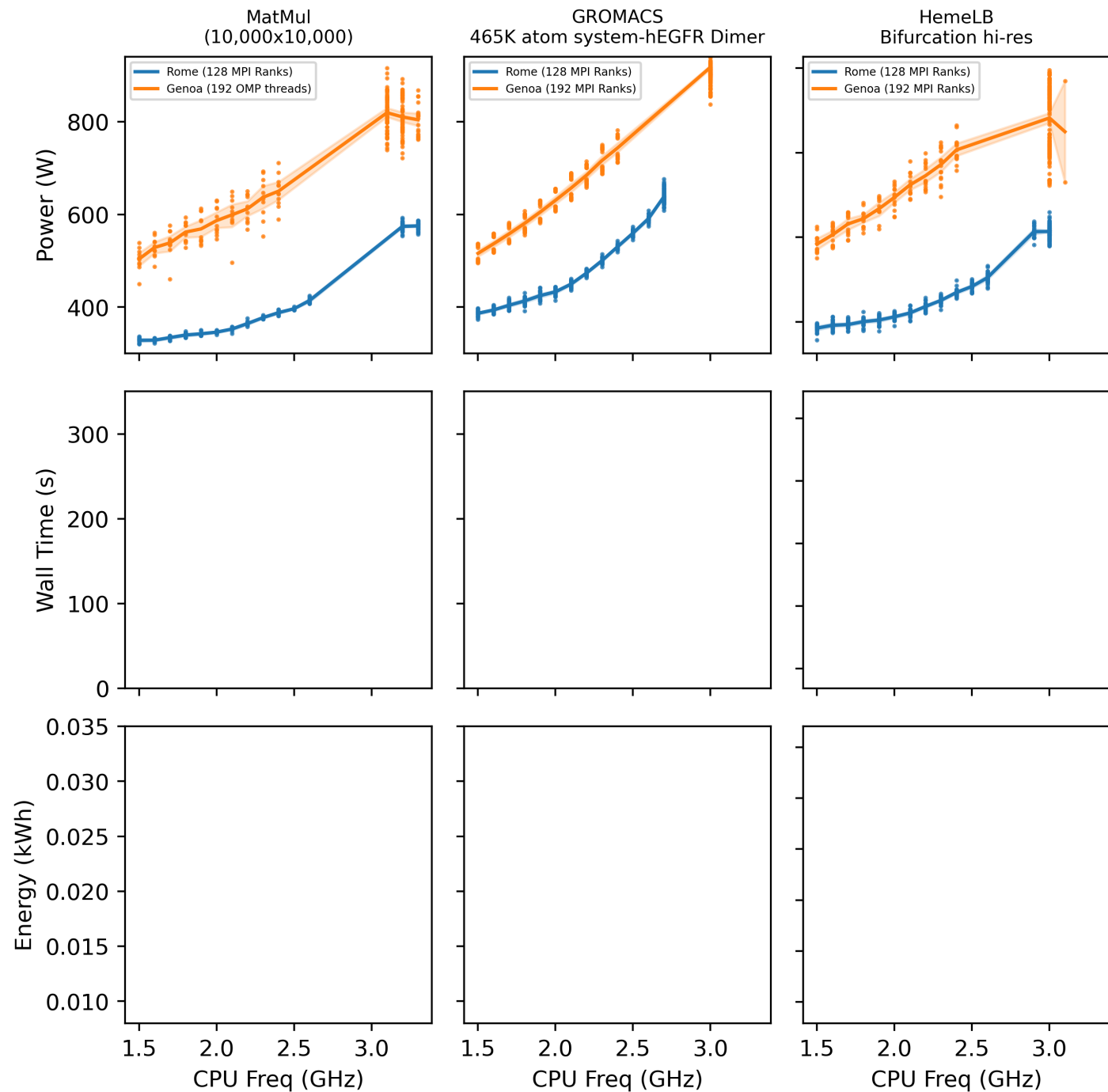
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Observations:

1. Genoa draws more power
2. Each application has a different “power draw signature”



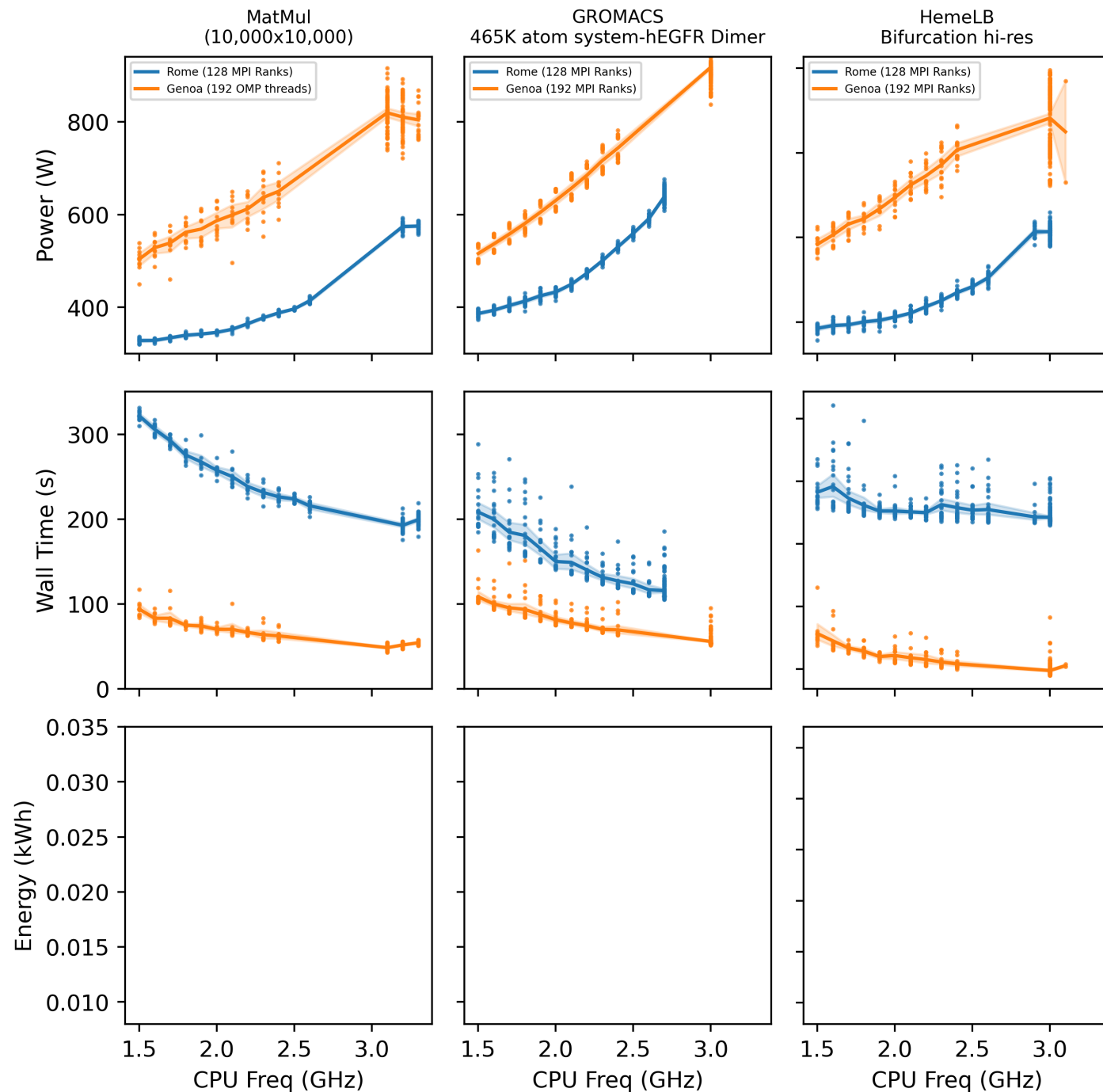
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Observations:

1. Genoa is more performant
 - More Logical cores to devote to problem
2. In the 3 cases, Boost does not have the similar effect in performance vs power draw. i.e. its performance increase is flat as compared to its power draw



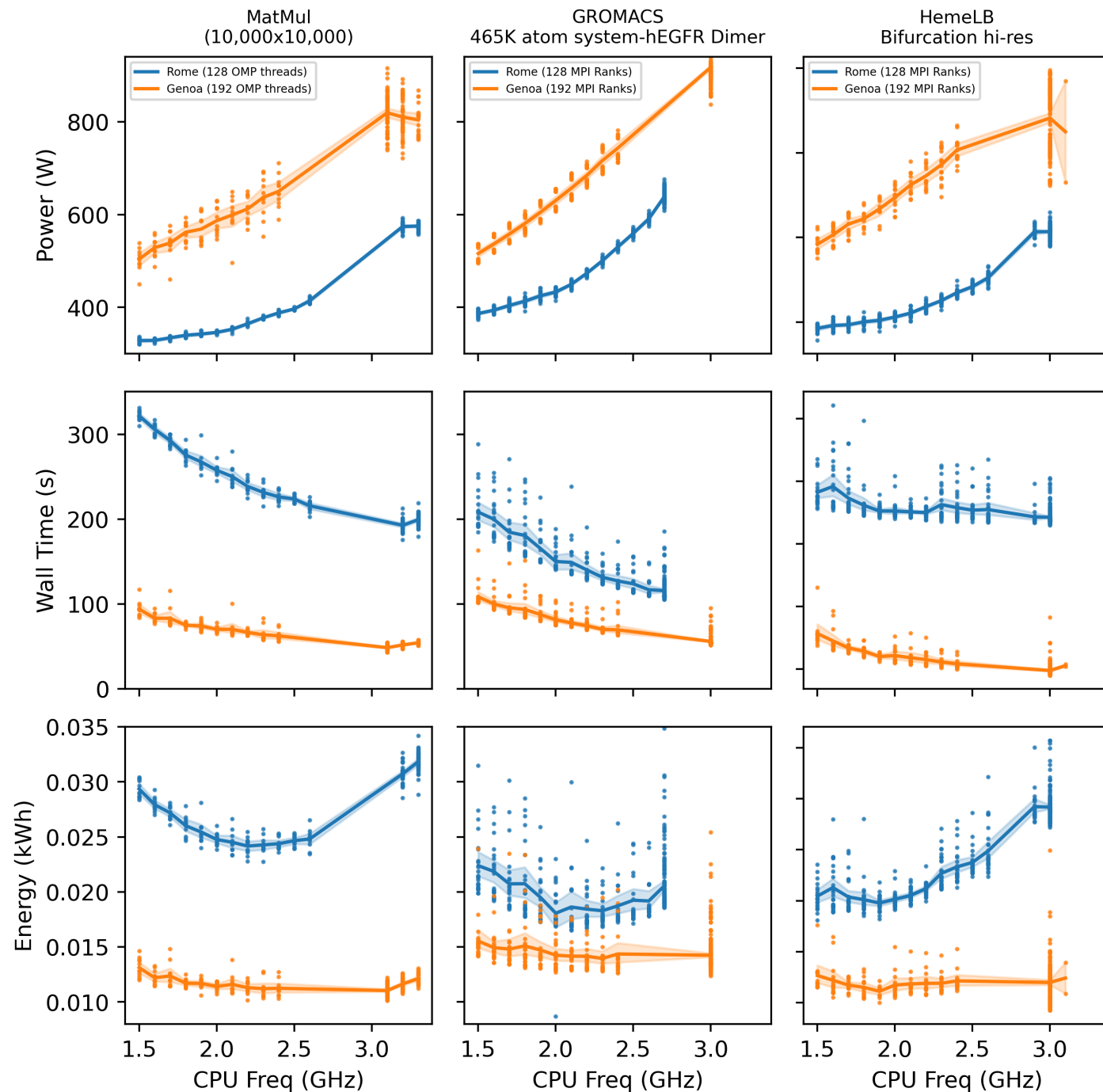
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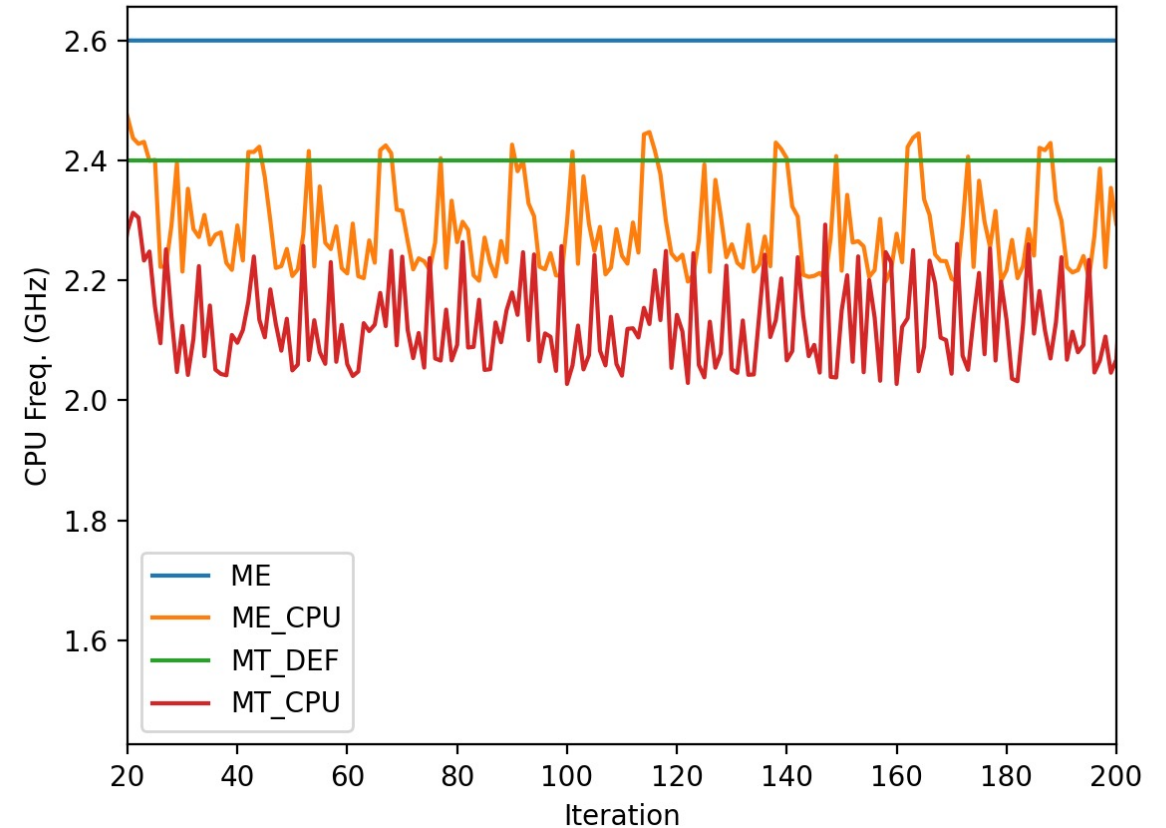
Observations:

1. Genoa is more energy efficient.
2. Each application has its own energy minimum.
3. **DVFS “by hand” is HARD!!!!!!**

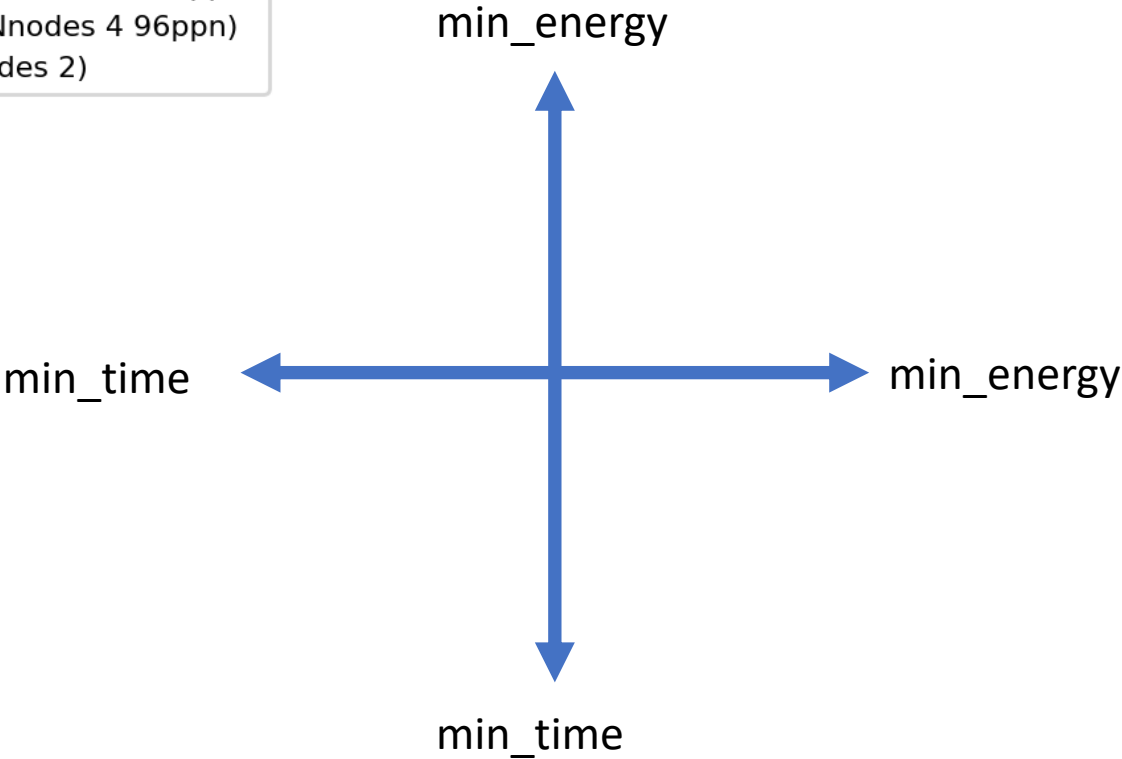
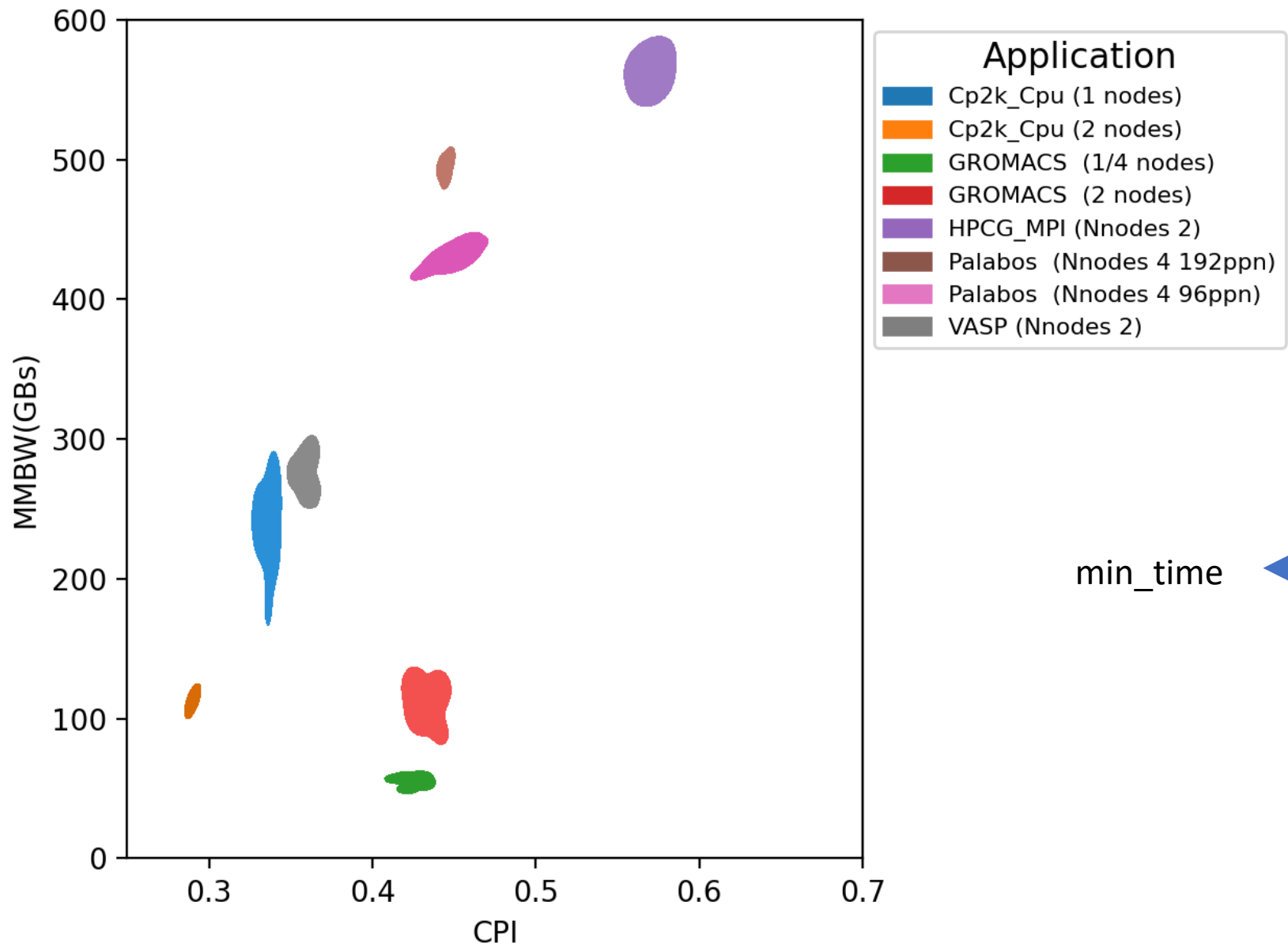


Application Optimization via EAR Policies

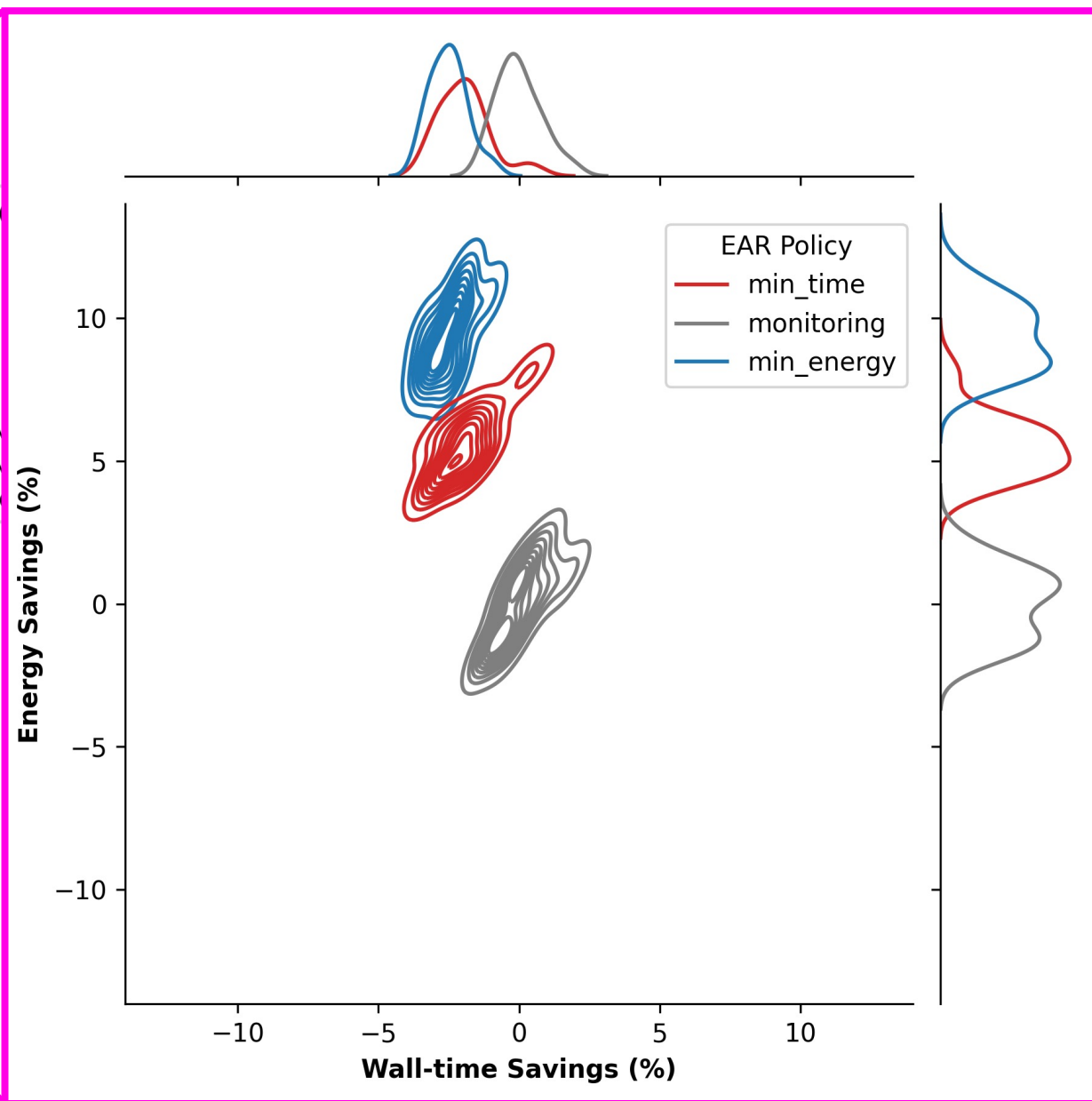
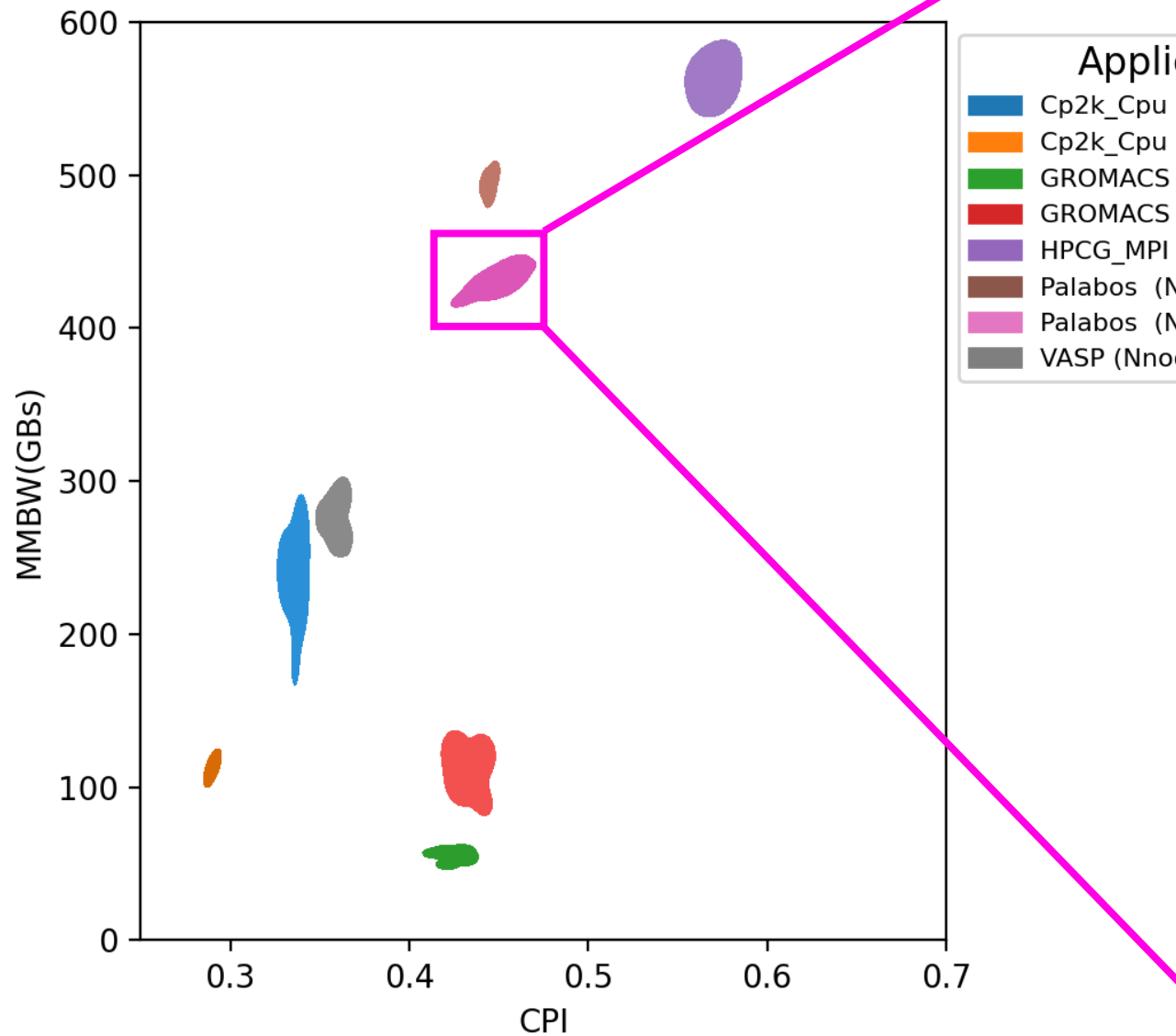
- monitoring
 - Does not affect the CPU Freq.
Only monitors applications.
- min_energy
 - Memory intensive applications
- min_time
 - CPU intensive applications



CPU Application characterization



Application characterization/optimization



Energy Aware Runtime (EAR)

Energy Aware Runtime (EAR) package provides an energy management framework for super computers.



Its Documented and available for use!!!

<https://servicedesk.surf.nl/wiki/display/WIKI/Energy>

Pages / ... / Energy

EAR example: GROMACS

❗ In this short example we will show you how to run a simple GROMACS benchmark with EAR enabled.

GROMACS (<https://www.gromacs.org>)

The HECBioSim Benchmarks (<https://www.hecbiosim.ac.uk/access-hpc/benchmarks>)

GROMACS A free and open-source software suite for high-performance molecular dynamics and output analysis.

HECBioSim benchmark suite consists of a set of simple benchmarks for a number of popular Molecular Dynamics (MD) engines, each of which is set at a different atom count. The benchmark suite currently contains benchmarks for the AMBER, GROMACS, LAMMPS and NAMD molecular dynamics packages.

- 1 Prepare the benchmark input
- 2 Prepare the SLURM job-script
- 3 Get energy and performance metrics report from your job

Prepare the SLURM job-script

Notice all that is special here is Lines 10 and 11. This is how you call the EAR runtime library (EARL).

Read more detail here [Energy Aware Runtime \(EAR\)](#) if you want more information on how EAR works.

```
1  #!/bin/bash
2
3  #SBATCH -p rome
4  #SBATCH -n 128
5  #SBATCH -t 00:20:00
6  #SBATCH --exclusive
7  #SBATCH --output=GROMACS_run.out
8  #SBATCH --error=GROMACS_run.err
9
10 #SBATCH --ear=on
11 #SBATCH --ear-policy=monitoring
12
13 module load 2022
14 module load foss/2022a
15 module load GROMACS/2021.6-foss-2022a
16
17 srun --ntasks=128 --cpus-per-task=1 gmx_mpi mdrun -s hEGFRDimer_benchmark.tpr
```

Obviously you need to submit it to the SLURM scheduler!!

So...

```
sbatch myjobscript.sh
```