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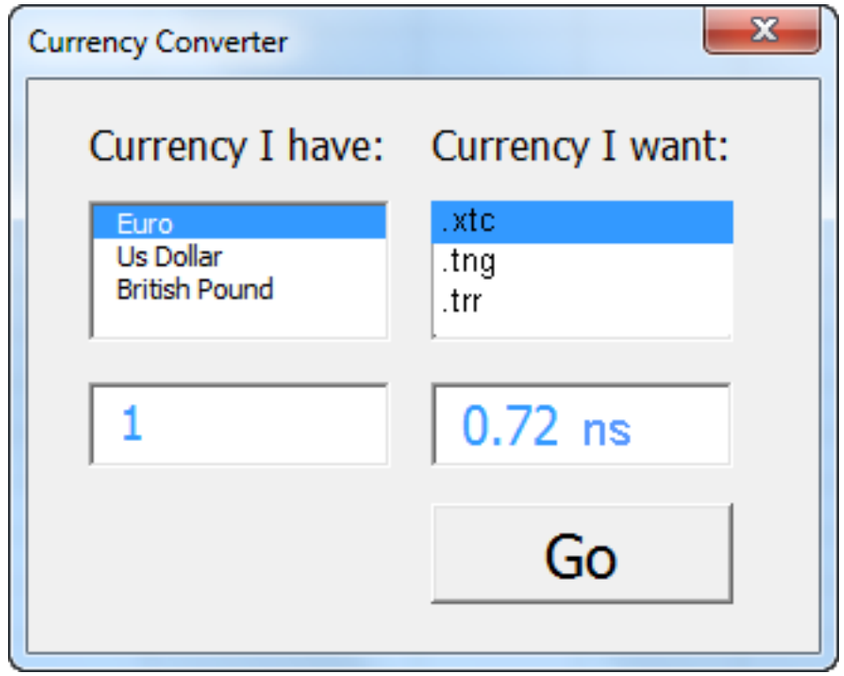
SAVING MONEY WITH GR MACS

Cost-efficient MD simulations 2018

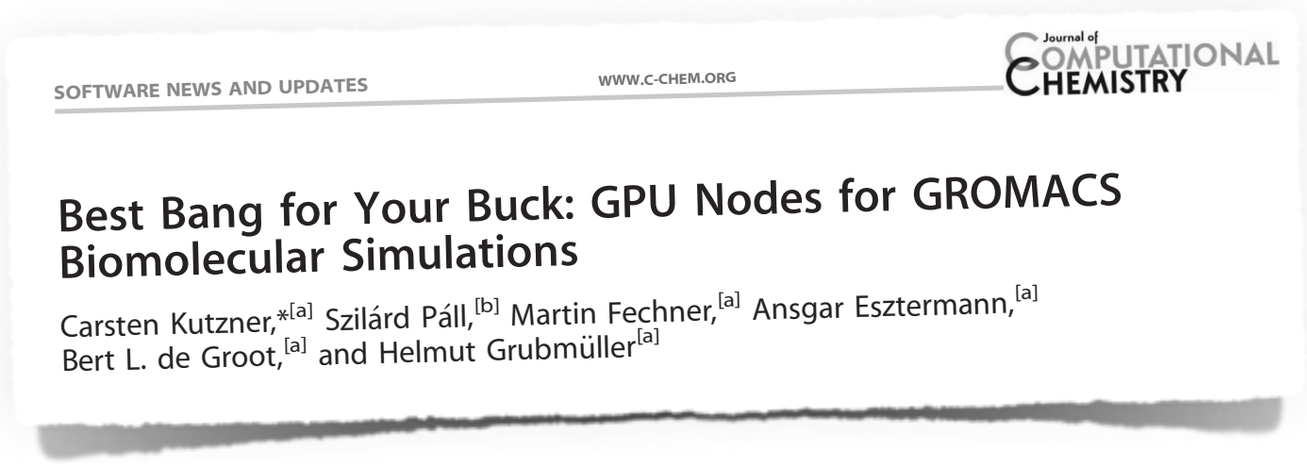
MOTIVATION

- from a fixed hardware budget . . .
- . . . produce as much MD trajectory as possible!
- use tax payer's money responsibly
- therefore, measure MD performance and get hardware prices in an ongoing effort



OUTLINE

- **2014:**



SOFTWARE NEWS AND UPDATES WWW.C-CHEM.ORG Journal of COMPUTATIONAL CHEMISTRY

Best Bang for Your Buck: GPU Nodes for GROMACS Biomolecular Simulations

Carsten Kutzner,*[a] Szilárd Páll,[b] Martin Fechner,[a] Ansgar Esztermann,[a] Bert L. de Groot,[a] and Helmut Grubmüller[a]

- **RECAP: what were our conclusions in 2014/15?**

- **UPDATE: hardware & software developments + their impact**

WHAT IS THE 'OPTIMAL' HARDWARE TO BUY?

WHAT DO YOU WANT?

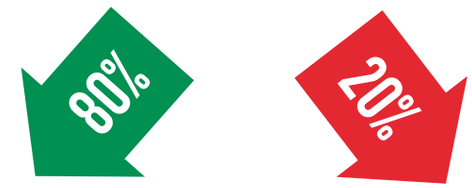
general-purpose cluster for all kinds of applications

- large RAM
  GROMACS uses 250 MB - 1 GB of CPU RAM per process
- nodes connected by a high-performance network
- double-prec. GPU performance
- large GPU memory
  even a 2M atom system requires only 225 MB GPU RAM

WHAT CAN WE SPARE?

maximize cost-efficiency by specialization

- GROMACS only



max. sampling, many separate simulations

single long trajectories

WE OPTIMIZE FOR HIGH THROUGHPUT

run these @ national HPC centers

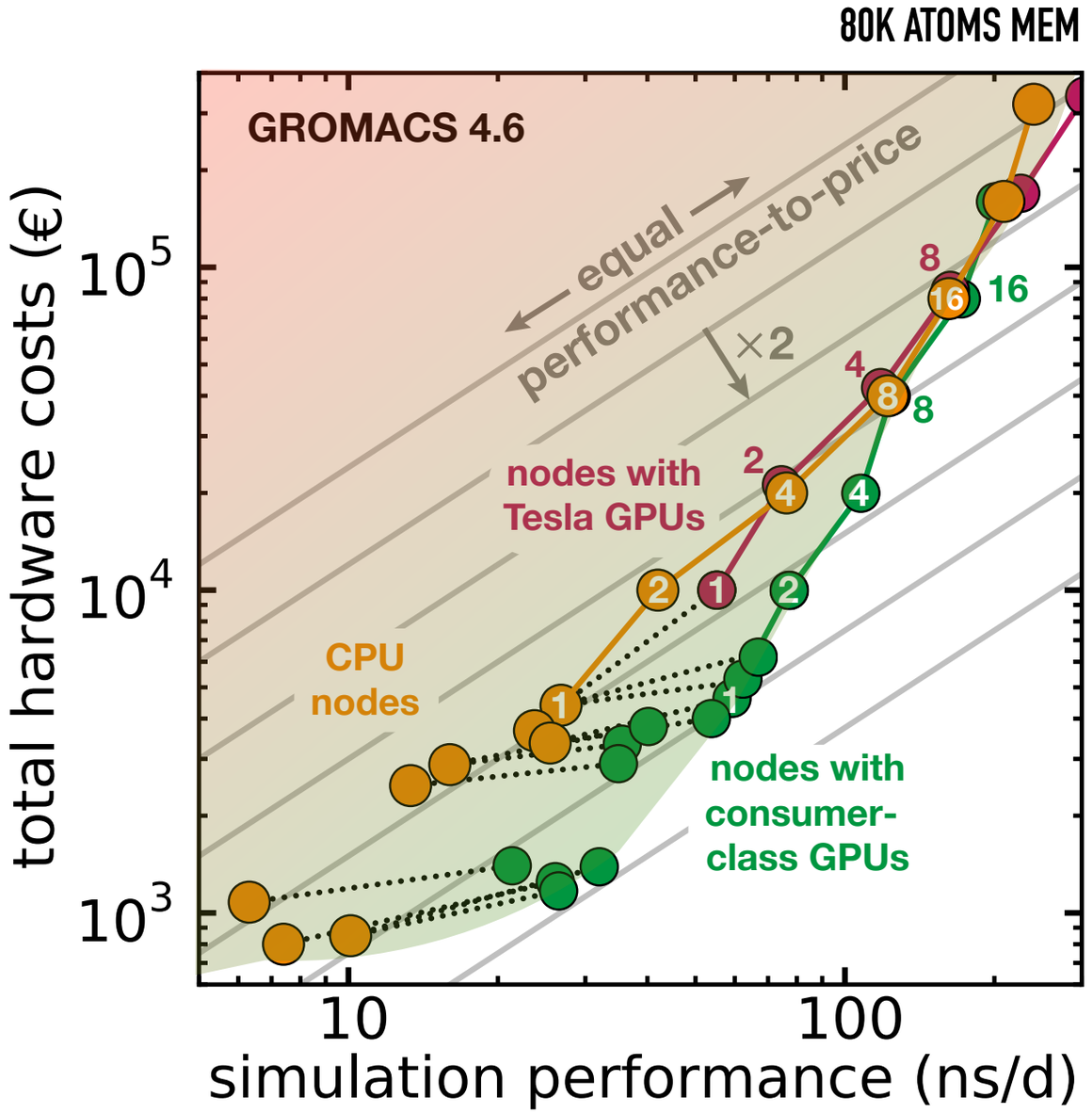
FIND OPTIMAL HARDWARE FOR GROMACS!

Our criteria:

1. high performance-to-price (P/P) ratio
2. low energy consumption
3. reasonably high single-node performance
4. low rack space requirements

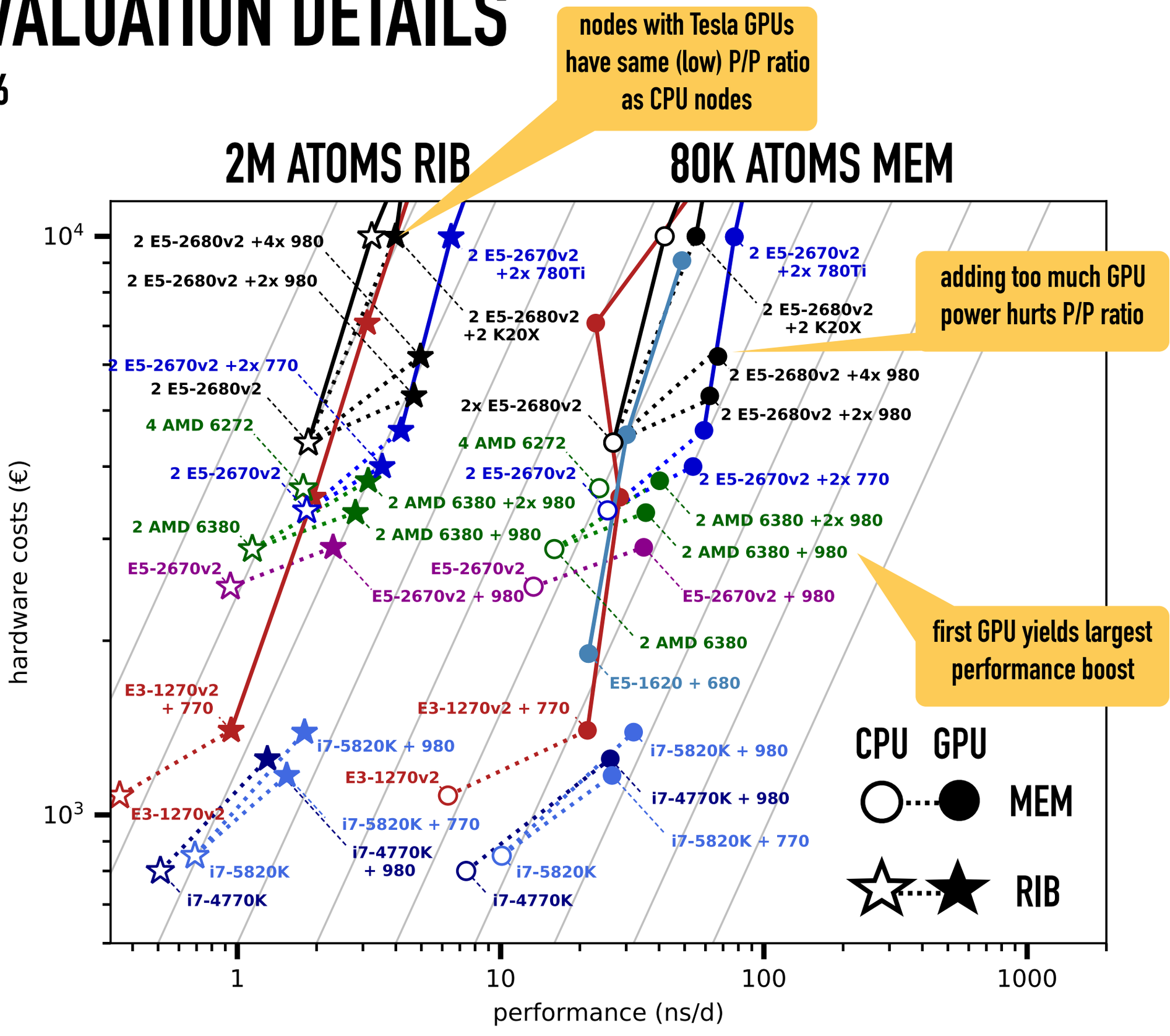
2014 EVALUATION SUMMARY

- get prices + benchmark GROMACS performance for >50 hardware configurations
- 12 CPU types + 13 GPU types
- 2 benchmark systems:
  - MEM 80k atoms
  - RIB 2 M atoms
- on each hardware determined fastest settings for running one simulation
  - # MPI ranks
  - # OpenMP threads
  - # separate PME ranks



2014 EVALUATION DETAILS

GROMACS 4.6



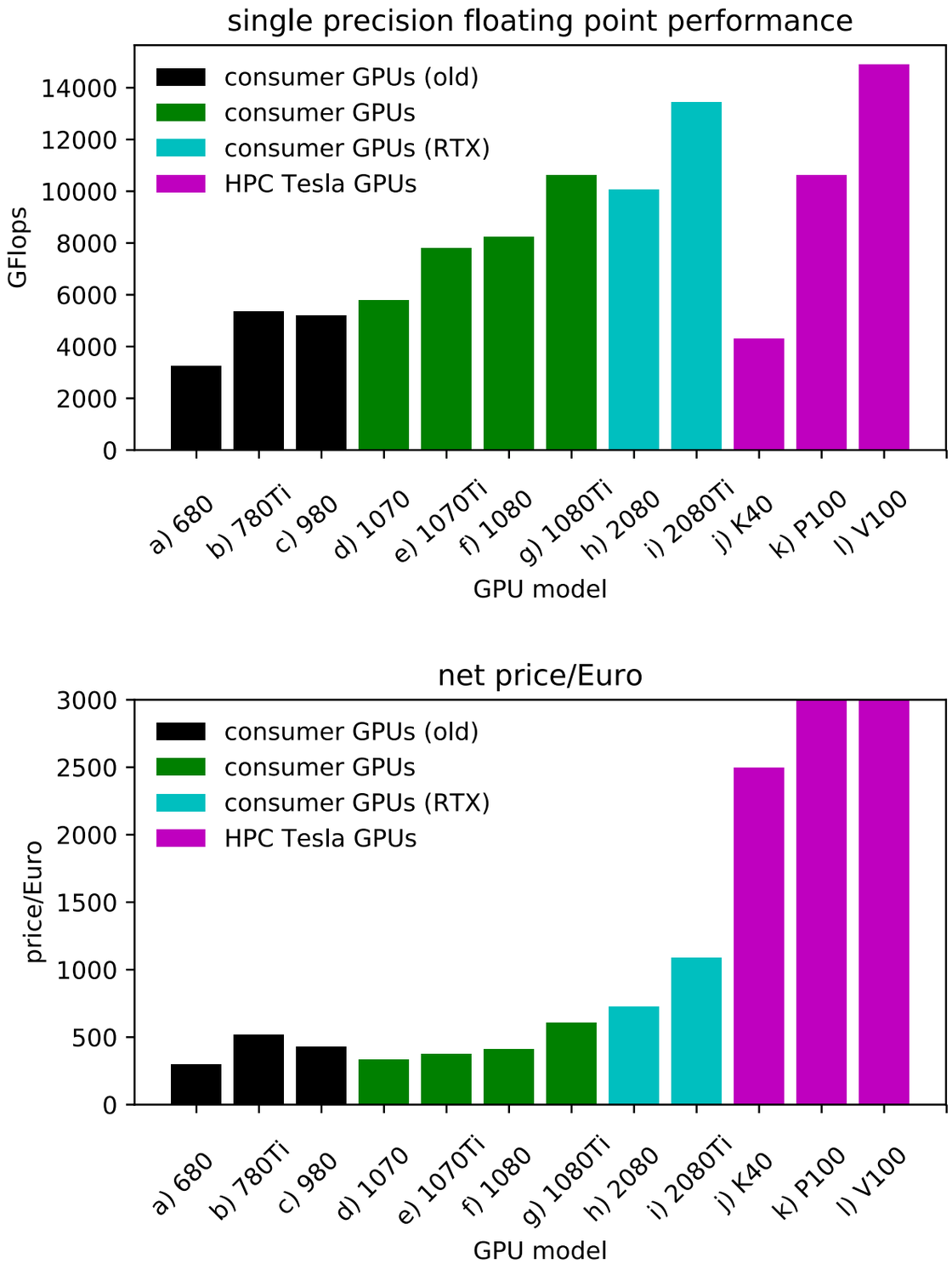
2018
WHAT'S NEW?

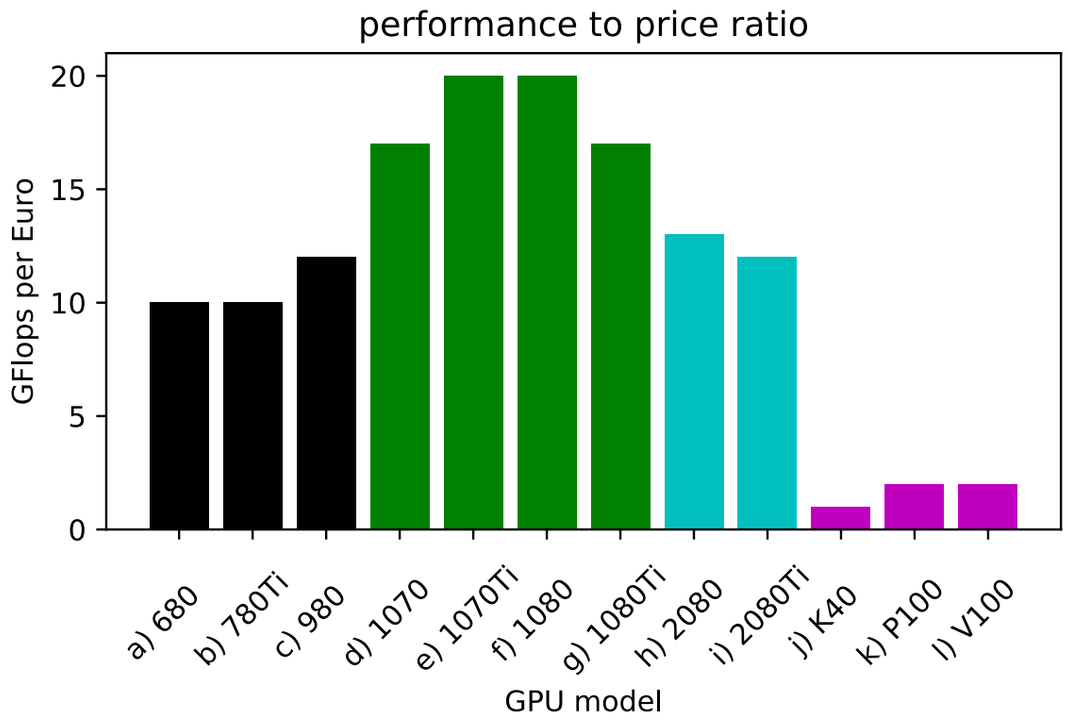
1. **Hardware:**
   GPUs with higher performance

2. **Software:**
   PME can be offloaded to the GPU
   (among many other features!)

3. **Benchmarks:**
   (Slight) change of protocol

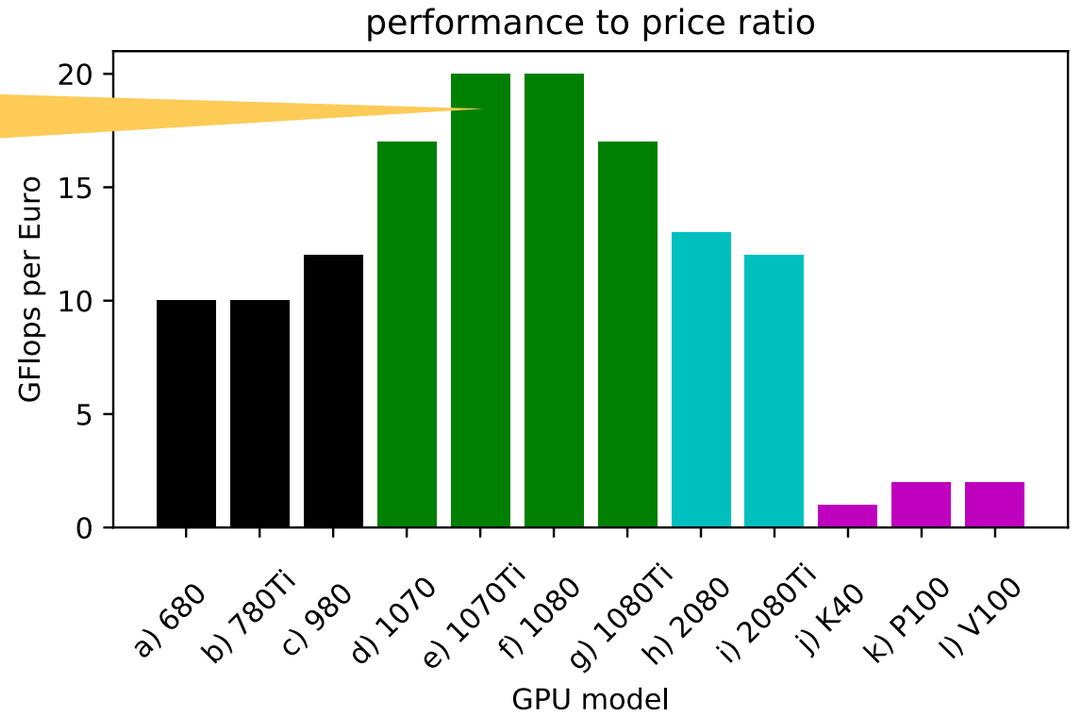
1. HARDWARE DEVELOPMENTS— GPUS 2014…2018

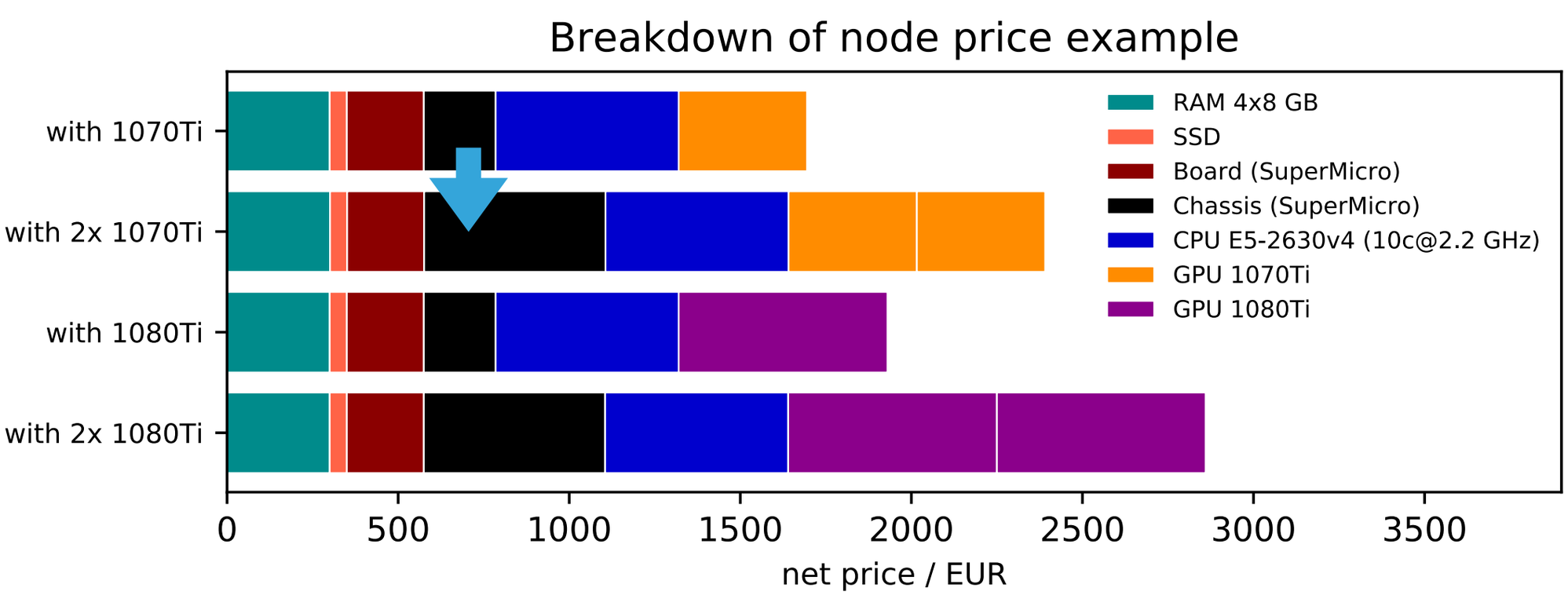




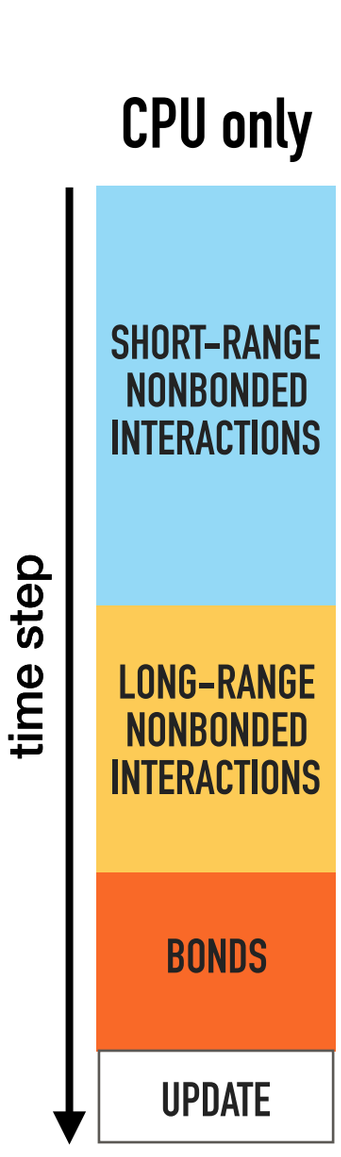
1. HARDWARE: BUILDING A GPU NODE

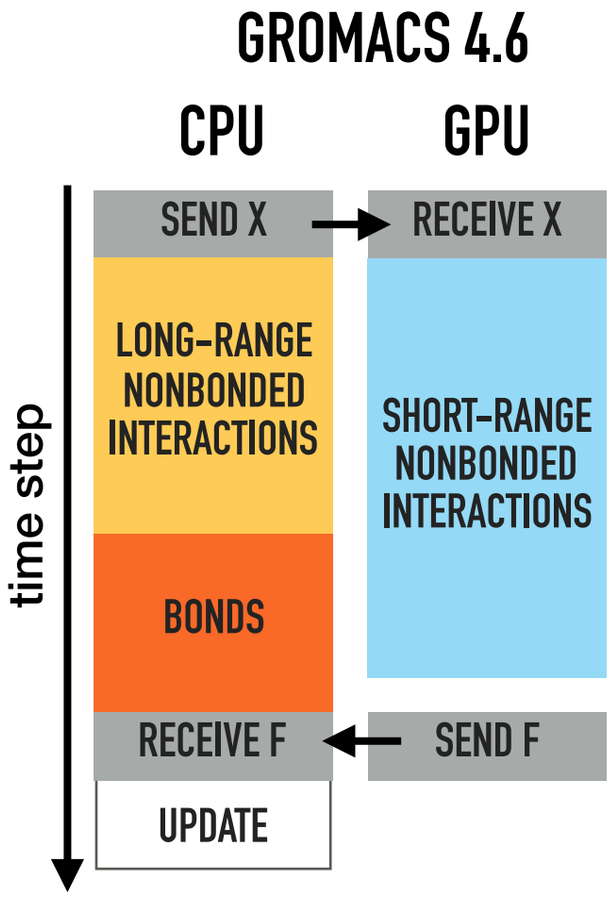
why not exclusively use GPUs with optimal performance to price (P/P) ratio?

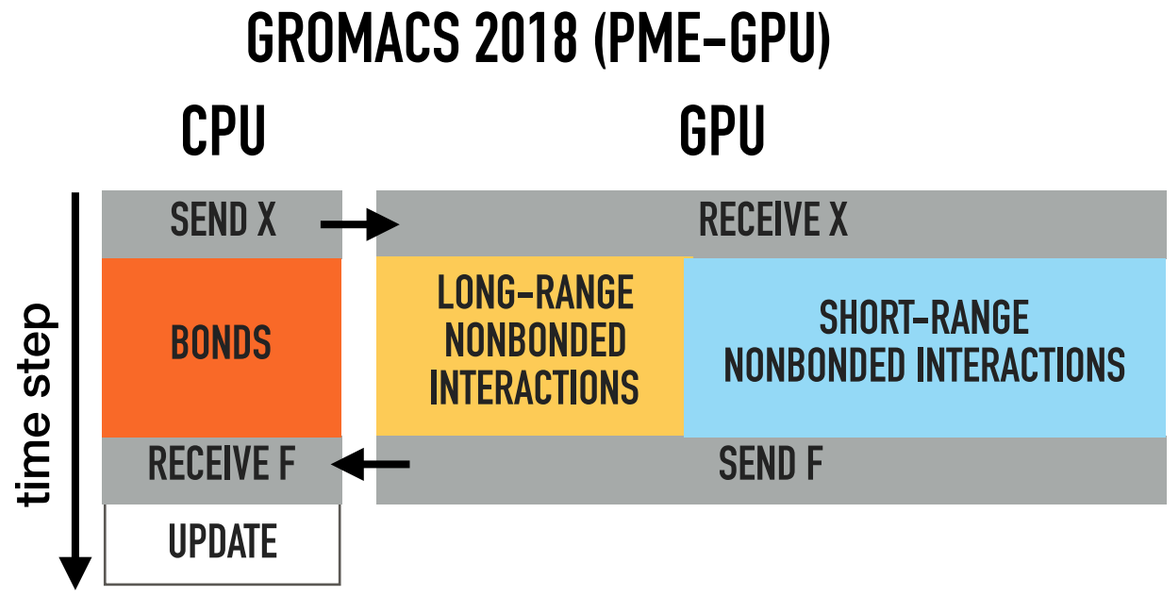




2. SOFTWARE: GPU OFFLOADING SCHEMES

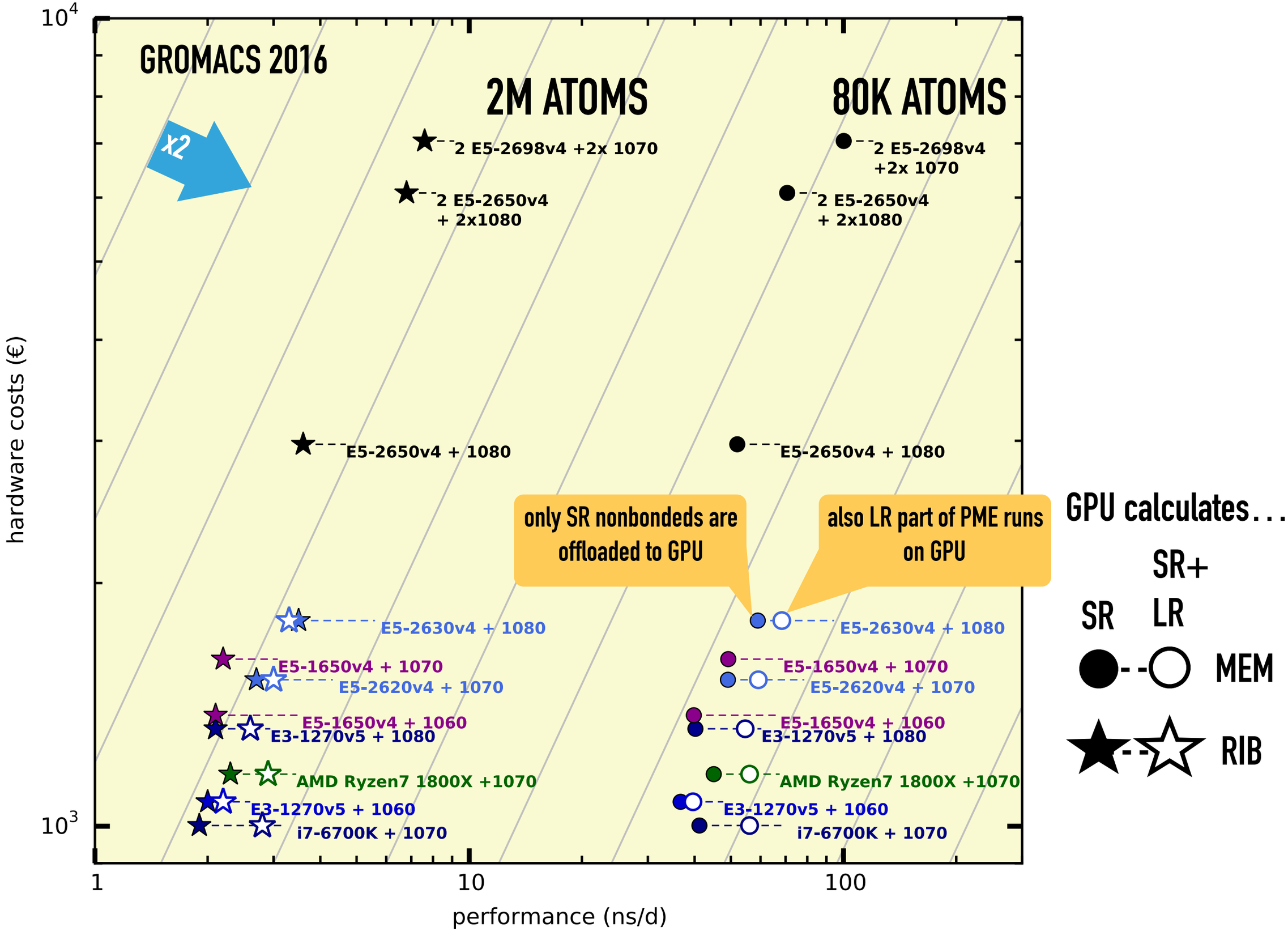






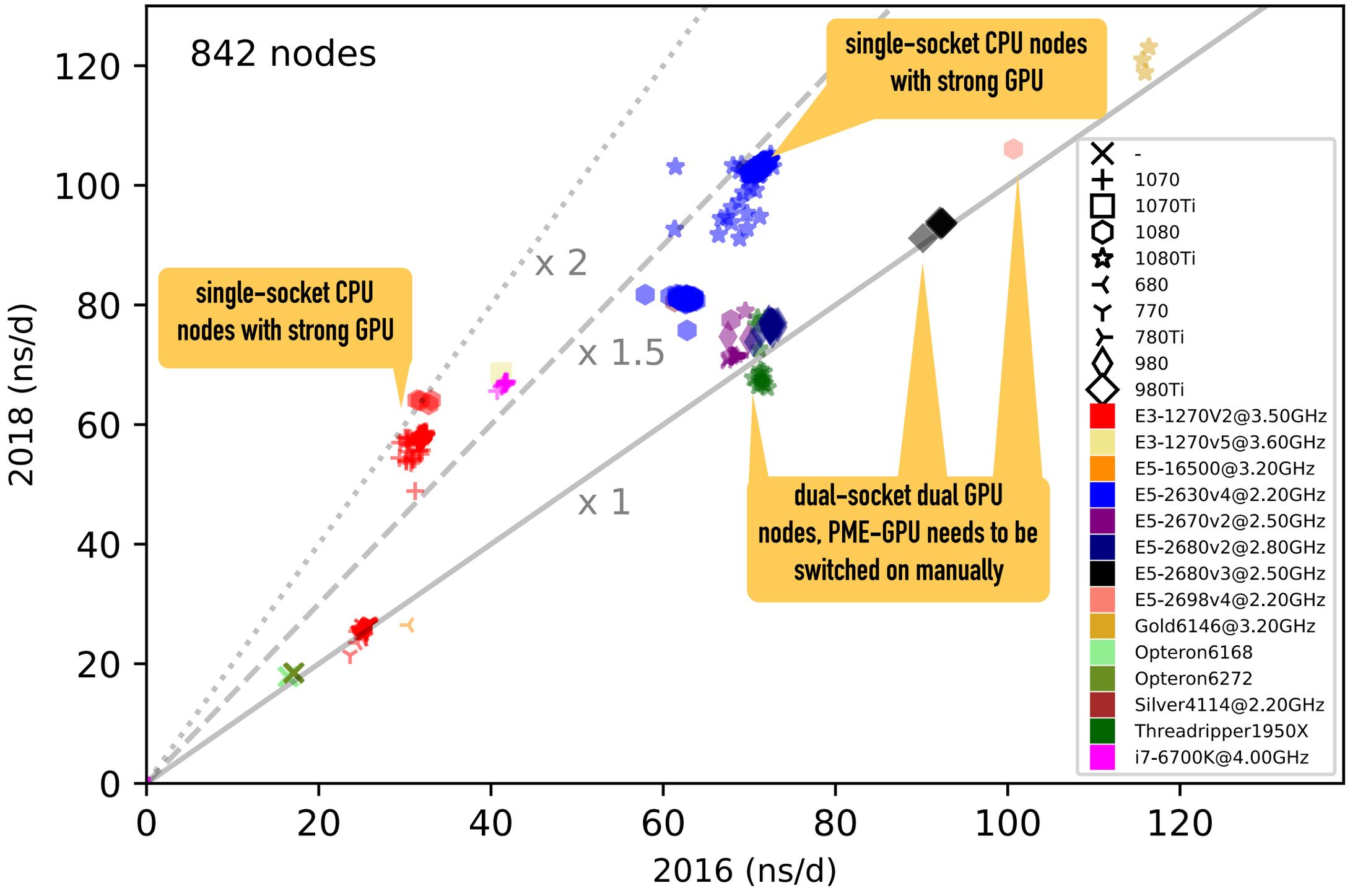
- offloading approach works best when CPU / GPU resources are balanced
- if a run is CPU-bound, more GPU power won't shorten the time step

2. SOFTWARE: PME ON GPU



2. SOFTWARE: PME ON GPU

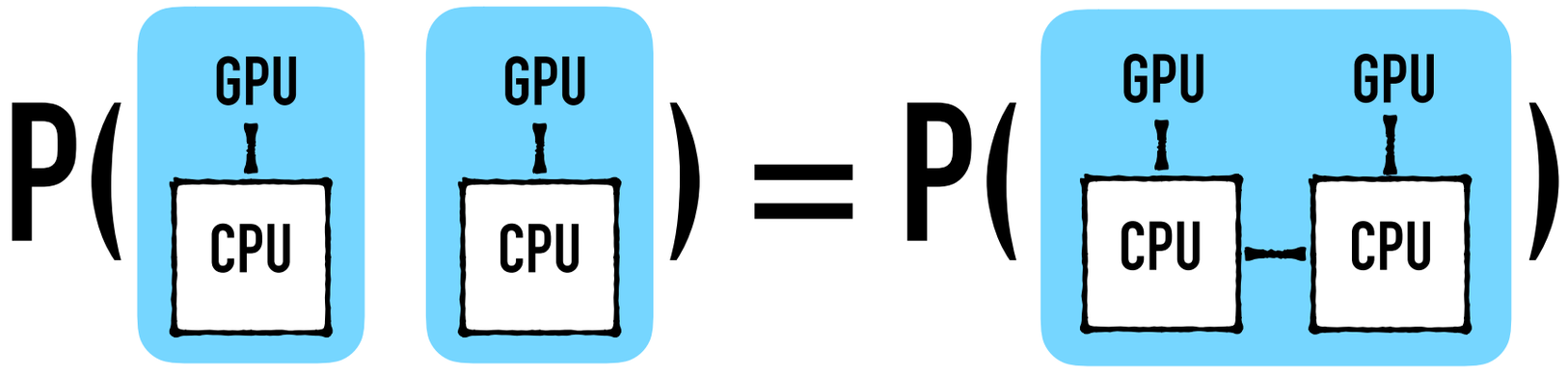
cluster health check using 80k atoms MEM benchmark

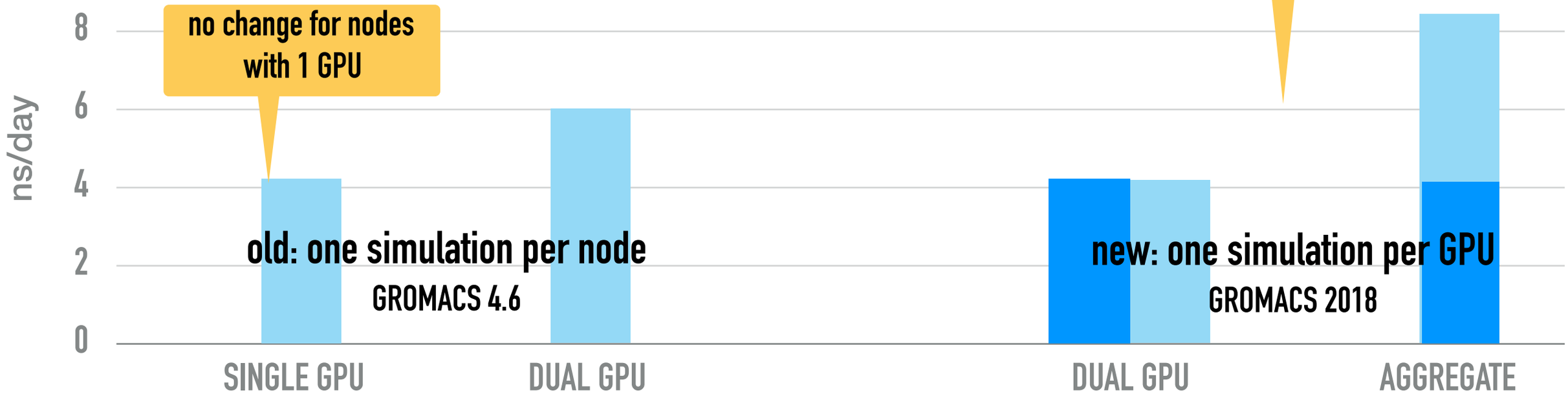


3. BENCHMARK PROTOCOL CHANGE – WHY?

We don't want to penalize the aggregation of compute power
(which may offer price and rack space savings!)

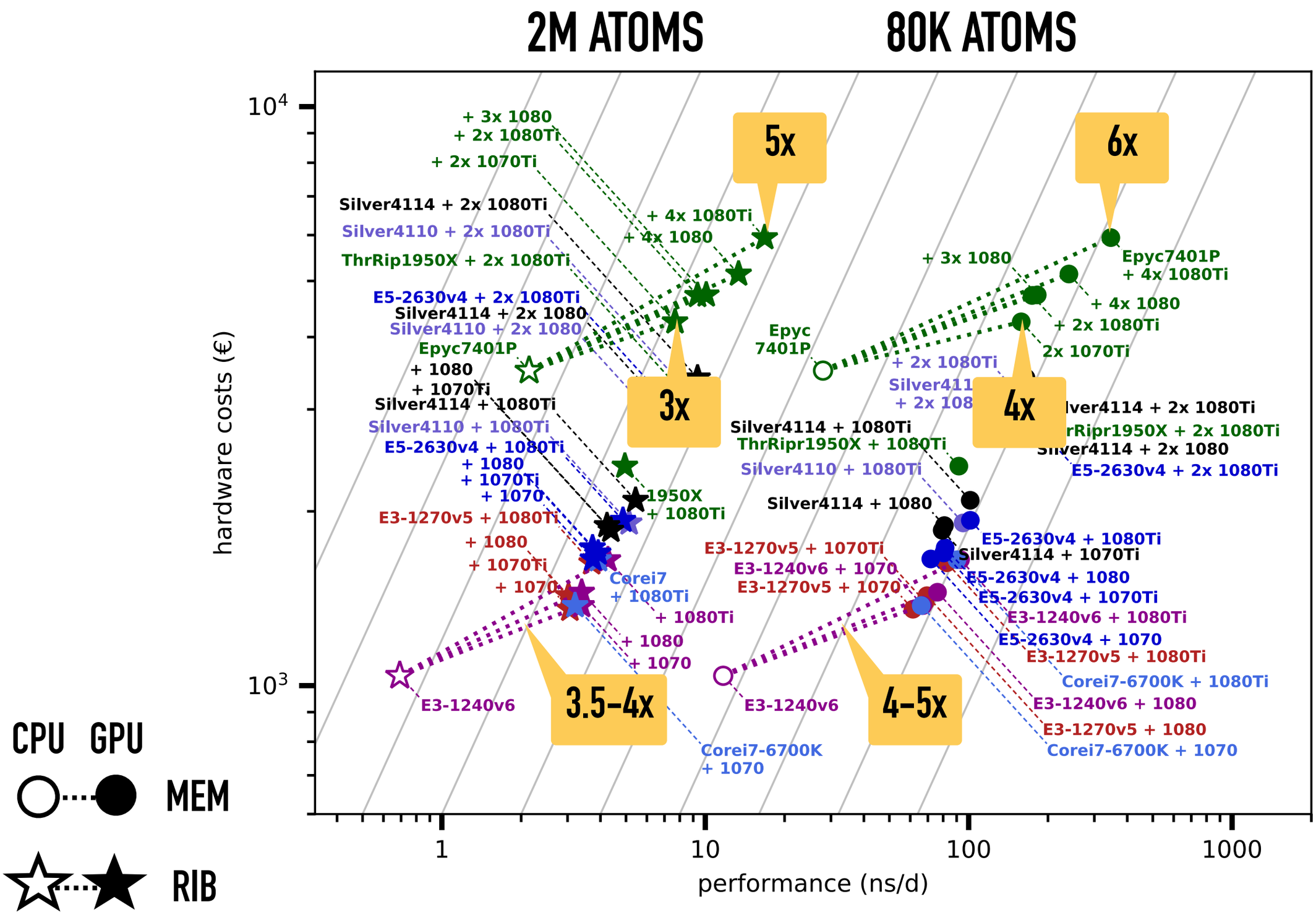
How do we measure the performance of a node? Ideally we get:





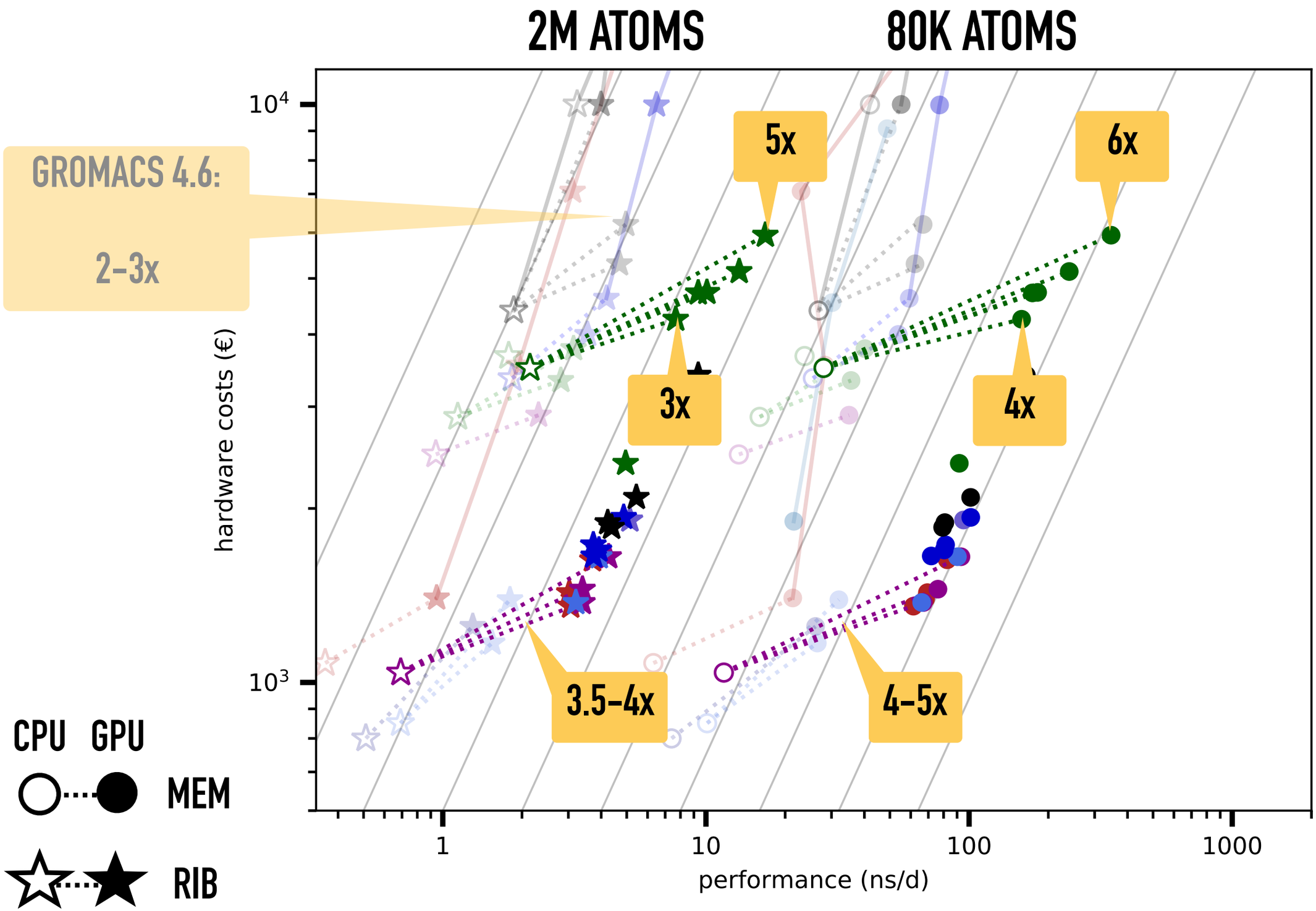
RESULTS 2018

PERFORMANCE TO PRICE 2018



4-YEAR PERFORMANCE TO PRICE DEVELOPMENT

2014...2018



ENERGY EFFICIENCY

ADD ENERGY COSTS TO THE BILL

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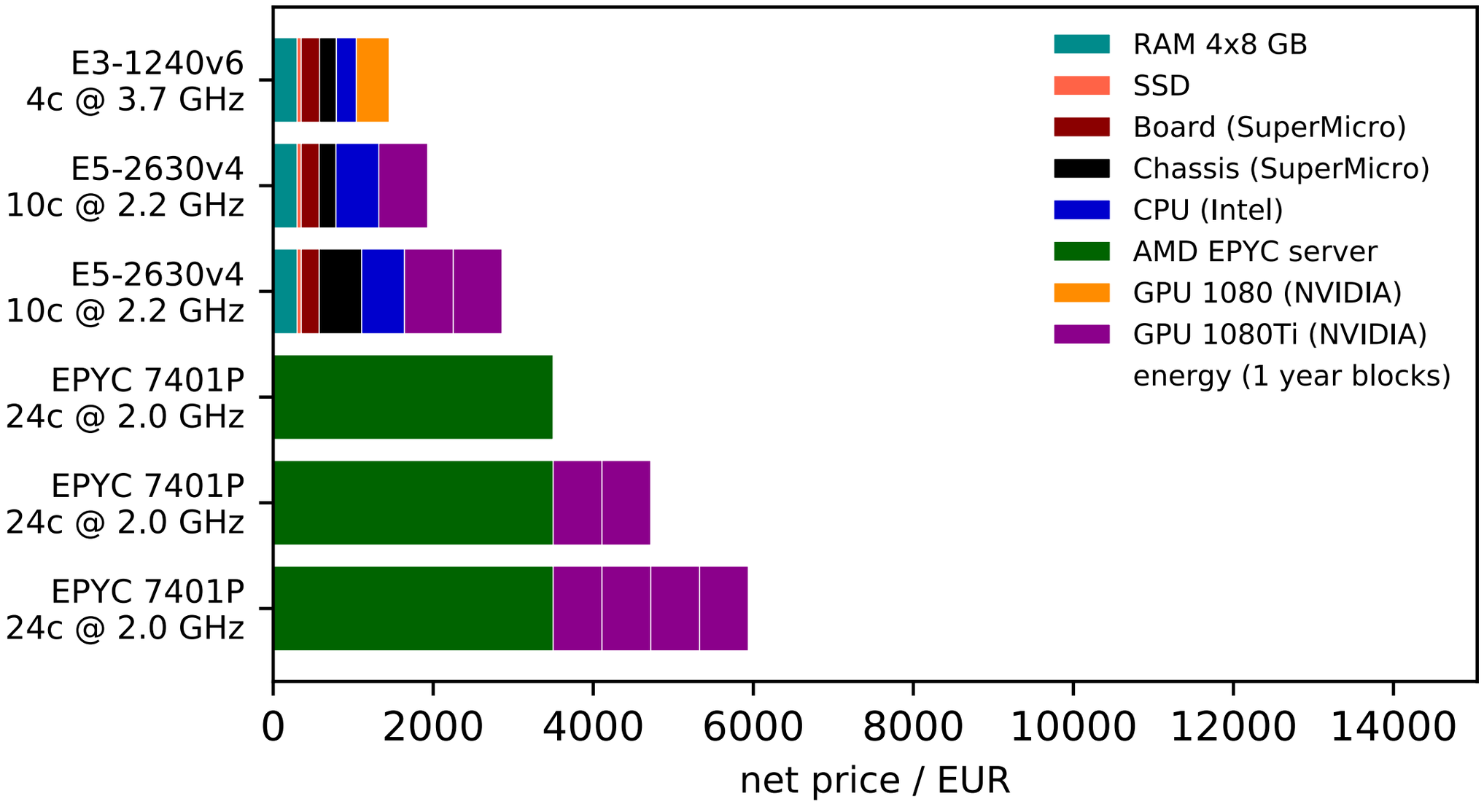
node costs taking into account energy + cooling (0.2 EUR / kWh) RIB



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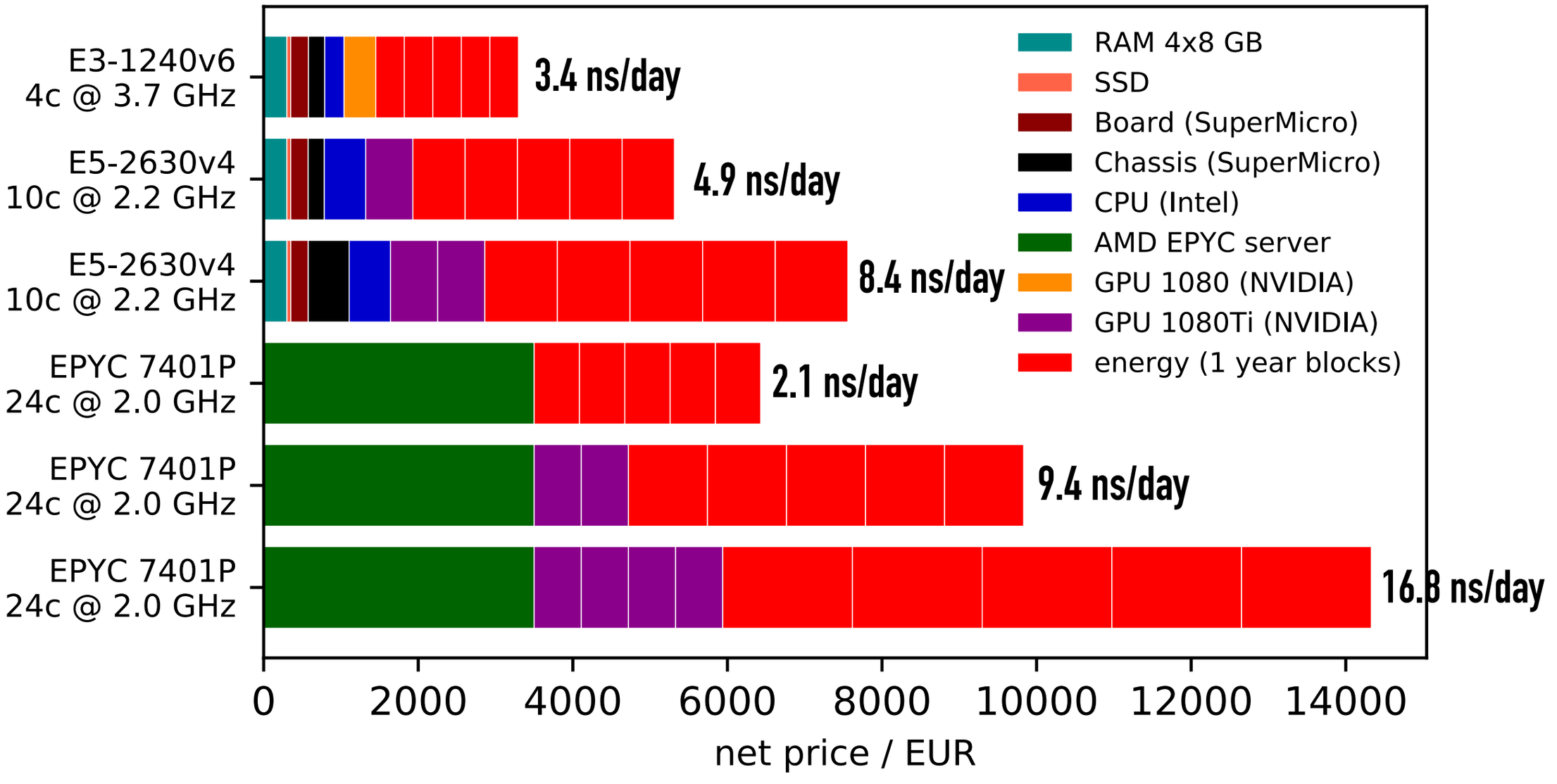
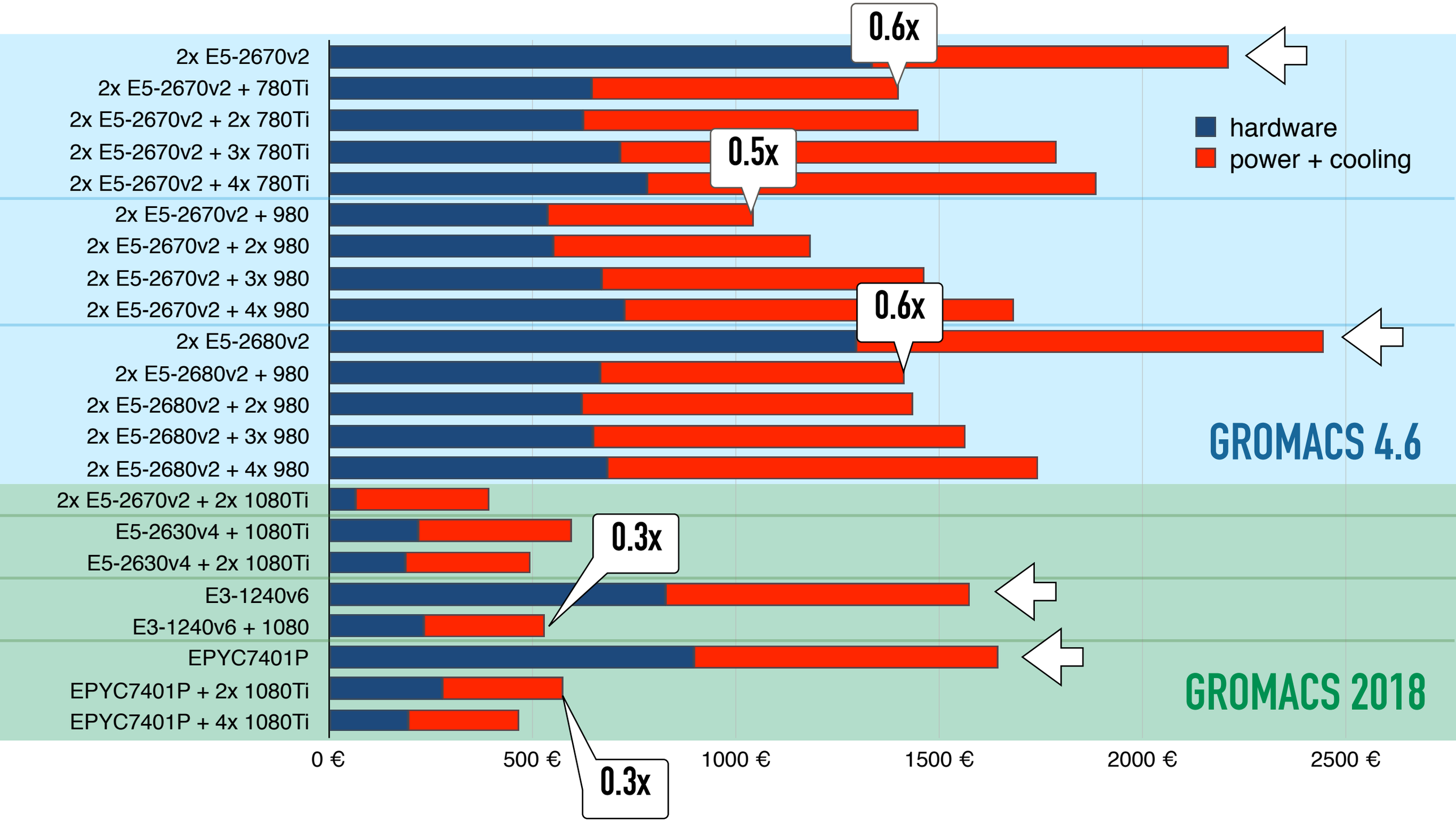


ENERGY EFFICIENCY

trajectory costs per microsecond RIB for 5 years of operation



ENERGY EFFICIENCY

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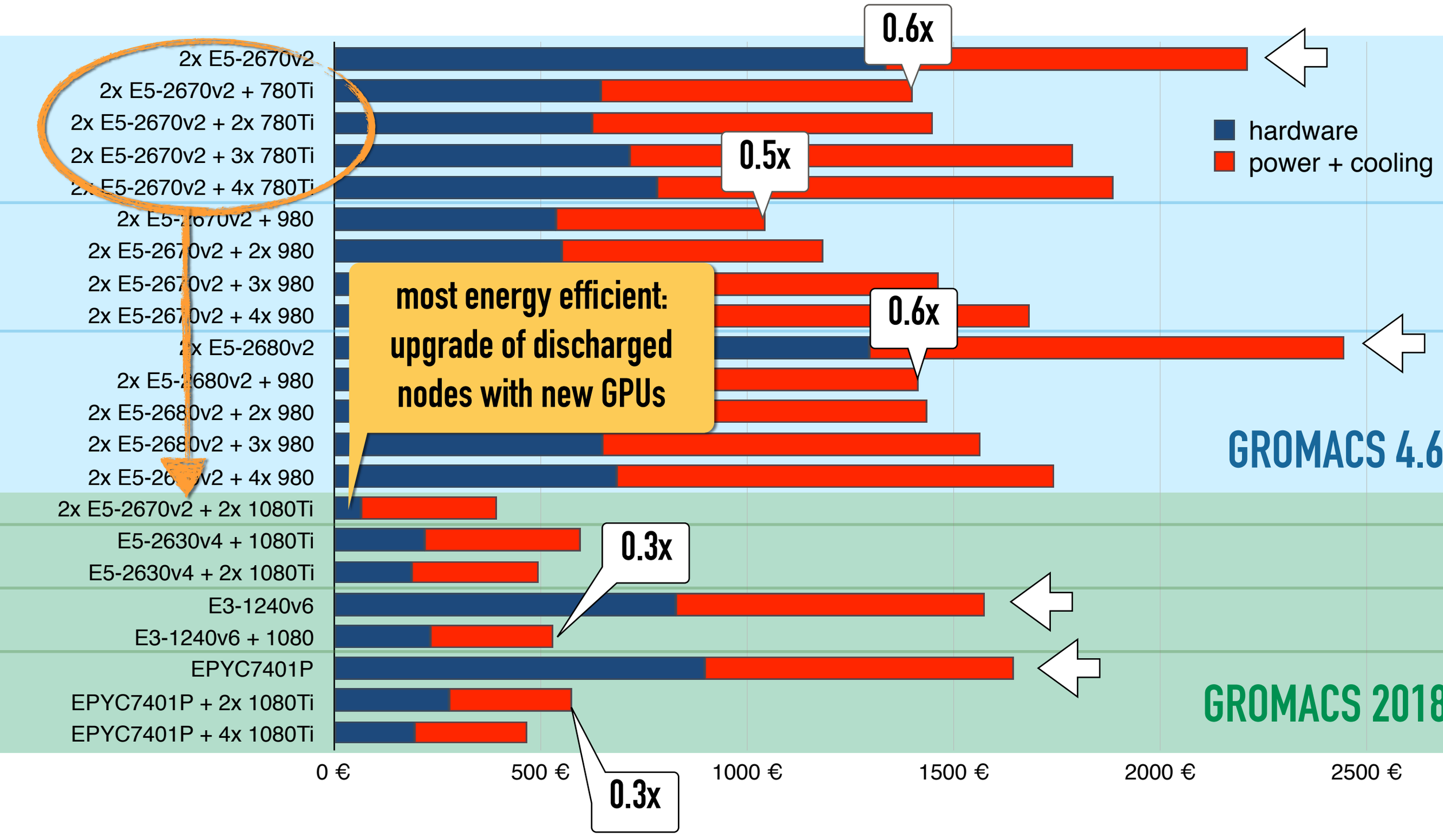


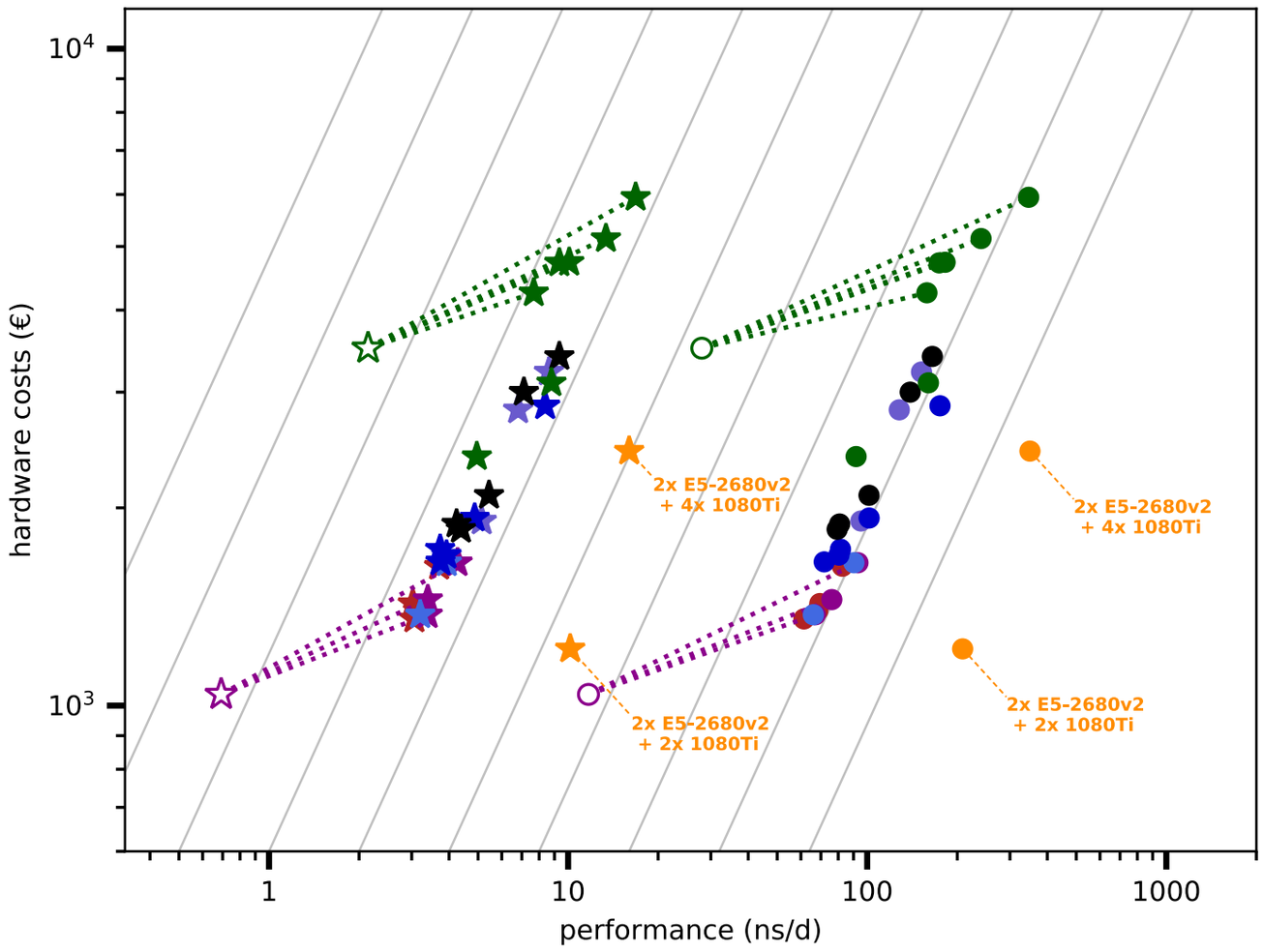
CONCLUSIONS

- compared to CPU nodes or nodes with Tesla GPUs,
  nodes with consumer GPUs yield significantly higher trajectory output per invested Euro
  - taking into account raw node price: 2–3 x for GROMACS 4.6, and 3–6 x for GROMACS 2018
  - including energy costs: about 2 x for GROMACS 4.6, and 3 x for GROMACS 2018

- PME on GPU...
  - ...moves the optimal hardware balance even more towards the GPU side
    (4–8 cores / 1080Ti)
  - ...allows to cheaply upgrade old nodes with state-of-the-art GPUs!

OUTLOOK

- upgrade old E5-2670v2 nodes (2x 10 cores @ 2.8 GHz) with 2 or 4 GTX 1080Ti.
- benchmark configurations with AMD GPUs (e.g. VEGA64)
- want to compare your own hardware and contribute to benchmarking? https://www.mpibpc.mpg.de/grubmueller/bench has various benchmark .tprs for download (CC licensed, also FE benchmarks)
- keep an updated list of benchmark results for the most recent GROMACS version



ACKNOWLEDGEMENTS

- the Grubmüller department
  - Martin Fechner, Ansgar Esztermann
- Szilard Pall (KTH)
- Markus Rampp (MPCDF)