Improving the Energy Efficiency of Large-Scale Scientific Simulations

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Overview

Context: Rising energy costs in HPC present significant challenges requiring novel solutions from both platform developers and application users.

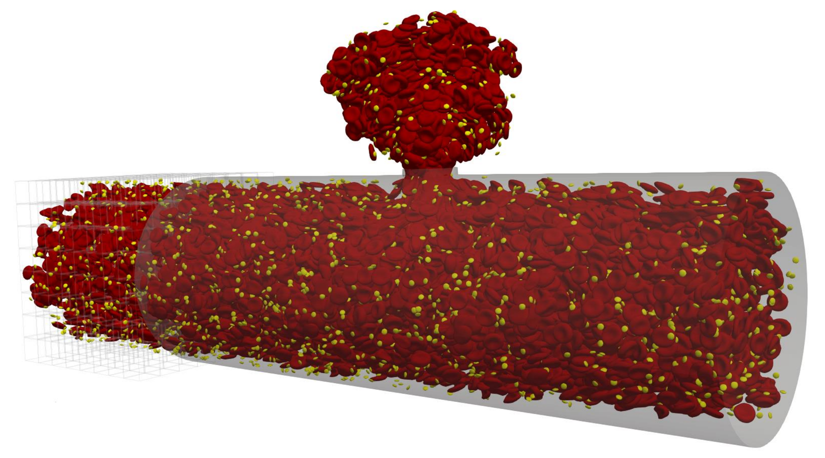
Goal: Focusing on large-scale scientific simulations, propose a method and tools to analyze and model performance, detect existing bottlenecks, and leverage on this information to improve energy efficiency,

Key contributions:

1. Systematic benchmarking of the effect of CPU features on HemoCell performance and energy efficiency [1].
2. Developed a methodology to build fine-grained per-process analytical performance models [2].
3. Proposed selective frequency scaling to improve energy efficiency in underutilized nodes [3].
4. Implementing a tool for on-the-fly workload modeling and energy optimization of large-scale applications [WIP].

Usecase

HemoCell (www.hemocell.eu), a coupled biomedical code for blood flow simulation. Blood is modelled as a set of deformable particles: red blood cells and platelets immersed in fluid.

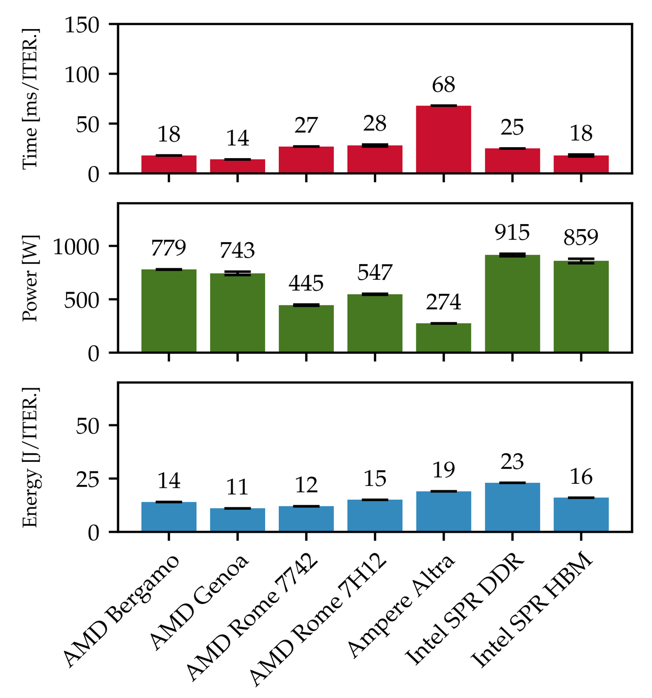


1. Benchmarking

Setup: Six different HPC CPUs with distinct key features, e.g.:

- *high memory bandwidth* (Intel),
- *high core density* (Bergamo),
- *low power draw* (Ampere),
- *high cache per core* (Genoa).

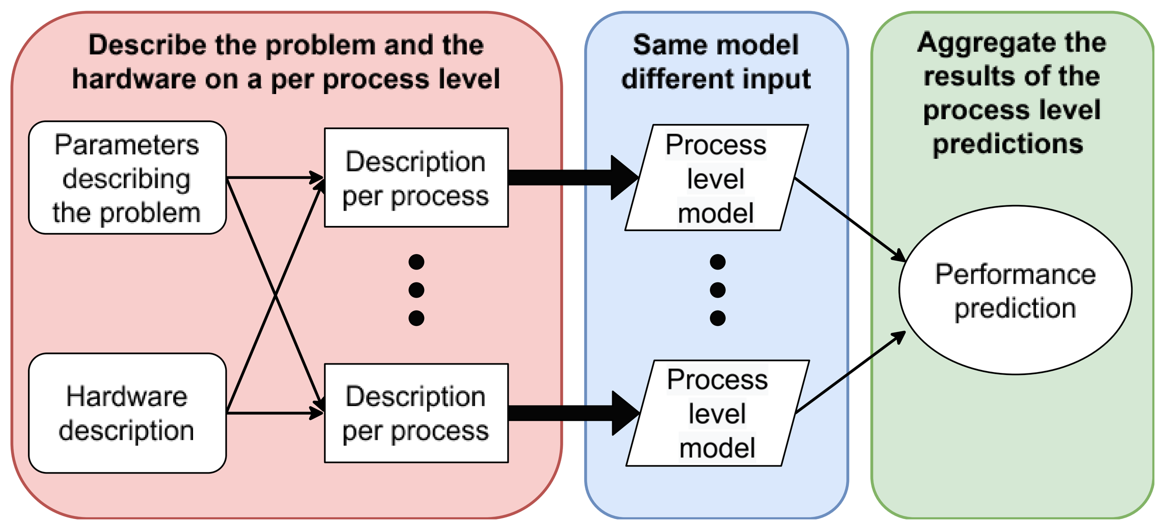
Take-Away: Increased cache capacity has the highest positive impact on both the performance and overall energy efficiency.



2. Analytical Performance Modeling

Modeling methodology: *(1)* Identify performance relevant code-sections and parameters; *(2)* Build symbolic analytical performance model; *(3)* Calibrate model using empirical data.

Model outline:

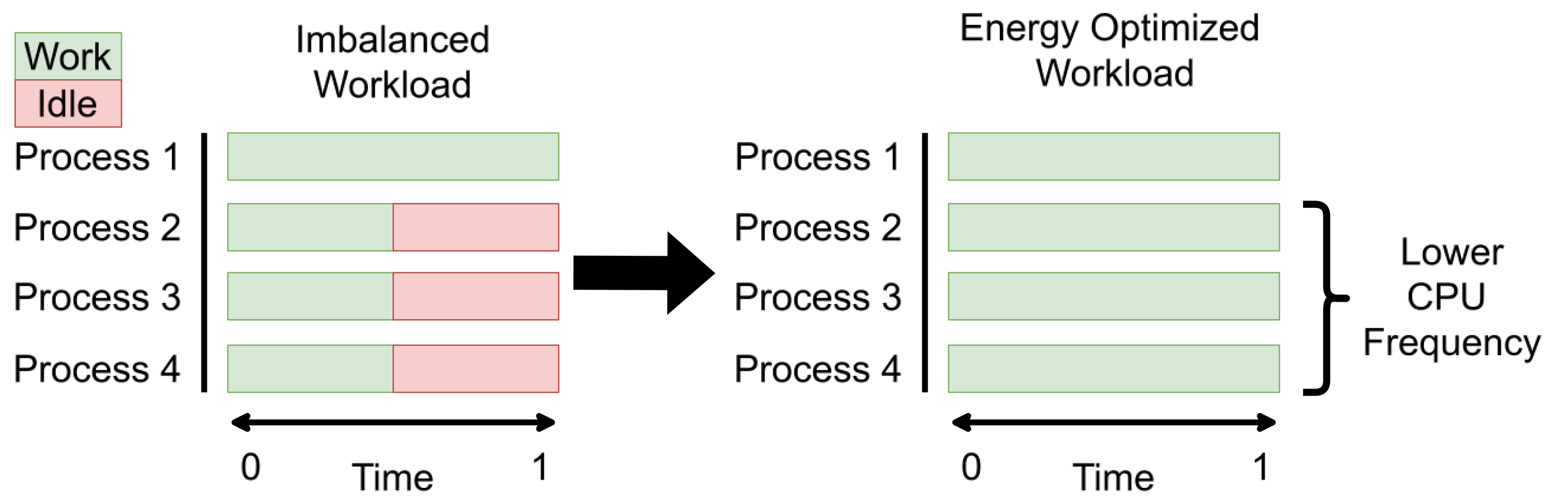


Results: The calibrated performance model is tested in simulation scenarios similar to (*balanced*) and highly different (*imbalanced*) from the calibration data:

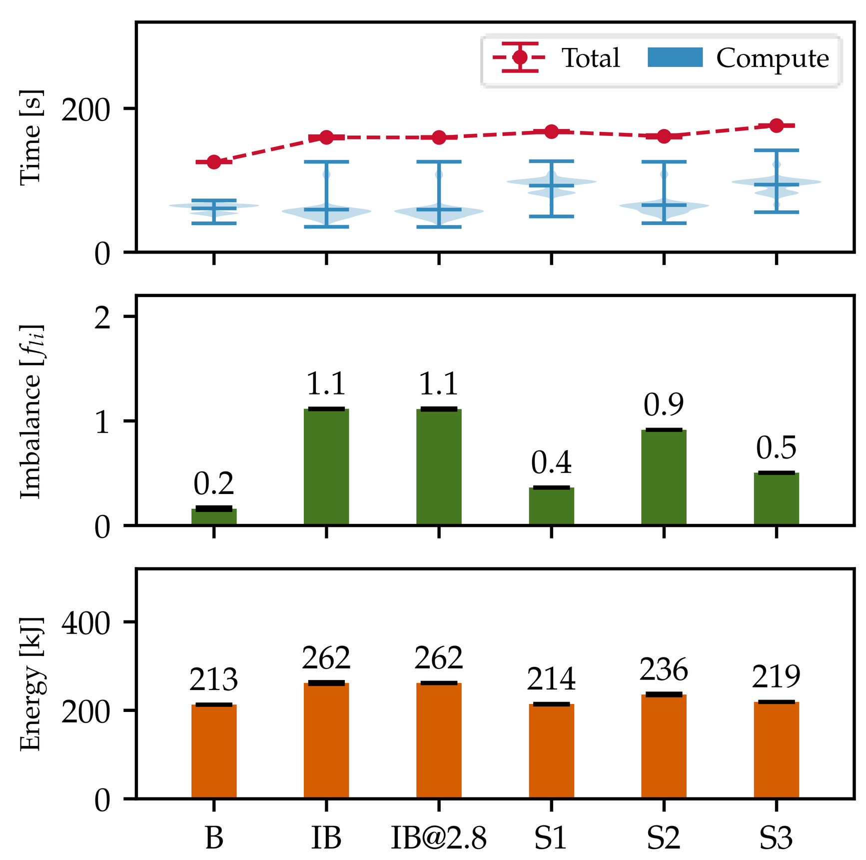
Scenario	Average Error	Maximum Error
Balanced	4%	13%
Imbalanced	10%	16%

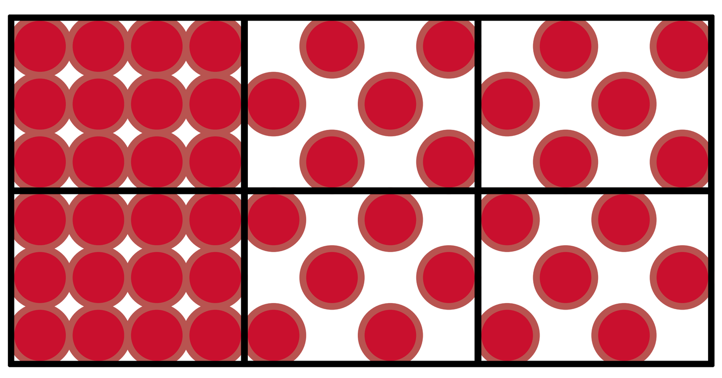
3. Energy Optimization Method

Method: Improving energy efficiency through selective frequency scaling of underutilized compute resources.



Results: Energy consumption is reduced by up to 23% in 16-node experiments with minimal impact on total runtime.





Strategy	Nodes 1-2	Nodes 3-16
Balanced (B)	1.5 - 3.35 GHz	1.5 - 3.35 GHz
Imbalanced (IB)	1.5 - 3.35 GHz	1.5 - 3.35 GHz
Imbalanced (IB@2.8)	2.8 GHz	2.8 GHz
Strategy 1 (S1)	2.8 GHz	1.5 GHz
Strategy 2 (S2)	2.8 GHz	2.4 GHz
Strategy 3 (S3)	2.4 GHz	1.5 GHz

4. Energy Optimization Tool

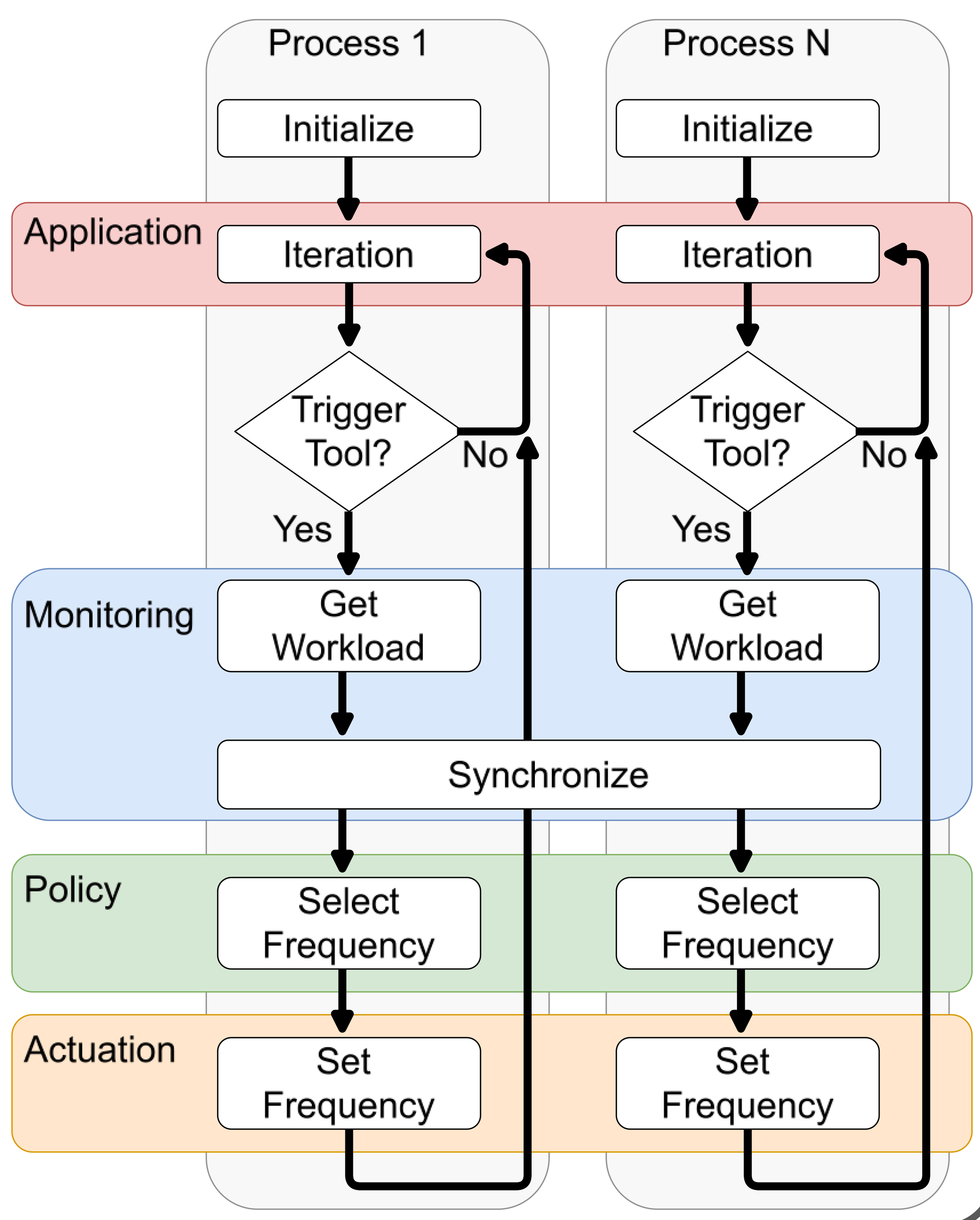
Goal: Implement a tool to detect load imbalance on-the-fly and optimize energy efficiency accordingly using our energy optimization method.

Implementation:
A lightweight C++ library consisting of three separate components.

1. Monitoring: Measure or model the workload on for each process.

2. Policy: Based on workload and available frequencies identify the optimal frequency.

3. Actuation: Interface with the HPC platform to set the chosen frequency.



More info ?

Get in touch!

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References

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[2] J. van Dijk, G. Zavodszky, A.-L. Varbanescu, A. D. Pimentel, and A. Hoekstra, "Building a Fine-Grained Analytical Performance Model for Complex Scientific Simulations," in PPAM'22, Springer International Publishing, 2023, pp. 183–196, ISBN: 978-3-031-30442-2. DOI: 10.1007/978-3-031-30442-2 14.
[3] J. van Dijk, G. Zavodszky, A.-L. Varbanescu, and A. D. Pimentel, "Embracing load imbalance for energy optimizations: A case-study," Accepted for publication at IPDPSWS PDSEC'25, 2025.