Improving the Energy Efficiency of Large-Scale Scientific Simulations

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I. Introduction

In June 2022, the top spot on the Top500 list was held by Frontier, the first true exascale supercomputer, able to achieve a peak performance of 1.102 exaflop/s. Researchers use supercomputers like Frontier for many applications in science and engineering, from astrophysics simulations to biomedical modeling and materials design. However, computing at large scale poses many challenges that the High-Performance Computing (HPC) community (i.e., the broad community of supercomputing-applications developers) needs to address. One of these major challenges is the increasing energy footprint of supercomputing.

Improving the energy efficiency of HPC platforms and applications is an important challenge that needs to be tackled by systems' and applications' developers together. HPC applications cannot only rely on hardware vendors and system designers to provide more and more efficient infrastructure. Instead, developers must also design and implement *more efficient applications*. In my research, *I focus on large-scale scientific simulations and propose methods and tools to analyze and model their performance, detect existing bottlenecks, and improve energy efficiency*.

II. Background and Related Work

My work targets a representative case-study: HemoCell, a simulation code used for modeling cell-resolved blood flow. In HemoCell, blood is simulated as a fluid with suspended particles. The fluid and particles are modeled separately and coupled together using an immersed boundary method. To enable parallelism, the simulation domain is decomposed into smaller subdomains, and each subdomain is assigned to a single MPI process. Each MPI process computes its own subdomain and uses peer-to-peer communication with its direct neighbors to keep halo regions up-to-date.

III. Contributions and Achievements

The goal of my PhD is developing a set of tools for improving the energy-efficiency of HemoCell and other large-scale parallel applications. The following paragraphs describes the three steps taken towards this goal, (1) performance benchmarking, (2) performance modeling, and (3) designing and validating a method for optimizing the energy efficiency of imbalanced applications using dynamic frequency scaling.

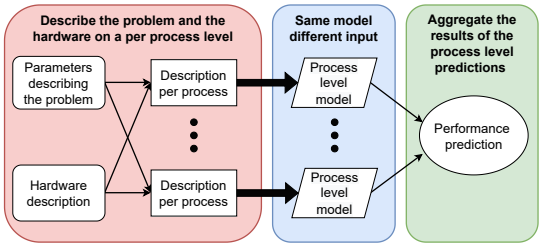

Fig. 1. Visualization of the per-process analytical performance model structure [2].

Benchmarking of HPC CPUs [1]

This study analyses the performance and energy efficiency of HemoCell across six HPC processors, including three emerging platforms with distinct architectural features, aiming to showcase the features with the most impact on performance and energy consumption. For example, we found that *AMD Genoa* scores the highest for both performance and energy efficiency metrics, outperforming processors with high-bandwidth memory (HBM), processors with significantly more cores, or low-power processors. We showed that the performance of *AMD Genoa* is primarily due to its large cache-per-core. The empirical findings from our cross-architecture evaluation lead to two main conclusions: (1) cache capacity per core represents the dominant architectural factor influencing HemoCell computational performance, and (2) optimization of runtime efficiency serves as the most effective strategy for improving energy efficiency metrics, with direct runtime reduction yielding proportional improvements in energy consumption characteristics.

Analytical Performance Model [2]

This work presents a methodology to construct per-process analytical performance models, see Figure 1. Our approach yields portable, fine-grained, and precise performance models that operate at process level. We use this methodology to build a model for HemoCell, and validate this model across multiple computational scenarios. For balanced workloads, the model achieves a maximum prediction error of 12.9%, with a mean error of 3.6%. When evaluated against imbalanced workload distributions, the model maintains robust predictive capability with a maximum error of 16.2% and a mean error of 10.2%. These results conclusively demonstrate that the

model, despite being calibrated using only balanced workload configurations, effectively captures and predicts performance characteristics for load imbalanced scenarios on single-nodes. The next step for this model is extending it to capture multi-node performance, this is still an ongoing effort. The current multi-node model can accurately predict computation cost in multi-node scenarios. However, the overall prediction is inaccurate due to communication costs modeling, which right now is still imprecise. This is something we are still trying to investigate and perfect.

Energy Optimization Method [3]

In this work we present a method to improve the energy efficiency of load-imbalanced applications. Our method leverages the observation that load-imbalance, when unavoidable, can be used for energy-savings. Thus, we exploit load-imbalance to dynamically adjust the CPU frequencies of underutilized nodes, thereby reducing energy consumption without impacting overall execution time.

To validate and assess the efficacy of our proposed methodology, we designed and implemented a comprehensive set of syntactic test cases that encompass the full spectrum of workload imbalance scenarios encountered within HemoCell. Each test case is systematically evaluated by comparing three distinct performance metrics (1) execution time, (2) energy cost, and (3) amount of workload imbalance. For each case we compare the theoretical optimal performance baseline, the performance under imbalanced workload conditions, and the performance achieved using our energy-optimized approach. We conclude that, by reducing processor frequencies on nodes with lighter computational loads proportionally to their workload, we can achieve substantial energy conservation: our results using HemoCell demonstrate energy consumption reductions of up to 23% (compared to the imbalanced setup), with negligible impact on simulation runtime. We also show that this method is robust across different types of imbalance in HemoCell.

A. Dissemination and Community Engagement

To share my research with the community and ensure continued open-access, all the data, tools, and code created for my work is freely available on Github, and is indexed on Zenodo [4]–[6].

In addition to publishing I have shared my research through presentations and posters on multiple occasions:

- PPAM 2022 (Presentation)
- CompSys 2021, 2022, 2023, 2024 (Presentation)
- ICT.OPEN 2021, 2023 (Poster)
- DUCOMS 2024 (Poster)

IV. Summary and Outlkook

The work thus far has build the foundations for a tool for improving energy efficiency energy of imbalanced large-scale applications. This foundations consists of extensive analysis of application performance, a methodology for building analytical performance models, and finally proving the efficacy of our energy optimization methodology.

Now we are focusing on the last step needed to complete this research: generalizing the energy optimization method in combination with the analytical performance model. Specifically, I am designing a framework that automates the entire process, from detection of load imbalance (using models) to actuation (using the load-imbalance DVFS), while investigating different DVFS policies and granularity.

This framework is build on three distinct components, (1) detection, (2) policies, and (3) actuation. For detection we use our analytical performance model [2] to provide a quick and accurate load-imbalance prediction, which we further use to drive the DVFS process. Next, we plan to devise and analyze different policies on how to respond, i.e., how can we determine the core frequencies that maximize energy efficiency (i.e., minimize load-imbalance) with limited impact on performance. Finally, in the actuation phase, we need to define and implement the mechanisms to change the core frequencies.

We plan to evaluate this framework on HemoCell, and investigate its impact on other simulations. We expect that our modular design will help adjust the framework for other HPC platforms and large-scale scientific applications.

References

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