### Tools for assessing and optimizing the energy requirements of high performance scientific computing software

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#### Abstract

Score-P is a measurement infrastructure originally designed for the analysis and optimization of the performance of HPC codes. Recent extensions of Score-P and its associated tools now also allow the investigation of energy-related properties and support the user in the implementation of corresponding improvements. Since it would be counterproductive to completely ignore performance issues in this connection, the focus should not be laid exclusively on energy. We therefore aim to optimize software with respect to an objective function that takes into account energy and run time.

# 1 The basic problem and static tuning approaches for its solution

To satisfy the demands from the scientific computing community, the established high performance computing centers provide a large amount of massively parallel computing hardware. One of the main challenges that the HPC centers have to face today is the cost of the energy required to operate this hardware which already amounts to about 30% of the total cost of ownership of a current HPC system, with a rising tendency [1]. Thus HPC centers will likely force their users to optimize their software with respect to its energy requirements. In this paper, we provide a brief survey of recent developments in this area.

An early strategy implemented by certain HPC centers [2] was to set the default CPU clock frequency of their systems to a value much lower than the highest possible frequency. This concept is based on the fact that the total power required by a compute job can be additively decomposed into a static

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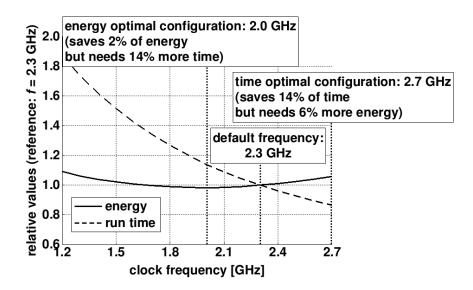


Figure 1: Relative energy requirements and run times for a typical run of the *Indeed* finite element code on SuperMUC.

component  $P_{\rm st} = {\rm const}$  (known as *idle power*) and a dynamic part that depends on f and on the voltage U as  $P_{\rm dyn} \sim U^2 \cdot f$  where, to obtain stability of the operation, U needs to be raised when f is increased. The job's total energy is  $E = \int_0^T (P_{\rm st} + P_{\rm dyn}) dt$ . An increase in f decreases the run time T, so the static component of the total energy decreases while the dynamic component may increase. Using a few test runs with typical input data sets, one tries to gain an impression of the nature of this dependence. For a specific example, Fig. 1 shows the result.

As expected, a moderate reduction of the clock frequency decreases the energy consumption but also significantly increases the run time. A straightforward application of the idea thus implies that the available hardware cannot be fully utilized, i. e. the number of program runs that can be executed during the system's life cycle is lower than it could be. To justify the hardware investment, it is thus not reasonable to focus only on energy. A more useful metric is the energy delay product EDP =  $E \cdot T^w$  where E is energy, T is run time, and w is a parameter weighting energy and run time according to the policy of the specific HPC center; typical values are  $w \in \{1, 2, 3\}$ . An optimization with respect to such a metric leads to a strategy that permits using higher frequencies in spite of possibly larger energy requirements if the run time savings are sufficiently large. Usually this is the case for compute-bound software like, e. g., many finite element codes. The CPU frequency is then fixed in advance for each code, and all runs of this code are executed with this predefined frequency. This approach is called static tuning.

Apart from the CPU frequency, other parameters of a program run such as, e. g., the number of OpenMP threads or the number of MPI processes, can also be tuned in an analog way in order to optimize the energy requirements.

## 2 Energy analysis with *Score-P* and the associated tools

Tuning and optimization has been part of the scientific computing software development process for a long time. The focus of these activities has traditionally been on the software's performance. A well established tool set for this purpose consists of the automatic trace analyzer Scalasca (cf. [3] or http://www.scalasca.org), the interactive trace analysis tool Vampir (see [4] or http://www.vampir.eu), the profile analyzer CUBE (cf. [5] or http://www.scalasca.org/software/cube-4.x), the profiling and tracing system TAU (see [6] or https://www.cs.uoregon.edu/research/tau) and the Periscope Tuning Framework (PTF) (cf. [7] or http://periscope.in.tum.de) for on-line analysis and tuning, and their underlying common measurement infrastructure Score-P (see [8] or http://www.score-p.org). Recently [9], the systems have been extended so that they can now also be used to analyze and optimize HPC codes with respect to energy related metrics.

A key observation in such an analysis is that most codes exhibit dynamism, i. e. their behavior varies over the run time. These variations can be exploited for optimization purposes. The tools listed above provide combined energy and performance measurements for each slice of the run time. On this basis, one can develop and implement dynamic tuning strategies, e. g. by adding commands to the code that change CPU frequencies, the degree of parallelism, etc. as required in the current situation.

A simple use case is a domain decomposition based finite element simulation. The simulation consists of a number of time steps; each subdomain's mesh undergoes an adaptive refinement. Then it is common for the workload to fluctuate between the processes associated to the subdomains (see Fig. 2). By setting the clock frequency for each process according to its current workload (i. e. according to the current number of elements in its subdomain), processes with a smaller workload can run at a slow clock speed, and hence require less energy, but still finish their task in sync with the other processes, so that the total run time is not negatively affected. Similar tuning actions can be implemented for, e. g., the number of OpenMP processes, thus saving energy by temporarily switching off some cores. Our tests indicate that static tuning increases the energy efficiency (in the sense of "energy-to-solution") by some 10%; we expect that dynamic tuning will lead to improvements of about 30%.

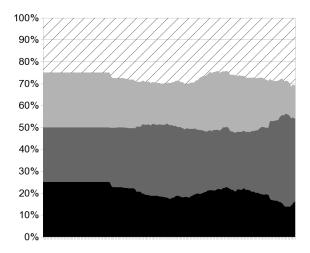


Figure 2: Distribution of work load over run time across four processes of a finite element simulation with domain decomposition and adaptive mesh.

### 3 Outlook: (Semi-)automatic dynamic tuning

Our next steps in the development of the analysis and optimization tools [10] aim at increasing the degree of automation. Specifically, a methodology has been derived that allows the user to define points in the code at which a change of run time parameters like CPU frequency of degree of parallelism is reasonable. Test runs will then be used to find optimal values for these parameters in certain situations defined, e. g., by the distribution of the workload or other suitable data. During production runs of the code, a runtime library will check the current situation at each switching point, find the situation from the test runs that matches best, and change the parameter set to the values identified as optimal for this situation. The implementation of this methodology is in progress. Our goal is to achieve an improvent of the energy efficiency in the range of 20% to 25% and to simultaneously reduce the programming effort in comparison to the manual dynamic tuning by 90%.

### Acknowledgement

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