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Towards Green Big Data at CERN

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Abstract

High-energy physics studies collisions of particles traveling near the speed of light. For statistically significant results, physicists need to analyze a huge number of such events. One analysis job can take days and process tens of millions of collisions. Today the experiments of the large hadron collider (LHC) create 10 GB of data per second and a future upgrade will cause a ten-fold increase in data. The data analysis requires not only massive hardware but also a lot of electricity. In this article, we discuss energy efficiency in scientific computing and review a set of intermixed approaches we have developed in our Green Big Data project to improve energy efficiency of CERN computing. These approaches include making energy consumption visible to developers and users, architectural improvements, smarter management of computing jobs, and benefits of cloud technologies. The open and innovative environment at CERN is an excellent playground for different energy efficiency ideas which can later find use in mainstream computing.

Keywords: Scientific computing, green computing, CERN, energy efficiency

1. Introduction

The Large Hadron Collider (LHC), which was used to discover the famous Higgs boson, started to run at CERN in 2010. During the first run, the CERN computing center stored up to 6 GB of data per second. The total need of

5 computing resources was around 200,000 CPUs and 40 PB disk space. The
6 second run of LHC started in June 2015. During this run, data is stored at
7 a maximum rate of 10 GB per second and CERN alone has allocated 140 PB
8 disk space divided between its data centers in Switzerland and Hungary [1].
9 The required computing resources for LHC data analysis are divided among 11
10 tier-1 and 155 tier-2 globally distributed computing centers by using the grid
11 computing paradigm [2]. Efficient management of these computing resources is
12 vital for the success of the project, which is foreseen to be active for the next
13 20 years.

14 From the physicist point of view computational speed is of prime impor-
15 tance to efficiently analyze the data and to enable progress on particle physics.
16 It is therefore important to consider both user needs and cost-efficient use of
17 resources when managing the computing infrastructure and training and en-
18 couraging users.

19 The energy efficiency of computing is receiving increasing attention (see e.g.,
20 [3] for a survey). For example, Van Heddeghem et al. [4] reported that data
21 centers worldwide consumed 270 TWh of energy in 2012 and this consumption
22 had a Compound Annual Growth Rate (CAGR) of 4.4% from 2007 to 2012. Be-
23 sides the expenses related to the data center energy consumption, environmental
24 aspects are also relevant. Therefore, the reduction of electricity consumption
25 for computing is important both from cost and environmental point of view.

26 The increased computational speed enabled by Moore’s law has for a long
27 time contributed to increased energy efficiency. If the same task can be com-
28 pleted faster and the power consumption remains unchanged, this obviously
29 results into energy savings. However, we are now in a situation where the com-
30 putational speed will no longer increase. While Moore’s law still increases the
31 number of transistors on chips, the computational speed of individual cores has
32 stopped growing [5]. As a result developers need to be able to better distribute
33 their workloads to take advantage of the increasing number of cores in net-
34 worked systems. However, according to Amdahl’s law [6] the distribution is not
35 a panacea, because the speed improvement of parallelism is limited by the parts

36 of the software that cannot be parallelized. Normally this has a negative effect
37 on energy efficiency but in some cases, due to the dynamic voltage and fre-
38 quency scaling (DVFS) [7], increased parallelism can even have a positive effect
39 on energy efficiency [8]. One conclusion of this is that instead of simply trying
40 to make the software run faster, and, as a result, become more energy-efficient,
41 we need to consider other ways to run the software in a more energy-efficient
42 fashion.

43 In this article, we take a holistic view of energy efficiency by introducing
44 three main roles, which can be recognized in the value-chain of scientific com-
45 puting: user, software developer, and data center operator. These three groups
46 are connected through the computing system they use/develop/operate even
47 though their aims and goals are often quite different and orthogonal. This
48 also naturally affects energy consumption. Therefore, we look at energy effi-
49 ciency from these three perspectives and form a holistic view of the scientific
50 computing ecosystem. We do this by combining the roles with a set of in-
51 termixed approaches, which we have studied in our Green Big Data project
52 (<https://twiki.cern.ch/twiki/bin/view/Main/GreenBigData>) to improve
53 the energy efficiency of CERN computing. Philosophically, we can say that
54 our research methodology is based on decomposing the whole system into in-
55 dependent subsystems, which can be optimized separately [9]. The result of
56 optimization is usually Pareto optimal, meaning that improving the system
57 from the view point of one role, would reduce its optimality for another role.
58 For example, allowing longer queueing times can make it possible to improve
59 the energy efficiency of the data center but it also reduces the service level of
60 the user.

61 The rest of this article is organized as follows: First, we give a review of
62 related work in energy efficiency in Section 2 and then introduce the reader
63 to scientific computing by reviewing the CERN computing problem (Section
64 3). In Section 4 we introduce the three roles/stakeholder groups in computing
65 and present possible technology solutions to improve energy efficiency related
66 to the functions of these groups. In Section 5, we discuss future possibilities

67 and identify potential targets for future research. Finally, conclusions are given
68 in Section 6.

69 **2. Related Work**

70 A large part of research in energy efficiency has focused on cloud data cen-
71 ters. For example, Dayarathna et al. [10] give a large survey of state-of-art
72 techniques in energy consumption modeling and prediction for Internet data
73 centers, and Shuja et al. [11] present several case studies demonstrating meth-
74 ods and techniques for sustainable data centers. Moreover, Mazumdar and
75 Pranzo [12] study server consolidation in cloud data centers by proposing a for-
76 mal formulation for the server consolidation problem and showing that using
77 a snapshot-based method it is possible to find efficiently near optimal server
78 allocations.

79 Another significant part of research focuses on hardware. For example Kar-
80 powichz et al. [13] study on energy-aware design in hardware, middleware and
81 software layers. They note that to get benefit on hardware development, a
82 holistic view to the whole system must be taken. This includes, for example,
83 developing power consumption models, measuring methods for energy efficiency,
84 modeling computing and network dynamics, multi-level control systems, energy-
85 aware scheduling and software development techniques.

86 There are also many studies on energy efficiency in high-performance com-
87 puting. For example, Rong et al. [14] review energy optimization technologies
88 in high-performance computing and propose a set of strategies to maximize
89 the efficiency and minimize the impact for environment. Further, Zakarya and
90 Gilliam [15] focus on energy efficiency on scientific computing systems. They
91 key findings are: 1) using system level technologies may actually increase en-
92 ergy consumption in clusters; 2) optimizing scheduling and resource allocation
93 in clouds can offer better results than consolidation using migrations; and 3)
94 turning off idle resources works well in clusters but may cause performance
95 issues in cloud when demands fluctuates.

96 There are also many other studies on resource management and scheduling
97 in scientific computing. Uddin et al. [16] evaluate three scheduling algorithms
98 to find the most energy-efficient one. The algorithms were implemented using
99 the CloudSim software to simulate IaaS cloud infrastructure. The results indi-
100 cates that the two phases power convergence (TPPC) algorithm [17] is the most
101 energy-efficient of the tested algorithms. Zhao et al. [18] propose an energy and
102 deadline aware scheduling method for data intensive applications. The method
103 is based on the idea of modeling data sets as a binary tree based on correlations
104 among them. This helps reducing data transmission. The second step of the
105 method is based on energy-aware scheduling minimizing the number of active
106 servers. Finally, Madni et al. [19] study resource allocation methods in their
107 review article. Their conclusion is that not all important parameters are taken
108 into account in current methods and improvements would be needed.

109 Energy-aware algorithms have been received a lot of attention during the
110 last years. Many of these algorithms aim at optimizing resource selection or
111 scheduling problems [20, 21, 22], while others focus on cloud computing [23, 24,
112 25] or networking [26, 27, 28].

113 Although most of the research on energy efficiency have focused on hard-
114 ware, infrastructure, or algorithms there are many studies on software devel-
115 opment, too. For example, Jagroep et al. [29] study how to make software
116 developers aware on energy efficiency. In their case study they followed two
117 software development projects and gave feed back to the developers on energy
118 and performance issues. The results indicate that increased awareness makes
119 the developers consider more on energy efficiency.

120 Energy-efficient operation is naturally highly important for major cloud ser-
121 vice providers (e.g. [30] for Google,[31] for Facebook). Although there are
122 commonalities, the key difference between big cloud operators and scientific
123 computing community is that in cloud providers are hosting services which often
124 require low latency to keep the interactive users happy. In scientific computing
125 single jobs can run for hours or even days and thus high throughput is often far
126 more important than shorter runtime. Therefore the architectural concepts are

not directly transferable between the two camps but a lot of the learnings can still be beneficial for both.

Moreover, scientific computing has been slow in adopting virtualization, containers, and other techniques which form the basis of commercial cloud services. One reason for the slow adoption has been the belief that all kinds of additional layers waste computing resources. However, some studies indicate that the performance difference especially with container technology is not very significant [32]. Moreover, the resource isolation of containers allows new ways to manage the computation and the possibility to store the entire computational environment in the container provides new opportunities for reproducible research [33]. Therefore it is likely that we see increasing adoption of container technologies in the future in scientific computing following the initial steps already taken [34, 35, 36].

3. Computing Challenge at CERN

In the 27 km long LHC ring particles are accelerated close to the speed of light. Two particle beams traveling in opposite directions collide at the detectors of experiments. There are three main experiments at LHC: CMS [37], ATLAS [38], and LHCb [39]. Each experiment has a custom made particle detector consisting of multiple layers of different sensors, which measure speed, charge, and other characteristics of the particles that are created in the collisions. While the number of monitored collisions is large, only some of them are selected for further studies. The first selection is made in real time by dedicated trigger hardware [40] in the experiment and the second filtering using a cluster of powerful computing servers [41]. The data from the selected events is permanently stored on the computing center. The raw event data is processed and converted into a reconstructed event, which is more compact and more suitable for analysis. The actual analysis phase then selects a set of events matching according to some criteria with the simulated events, which, based on theoretical models, try to anticipate what should be happening in the collisions. In order to under-

stand physics phenomena and get statistically significant results a huge number of measured events must be compared with simulated events.

A single high-energy physics analysis job processes millions of events. The work can be parallelized easily because each event can be analyzed independently. Normally, each analysis job starts around 600 - 1,000 separate processes each of which analyzes a subset of total events. Physics events are stored in database like repositories called ROOT files [1]. A typical ROOT file is about 100 - 300 MB in size and contains 700 - 2,000 events. An average analysis job would pass through 15 million events that are stored in 35,000 files.

Originally, the huge computing needs of LHC were handled by the grid computing model (see e.g., [42] for an overview). For this purpose, large R&D projects were launched in early 2000 [43, 44]. Initially, achieving the required computing power was the only target and the importance of minimizing energy consumption was not understood yet. Some years later, however, offering enough power started to limit the number of servers that could be installed in the CERN data center. Outsourcing a part of capacity to another data center to Hungary using cloud technologies was found as a working solution. Moving from grid to cloud offers new possibilities for energy optimization such as consolidation of computing [45] either automatically or through human expertise.

So far the increasing need for computing power has been satisfied by purchasing more hardware and by performance improvements. Moreover the computing has been distributed to multiple locations with grid and cloud technologies. Until recently Moores law has handled the increasing computing needs quite well and the power efficiency has improved at least at the same rate as computing power. But as computational needs continue to grow and keeping up with Moores law is increasingly difficult, new ideas and technologies are needed.

Scientific computing at CERN is an interesting case since the problems are real, the amount of data massive, and the atmosphere at CERN like in the science community in general, is receptive to new ideas. An idea tested in the challenging environment of CERN has a good possibility of being useful elsewhere. The most known example of this is the World Wide Web [46], which

187 has its roots in CERN. However, it is important to keep in mind that there
188 are differences between scientific and general computing environments. For in-
189 stance, power proportional computing is useful in many areas in the computing
190 industry [47], but its impact on scientific computing at CERN is small since
191 there are enough computing tasks to keep the batch processing queues full and
192 the servers busy all the time. Obviously, this does not alone mean that CPU
193 utilisation would be 100%, since there can be latencies, for example, because of
194 waiting for I/O. However, high CPU utilisation can be guaranteed by slightly
195 over committing CPU resources [48]. Moreover, long computing times spanning
196 hours or days are a norm in scientific computing while interactive applications
197 naturally require rapid responses.

198 **4. Three Roles in Energy Efficiency**

199 Generally, green computing has been seen as a technical solution and there
200 are plenty of methodologies and technologies for improving the energy efficiency
201 of super computing clusters [49, 50]. However, in many cases, the motivation for
202 investing in energy efficient technologies remains quite low. For example, quite
203 often hosting charges in data centers are based on the amount of electricity used.
204 This clearly demotivates the company running the data center in the effort to
205 save energy in its computing infrastructure. However, improving other parts of
206 the infrastructure such as cooling still makes sense. Partially for this reason,
207 the PUE index [51] is a commonly used key performance indicator for energy
208 efficiency. Or, in some other organizations, the electricity bill for computing is
209 still very small compared to other costs such as rent, personnel, etc. Optimizing
210 computing systems for energy efficiency can also increase risks in operational
211 failures or make those risks more pronounced. For example, a hardware failure
212 of a virtualized server running several services can have a negative impact for
213 many customers.

214 In scientific computing, like at CERN, we can recognize three different groups
215 of actors: 1) Users, that is, scientists solving their problems by running scientific

216 software packages on computing clusters, 2) Developers of scientific software
217 packages, and 3) Operators of the computing clusters and the data center. Based
218 on this classification, we can form three different and mostly orthogonal views
219 of energy efficiency:

220 **End user view** How can a scientist using computational methods in his/her
221 research improve energy efficiency and avoid wasting resources or energy
222 (Section 4.1)?

223 **Software developer view** How can energy-efficient software be written for
224 complex multi-core-multi-user systems? What can the software developer
225 do to improve the energy-efficiency of the code (Section 4.2.2) and what
226 kind of tool support would help in this (Section 4.2.1)?

227 **Data center management view** How can resources be managed in an opti-
228 mal but still fair way? How can we influence energy spending by better
229 scheduling and allocating work loads in a data center locally (Section 4.3),
230 and also globally by dividing the work between multiple data centers in
231 an energy optimal way (Section 4.4)?

232 A way to study the efficiency of scientific computing is to look at the ra-
233 tio between computing outcomes and expenses. Computing expenses can be
234 classified into hardware, electricity, and personnel costs, as well as the impact
235 on the environment. While the three first costs are easy to measure, the en-
236 vironmental impact is a more hidden factor. Fortunately, through electricity
237 pricing the common objectives of minimizing energy expenses and minimizing
238 the environmental impact have strong synergies.

239 The outcomes of computing are more difficult to measure than its costs.
240 Obviously computing is done for a goal but quantifying the value of computing
241 results is difficult as well as comparing the values of different computing out-
242 comes. Therefore it is difficult to come up with useful measures of efficiency
243 by simply dividing the value of computing output with the computing costs.
244 CPU time is often used as a substitute measure of computing output although

245 it does not indicate how efficiently the implemented algorithms work and use
246 the available resources. There are also a lot of trade-offs: for example, between
247 the computing speed and the cost (i.e., electricity or CO2 emissions).

248 Keeping in mind the limitations that arise from the difficulties of exact
249 metering, in the following subsections we study how different solutions can help
250 the actors in the roles of end users, developers, and data center managers to
251 improve the energy efficiency in the parts of the computing system they can
252 influence.

253 *4.1. User View for Energy Efficiency*

254 While technical solutions in computing hardware form the basis of energy
255 efficiency, the way computers are used also plays an important role in energy
256 efficiency. Efficiency, meaning optimal usage of available resources and avoid-
257 ing generating waste, is a widely-studied topic in operations and production
258 management [52] but it is usually understood in a narrower sense in scientific
259 computing, where the main target is optimising the computing speed. One
260 particular challenge is to motivate users to write and run their programs in an
261 energy-efficient way. The users are focused on getting the results they need and
262 not on looking at the bigger picture. For example, creative ways to greedily
263 use the computing resources for gaining an advantage over other users, such as
264 running multiple parallel tasks for solving an optimization problem and picking-
265 up the best solution, or bypassing the cluster’s scheduling system by using so
266 called pilot jobs [53] for reserving resources [54], are clearly not be the most
267 energy-efficient way.

268 It is however natural for a single user to minimize both the set-up and run
269 time of his/her own application. However, this seldom results into the best
270 total (energy) efficiency for the whole user community. If every user behaves
271 in this way, everyone has less resources available. In closed communities, such
272 as among CERN scientists, these issues could be alleviated by better training
273 and also by introducing tools giving feed-back to the users on the energy and
274 computational efficiency of their applications. Usually people want to reduce

275 the environmental impact if it is not too difficult or costly for them [55].

276 How can the users be motivated to save energy? The following could possibly
277 provide some incentives:

- 278 • Moving to energy based accounting and billing.
- 279 • Offering benefits to energy-efficient users. For example allocating higher
280 priority for their jobs or giving them the most powerful hardware.
- 281 • Promoting environmental awareness and making it possible to schedule
282 jobs based on the availability of green electricity.

283 *4.2. Software Developers View*

284 For the software developers we can identify at least two methodologies for
285 improving energy efficiency: 1) making energy consumption visible and 2) ad-
286 vising them to use optimal methods for the architecture at hand. These are
287 studied in the following sub sections.

288 *4.2.1. Energy Profiling*

289 As far back as in the 19th century Lord Kelvin observed that "...when you
290 can measure what you are speaking about, and express it in numbers, you know
291 something about it; but when you cannot measure it, when you cannot express
292 it in numbers, your knowledge is of a meagre and unsatisfactory kind" [56]. Tom
293 DeMarco applied this to software development by famously stating that "You
294 cannot control what you cannot measure" [57].

295 The observation also applies well to the energy consumption. Most develop-
296 ers do not have any idea how much electricity it takes to run their application.
297 In comparison to computing speed, the energy-spending of computing is hard
298 to detect. In mobile devices consumers are sensitive to power consumption,
299 because of the frequent need to recharge influences the comfort of using the
300 device. However, in data centers this is not the case and therefore, the energy
301 consumption of computing is generally beyond the interest of a typical software

302 developer or end user. Obviously the electricity bill of the data center is in the
 303 interest of the IT managers, but the link to the developer is typically weak.

304 An obvious way to make developers consider the energy efficiency of their
 305 code is to make energy spending visible. There are multiple ways to achieve this.
 306 First, tools like RAPL (Intel technology for programmatic access to counters
 307 giving the energy spending of the processor chip [58]) or smart power sources
 308 allow programmatic access to counters that keep track of spent electricity [59].
 309 In this way we can easily monitor the electricity consumption of the computing
 310 server (or even some smaller units like CPU or memory) but it is hard to know
 311 the share of a single job’s electricity consumption relative to the overall energy
 312 consumption of the computing facility. Furthermore it is difficult to identify
 313 how different parts of the software use the energy.

Figure 1: An example of measurements taken by the performance and energy profiling tool.
 [60]

314 To make the energy usage more visible to the software developers, we im-
 315 plemented an energy profiling functionality to IGProf [60]. IGProf is an open
 316 source profiler developed initially at CERN [61]. With its energy profiling fea-
 317 tures, it is able to report the amount of energy consumed in each function [62] in
 318 addition to the processing time. The essence of the energy profiler is the RAPL
 319 measurements, which tell how much energy has been consumed between con-
 320 secutive readings, and a mechanism to allocate the energy reading to different
 321 functions.

322 While the energy profiler is operational and the concept works, it still has
323 two main challenges. First, the granularity of energy measurements is rather
324 coarse, around 1 ms. Therefore, it is difficult to allocate the spent energy to the
325 proper functions because a program typically executes thousands of function
326 calls before RAPL updates the energy counters. An option used by Hähnel
327 et al. [63] is to artificially spend time in a function until the next reading
328 is available. However, this has the drawback of making the execution of the
329 software extremely slow. An alternative option is to rely on statistics: if the
330 same code is executed multiple times, the energy readings should over time
331 accumulate to those functions that are responsible for the consumption.

332 The second problem with energy profiling concerns the value of separate
333 energy readings. In many cases there is a very strong correlation between energy-
334 spending and processing time and therefore it is reasonable to ask what is the
335 added value of energy profiling. However, while the correlation is strong we
336 can still see cases where the time and energy do not exactly correlate. In those
337 cases the energy profiler is able to give additional insight beyond the regular
338 performance profiles.

339 In summary, there is still no way to accurately estimate the energy consump-
340 tion of each function or line of code. The present trade-off between accuracy
341 of energy estimation and the effect on the execution time needs to be replaced
342 with a viable solution. Furthermore, accurate energy estimates are also difficult
343 to achieve because the energy consumption depends on what other applications
344 are running at the same time. Also, another program competing for the same
345 memory and cache resources will influence the energy consumption. However,
346 even indicative estimates are likely to be helpful.

347 4.2.2. *Software architecture implications on energy-efficiency*

348 The key to computational efficiency is the quality of used algorithms. How-
349 ever, even with an optimal algorithm, its implementation must follow the con-
350 straints of the run-time environment to maximize performance and energy ef-
351 ficiency. Especially, the way in which the software accesses data stored in the

memory has a significant impact on performance and energy spending.

At the core level, the processor executes calculations on values stored in its registers. Fetching a value from the RAM to a register takes approximately 100 clock cycles. Therefore multiple levels of faster cache memory are utilized to prefetch data from the slow RAM to a faster cache, so that the register load can happen in only around 10 clock cycles. To produce this speed-up, cache prefetching algorithms must correctly predict future data access needs. If a value that is not in cache is needed, the cache needs to prefetch the contents of memory in the accessed region and the processor will stall waiting for the memory load to complete.

The speed disparity between registers, cache, and RAM has a major effect on the computing speed, and, through speed, on energy consumption. While the effect of object-oriented programming to memory use has already been investigated and well understood in the 1990s [64], the problem is becoming even more visible today, since the difference between the computing speed and memory access speed is significantly larger in modern processors than it was previously. Therefore, the efficient use of the cache is even more important today [65].

Optimizing cache prefetching involves designing data layout in memory to match processor cache design. When a cache miss occurs, the cache controller fetches a block of memory around the accessed location. The size and alignment of the block, called a cache line, depends on the processor. A typical cache line is 32 words, or full register sized data items, starting from the preceding memory location whose address is divisible by the cache line size. Data layout in memory should therefore be consecutive words, packaged in cache line size sequences that are also referenced with high locality by the functional instructions in temporal proximity.

To quantify the importance of proper order of accessing memory, we performed a simple test with a large table of C++ instances [66]. When we accessed the instances (to perform a XOR operation) in the same order as they were created, the speed was around 4x faster than if we accessed the same instances in a random order. Accessing the instances in exactly the reverse order

383 from their creation fell between these two extremes.

384 To further minimize computing effort, we notice that some functional in-
385 structions are more efficient than others, but these instructions can only be
386 used when data is in specific registers and in a specific format. For example, a
387 matrix multiplication can be implemented using traditional looping over a two-
388 dimensional array, or by preloading the array to suitable registers and using
389 a single-instruction-multiple-data (SIMD) instruction. Compared to classical
390 looping over array, SIMD instructions have some set-up cost as multiple data
391 items need to be loaded in suitable registers, but their execution can be an order
392 of magnitude more efficient both in time and energy consumed. When data is
393 suitably prepared so that SIMD instructions can be utilized, multiple results
394 can be calculated per clock cycle.

395 There are also some special challenges related to scientific computing. For
396 example, a problem with floating point numeric computing is that the results
397 can be different depending on compiler version and operating system. For in-
398 stance, Baloolan [67] compared codes for electromagnetic wave simulation and
399 found code compiled with the same compiler produced different results when
400 running in Windows and Linux environments or in different Windows XP ver-
401 sions. The underlying reason is the floating point calculations way they have
402 been implemented [68]. Even if there are standards for floating point encodings
403 and functionality [69] subtly differences in e.g. computation order or processor
404 use can still cause different numeric results from the same computing [70]. Hayes
405 et al. noticed a similar problem when running the same simulation software in
406 two different hardware [71]. The unfortunate consequence of this is that taking
407 into use newer, more optimal compilers is not possible. The big investment
408 over the years to ensure that the physics computing codes produce the cor-
409 rect answers would be partially wasted and the results of the new calculations
410 could not be trusted without extensive analysis and verification. Therefore the
411 key physics software is stuck with the old compiler versions which are not able
412 to take advantage of advanced possibilities of modern processor architectures.
413 This is one instance of risk avoidance, which is also visible in other software

414 improvement actions. The threshold is high to modify old, thoroughly tested
415 and validated code only for better performance.

416 In the CERN case, a lot of the code is old and developed at a time when
417 the processor architecture did not support the features of modern processors
418 described above. In a typical use case, the data in ROOT format files is used to
419 construct C++ objects in RAM [72]. The object oriented design of the low-level
420 data manipulation software enables high-level abstractions in application code,
421 provides clear interfaces between components, and thereby supports coopera-
422 tive work. Unfortunately, it also distributes the data items in non-consecutive
423 locations in memory, in a format that is not directly suitable for use by SIMD
424 instructions. The data items are not packed in cache-efficient blocks and, due
425 to the data hiding pattern, the algorithm implementations can not consider lo-
426 cality of reference for data item accesses. The unfortunate result is that the
427 processor spends a lot of time waiting for memory accesses and efficient SIMD
428 instructions can not be used. The challenge is to write the software providing
429 a high-level abstraction interface for the users, while still handling data effi-
430 ciently in memory, and adapting the handling to the type of processor where it
431 is scheduled to run.

432 It is well understood that software tends to increase in complexity as a result
433 of late-lifecycle changes making it harder to modify and forcing an architectural
434 restructuring over time. Williams et al. [73] review the work on this phenom-
435 ena sometimes called code decay, software aging, or architectural degeneration.
436 Most of the work deals with how new and changing functional requirements
437 cause code complexity to increase. In early and influential work on software
438 evolution Lehman [74] observes that hardware change is one of the reasons for
439 code decay. However, hardware change and how to develop software which is
440 able to improve efficiency by using the novel opportunities of new hardware
441 technologies has received less attention than changes arising from functional re-
442 quirements. The study by Kuusela [75] is an attempt to consider how to create
443 an architecture that is adaptive to hardware changes. However, in most cases
444 the adaptation to hardware is seen as a way to make the system work in another

445 hardware platform.

446 Our observation is that bringing the software to work on a new platform
447 can sometimes be easy but more work is needed to get the software work effi-
448 ciently with the opportunities and characteristics of new hardware platforms.
449 Therefore, an ideal architecture should be resilient both to new functional re-
450 quirements as well as to new hardware opportunities. Brown et al. [76] discuss
451 how changes done for improvements in one dimension create an architectural
452 debt in other dimensions. The debt, as seen in additional complexity or non-
453 optimal performance, has to be "paid back" as a later development step. We
454 think that this theory applies well to the CERN case where the functional and
455 other requirements lead the development. The performance problems initially
456 felt to be secondary but as time goes by they become more visible. The same is
457 even more true for the energy spending of the software. It is only recently that
458 the electricity spending has become a bottleneck.

459 In conclusion, an energy efficient software architecture must provide the
460 interfaces that users need to define their application level logic, while providing
461 an efficient data manipulation and processing layer underneath the high-level
462 interface. This data manipulation layer either needs to be sufficiently adaptable
463 to runtime environment, or variants of the layer needs to be available for a smart
464 scheduler that is able to choose the correct software version for the current
465 runtime environment.

466 In the case of CERN, adapting the current software towards a more energy
467 efficient architecture is a major challenge because of the large amount of code
468 and the long legacy in software development. Even if we understand what
469 the energy-optimal architecture would be, reaching that goal is a slow process.
470 From the software design perspective the direction of the required changes is
471 clear, but from a software engineering perspective it is not obvious how the task
472 could be achieved. Although software re-engineering has been widely studied,
473 for example in several EU funded projects such as [77], it is a time consuming
474 and complex process. Empirical study of industrial software refactoring [78]
475 indicates that developers tend to fix concrete coding issues and improve the

476 maintainability of their code. Because energy-efficiency is largely invisible to
477 the developers, it is unlikely that it would be considered in ordinary refactoring.
478 Explicit targets and resources for its improvement would therefore be needed.

479 *4.3. Data Center Management View*

480 In this section, we change our perspective beyond the efficiency of a single
481 piece of software and investigate the problem of how to process a large set of
482 jobs efficiently. While most of the existing work on high performance computing
483 focuses on optimizing the processing time of individual computing jobs, we now
484 try to optimize the energy consumption and the total processing time of the set
485 of jobs by choosing an optimal scheduling policy. In what follows, we assume
486 that jobs (the programs to be executed) can be treated as black boxes without
487 detailed understanding of the internals of them. This means we also change the
488 perspective from what software developer can do, to ideas, which can be applied
489 by the workload management at the data center.

490 The computing clusters can be seen as production resources processing jobs
491 consisting of numerous tasks [79]. The tasks can be processed by different
492 resources, and finally the jobs are assembled together to be delivered back to the
493 cluster customers. Operating such a cluster has its own cost structure related
494 to capital invested, energy consumed, maintenance work, and facility related
495 costs. Based on this, we can apply operations management principles used in
496 manufacturing such as minimizing the lead time, waste, and inventory, and
497 maximizing the utilization and output to improve productivity and minimize
498 the energy consumption.

499 Following the operations management approach [52], the efficient manage-
500 ment of computing resources is based on the following principles:

- 501 1. Modeling the computing system as a manufacturing unit applying well-
502 known operations management theory (e.g. [80, 79]).
- 503 2. Measuring performance using meaningful indicators (e.g. [81]).
- 504 3. Managing the resources in a way that maximizes the energy efficiency and
505 output (e.g. [48, 82]).

506 In the following sub sections, we discuss these principles in more detailed.

507 *4.3.1. Modeling Energy Efficiency of Scientific Data Center*

508 Since a data center or a cluster closely resembles an industrial production
509 unit, we can apply operations management principles, such as minimizing the
510 lead time, waste, and inventory and maximizing the utilization and output, used
511 in manufacturing to improve computing cluster productivity and minimize its
512 energy consumption. However, not all principles from manufacturing directly
513 fit in computing clusters. For example the law of variation, stating that all
514 variability reduces efficiency, is not actually true in computing [79].

515 In practice, our approach is based on collecting and analyzing log data on
516 a computing cluster at CERN [79]. When analyzing the data, we noticed, for
517 example, that wall clock processing times of jobs are 15 to 50% longer than
518 the actual CPU times. Since the cluster configuration was set to process one
519 job per CPU core, this means that there is a bottleneck slowing down the
520 computing process. The most obvious bottleneck is I/O access to the disk or
521 network. Furthermore, the memory utilization of jobs was only about half of
522 the CPU utilization rate. One reason for this is an irregular memory utilization
523 curve of particle physics jobs. Based on this observation, we assumed that
524 reasonable overloading can help and throughput can be improved and electricity
525 consumption reduced by increased multitasking, i.e. processing more than one
526 task per CPU core in parallel, and mixing heterogeneous tasks in parallel while
527 multitasking.

528 *4.3.2. Technologies for Measuring Energy Efficiency*

529 There are several indicators for measuring the (energy) efficiency of data
530 centers [83, 84]. Probably the most commonly used is the Power Usage Ef-
531 fectiveness (PUE), measuring the ratio of power consumed by ICT equipment
532 compared to the total power of the data center [85]. It measures the energy effi-
533 ciency of the overall infrastructure, but it does not indicate whether ICT services
534 run efficiently. Therefore, other performance indicators have been suggested, for

535 example for measuring useful work per unit of energy [86].

536 Since all components of the computer use energy even when idle, and they
537 also have an optimal utilization rate, the optimal case would be using all com-
538 ponents in their energy-optimal rate all the time. For most of the components
539 the highest energy efficiency is reached when utilization is high but not too close
540 to 100%. For this purpose we [81] have developed the energy-efficient utilization
541 indicator (EEUI). This indicator gives a weighted average of energy efficiency for
542 all components of a computing unit (single server to data center). Using EEUI
543 as a guide to run computing resources optimizes both throughput and energy
544 efficiency. However, a challenge using the EEUI indicator is the need for power
545 measurements in a server or even server component level. Fortunately, measur-
546 ing, or estimating, power values is becoming possible through technologies such
547 as RAPL [87], which was discussed more thoroughly in Section 4.2.1.

548 *4.3.3. Technologies for Energy-efficient Management of Computing Resources*

549 This final step in our approach is probably the most difficult one answering
550 to the following question: How should workloads be scheduled for different
551 computing servers so that the processing remains energy-efficient and gives the
552 optimal throughput? Good allocation involves several practical issues. For
553 example, the number of parallel tasks in a server is limited by physical resources,
554 especially by the main memory. Another challenge is that the workload is not
555 stable but constantly changes. Thus, static scheduling would lead to a non-
556 optimal solution [82, 48].

557 For scheduling, we can use the following criteria: 1) a task uses a minimal
558 amount of energy, and 2) the total throughput is maximal. These goals can be
559 contradictory but usually the maximal or near maximal throughput also gives
560 the minimal energy consumption per processed task. As far as the clusters are
561 concerned, the problem can be divided into two independent steps assuming
562 that cluster nodes are homogeneous:

- 563 1. Finding the optimal load combination for the computing node.

564 2. Scheduling jobs to the computing nodes in such a way that all computing
 565 nodes are as close as possible to the optimum state.

Figure 2: An example how the number of parallel jobs affects throughput and energy efficiency [48].

566 The efficiency and energy consumption of computing servers depends on the
 567 load level as illustrated in Figure 2 when CMS data analysis application [88]
 568 was run. If the workload is heavy enough to keep all servers busy, the optimal
 569 number of parallel jobs running on a computing server can be estimated, for
 570 example, by the fuzzy logic-based algorithm [82]. The algorithm dynamically
 571 adapts the memory threshold for submission of jobs based on the overall load. In
 572 this way, it is possible to keep memory consumption stable with different work-
 573 loads while achieving significantly higher throughput and energy-efficiency than
 574 using traditional fixed number of jobs or fixed memory threshold approaches.
 575 The test results showed that at best, the memory-based scheduling with fuzzy
 576 tuning improved throughput by over 150% and reduced energy consumption
 577 around 50% compared to one job per CPU core scheduling. Mixing CPU and
 578 I/O intensive jobs improved both throughput by 10-20% and energy efficiency
 579 by 5-10% compared to running single types of jobs only.

580 For situations where the intensity of the workload fluctuates a lot, we can
 581 apply dynamic workload management, meaning that the allocation of computing
 582 tasks running on virtual machines (VM), to servers can be changed during
 583 processing. For this purpose, we developed a methodology and prototype system

584 for the load based management of virtual machines in an OpenStack cluster
 585 [89]. The novelty of this load balancer is to use specialized, energy-efficient
 586 servers (park servers) for storing idle virtual machines in addition to the active
 587 monitoring of resources and the load based active management of VMs in the
 588 physical cluster. Since the park server is used to store idle VMs its over-commit
 589 ratio can be high while actual computing servers used by active VMs have one-
 590 to-one mapping of virtual to physical resources. The load balancing algorithm is
 591 based on live migrated VMs as follows: 1) move idle VMs to the park server; 2)
 592 move a VM from the park server to a computing node when it becomes active;
 593 3) consolidate active VMs within the cluster to minimize the number of active
 594 servers. Our tests with real hardware indicated potential energy savings of 9%
 595 to 48% and the simulation results showed that in large installations the energy
 596 efficiency could be improved by up to 40%. Naturally, the energy savings of the
 597 active management greatly depend on the workload and its fluctuations.

598 *4.4. From Energy Saving to Proper Timing of Energy Use*

599 An important observation in energy-efficient computing is that saving energy
 600 is not the only goal. Often it is more important to use the energy at the right
 601 time in the right place. Demand management [90] is a hot topic in the electricity
 602 sector and scientific computing could be a component that brings additional
 603 elasticity to the demand. In electricity grids the supply and demand have to
 604 meet at each time point and scientific computing could be one way to very
 605 rapidly react to imbalances in supply and demand.

606 Especially with renewable energy sources the energy supply and price can
 607 vary a lot. There have been extreme cases for example in Germany and Denmark
 608 where the price of electricity has been negative. The obvious but not very useful
 609 way to take advantage of this is to time the computing so that it is done when the
 610 electricity is free or cheap. The problem with this approach is that scientists are
 611 eager to get results and therefore they are not willing to tolerate very long wait
 612 times. Moreover, it is questionable whether an investment in computer hardware
 613 that is only used when cheap energy is available, makes enough economic sense

614 these days when the electricity price is generally low.

615 A set of more interesting ideas is based on the observation that often it is
616 easier to move computing tasks than to move electricity. Therefore the goal
617 could be to move the computing tasks to places which have abundant energy.
618 Researchers have already explored cases of optimally moving the computing to
619 different countries or regions depending on the variable electricity prices (see
620 e.g. [91, 92, 93]).

621 In our own work, we have studied the idea of spending the spare energy of
622 a house equipped with renewable energy sources for computing as described in
623 [94]. The development is based on the fact that it is not straightforward to
624 decide what to do with the extra energy generated, for example by solar panels.
625 This issue can exist for example on a sunny day when the home is empty. The
626 conventional possible alternatives include selling spare energy to an electricity
627 company, storing it locally, or in the extreme, wasting it completely. However,
628 all of these have they shortcomings. Therefore, we have developed a computing
629 server which uses the spare electricity in a home to perform computing. This
630 allows the homeowner to earn money by selling computing services instead of
631 selling electricity back to the grid. Scientific computing workloads could be
632 excellent candidates for such calculations since they can often tolerate the delays
633 that arise because of the unpredictable availability of the computing services.

634 5. Towards a More Energy-Efficient Future

635 In this section we discuss ideas and observations for improving energy effi-
636 ciency in scientific computing and computing in general. First, it is important
637 to have a holistic view. Different actors, as we have described in this paper,
638 have different viewpoints and different sets of options to influence the energy-
639 efficiency of computing. In addition to focusing on improving a single perspec-
640 tive it is essential to understand how the different views coexists and influence
641 each other. It is also essential to analyze the computing system as a whole and
642 to find the most promising opportunities to be implemented. Taking advantage

643 of expected benefits requires work: it includes making changes to the existing
644 legacy systems, developing new ways of working, and inventing new methods
645 to manage computing. A large part of this work can be done in parallel. Only
646 through gradual progress on multiple frontiers, we can gain concrete advances,
647 since any single breakthrough alone is unlikely to have a dramatic effect but
648 accumulating the effects of several improvements will be important.

649 In this paper, we introduced three groups of methods for improving energy
650 efficiency of scientific computing presented in Section 4: 1) promoting green val-
651 ues to the users, 2) offering tools such as energy profiling and energy-aware ar-
652 chitectures for developers, and 3) monitoring and optimizing tools and methods
653 for data center operators. Although these methods have similarities to proven
654 techniques used in traditional manufacturing such as the continuous improve-
655 ment paradigm [95] emphasizing visual control and the theory of constraints
656 focusing on process bottlenecks [96], our examples also show that a scientific
657 computing system should not be managed as an automated factory but it is
658 an interactive system among the shareholders. For example by providing the
659 user with feedback on the resource usage and energy consumption along with
660 the yield (processed jobs in time per available processing time) may change
661 user behavior towards a more resource intensive and energy efficient use of the
662 facility. At the same time, a developer who realizes through visual reporting
663 which functions of the software are most used, may direct his efforts to further
664 develop those key functions to be more efficient and faster. This follows closely
665 the bottleneck approach, which aims to remove process constraints to reach a
666 swift, even flow [97] in the value adding process. Moreover, data center man-
667 agement could be directed, for example, by showing key performance indicators
668 on resource utilization. According to operations management principles, the
669 practical version of the law of utilization indicates that lead times and work in
670 process will increase radically when a threshold level is passed [52].

671 On the other hand, we must remember that, as operational entities, data
672 centers radically differ from the traditional supplier-customer relationships in
673 manufacturing and service industries. In these industries partnerships are crit-

674 ical to success, meaning that in supply chains suppliers and customers share
675 information, plans and the additional business environment related knowledge
676 to improve efficiency and responsiveness. In the computing center context the
677 triangle of stakeholders, namely the users, developers, and data center opera-
678 tors seldom discuss with each other. This can reduce efficiency, since scientific
679 computing systems are often custom-made systems which would benefit infor-
680 mation sharing among the stakeholders. There is no genuine partnership or
681 unity, which would on its own improve the situation like in supplier-customer
682 quality circles [98], where different parties systematically and with objective
683 methodology improve the overall system performance.

684 As we have discussed above there are still many open issues in the quest
685 for greater energy efficiency. While our work and that of other scientists in the
686 area is touching some of these issues, a fair number of unsolved problems exist.
687 One important outcome of our work in this area is a clearer understanding
688 of important research problems to tackle. We have collected the major open
689 technical challenges covered in this article in Table 1. The first column of the
690 table describes the challenge, the second one explains its importance, the third
691 one indicates possible difficulties and the last one gives examples on studies
692 towards possible solutions.

693 Besides the somewhat well understood possibilities there are naturally a mul-
694 titude of other future possibilities such as photonic, biomolecular, and quantum
695 computing (see e.g. [116, 117, 118]).

696 While each of the ideas discussed in this article works separately the best
697 results can of course be attained if they would be used in an integrated fashion.
698 However, this is very challenging to achieve in practice. The massive amount of
699 legacy software would need to be adapted to the new environment. Considering
700 the different aspects would make software development harder, and in scientific
701 computing most of the software is developed by scientists who are experts in
702 physics but not necessarily in software development. Furthermore, considering
703 the amount of time that is needed to develop and deploy integrated solutions
704 the world may change and new, unanticipated options, may become available.

705 Therefore a perfect future solution is an illusion. It is good to have a vision and
706 take steps in that direction but at the same time admit that in real-life reaching
707 the ideal target may be challenging.

708 **6. Conclusions**

709 Improving the energy efficiency of computing systems is becoming more and
710 more difficult since simple technical solutions and replacing the computing hard-
711 ware with next generation models does not offer as much improvement it used
712 to. Therefore, other solutions are needed and, for example, optimizing parts
713 other than hardware of computing systems still offer a large potential for im-
714 provement. In this paper, we studied how the computing system can be seen as
715 a value chain of three main roles: users, software developers, and data center
716 administrators. Using this grouping, we introduced a set of potential technolo-
717 gies and methodologies for improving the energy efficiency of each of these roles.
718 This makes it possible to recognize the bottlenecks of the system and focus on
719 removing those bottlenecks.

720 The high energy physics community is a global family of researchers and
721 experts working on the experiments to detect new particles generated by the
722 colliding beams in the LHC. To reveal the elementary levels of matter from these
723 collisions requires massive computing infrastructure and multitude of skills to
724 master. Therefore, information technology has always played an essential role
725 [119]. The community works in distributed manner through globally spread
726 institutes, which all share their own political and computational habits, but
727 still striving towards common scientific goals. The spirit is similar to open
728 source societies, where transparency and rough consensus drives the collabo-
729 ration. Complex system development requires architectural control, which is
730 balanced by technological memorandum of understanding to which developers
731 commit and which is continuously scrutinized through a social network and fre-
732 quent collaboration meetings. This facilitates also global and fast dissemination
733 of different results produced by the community.

Table 1: Summary of selected technical challenges towards more energy-efficient future

Challenge	Motivation	Difficulty	Studies towards possible solutions
Accurate and non-intrusive way to estimate energy spending at function or line-of-code level	Making it possible for the developer to know where in the program code the energy is consumed.	Too coarse granularity of energy measurements	[60, 99]
Methodology to see how energy consumption varies when code is modified	In this way, alternative designs could be tested and 'energy bugs' could be recognized	Software energy consumption is influenced by external factors like other applications running at the same time	[100]
Measuring energy consumption of a computing job	Users would be more motivated for saving energy if its usage is visible	Other applications and utilization of the resources make it difficult to map the energy to a single application	[101]
Automatic methods for taking benefit on heterogeneous hardware	Code could benefit energy optimizations of different architectures and applications run in the optimal hardware	Although relatively easy for similar architectures, using e.g. GPUs requires writing memory management etc.	[102, 89, 103, 104, 105, 106]
Appropriate software architectures, which have proper balance between efficiency and other needs	Software systems tend to live and evolve for decades. Easy adaptation to new needs is essential. At the same time efficiency is important when amount of analyzed data grows	Anticipating the aspects that are relevant for future is hard.	[107, 108, 109]
Incentives for scientists to develop energy efficient code	Prices of ICT components are continuously decreasing while electricity production remains a bottleneck	Little tradition in teaching and developing energy efficient code and systems in scientific computing	[110, 111, 112]
Large-scale energy driven distributed computing	Bring computing to locations with plentiful energy (with renewable production energy availability will increasingly fluctuate)	Grid and cloud systems not designed for easy geographic migration of computing	[113, 93, 114, 115, 94]

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