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Partnership for Advanced Computing in Europe

HPC Infrastructures Workshop #10

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Abstract

The 10th European Workshop on HPC Centre Infrastructures was hosted by PSNC and held in Poznań, Poland, between 20 and 23 May 2019. BSC, CSCS, CEA, LRZ, PDC-KTH, and PSNC have collaborated in the committee organising the workshop. The workshop, upon invitation only, with participants from Europe, America, Australia, and Asia, brought together experts from the HPC facility management side with experts from companies developing and bringing technologies to the market relevant for energy-efficient HPC and energy-efficient HPC facility management in particular.

The workshop covered a broad range of topics, ranging from cooling technologies to the provisioning of electricity, and from overviews of standards and certification to the management, storage, and analyses of the large streams of heterogeneous metrics that are crucial for the efficient operation of modern HPC datacentres. Several presentations from supercomputing sites gave an insightful look into the "kitchen" of their facility management, explained the challenges they had faced and in what way those were tackled, and gave an overview into their roadmaps for the near future. The PRACE closed session, held at the end of the workshop, gathered attendees from PRACE Tier-0 and Tier-1 sites and gave the opportunity for exchanges between experts from the European supercomputing sites.

This paper summarises the presentations and discussions held at the workshop and identifies major trends in the field of the HPC centre infrastructures.

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Introduction

The 10th European Workshop on HPC Infrastructures was hosted by PSNC and held in Hotel Andersia, in Poznań, Poland, from 20 to 23 May 2019. BSC, CEA, CSCS, LRZ, PDC-KTH, and PSNC have collaborated in the committee organising and assembling the programme for this workshop. Some PRACE-5IP Work Package 5 (WP5) manpower, as well as PRACE aisbl sponsorship, was used for the preparation of the workshop. Additional sponsorship was provided by CEA, CSCS and GCS. The programme committee consisted of the following members:

- Javier Bartolomé Rodriguez, BSC, Spain
- Ladina Gilly, CSCS, Switzerland
- Herbert Huber, LRZ, Germany
- Norbert Meyer, PSNC, Poland
- Michael Ott, LRZ, Germany
- François Robin, CEA, France
- Gert Svensson, PDC-KTH, Sweden

The workshop, upon invitation only, was very successful, with 74 participants, coming from Europe, America, Australia and Asia. Among participating parties, there were PRACE-related datacentres, large government-funded non-European HPC sites, commercial datacentre providers, companies aiming to HPC relevant technologies for cooling and heat re-use, and experts from HPC equipment vendor labs.

The proceedings of the workshop, the facts and insights presented during its sessions, are summarised in this paper, to be accessible to a wider audience of HPC facility management and datacentre management experts. The sites represented are often early adopters of or experimenters with new technologies and procedures. Their evaluations and accounts of problems encountered and solutions experimented are valuable for professional peers. The intention to learn collectively from problems encountered during datacentre operations was fully honoured. Several presentations from datacentre sites gave insightful and unabashed looks into the peculiarities of their facility management, problems encountered, and the struggles and various solutions tried to overcome these.

Figure 1: Participants of the 10th European Workshop on HPC Infrastructures

The themes we focussed on during this workshop work were immersion-cooling, standards relevant for HPC and HPC facility management, energy, future technologies, tooling for facility management, and developments concerning EuroHPC. The role of system integrators, vendors of HPC systems, was different from their role in previous workshops where they used to give an overview of their current products, mostly with a focus on the energy-efficiency and requirements for power and cooling of their current systems. The judgement of the programme committee was however that such overviews and the discussions they entice in practice tended to be somewhat constrained by the lack of non-disclosure agreements. Representatives from vendors on this workshop focussed more on technologies for a slightly more distant future.

The PRACE closed session, held at the end of the workshop, gathered attendees from PRACE Tier-0 and Tier-1 sites. Several site representatives gave an update on specific datacentre infrastructure. The PRACE closed session gave the opportunity for exchanges between experts from the assembled PRACE sites.

The workshop made possible an assessment of the situation in Europe in terms of best practices in facility management, infrastructure design, and initiatives to strengthen Europe's role in HPC and HPC technology development.

Session I - Site updates, chaired by Norbert Meyer

This session contained two presentations with site updates on developments in two very large HPC sites (Japan and the USA). The session concluded with a third presentation giving a preview of an ongoing survey on standards for HPC datacentres.

Facility enhancement and operations for post-K computer systems

Fumiyoshi Shoji, RIKEN (Japan)

RIKEN is Japan's largest and most comprehensive research organisation for basic and applied sciences. Founded already in 1917, RIKEN today encompasses a network of world-class research centres across Japan, with campuses in Wako, Tsukuba, Yokohama, and Harima. Kobe is the site that houses the K computer, which ranked at 1st place of the HPC systems Top500 lists of June and November 2011. It was the world's first HPC system that achieved a measured High-Performance LINPACK (HPL) performance of over 10 petaflops.

Figure 2: RIKEN site at Kobe. In the front, left, the chiller building; in the front, right, the power substation; in the back the computer building, with the research building left next to it

K computer

The K computer was developed in a collaboration between RIKEN and FUJITSU in a Japanese national project. Design and construction of the system and its supporting facility was quite a long-term process. Design of the system started in January 2006. Design and construction of the supporting facility commenced in 2007 and was completed in 2010. The system has now been in production for more than eight years: from 2011 until September 2012 early adopter programs ran on the K computer. After that, the K-computer was available for shared use and has been Japan's HPC flagship system, figuring as an indispensable tool in many science and engineering projects.

One explicit part of the mission of RIKEN Centre for Computational Science (R-CCS) is to manage the operations and enhancement of the K computer. Another explicit part is to plot and develop Japan's strategy for computational science, including defining the path to exascale computing. The K computer is to be replaced. Not only is its design, as a system without accelerators, getting outdated. After so many years, its operation is becoming increasingly difficult. The role of open source in scientific computing has grown tremendously since the design and construction of the system. However, there is no open source software eco-system readily available for the K computer, so building and maintaining new applications and tools, as well as doing security upgrades, is becoming more difficult and laborious. In addition, many key hardware components used in the system are approaching end-of-life – which has a considerable impact on hardware maintenance.

A phased termination of services of the K computer started in August 2019. Its successor system – provisionally named "post-k" - is planned to become fully operational as a production system for shared use in 2021. RIKEN has set up an information site at https://postk-web.r-ccs.riken.jp/index.html with detailed information about the design of the system and the progress of the project that will be very regularly updated.

Post-K system overview

The performance target for the K computer was to become number 1 in the Top500. This is not a goal with the new system and its overall performance target is not specified in terms of peak flops, as measured by the Linpack benchmark, but rather in terms of application performance: the post-K system is to be at least 100 times faster than the K computer for several key applications, taking tuning of these applications into account. RIKEN has, in fact, distinct speedup targets for many applications: a weather prediction system application and a molecular dynamics application are expected to be over 120 times faster. However, for example, for large eddy simulations, a speedup factor of 25 is expected. An important condition is that the system must be able to reach its application performance targets within a power consumption of 30-40 MW. Power management and power monitoring capabilities figure prominently in the design of the system. Users and administrators will be able to control power optimisations functions that change hardware configurations, via a Power API.

The system will comprise over 150.000 nodes that come in two types: compute nodes and I/O + compute nodes. One feature of the latter type is that it will be equipped with a local high-performance solid-state disk with a capacity of 1.6 TB. The CPUs architecture of nodes is an ARM-based 7-nanometre technology design with specific extensions by Fujitsu (see also the remarks pertaining to architecture in the table shown in Figure 3).

The node high bandwidth and low latency interconnect between the nodes, "Tofu D", is a further development by Fujitsu of the Torus Fusion (Tofu) interconnect that was used in the K computer. Figure 3 details further hardware characteristics of the node architecture, including the bandwidth of its interconnect interface.

Post-K system facility operation

The Kobe facility has on-site gas turbine power generators, and absorption chillers as well as centrifugal chillers for cooling. The resources for power and cooling of the current facility infrastructure must be reused as much as possible. For providing the electricity, mainly transformers and power distribution units have to be added. For cooling, centrifugal electrical chillers have to be added. The Water/Air cooling ratio has to be increased from 7:3 to 9:1.

One challenge for RIKEN is to orchestrate the construction of the new system, the adaptation of the facility, and the shutdown of the current K computer in such a way that; on the one hand delivery targets for the new system are met without on the other hand obstructing too much the provision of compute resources to the scientific computing community that RIKEN aims to serve.

	Description	Remarks
Architecture	Armv8.2-A SVE 512bit SVE: Scalable Vector Extension	With the following Fujitsu's extensions: Hardware barrier, Sector cache, and Prefetch
Core	48 cores for compute and 2 or 4 cores for OS activities	4 CMGs (NUMA nodes)
	DP: 2.7+ TF, SP: 5.4+ TF, HP: 10.8+ TF	
Cache	L1D: 64 KiB, 4way, 230+ GB/s (load), 115+ GB/s (store)	per core
	L2/CMG: 8 MiB, 16way L2/node: 3.6+ TB/s L2/core: 115+ GB/s (load), 57+ GB/s (store)	
Memory	HBM2 32 GiB, 1024 GB/s	
Interconnect Interface	Tofu Interconnect D (28 Gbps x 2 lane x 10 port)	
I/O	PCIe Gen3 x16	
Technology	7nm FinFET	

Figure 3: Post-K system, summary characterisation of the compute node

Another challenge is the handling of power consumption fluctuations to be expected when the post-K system runs in the so-called "large scale job mode". The post-K system will have two modes of operation:

1. Normal mode, in which the system is utilised by a large number of smaller jobs. In this mode, the power usage fluctuations occurring in many unrelated jobs are expected to cancel out each other largely. Power fluctuations are estimated to be within a 10% range. In addition, the power saving functions of idle nodes are expected to contribute a reduction of overall power usage of 5-10%.
2. Large-scale job mode is the mode of operation that is planned to occur up to three days per month in which few huge jobs are run that utilise a very large part of the system. In this mode with power-saving functions enabled, the gap between idle and peak moments can become as large as 26 MW. If the power-saving functions are disabled, the width of the gap can be reduced to 8.3 MW.

Fast fluctuations of this size simply cannot be dealt with by a substantial part of the power and cooling infrastructure. Especially the cooling capability for a quick change of heat load is limited. The bulk of the cooling capacity is provided by 4 absorption chillers with a total cooling capacity of 23.92 MW. However, these need a time-interval of 1.5 to 2.5 hours from activation to full capacity. If they are already on, they still need about 45 minutes to go from minimal to maximal capacity. The centrifugal chillers are quicker: they need about 20 minutes from activation to full capacity. In addition, if they are already on, they need 4 minutes to go from minimum to maximum capacity. RIKEN has decided that in large scale job mode the power saving function must be off, otherwise the possible gaps between lowest and highest power level cannot be bridged by the electrical chillers.

Power capping and forecasting of the power usage of the job from job history data, and preparing additional chillers when needed, will be an essential part of operating the system in large job mode. A preview process will be institutionalised to help identify a precise enough power profile of jobs to be run in this mode:

1. The user must execute a small version – up to 10% of the full system – of the large-scale job before the large-scale mode period.
2. The resulting power profile of that job is analysed and based on that analysis, the decision is taken whether or not to admit the job at full scale in large job mode.
3. If power usage nonetheless exceeds expectations, a monitoring system will terminate such a job automatically.
4. At the blade level, an FPGA-based power capping can decrease the CPU clock frequency, per unit of 16 compute nodes, when power consumption exceeds a limit predefined limit. If that does not help, the unit can also shut down the 16 nodes that it controls.

Benefits and challenges of warm water cooling at scale

Jim Rogers, Oak Ridge National Laboratory (USA)

From 2004 up to 2018, HPC systems at ORNL relied on the supply of cold water by the facility and were operated with an annualised power usage effectiveness (PUE) of about 1.4. Only since 2018, with the advent of Summit, ORNL is making the transition to cooling by means of water with warmer temperatures supplied by the facility. Table 1 shows the HPC flagship systems operated at ORNL, from 2004 up to 2018. The table documents a more than thousand- fold growth of compute capacity. In addition, from a mechanical perspective, lots of innovations went into these machines. However, the basic cooling principle of all these machines remained the same, viz. blowing cold air over hot components and subsequently capturing the heated air to transfer the heat to water. Titan did this in a more efficient way than its predecessors did, but the cooling of Titan required the supply of cold water as well, with a temperature of about 5.5°C.

1st year of operation	Machine	Compute capacity (in TF or PF)	
2004	Cray X1E, Phoenix	18.5	TF
2005	Cray XT3, Jaguar	25.0	TF
2006	Cray XT3, Jaguar	54.0	TF
2007	Cray XT4, Jaguar	62.0	TF
2008	Cray XT4, Jaguar	263.0	TF
2008	Cray XT5, Jaguar	1.0	PF
2009	Cray XT5, Jaguar	2.5	PF
2012	Cray XK7, Titan	27.0	PF

Table 1: Air-cooled HPC machines operated at ORNL

The cooling of all of these systems is 100% chiller-based. With Titan, all options to optimise chiller-based cooling, not just the low hanging fruit, had already been applied. The operation of the 27 petaflops machine results in an annual electricity cost of more than eight million US Dollars. About a quarter of that electricity budget goes into the running of the infrastructure needed to get rid of the waste heat produced by the system.

The Summit System

A larger successor to Titan, with still affordable operating cost, was only feasible if the reliance on traditional chillers could be decreased very substantially, that is traditional chillers would only be used during the hottest season in the year. With the request for proposal (RFP) for Summit, the HPC vendors were forced to come up with a system that could be operated with facility supplied cooling water with an inlet temperature of at least 21°C. The system should also be room neutral, or nearly room neutral.

The resulting machine is cooled by a combination of direct on-package cooling and rear door heat exchangers (RDHX). The CPUs and GPUs of Summit use cold plates. Dual inline memory modules (DIMMs) and parasitic heat-loads, mainly from the power supplies, in the compute nodes are cooled by RDHX. Storage and network cabinets are completely cooled by RDHX.

The temperature of the facility supplied water is now at 21°C and the system is about 95% room-neutral. With a flow rate of 12,500 litres/minute, the return temperature is 29°C. ORNL started with an inlet temperature of 19°C and a higher flow rate, and slowly have driven the flowrate down and the temperature difference between inlet and outlet temperature up.

The annualised PUE for Summit is 1.1. Contribution to the cooling by chillers is limited to about 20% of the hours of the year. A new primary cooling loop (green circuit in Figure 4) uses “Econo” heat exchangers that get their cooled water from evaporative cooling towers on the roof. On hotter days, when the water that comes back from the roof has a temperature above 21°C, the water supplied to Summit (red circuit in Figure 4) is further cooled down by "Trim" heat exchangers. "Trim" heat exchangers get their cooling capacity from the already existing chiller-based cooling plant (blue circuit in Figure 4) that provides the cold water that is used to cool Titan and other cold water-cooled equipment. The water temperature monitoring, and the decision whether or not to involve the cold water loop are all fully automated. Apart from reduced operational costs, this allowed for an easier and more reliable design of the facility to support the system, and in turn drives down capital expenditure. With no additions to the existing chiller-based cooling plant being necessary, the new facility design is essentially reduced to pumps, evaporative cooling, and heat exchangers. For future machines, a chilled water infrastructure may not be necessary at all.

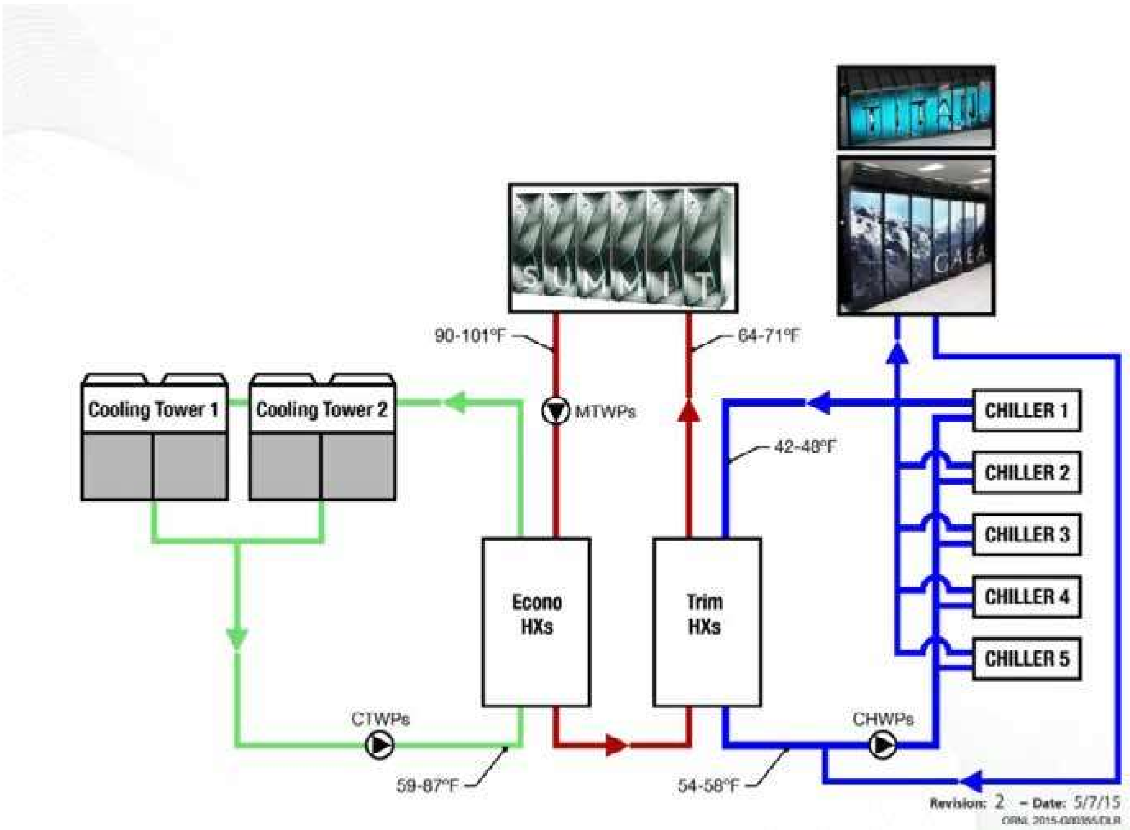

Figure 4: Cooling loops at ORNL used by Summit

An interesting observation is that the annual electricity cost for operating the 200 petaflops system Summit is at least a million US Dollars lower than the annual electricity cost for operating the 27 petaflops system Titan. However, even if a more efficient cooling system contributes to this result, this is in large part due to the increased compute capacity per Watt of the computational components in the machine. Titan could deliver about 2 gigaflops per Watt, Summit can deliver about 14 gigaflops per Watt. In both systems, the bulk of the compute capacity is delivered by their GPUs (see Table 2).

System:	**Titan, 2012 Cray XK7**	**Summit, 2019 IBM Power 9**
CPUs:	18,688 AMD Opterons	9,216 IBM Power 9s
GPUs:	18,688 NVIDIA GK 110 GPUs	27,648 NVIDIA GV100 GPUs
Aggregate GPU performance:	90% of 27 petaflops	95% of 200 petaflops
Flops per Watt:	2 gigaflops/Watt	14 gigaflops/Watt

Table 2: Titan and Summit compared for their compute capacity and flops per Watt

Handling 470,000 metrics per second real-time

The hard part about running systems at the scale of Summit or even larger systems is the overwhelming amount of monitoring data that have to be taken into account for safely running the system. For Summit there are roughly 470,000 metrics per second that have to be processed. The CPUs, GPUs, and many other components that have very specific conditions under which they operate best. When experimenting with changing the inlet temperature of cooling water, or changing the flow rate, a comprehensive and reliable monitoring system has to be in place to make sure that undesired effects are discovered quickly. The ultimate ideal is that the system runs itself. I.E.: that monitoring data are fed back to control systems to enable corrective responses to a variety of events. The metrics range from metrics that pertain to weather conditions in the Oak Ridge area to metrics describing the conditions in the water flow system, and from data from the IBM LSF batch system to the 99 metrics per node per second that are obtained from the IBM OpenBMC framework. ORNL has invested about nine months of work to create a system that collects, stores and processes all these data.

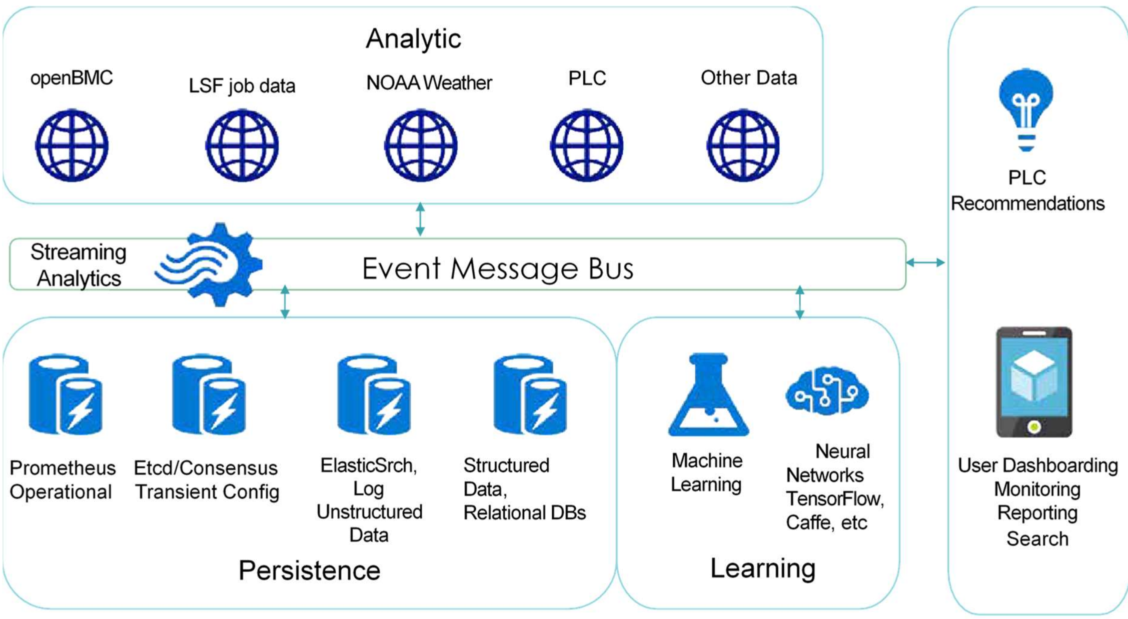

Figure 5: Summit monitoring, analytics, reporting and dashboards

The system is designed as a distributed stream processing system able to handle multiple large real-time data feeds from multiple producers. Figure 5 presents a high-level overview of the system, with an Apache Kafka message bus as the heart of the system. Grafana has been used to create dashboards, insightful high-level graphics spatial overviews, such as heat maps of the system and visual representations of cooling metrics of the system.

Post Summit: Frontier

The HPC power budget continues to grow. Summit has a design point for over 12 MW, though, in practice, it consumes about 6 MW most of the time and up to 9 MW for very compute-intensive high loads. The design point of its successor is however about 30 MW. The RFP for Summits successor, Frontier, planned for the 2020/2021 timeframe, targets an aggregate compute capacity of 1.5 exaflops and aims to drive the temperature requirement for facility supplied water up to the 30°C range, at which RDHX cooling is no longer very feasible. Nearly all of the cooling capacity must come from custom mechanical on-package cooling technology. This system must be able to operate with almost 100% of evaporative cooling the whole year through and be more than 95% room-neutral. Some auxiliary ventilation and air conditioning to deal with the less than 5% residual parasitic heat in the computer room are allowed.

To push vendors to innovative power usage effective designs on the mechanical side the RFP for Frontier contains:

- The requirement that the inlet temperature for the facility cooling water is no less than 21°C, with a preference for 32°C;

- Demands for on-packaging or system-wide cooling solutions that substantially reduce or eliminate waste heat ejection back to the facility (i.e.: “room-neutrality”);
- Demands that minimize the impact of any air-cooled systems on the facility environment (i.e.: even with a great design for the compute nodes, there will be “pesky” storage and infrastructure devices that are air-cooled; indicate how the waste-heat of these is going to be managed).

Water chemistry

One of the main challenges when dealing with warm-water cooling solutions is the requirement for the continuous management of the water chemistry to maintain acceptable water quality. E.g. fungi might grow in the water and eventually cause blocking of cooling channels in cold plates. Depending on what you must chase – fungi, algae, anaerobic or aerobic bacteria – there is a choice of biocides to add to the water. However, IBM is very strict about the generally very low levels of substances that may be present in the water.

PRACE Survey of standards for HPC datacentres

Gert Svensson, PDC, KTH (Sweden)

PRACE will produce a white paper on standards for HPC datacentres. The paper will address to what extent leading edge HPC is a suitable area for standardisation and what standards should be taken into account. One of the important activities that provide a background for this white paper is a currently still ongoing survey among datacentres run by PRACE members that inquires what the centres consider the most important standards that they adhere to now, and what their experiences are with practising these standards. So far, 11 datacentres have responded – which is not enough to base any statistical conclusions on, but from the preliminary results, some noticeable patterns do emerge that were not envisaged when the survey was initiated.

A couple of standards are mentioned quite often by the respondents of the survey:

- Computer hall standards: ANSI/TIA 942, EN 50600, EU Code of Conduct
- Tier rating and classification of computer halls: Uptime Institute, ANSI/TIA 942
- Technical know-how and best practices: ASHRAE standards
- Quality Management: ISO 9000
- IT Service Management: ISO 20000, FitSM, ITIL
- IT Security Management: ISO 27000
- Energy Management: ISO 50001

Mentioned as well, but far less, are technical standards that cover norms for types of datacentre equipment, such as uninterruptible power systems (IEC 62040), batteries (IEC 62485), and cabling (ISO/IEC 11801, EN 50173).

A very practical reason to report on the rather preliminary results of the survey is to discuss with the participants of the workshop what should be the focus of the white paper. On the one hand, most of the datacentres appear to give a rather prominent place to general management standards rather than the technical standards. On the other hand, such standards are hardly specific for HPC. It is still to be decided whether the whitepaper should focus on these standards.? In any case, it would be interesting to know *why* management and classification standards are more mentioned than technical standards and norms are.

Standards, guidelines, and ratings pertaining to datacentre infrastructure

The EN 50600 European Datacentre Standard, created by CENELEC, the European Committee for Electrotechnical Standardisation, is a modular but quite comprehensive standard that focusses on physical security and availability of power and mechanical systems. Part 1 deals with general aspects for design and specification of datacentres. Part 2 deals with physical aspects of structural issues related to the building: construction, power distribution, environmental control, cabling, and security systems. Part 3 deals with management and operational information. Part 4 deals with efficiency aspects such as key performance indicators for power usage effectiveness and renewable energy. This standard has a certification program.

The UPTIME institute is well known for its “four-tier rating” of computer halls. A higher tier denotes a higher level of redundancy, resilience and fault tolerance of a datacentre infrastructure. The institute is the sole certificate body for rating datacentres according to their detailed norms for the several tiers.

The origins of the ANSI/TIA 942 are in the telecommunications industry. It started as a cabling standard but has developed into a standard covering all aspects of the physical datacentre: site location, architecture, security, safety, fire suppression, electrical and mechanical aspects, and telecommunication. It has a classification and rating system, comparable to that of the Uptime Institute, and it has a program for certification by independent bodies.

By contrast, the EU Code of Conduct for Computer halls, for the most part, is more a high-level specification of what datacentres are expected to strive for. But the code of conduct is complemented with a selection of more detailed best practice guidelines in several areas such as datacentre utilisation, management and planning, IT equipment and services, datacentre equipment datacentre power equipment, cooling, monitoring and datacentre building.

The guidelines published by the American Society of Heating, Refrigerating and Air-Conditioning Engineers (ASHRAE) are generally highly regarded as practical standards concerning cooling aspects, done by engineers for engineers.

General IT management standards

ITIL, FitSM, and the abovementioned ISO standards for quality management, IT service management, and IT security management, though having different focuses and varying in level of detail, have considerable overlap. Furthermore, they all have a more or less process-oriented view – which is also true for the ISO energy management standard. Typically, a continuous iteration of a "plan-do-check-act" cycle, as schematically represented in Figure 6, is advocated and constitute the core of the methodology to achieve better energy management, better service management, and security management.

This process orientation seeks to achieve a regularly adjusted, formal measurable definition of what "better" means in these different areas of management. Regular internal audits that check whether formalised processed definitions are adhered to in daily practice are an important integral part of most of these standards. For some of these standards, organisations can be certified, but for example, for FitSM only individuals can be certified as professionals that know how to follow due process as outlined by the standard.

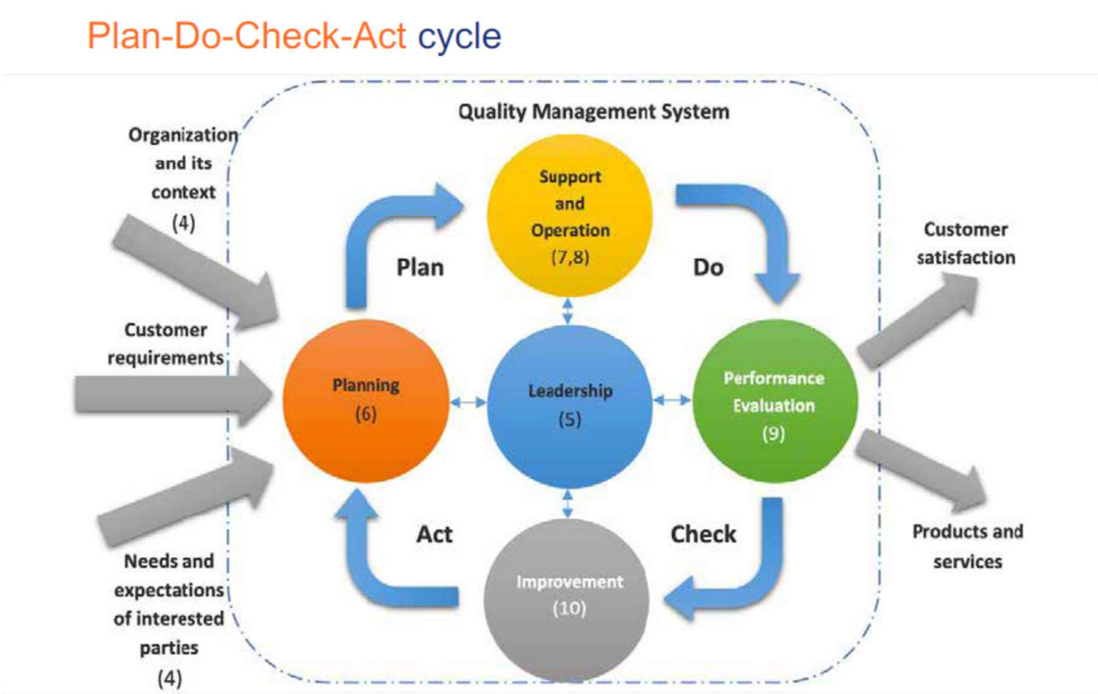

Figure 6: The Plan - do - check -act - cycle

Session II – Immersion Cooling & 'Lighting Talks', chaired by Michael Ott

This session contained two presentations on immersion cooling: one from a company producing immersive cooling solutions, explaining their product. And another one from an early adopter of immersion cooling, telling about their experiences.

The session was concluded with a number of 'lightning talks'. 'Lightning talks' were introduced as a new, experimental, part of the programme of this year's workshop. The concept is very simple: participants can sign up to pitch an idea, or present a message, in five minutes at most, ideally with the help of a single slide.

Immersion cooling, high-performance cooling for HPC

Daniele Rispoli, Submer

Submer is a company, based in Barcelona that produces immersive cooling solutions for computer systems. Submer predicted that by 2023 at least 50% of all HPC deployments will be liquid-cooled. For years, the basic way of cooling IT equipment was by blowing cold air through the heat-producing components. This may be relatively easy to implement, but it is not the most efficient way to do cooling, as air is not very good at picking up the heat and transporting it. For various reasons, ranging from the cost of real estate and floor space to power efficiency and performance of the IT equipment, the density of systems is increasing. And with increasing power density in the racks, the inefficiency of air cooling increases. With an average power density greater than 7 kW per rack the space utilization necessarily must go down below 50%.

Liquid cooling enables high rack densities, but there are various approaches for deployment of a liquid cooled solution, with each bringing in its own advantages and disadvantages. The most common examples include:

- Direct to chip liquid cooling (DLC), generally with water
- Liquid immersion cooling (LIC)

One of the advantages of DLC is that conventional form factors and orientation of equipment are maintained. Another is that it has already been adopted by quite a few original equipment manufacturers (OEMs). The dissipation capacity of DLC is much better than that of air; however, DLC does not dissipate the heat of all components uniformly. Because of this, some components still need air cooling, and both air cooling and a water cooling infrastructure are needed. The risk of leakage, direct spillage of water on critical components is an additional drawback of DLC. There is also a considerable risk of vendor lock-in, as a high-level tailoring to specific components and motherboards is required.

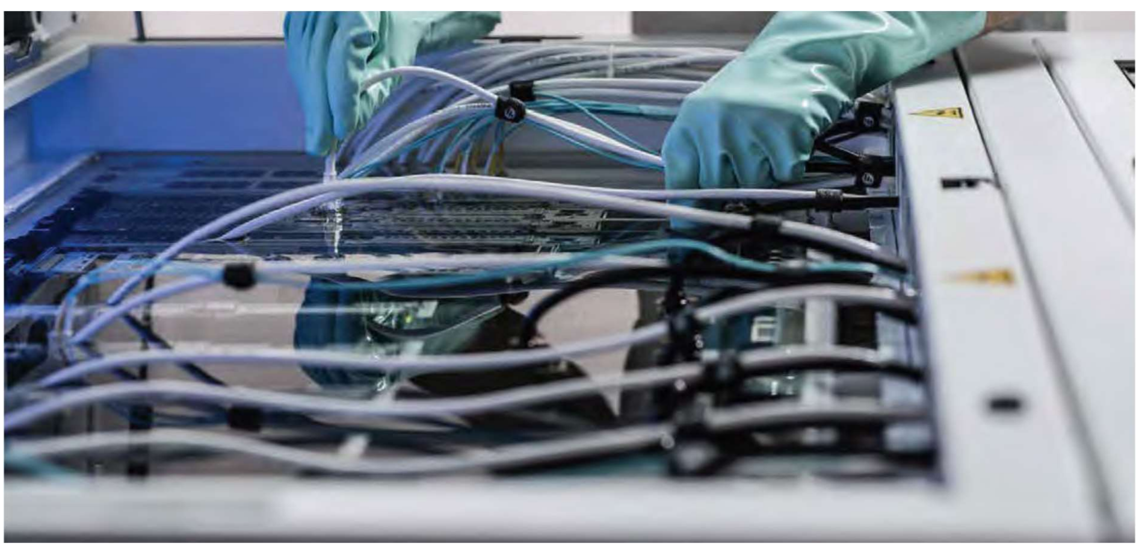

Figure 7: A Submer "SmartPod" container

An advantage of LIC is that it does dissipate the heat of all components uniformly. Submer also finds a significant increase in hardware life span and a significant reduction of hardware failures to be among the advantages: there are no moving parts, no dust particles, and no vibrations. There is less thermal and mechanical stress due to the uniformity provided by the liquid and its viscosity. Build costs are low, as immersion cooling systems are rapidly deployable in “raw” space, without the need for raised floors or a lot of piping. The cost of retrofitting LIC in existing datacentres thus is low. The operational expenditure is also lower, compared to air-cooling, and the resulting environment is nearly silent.

The main disadvantages, according to Submer, are the unconventional form factor and orientation: racks are placed horizontally rather than vertically. Furthermore, there is a perception and mind-set barrier to overcome. There is, for example, fear to lose the warranty on expensive equipment when it is submerged. To overcome this, Submer is involved in many programmes to get their cooling solution certified to work with the products of many IT equipment companies.

The choice of coolant is very important. The coolant used by Submer is an in-house developed synthetic fluid specifically crafted for electronics immersion cooling. It is a single-phase coolant. So there are no state changes. Circulating the coolant through a heat exchange dissipates the heat. There is no cooling by evaporating the coolant involved, so the system can be simple, does not need to be sealed to prevent hazardous fumes. The Submer equivalent of a rack is the SmartPod (Figure 7): a container that allows for 100 kW of heat dissipation. Typically, the containers are connected to a closed loop of an adiabatic cooling tower on the roof.

The characteristics of the coolant used by Submer avoid many of the problems that are often associated with immersion cooling. The coolant is eco-friendly: it is clear, odourless, biodegradable, non-corrosive and non-toxic. It is dielectric and practically non-flammable: its flash point is above 159°C. It is innocuous to compatible OEM and commodity hardware and fully compatible with submerged fibre-optics.

Some in the audience questioned the serviceability and accessibility of components of immersion systems. Submer’s SmartPods are equipped with a system designed for easy lifting blades out of the container without spilling any coolant. Questions from the audience also display some doubt as to whether the system can cool ultra-dense chips, of about 400 Watts in the form factor of a CPU. Contrary to other immersion cooling systems on the market, it is pointed out that Submer’s solution actively forces the distribution of the liquid and does not rely merely on convection to circulate the liquid. Therefore, Submer’s immersion containers should be able to handle such concentrations of heat much better.

Immersion cooling with white mineral oil

Ernst Haunschmid, TU Wien, Vienna Scientific Cluster

The Vienna Scientific Cluster (VSC) operates several cluster systems that provide HPC resources and services to its partner universities and, on pay per use basis, to various academic and non-academic parties as well. VSC has been an early adopter of oil-immersion cooled systems. VSC’s interest in the immersion cooling was, in fact, triggered at the third edition of this very workshop in 2011, by a presentation by Green Revolution Cooling (GRC). At that time, the VSC operated a cluster with water-cooled rear doors and a hybrid cooling system: with outdoor temperatures up to 15°C it could be used chiller-less, but with higher outdoor temperatures, chillers had to be used, which drove up the power used by the facility. This was the case roughly from the beginning of May until the end of September. VSC, looking for ways to improve their PUE, found the case made by GRC for the high efficiency of immersion cooling very promising. A first prototype system was installed in January 2012 and extensively evaluated for more than two years. Compute nodes under full load were tested with oil temperatures up to 75°C. A fair number of power supplies failed in the period, but generally, VSC was very satisfied with the cooling solution.

However, when tendering for the next system, VSC doubted whether specifically asking for an immersion cooling solution, or stating a preference for an immersion cooling solution, in their RFP would be advantageous for them. Many potential vendors stated that they would not offer and support an immersion cooling system. VSC had some difficulty deciding whether they should perhaps expand their hybrid, chiller-based cooling infrastructure expanded after all. The alternative - an investment in a new dry-cooling, free cooling infrastructure – was more promising. Eventually, VSC tendered without a preference for immersion cooling or another cooling technology, using computational power, capital expenditure and operational expenditure over five years as selection criteria. Tendering for a cooling infrastructure would happen afterwards, separately.

It turned out that two offers were immersion cooling based. The contract was awarded to one of them: ClusterVision offered a system with oil-based immersion cooling provided by GRC. The system, with 2020 Supermicro-based compute nodes and an Intel dual-rail QDR InfiniBand interconnect, was installed in the summer of 2014. More than 32,000 litres of white mineral oil were used in the containers of compute nodes. An additional 5000 litres were present in spare parts. The room itself had no air cooling. Temperature in the room could go up to 45°C. The InfiniBand Core is located in a single air-cooled rack. Storage and management nodes are located in a separate nearby room. There are 23 containers, each with 38 vertically aligned rack units. Each container houses

96 compute nodes, 12 IB switches and 2 Ethernet switches. There are two compute nodes per blade. The blade has two motherboards, two IB controllers, and two power supplies – nothing else. Fans are disabled by firmware.

The containers are quite deep and therefore not so easy to maintain, and a lot of power cables are coming out of the containers (Figure 8). Due to space limitations, the pump modules for the coolant were placed under the raised floor (Figure 9) – a first for GRC to do that. There is quite a lot of piping – a mixture of steel and plastic pipes, not compliant with any standard for welding or gluing them together – from the pumps to the containers. Two heat exchangers in series for heat transfer from oil to water. There is oil flow within the containers, and to and from the containers.

The system posed many challenges. The coolant, white mineral oil, is flammable. The flashpoint, at 180°C, is high, but fire prevention, fire detection, and fire extinguishing system are all needed. With oil, there is a need to deal with oil disposal and filter replacement. Several oil leakage prevention measures must be taken, and capillary effects through cabling may still cause dripping of oil. Cables may get really stiff and have a high risk of breaking. Serviceability is hard and gets harder over time. To get a full warranty on all components is a challenge too.

Optical cables may fail when fully submerged. VSC observed that particularly the transceivers, converting optical to electrical signals, had a very high risk of failing when fully submerged. This, however, turned out to be true of the used array Vertical-Cavity Surface-Emitting Laser (VCSEL) transceiver technology, which had been used for all cabling. However, tests with an alternative technology – silicon photonics – showed no such failures over a period of two years.

VSC's experience is that fully immersed high-speed network switches are not a good idea - though they have not been able to find a root cause directly linked to oil immersion for the comparatively high number of failures in switches.

Figure 8: Containers with many power cables sticking

Figure 9: Non-standard piping under the raised floor

There have been very few events of leaking large quantities of oil. There was however one major incident at which, after an improper replacement of a filter element, more than 300 litres of oil leaked out. There is also constant dripping of oil, mainly through power cables, causing the raised floor to be slippery and oil dripping through tiles and sometimes causing defective electrical cabling of which the isolation was affected. Over a period of five years, the gradual leakage of oil adds up to a considerable loss of over 1700 litres.

VSC's experience is that of an early adopter: finding massive room for improvements whilst using the system. Immersive cooling is still a valid option and its implementation has matured. Many improvements have already been implemented in newer systems. A particular weak aspect of their immersion cooling was the placement of so many components outside of the container and the low quality of the piping.

With the immersive system having reached end-of-life VSC has tendered for a new HPC system. The evaluation of offers has been based on compute power and total cost of ownership for a period of five years. The contract has been awarded to EDV-design, a company based in Germany, with an offer based on a Lenovo direct water-cooled system.

'Lightning Talks'

GEOPM

Jonathan Eastep, Intel

GEOPM - "Global Extensible Open Power Manager" - is an open source and community collaborative project started by Intel. GEOPM is a runtime technology for power management that aims to improve both application performance and energy-efficiency of HPC systems. Production release 1.0 has been completed in April 2019. Utilising GEOPM, up to 30% application speedup when power capping, and up to 47% energy savings with minimal runtime impact, have been achieved.

We have entered an era in which the performance of large scale systems is constrained by power costs. At some sites the limiting factor is the cost of expanding the infrastructure providing power and cooling to the system. At others, there is a limited budget to buy the electricity required to run the system. GEOPM is being developed to make more effective use of the limited power that is available. This is achieved by taking a more dynamic approach to power management than is conventionally done in HPC. It profiles the application's power usage over time and looks for patterns. GEOPM seeks to predict how application behaviour will look like in the future and then proactively uses the controls that the software and hardware have for power management. Techniques from control systems and machine learning are used to achieve the predictive goals.

HPC applications often have distinct recognisable phases and it is worthwhile to anticipate phase's changes of analysed applications and adjust the "power knobs" of the system accordingly. But GEOPM can also optimise globally, across the many processors that are used simultaneously. It can detect that some processor is running slightly slower than its peers and is constraining efficiency of the applications because they always reach a global synchronisation barrier last. GEOPM can dynamically compensate for that by steering more of the available power budget to the processors that are on the critical path and holding up the application. By balancing the power across nodes, the performance is equalised. To prevent that such global optimisation becomes intractable on larger systems, it is designed to operate via a tree-hierarchical design.

The system is designed to support extensions and ports via plugins. New optimisation strategies or ports to new hardware happen frequently. Intel is working with many system integrators to make GEOPM usable for many platforms, including platforms that are not even Intel-based.

Rack-integrated adsorption cooling

Matthias Hoene, Fahrenheit

Adsorption cooling utilises the energy in hot water, stemming from the heat produced by the CPUs of a machine, to produce cold water. The principle has been convincingly applied at large scale, in systems at LRZ, and has been reported and explained in earlier workshops. Deploying adsorption at the machine and room level can be quite complicated, as there are three distinct water circuits to deal with: the hot water circuit picking up heat from the CPUs, the cold water distribution circuit delivering a coolant to the air cooled systems, and the re-cooling loop to a dry or hybrid re-cooler.

Fahrenheit has tuned and tweaked the technology. It has evolved to the point where it is possible to produce a downsized version, a rack-integrated adsorption cooling system, which is just as efficient as a large-scale adsorption cooler. The packaging in a rack offers substantially lower complexity of the deployment, and hence faster deployment and less planning.

A few variations are possible. One is to mix air-cooled and hot water-cooled nodes in the rack with the downsized adsorption cooler. In this setup, the rack is room neutral: the hot water-cooled nodes cool the air-cooled nodes. Another way is to have only hot water-cooled nodes in the rack with the adsorption cooler. The rack can blow cold air into the cold aisle and thus contribute to the cooling of air-cooled neighbouring racks with air-cooled nodes.

Intel Innovation to accelerate the path to exascale

Mani Prakash, Intel

Doctor Mani Prakash, a senior principal engineer at the Intel datacentre group, pointed out that Intel's path to exascale strategy has six pillars, for the inside of the process technology in chips to the outside of presenting an API to programmers:

1. Power: new process technologies, with more energy-efficient designs and 3D packaging
2. Performance: applying a diverse mix of scalar, vector, matrix, and spatial architectures
3. Memory: development of in-package memory and persistent memory
4. Interconnect fabric: high-performance fabrics, silicon photonics technology
5. Reliability: aiming for system level fault tolerance
6. Programmability: development of OneAPI, a single software abstraction CPUs and GPUs

The main product lines in which these developments are brought to the market are the Intel Xeon processor, the Intel X^e compute architecture, and Intel Optane persistent memory.

Using machine learning for datacentre cooling infrastructure efficiency and power prediction

Hayk Shoukourian, LRZ

LRZ's strategy for improving energy-efficiency is to take into account all four main aspects of power consumption - "pillars" - in a typical datacentre. Goals are set for each of them, and an integrated approach towards data collection and data analysis is pursued. The four pillars and their goals are:

1. Building infrastructure, providing electricity and cooling capacity: improve key performance indicators (KPIs)
2. HPC and auxiliary (storage, network) system hardware: reduce hardware power consumption
3. System software, in particular the batch system software that schedules applications to run: optimise resource usage, tune the system
4. Applications: optimise application performance

Figure 10 shows a schematic representation of the global optimisation strategy over all four pillars.

The application of that strategy requires a tool that is able to continuously collect and process the data from all the four pillars. Such a tool is not readily available in the market. For a number of years LRZ has been developing and using their own all-encompassing power data aggregation monitoring toolkit, called PowerDAM: Power Data Aggregation Monitor [1].

To cope with the huge variety of relevant data sources and their possibilities for data extraction PowerDAM is designed as a highly modular system that deploys custom agents, plug-ins, that put time series of power relevant variables, into a single database system. Depending on what is a more feasible implementation for a given point-of-interest and to-be-monitored entity, the agents can either push the required data or PowerDAM is capable of pulling the data, i.e. acting as an initiator of data collection. Ultimately, the values are obtained from various sensors at the infrastructure level, from HPC systems HW and system SW (e.g. batch system), etc., with which particular agents interface.

Starting from 2012, users at LRZ can query the overall energy/power usage of their applications using PowerDAM. This monitoring toolkit also contains procedures for data-processing and analyses that enable LRZ to have accurate continuous reporting on aggregate system level and datacentre level KPIs, such as overall power usage effectiveness (PUE), coefficient of performance (COP) for the cooling infrastructure, and energy re-use effectiveness (ERE), etc.

[1] https://www.sciencedirect.com/science/article/pii/S1364815213002934

The capabilities of PowerDAM, have progressed from data collection and monitoring, via analyses of power usage profiles of applications, to prediction of power consumption. LRZ has an electricity contract with an upper and a lower band of power usage. Electricity is cheapest whenever the usage remains between the two bands. If the usages drops below the lower band, or rises above the upper band, a financial penalty is incurred. Being able to predict overall aggregate power usage thus helps reducing cost.

The other main power-hungry component, beside LRZ's flagship HPC system SuperMUC, is the cooling infrastructure. Reliable prediction of the power usage of the cooling infrastructure was obtained using both analytic methods and machine learning methods. Using the PowerDAM data, LRZ is now capable of predicting the efficiency of its warm-water cooling infrastructure, the associated power consumption, and other, datacentre-level KPIs.

The talk provided an update on the initial approach, presented in https://ieeexplore.ieee.org/document/7965143/, illustrating the improved accuracy and anomaly detection use cases. The proposed approach was tested on a 1,5 year operational data that was not available to the model during its training and validation phases.

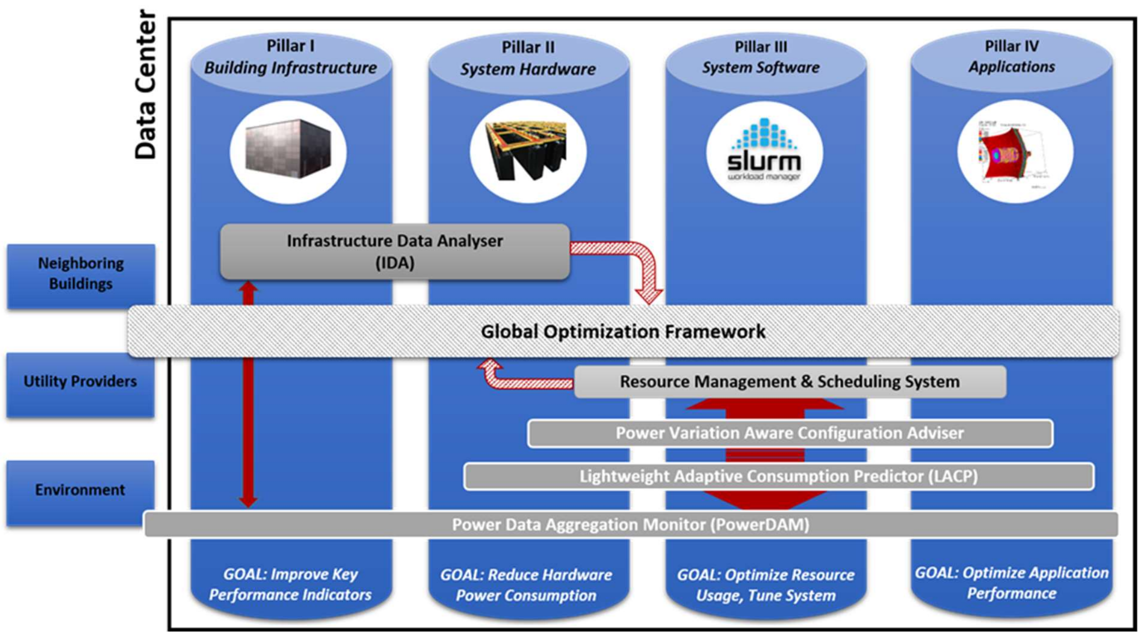

Figure 10: The four pillars of the LRZ strategy for energy-efficiency optimisation

HPC's impact on data centres in the private sector

Sammy Zimmerman, HPE

Zimmerman has been working with HPC customers, which are often government-funded, as well as with customers in the private sector. The trend - "trail blazed" to a considerable extent by the members of the workshop - is now catching on in the private sector, in enterprise HPC. Large customers in Texas, California, the Middle East, and Asia, that cannot be named, are now embarking on projects to build warm-water cooled, or at least liquid-cooled, datacentre infrastructures.

The next important step, according to Sammy Zimmerman, is to improve communications between datacentre procurement teams and teams that tender for machines themselves. Again, workshops like this one, have taken the lead in that as well. The private sector is eager to pick up the best practices developed in this community.

Sessions III - Site visit to PSNC, chaired by Norbert Meyer

The session consisted of an introduction to PSNC and an explanation of its role in Poland for HPC as well as for other services. The participants visited the new PSNC datacentre.

Introduction to PSNC

Norbert Meyer, PSNC

Poznań Supercomputing and Networking Centre (PSNC), affiliated with the Institute of Bioorganic Chemistry of the Polish Academy of Sciences, was established in 1993 in order to build and develop the IT infrastructure for science in Poland. This infrastructure includes the city fibre-optic network in Poznań, High-performance Computing and the national scientific broadband network PIONIER.

PSNC is a multifunctional institute. It provides computing power and archive systems as well as the internet and network services on international, domestic and local levels. It is also a research and development centre for new generation computer networks, modern applications, portals, parallel and distributed computing as well as network and system security. PSNC is involved in the integration and implementation of scientific research results via developing services for public administration, healthcare, education and the social area, and it is a centre for meta-computing.

The High-performance Computing centre within PSNC provides computing power, disc space and archiving systems for science, business and public institutions. A number of the systems it hosts have entries in the TOP500 list. PSNCs computing capacity includes systems with distributed and shared memory of varied architectures (parallel vector, multi-processor SMPs and clusters) connected with fast local networks (InfiniBand, Ethernet).

Datacentres

PSNC operates two datacentres (DCs) located near and in the Poznań city centre.

1. The new BST building (construction finished Q2 2015), is located at Jana Pawła II street, about 6 km from the Poznań city centre, near the Poznań University of Technology. The building has three floors, two of which are computer rooms with a total floor space of 1626 m^2. The third floor, the basement, hosts technical rooms.
2. An older datacentre is located at the Polish Academy of Science building in Wieniawskiego street, in the city centre, it has 320 m^2 of floor space. This datacentre equipped with a fully redundant power supply system. It is connected to two independent sources and protected by UPS and back-up power generators. The datacentre has direct 100 Gbps connections to the Polish national fibre optics network (PIONEER) and direct high bandwidth connections GÉANT – currently 10 x 40 Gbps.

There is a high level of connectivity between the two datacentres. Dozens of dark fibres connect them. Most of these are used for 100 Gbit ethernet connections, but other technologies, such as InfiniBand and Fibre Channel, can be implemented as well. For a number of services, the BST location functions as the primary DC, while the Wieniawskiego street DC is used as a backup location.

Access control

Both DCs have installed fine-grained access control systems that allow for access rights management of different sections of the DCs. In the BST datacentre, there are over 30 distinct security areas. Access of personnel to various sections of the building can be, and is, granted on a strict functional need-to-have basis.

Fire protection

The DC rooms are secured against fire passively and actively. The system consists of the following components:

- A main switchboard;
- Very early smoke detection apparatuses (VESDA);
- Standard optical smoke detectors;
- HI-FOG fire extinguishing system.

The VESDA device continuously sucks air from the monitored rooms. Smoke particles are detected by means of laser technology. The system is able to detect the embers of a fire at a very early stage, which gives the possibility of minimising the side effects.

HI-FOG is a fire extinguishing system using water mist under high pressure. Thanks to the efficient cooling and prevention of spreading the fire area, firefighting using water mist minimises danger to the people in the fire area. Thus, HI-FOG system facilitates the operation of the fire department and allows safe evacuation of people. It is also more cost-efficient than gas-based fire extinguishing systems. The HI-FOG systems use less than 10% of the amount of water used during firefighting with a conventional sprinkler system. This is important as costs caused by flooding in case of conventional fire protection systems often exceed the losses caused by the fire itself.

24/7 monitoring of network connectivity, datacentres, machines, and services

PSNC is an operator of the Polish NREN 'PIONEER' and its network operating centre (NOC) is run by a team of operators in shifts, providing 24/7 service. The NOC also takes care of the proper operation of the Poznań city network services, POZMAN, and supervises international network links. However, the NOC monitoring facilities are used for more than monitoring the network per se and play an important role in the monitoring of the DCs. The availability of the HPC system and data management systems operated by PSNC are also monitored by the NOC. It takes care of both the low-level infrastructure components, such as network, servers, and datacentre elements, and the high-level elements, such as database engines, filesystems, web and HPC servers and other services.

Within the NOC, PSNC also performs activities related to device installations, configuration of new connections, monitoring all resources in the POZMAN and PIONIER networks, bandwidth measurement, receiving and handling reports about network performance and security incidents.

The NOC is equipped with workstations running the HP OpenView Network Node Manager. This software, along with home-grown solutions, is used for continuous status checks of the infrastructure and monitors its usage. In particular, continuous monitoring of bandwidth usage in the networks is carried out by a Multi Router Traffic Grapher (MRTG) tool.

Cluster EAGLE

The cluster 'EAGLE' is PSNC's HPC flagship system. Deployed at the beginning of 2016, it ranked at number 90 in the TOP500 list of June 2016. It is an important element of large-scale computing for Polish science and business, which enables research, simulation, and analysis of problems that, due to their complexity, can only be considered in large computing centres. The compute capacity of the system is about 1.7 petaflops. EAGLE has a 56Gbit/s InfiniBand FDR interconnect and comprises 1300 compute nodes equipped with 33,000 cores and 150 terabytes of operating memory (RAM) in total. The system is connected to 47 petabytes of storage.

EAGLE (Figure 11) is a liquid-cooled system. Hot and cold aisle isolation is applied to take care of residual parasitic heat. Part of EAGLEs waste heat is used to heat the PSNC building.

Figure 11: EAGLE racks in the BST datacentre

Session IV – Energy, chaired by Herbert Huber

The session started with a presentation about hydrogen-powered HPC and continued with a talk about the stability of the power grid for HPC installations and concluded with a presentation on how UPSs can be used for frequency regulation in the power grid.

Hydrogen-Powered HPC at NREL

Kevin Regimbal, NREL

Kevin Regimbal from the National Renewable Energy Laboratory (NREL) in Colorado, USA started the session by giving a presentation on how NREL has done experiments with powering their HPC infrastructure with a complete hydrogen infrastructure. NREL is an organisation with over 2000 employees and operates a campus as a living laboratory in many areas of renewable energy. The experiments they have done with hydrogen touch on many of the laboratory's key areas like storage of energy from solar and wind, vehicle technologies with hydrogen-powered cars, building and HPC technology. The idea is to build a proof-of-concept "hydrogen-based", carbon-free, datacentre utilising renewable energy sources, electrolysers, hydrogen storage, and hydrogen fuel cells as the key building blocks. Hydrogen is suitable for this since it is already in wide industrial use. The cost of hydrogen production is also expected to decrease when results of current and future research are utilised in fuel cell production.

The fuel cells used in the NREL experiments are coming from the automotive industry (Mercedes Benz). This has several advantages like:

- Robust and modular system, 65kW building block;
- Possible future volume production;
- Fast dynamic response;
- Long life;
- Silent operation, zero local emissions (no CO^2).

Safety is a critical consideration when running a hydrogen-powered device in a datacentre. The team completed an extensive analysis, planning, engineering and lab testing before hydrogen equipment was installed.

The fuel cell in the computer centre is connected to the HPC system with a 380 V DC power bus. The bus is also connected to batteries and a UPS so that the HPC system can operate on batteries if the fuel cell is off.

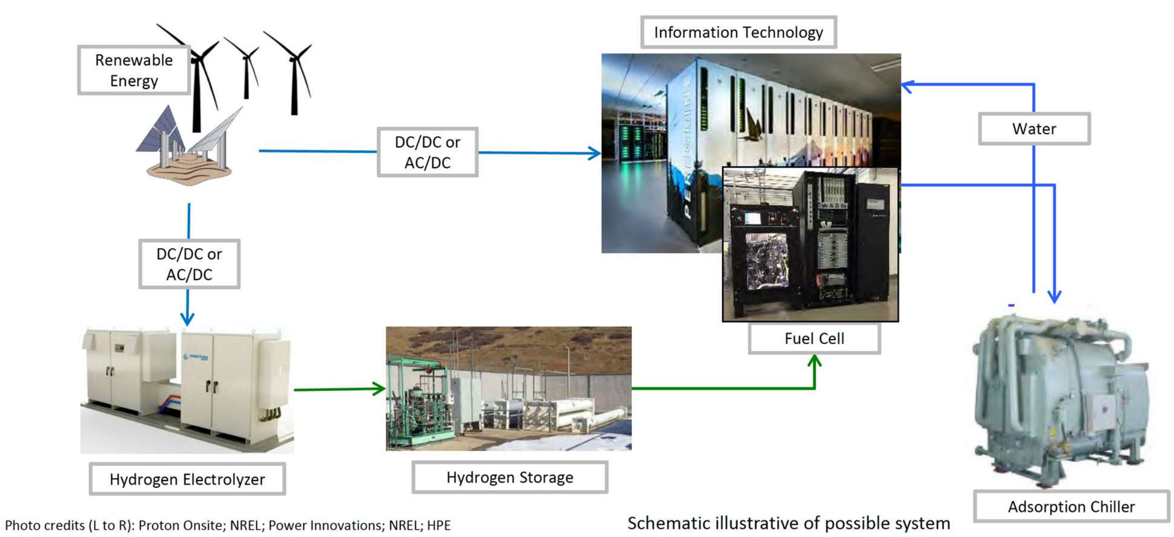

Figure 12: Schematic illustration of a complete hydrogen-powered HPC system

NREL is looking at the entire chain for a hydrogen-powered datacentre infrastructure. Figure 12 gives a schematic illustration of the interrelated aspects and components. At least the following aspects, listed below, are involved:

- Electrical power production with solar panels or wind power to provide the electricity needed for hydrogen production by means of electrolysis;
- Hydrogen production via electrolysis;
- Hydrogen storage in gaseous form;
- Distribution in hydrogen pipelines
- Transformation by a fuel cell to electrical power locally in the computer centre;
- The heat from the fuel cell can be used in an adsorption chiller to cool the HPC system.

To provide an overview of the various advantages and disadvantages of current hydrogen fuel cell technology, NREL has compared various costs and other aspects involved in using a 1 MW fuel cell facility to using a 1 MW diesel generator. Table 3, below, summarises the comparison.

1-megawatt generator needs about 273 litres of diesel fuel per hour	1-megawatt fuel cell needs about 70 kg of H^2 per hour
Generator Purchase Costs are about $100 / kW	Mobile PEM [2] Fuel Cell Purchase Costs are in the range between $60-$230 / kW [3]
Fuel Storage Infrastructure: ~$.35 / kWh	H^2 Storage Infrastructure: ~ $70 / kWh
Lifespan: 15,000 to 50,000 hours	Lifespan: 5,000 to 40,000 hours
Fuel: 1 gallon (4.5 litres) costs ~ $3.00 + delivery	Fuel: 1 kg costs ~ $2.00 (SMR[4]) + delivery
Limited use: testing & emergency power	No use limitations (peak shaving)
Start time: 30-60 seconds	Start time: a few seconds
Loud	Nearly silent
Exhaust: carbon dioxide, water, and nitrogen, nitrogen oxides	Exhaust: water & water vapour
Location: outdoor	Location: outdoor or indoor: UPS room, in row, in rack

Table 3: Comparing a 1 MW diesel generator with a 1 MW hydrogen fuel cell

Case Studies of HPC power grid integration

Grant Stewart, LANL

Grant Stewart, from Los Alamos National Laboratory (LANL) USA, that houses one of the largest HPC facilities in the world, talked about HPC power grid integration. The presentation was based on a forthcoming paper by the Grid Integration Team of the Energy Efficiency HPC Working Group[5], which is led by Grant.

The fast variation of the power requirements of modern large HPC systems can have catastrophic effects on the power grid, such as voltage drops or equipment failure. In recent years, the attempts to make HPC systems more energy-efficient have increased this power variation. In the phases of an application run in which less computational power is needed, power consumption now can be reduced accordingly, and this can be done in a very short time interval. Conversely, computers are now capable to shift to maximum clock speed when the application needs it, very fast as well. As to the question whether the surrounding power-providing environment can deal with that, your mileage may vary considerably, depending on the local circumstances.

Utility power grid operators may have to adapt to this situation, but this can take 5-10 years to do so. To understand the problem and plan for a feasible solution in due time is highly important. As an example: in "LRZ SuperMUC

[2] Polymer Electrolyte Membrane
[3] https://www.energy.gov/sites/prod/files/2017/06/f34/fcto-h2-fc-overview-dla-worldwide-energy-conf-2017-satyapal.pdf
[4] Steam Methane Reforming
[5] https://eehpcwg.llnl.gov/

Phase 1, (Huber, presented at 5th European HPC Infrastructure Workshop, 2015) a 1.9 MW, power fluctuation, resulted in a 9% voltage drop of the utility power (see Figure 13).

A highly simplified view of Power Engineering was presented were the Resistance (Ω) in a DC circuit is compared with the impedance (Z) in an AC circuit. The impedance is the sum of the resistance and the capacitive or inductive reactance. In the same way, the apparent power is the sum of real power and reactive power.

The Power Factor (PF) is Real Power/Apparent Power and should be as close as possible to 1. A good PF is greater than 0.95.

In AC circuits, the impact of reactance is normally much larger than the impact of resistance (length & conductor size). Underground placement of cables gives more capacitive reactance than overhead placement while motor loads give more inductive reactance. The reactive power (VAR) can either be leading or lagging but for static situations, it can be compensated quite easily for example by shunt capacitors.

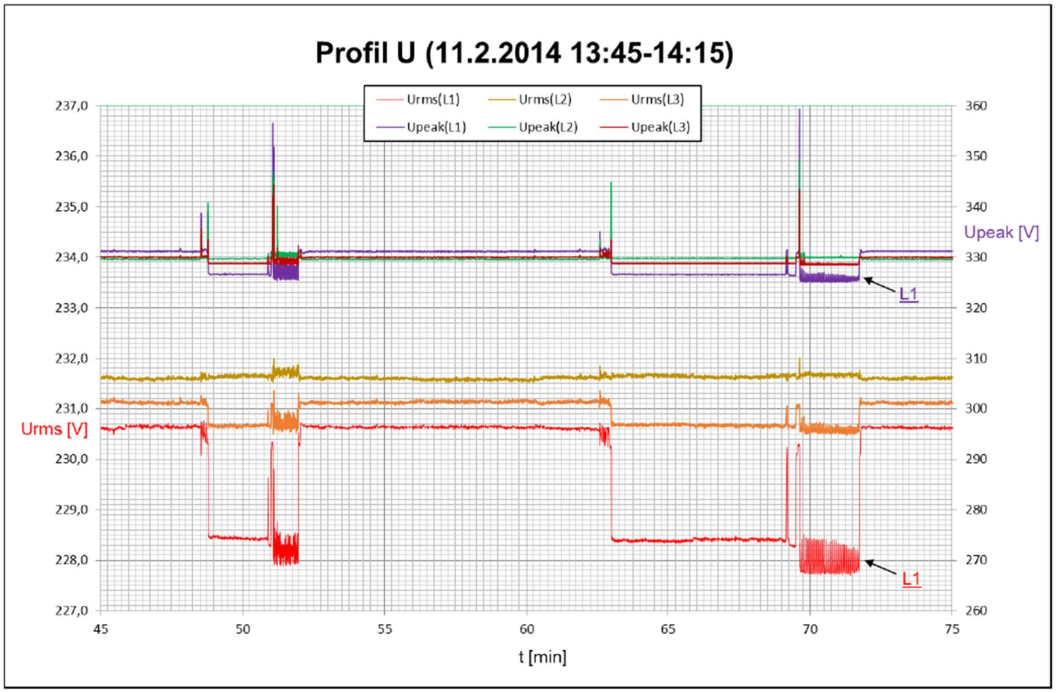

Figure 13: Effect of power fluctuations of SuperMUC, LRZ, Germany, measured by means of repetitive application (SeisSol) runs on four SuperMUC Islands

Circuit "stiffness" is defined as the ability to rapidly stabilise the voltage after an abrupt power-flow change to minimise voltage drop. Stiffness is associated with higher fault current availability and a lower impedance power flow path. However, high fault currents can be dangerous to workers and equipment. To reduce the fault current, the following type of equipment can be used:

- Current limiting fuses;
- Series reactors;
- Current limiting reactors.

Figure 14 shows which combinations of under- or overvoltage and the duration of the condition, which are dangerous for equipment. The green areas represent the combinations that are bad for the computer equipment. In the No Damage Region, the computer simply stops but the hardware should be intact while in the Prohibited Region there is a big risk of equipment failures.

In a dynamic situation, there are several ways to control the reactive power:

- Shunt capacitor banks can be automatically switched in or out to make step-function changes in power factor (slow);

- Advanced power transformers can have automatic tap changers that control output voltage (slow);
- Generators can have an exciter that can be adjusted to manage the power factor and regulate the voltage (very fast);
- Static VAR Compensator (SVC) or Static Synchronous Compensator (STATCOM), devices that automatically controls the voltage by generating leading or lagging VARs (very fast);
- Smart inverters on battery bank or photovoltaic array can provide VARs support and voltage control (very fast).

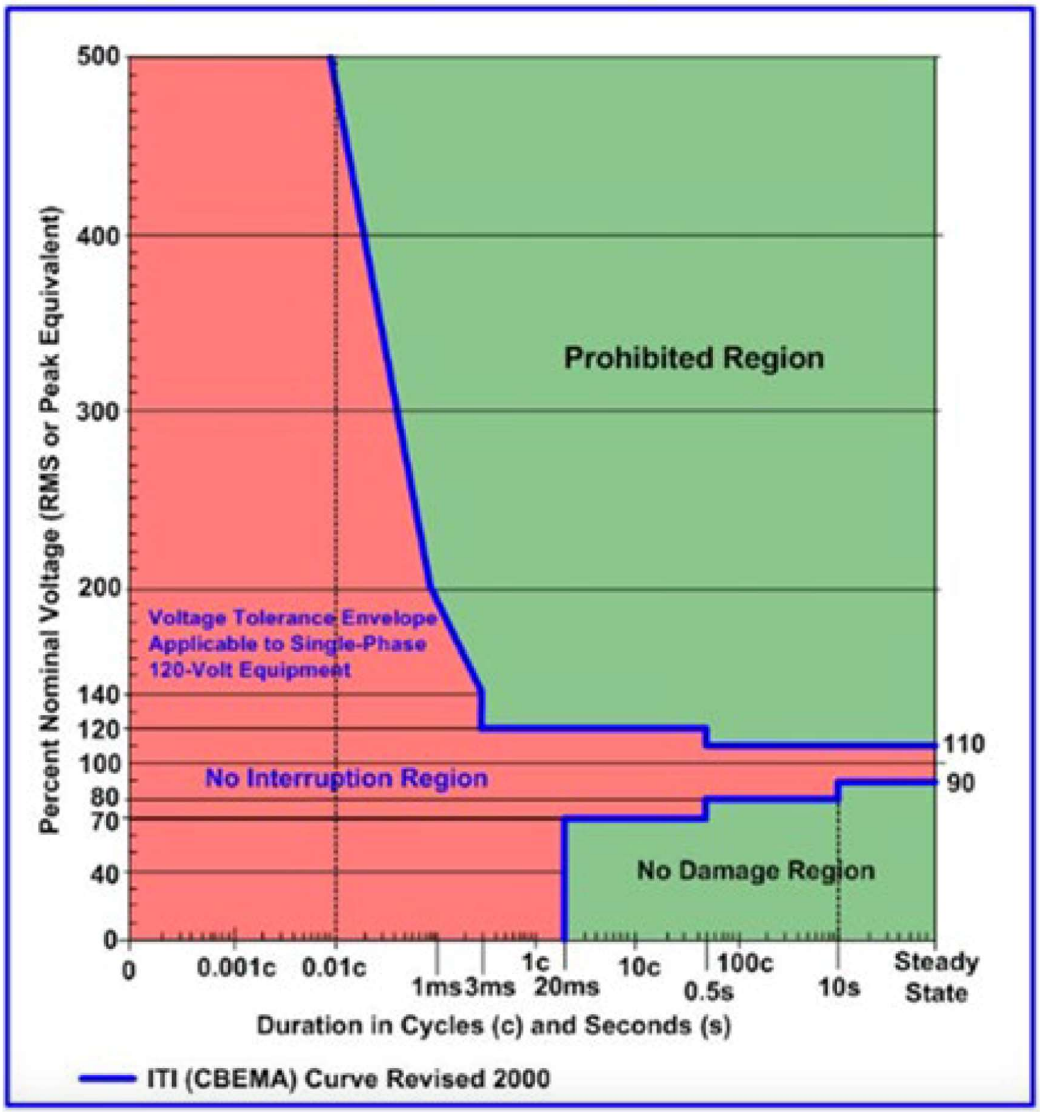

Figure 14: Computer and Business Equipment Manufacturers Association's (CBEMA) standard

Several cases from real-world HPC centres were presented ranging from quite simple power grid solutions to the very advanced setup in Figure 15.

The overall conclusions were that:

- The power supply infrastructure necessary for large HPC systems is expensive and takes 5 - 10 years to develop;
- Each site has a unique grid setting that is an artefact of its development over the years;

- Optimised planning for a supercomputer and its supporting power grid requires a clear understanding of grid stiffness characteristics and of the magnitude and ramp rate of dynamic power fluctuations.

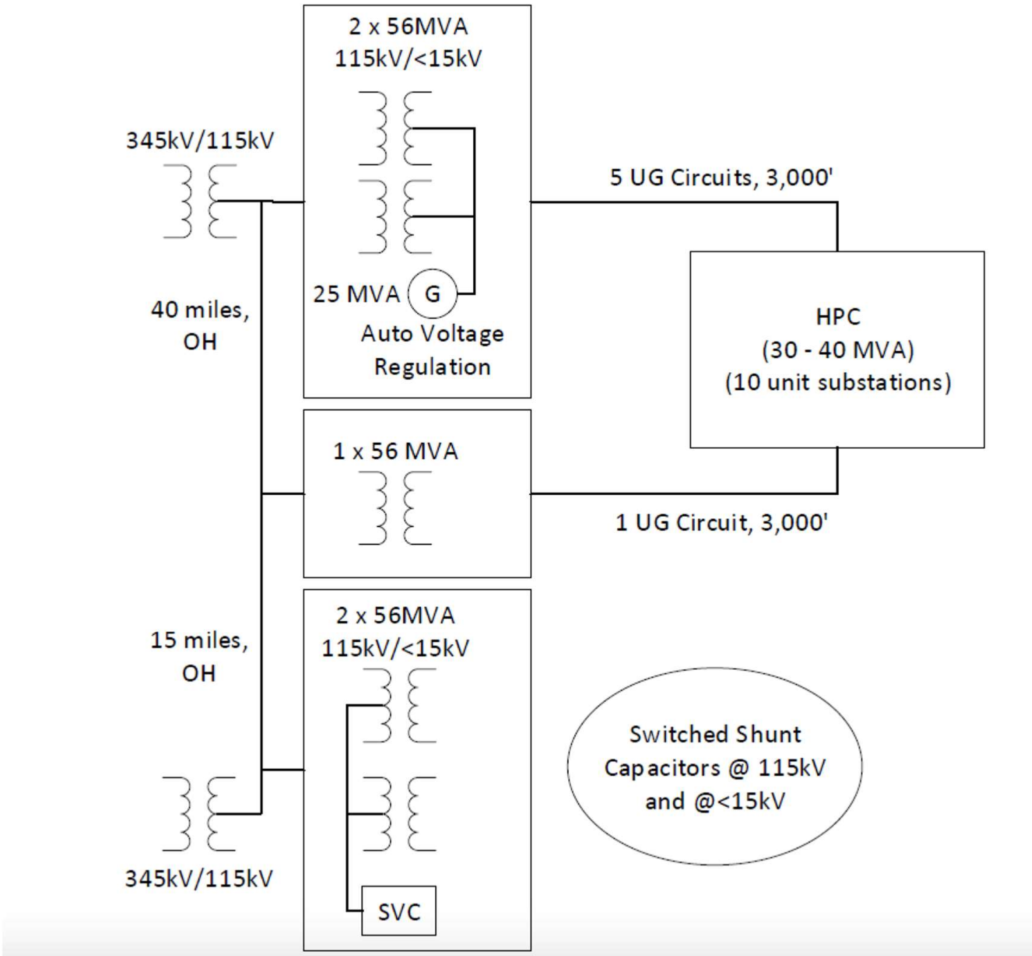

Figure 15: Advanced HPC facility with several ways to compensate for fast variations.

Use of UPS for demand response and frequency regulation

Janne Paananen - Eaton

The talk started with Janne Paananen from the UPS manufactory Eaton Finland explaining that the ICT sector would consume more and more energy and that everyone wanted power from renewables and carbon-free sources like wind and solar power. The big question is how to manage the variation in the amount of energy that is produced and how to manage any disturbances in the power grid resulting from the variations in production or from the variations in usage and demand. It is the transmission system operator's role to maintain the balance in the power system, but they might help with that in the future.

The idea is to stabilise the system frequency by releasing and absorbing energy if the energy is too low, respectively too high. In traditional systems, this has partly been done by using the inertia of spinning mass in power plants and factories. Newer power grids, due to larger variation in renewable energy production and modernisation of motor loads, will have faster and higher frequency variations and it will be more challenging to contain the frequency. The presentation focused on the fast frequency control where UPSs are useful. For slower frequency regulation, other methods exist like regulating the power production or start new power generation units.

Most people think of UPSs functioning as depicted in the left part of Figure 16. In fact, most modern UPSs are more flexible than that and can send energy bi-directionally, as shown in the right part of the figure. This means that energy can be sent out to the grid if help is needed to stabilise the grid by taking energy from the batteries.

How frequency control is done varies among power grids. In Europe, frequency control is done by listening to the local frequency in the grid. If the frequency goes down, energy is sent out to the grid. In the USA the need for power is sent by a special signal to the UPS.

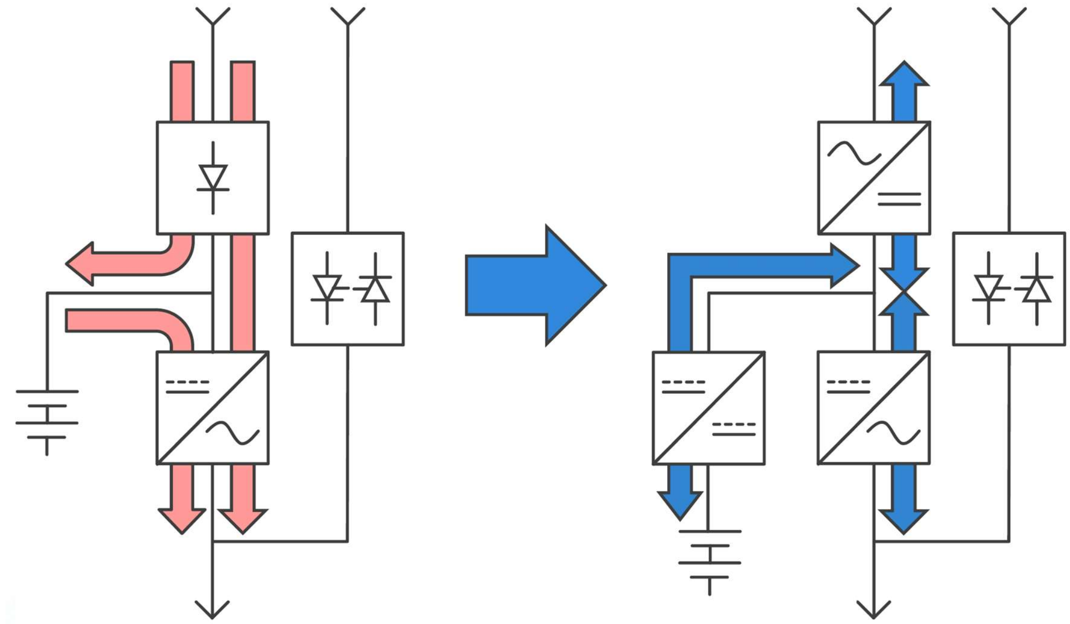

Figure 16: Schematics of normal UPS operation (left) and a mode to transfer energy bi-directionally (right)

If the frequency goes up, there is a need to consume more power to stabilise the grid. In this case, the UPS can load the batteries if they are not already fully loaded. For such a system, the batteries are only charged up to the point that they can maintain the critical load for the specified time. Therefore, to be able to use the batteries for frequency control, the batteries need to be somewhat larger than required otherwise. In addition, if the system is set up to balance, very small frequency variations the batteries will be charged or discharged very often, and lead-acid batteries are very sensitive for that kind of use, so nickel-cadmium batteries fit better for this kind of use. It is claimed that with proper UPS technology the UPS can take part in fast frequency control without increasing the risk for failures of the critical load.

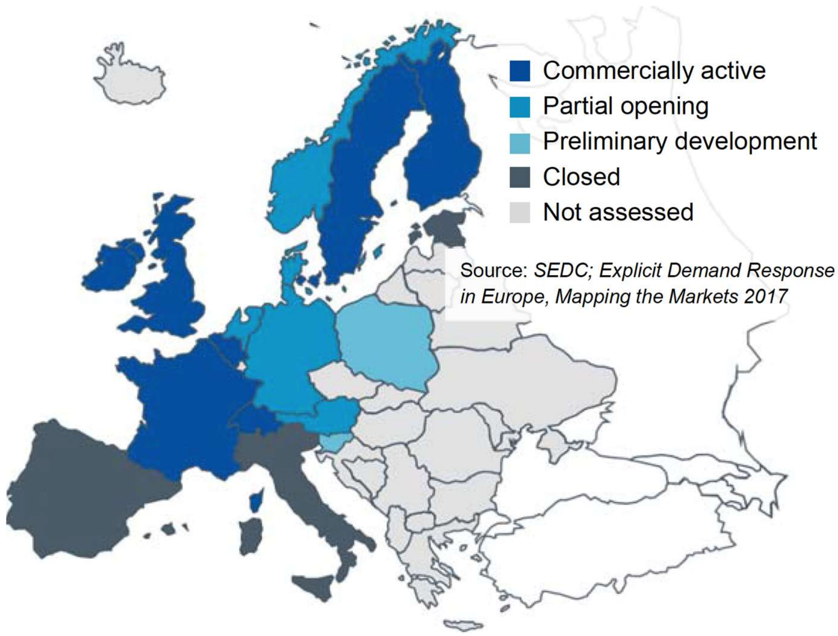

Figure 17: Map of the various levels of openness for demand response of different markets in Europe

Power generation companies generally are willing to pay for fast frequency control services thus provided to them and at least compensate for the additional cost of the extra size batteries and the UPS. Particularly in more open markets, the fee can be considerably higher than the mere compensation of the cost for oversizing the UPS and its batteries: a figure of 70,000 Euro/MW per year was mentioned. Figure 17 shows the status of different markets in Europe in 2017. To facilitate the operation of the market with many parties and potential parties, aggregator companies are used that can play a broker-like role. They collect a large number of devices that can be used for frequency control and can negotiate the price with the power company and handle all practical details. Among the devices are both UPSs and generators. Typically, a UPS is fast, but can play its stabilising role only for a limited amount of time. A generator has a slower reaction time, but typically can sustain its regulating role for much longer.

In conclusion, this technology is already ready to be used with modern UPSs where there is an open market.

Session V – Future Technologies & Certification, chaired by Gert Svensson

The session featured two presentations on future technologies: one on the feasibility and added value of using machine learning to improve the energy efficiency of datacentres, and one on possible next-generation computing technologies such as quantum annealing and approximate quantum computing. The session was concluded by an overview of the certification process as gone through by a commercial datacentre provider.

Artificial Intelligence / Machine Learning in Datacentres; Further Improvements of Energy Efficiency?

Ingmar Meijer, IBM Research, Zürich

Impetus for the work presented was a 2016 press release from Google about the DeepMind AI reducing their datacentre cooling bill by 40%. Expressed as a percentage that is impressive, but what does it mean in practice? In the same year, Google published a PUE number of 1.12 for their DCs and an educated guess puts the cooling part of that around 0.06. Therefore, a 40% reduction thus translates to a PUE improvement of 0.02.

For a new commercial datacentre (2200 m^2, 3.5 MW) built in Germany, IBM collected and validated very accurate electrical and thermal data from many well-calibrated sensors in the datacentre. IBM built a model of the datacentre, a 'digital twin', to investigate how much outcomes of machine learning could improve the PUE. The model is used to simulate the behaviour of the datacentre in several respects and includes functions for the datacentre's power usage, the temperature in the datacentre's cold aisles, and the pressure – or volume flow – in the datacentre's cold aisles. The datacentre's power usage is as a function of the IT load, the outside temperature, and the set points of the various components of cooling equipment: CRAHs, pumps, chillers, cooling towers. This is a complex non-linear behaviour. Machine learning is used to map this function onto a deep neural network that approximates this non-linear function. In the model presented, the water pumps and the chillers were the main targets for optimisations.

Hydrodynamic behaviour of pumps is dependent on pressure and volume flow. Given a certain amount of heat that has to be removed, the volume flow needed cannot be changed much, so the pressure remains as a variable. However, the pressure differential also affects how efficiently other components work, like CRAHs for example. Therefore, it is a fairly common practice that the set points are set to safe values with margins during installation and never changed afterwards.

For a new datacentre, the modelling and machine learning techniques can be used both when bringing up the datacentre, and afterwards, during normal operations. Designing the datacentre is still done by humans. The machine learning system optimises the settings on the selected equipment. Operators dislike changing set points in a working datacentre, so the best time to experiment with parameters is during the initial bringing up of the datacentre. During normal operation, the model can still be trained by slowly changing set points, which is also an option for an existing datacentre.

In the datacentre modelled by IBM, it was found that using set points from the trained model instead of the standard ones gave a 25% improvement (PUE 0.08) in chiller mode and 60% (PUE 0.02) in free-cooling mode.

A well-trained model can also predict maintenance, such as heat exchanger cleanings. Choosing which parameters to include in the model is dependent on both goals and intuition. Since the parameter space is so large, some domain knowledge is needed to identify features and prune the search space for the model. The datacentre referenced in this presentation had eight weeks allocated for measurements and training during the bring up.

Initially, only the pumps and chillers were included, since they had the largest share of power consumption. At the end of the period, the cooling towers were added.

In summary, this approach appears promising, but the digital twin model needs to be refined and verified for more datacentres. Operators need to ensure that their datacentre has well-calibrated reliable sensors in place to feed such a model with correct data.

Quantum computing with near-term quantum devices [6]

Historically, steady improvements in transistors have driven the computer industry for several decades, but in recent years the pace of making further improvements along these lines has slowed down. Three predicted and promising next generation technologies are: 3D / hybrid systems, neuromorphic computing and quantum computing (QC). These are not independent pillars but, combined with traditional computing technologies, make up the future of computing by leveraging individual strengths for specific applications.

QC is seen as a technology for solving currently intractable problems that scale exponentially. In QC the quantum properties superposition and entanglement can be used to create a single N-bit input state with all 2^N binary possibilities to be operated on simultaneously. To get the result, a measurement is performed which reads a single classical state that is chosen from a distribution determined by the quantum result. Special quantum algorithms, employing entanglement, are needed to obtain the correct result with high probability and multiple runs are required to find e.g. the state with lowest energy in an optimisation problem. Shor's factoring algorithm is an example of an algorithm, where exponential speedup can be expected over currently known classical methods. In this case, significant quantum hardware resources (millions of qubits) will be required to solve relevant problem sizes. However, if technological progress continues, it is expected that insights into useful problems already will be gained with a few hundred 'good' qubits.

The state of a qubit can be any point on the so called Bloch sphere. A state at the equator of this sphere is an equal-superposition state (0 and 1 at the same time).This is what allows representing many values at once (N qubits span a 2^N dimensional vector space). Information represented therefore scales quickly with the number of qubits and accurately representing the state of 256 qubits in conventional memory would require more bytes than atoms in the universe.

Different types of quantum computers exist:

- *Universal quantum computing*
  The ultimate goal of QC research. This approach will require error correction of qubits. Current error correcting codes have a huge overhead with on the order of 10^4 qubits needed to represent one 'logical' or error corrected qubit.

- *Approximate quantum computing*
  Focus of current IBM research. This approach tries to minimise errors, but does not have that many qubits. It is a hybrid approach, using QC exponential space and classical computing to optimise. It is Believed that 50-100 low error rate qubits can suffice to provide quantum speedup for some problems. The quantum hardware is of the same type as for universal QC.

- *Quantum annealing*
  Can be used for optimization problems and is easier to implement. The approach is more limited in problems that can be addressed, doesn't care about errors and can use quantum tunnelling to find global optima of Ising-type problems.

IBM has 14 quantum systems in the cloud which their partners and the public can use. Quantum processors with up to 16 qubits are freely accessible for everyone and processors with up to 53 qubits are available for their partners. Qiskit is a development framework that creates an interface with support for Python and other higher level interfaces such as e.g. for quantum chemistry . The software stack is being developed in parallel with the hardware and already now provides the possibility to test small algorithms, using simulation backends on classical hardware or the currently available processors. The development of new quantum algorithms is an important current field of research and one of the key areas pursued at IBM. The transition to QC cannot be made simply be

[6] Like all summaries, the summary of this presentation was produced by, and is the responsibility of, the authors of this paper. The name of the original presenter at the workshop, and his or her organization, are not mentioned here, to avoid any suggestion that the summary is published in their name, or in any way is formally endorsed by them.

recompiling old codes. It is important to understand the differences to classical codes and processors and prepare for this new technology. A skilled workforce is needed for this, leveraging progress in software and hardware to guide the field.

QC is done using logic gates in a similar manner as classical computing. Programs are compiled into a quantum circuit. Currently the hardware is limited by the error rate of the quantum gates. The number of sequential gates needs to be minimised and error mitigation must applied. Improving error rates is thus an active field of research. IBM uses superconducting circuits as their main technology. They are fabricated on silicon substrates and use superconducting layers to create microwave resonator circuits. A non-linear inductor, the Josephson junction, is combined with these microwave resonators to create qubits. The two levels used to represent 0 and 1 are typically separated by 5 GHz, which, temperature-wise, is a difference of 240 mK. Due to this very small difference the qubits need to be shielded and kept at a temperature of 10 mK to minimise interference caused by noise and thermal radiation. On current hardware all quantum gate operations in a circuit need to be executed within 100 µs before errors due to noise start to mask the result. A single gate needs about 100 ns to perform its operation.

Cooling quantum processors is not the real challenge, since they don't dissipate any significant heat. They are placed inside a dilution refrigerator with temperatures of 50K, 3K, 0.9K, 0.1K and 10 mK on different stages from outermost to innermost. Keeping the lines that go into the system cold, and preventing that they introduce heat into the system, is much more challenging. No scalable solutions using warmer temperatures are known but current cooling systems should easily be able to cool hundreds of qubits.

Compressors (placed far away) provide helium at 50 bar, for initial cooling down to temperatures of 50 K and 3 K. Subsequently a mixture of ^3He and ^4He is used in the dilution process to bring the temperature further down, to 10 mK. This is well-proven technology where the mass of the system determines the cooldown period. The cooling solution is also robust, in that power outages of a few minutes for the compressors are tolerated before the temperature starts rising.

Power consumption is around 10 kW for the gas handling and compressor, but can both be optimised and could also support many more qubits than today. Control and measurement use the most power for the system itself, around 100 W/qubit. It should be possible to bring this down to less than 10 W/qubit in the future, with more specialised generators. Currently it is not known how much power will be needed for error correction in larger systems.

There has been much progress over the last decade to extend coherence times, but QC is still a grand challenge type of problem, albeit one with a clear roadmap. The computing industry is still in the learning phase and it may take another 10 years before we see QC outperform classical systems on commercially relevant problems. Nevertheless it is important to prepare, to get ready now. Applications envisioned are those that are intractable today: Quantum chemistry, simulating large electron systems (50+ electrons), optimisation, finance, etc.. Quantum computing together with next generation HPC and neuromorphic computing architectures is expected to be an important pillar of the future of computing.

Datacentre facilities and infrastructures certification according to EN50600

Michał Jakś, Talex S.A.

Talex is a publicly traded commercial Polish datacentre operator with datacentres in Poznań and Wroclaw. Customers include banks and financial institutes, which require security certifications from suppliers for legal and regulatory reasons. Many different certifications exist and over the years Talex has been certified for ISO 9001 (2001), ISO 27001 (2005), ISO 20001 (2012).

At the end of 2017, Talex started working towards EN50600 certification for its two datacentres, completing the process in under a year (September 2018). The only other datacentre in Europe to be certified before these two was one in Austria. In fact, no Polish certifier was available at the time. An Austrian certifier was used instead. EN50600 became the ISO 22237 standard in April 2018, which also was a reason for choosing this standard.

As a standard, EN50600 is divided into different parts that in turn have different classes to target. It is possible to target different classes for each part. The standard references about 50 other European standards, so it is quite wide. What Talex wanted to achieve, was driven by customer requests:

- Physical security – class four (highest)
- Availability – class four (highest)
- Energy efficiency – class three (highest)

Since both buildings were already built, the requirements on neighbouring area and traffic could have been an issue but luckily posed no problems. The main challenge in meeting the requirements was the building in Wroclaw which was built in 1941 and is a historical building. Windows are not allowed in the datacentre walls for class four, but the exterior of the Wroclaw building could not be changed. To solve this problem, new walls were erected inside to create a building within the main building. More than 20 doors were replaced to provide enhanced protection against fire and break-ins.

Power redundancy and fire protection requirements mean that two separate providers are needed, each with separate transformers and secondary distribution within the datacentre building, all in separate fire zones. These redundant feeds first meet in the room where the IT equipment is.

Many sensors (temperature, humidity, particles, CO, etc.) are needed to fulfil the environmental control part of the standard. The location of all sensors in equipment needs to be known, including vendor boxes that might otherwise be black boxes, to be able to satisfy the auditors.

Separate meet-me rooms are needed for connecting to telecommunication operators and also the full separation of the data cable paths to the IT room. Inside the IT room, there is also a requirement on how the communication racks are placed.

Rooms inside the facility needed to be classified according to EN50600 standard. Firefighting systems and single person interlocks for movement of staff need to be in place for rooms rated for higher classes.

Cost-wise the construction work in Wroclaw was the main investment, with smaller changes needed in Poznan. To fulfil telco separation some old DC space was converted into a meet-me room. Ten man-days per facility were used for the auditing before the certificate was issued with the auditor billing around 150 EUR/hour.

Session VI – Tools and EuroHPC, chaired by Javier Bartolome

Integrated datacentre monitoring with DCDB

Michael Ott, LRZ

LRZ's global datacentre energy optimisation strategy is based on a four-pillar framework[7]. The first pillar focusses on the building infrastructure with the goal to improve the PUE. The second pillar deals with the HPC system hardware and targets the reduction of hardware power consumption. The third pillar focusses on the HPC system software with the goal to optimise resource usage by tuning the system. The fourth pillar consists of the HPC applications and strives for optimisation of application performance.

In the first pillar, one can optimise such things as the power draw of compression chillers and fans on the cooling towers and the whole infrastructure. On HPC system hardware side, the latest generation of processors deliver more flops per watt. With respect to the HPC software stack, anything from batch scheduler to HPC to for example the GPFS file systems need to be optimised. The biggest leverage is in optimising the application performance.

In each pillar, some useful work more or less confined to the pillar can be done. However, for best results, there is a need to consider all the pillars together. At LRZ, already several actions have been taken towards global energy-efficiency optimisation. LRZ is a pioneer in direct-liquid hot-water cooling with free cooling most of the year. Heat reuse is implemented by using waste heat for heating offices and for driving adsorption chillers. In such constructions, infrastructure gets tightly coupled to the machines it hosts.

To discover and investigate opportunities for global energy optimisation, broad instrumentation for all components in all pillars is required. However, it is not sufficient: trying to correlate data from various sources, with different timestamps and different time intervals, and so on, can be a total nightmare if you have to do this on a case-by-case basis, using an Excel spreadsheet to do the analyses. So what is positioned at LRZ in the middle of all high-frequency and high-resolution monitoring at LRZ is the datacentre database system (DCDB). The DCDB is a framework for continuous and holistic monitoring, from facility to applications combining the data from the four pillars of building automation, IT devices, operating system and application performance.

DCDB is modular, distributed, scalable and extensible architecture. It started out with data on the building infrastructure, building automation systems and IT devices. Now it also includes data on the level of the operating system and data about application performance. Apache Cassandra is used as distributed and scalable noSQL database for storage backend. NoSQL is appropriate: as most of the time, there is no need for complex complicated queries, but just a number of aligned time series for a selection of sensors. Grafana is used for visualisation.

[7] See also Figure 10: The four pillars of the LRZ strategy for energy-efficiency optimisation.

Cassandra is able to scale with multiple databases and servers if needed. There is also integrated data-analytics framework. DCDB is open source by GPLv3 and has a publicly accessible gitlab instance at https://dcdb.it.

The software architecture of DCDB consists of DCDB pusher, DCDB collect agent, and database itself. The pusher gets the data from compute nodes, and other nodes, via plugins and delivers the data to collect agent via the MQTT protocol. The collect agent can get data from sensors and all data is delivered to the Cassandra database. Both the pusher and the collect agent have user and administrative interfaces implemented with a REST API that avoids the need for root access to the system. You could have pusher running in a compute node and give user access to the REST interface to see node in band sensor data securely. The data is pushed out to the Cassandra database from where it can be queried via libdcdb, a well-defined API that has all the necessary functions available.

There are two different sources: in band and out of band. In band sources are for example Linux perf_events as API to the linux kernel performance counters and a plugin for linux sysfs as text file grep. A plugin for GPFS to read the statistics of parallel filesystem is also available as well as an Omnipath fabric plugin. Out of band data sources are ipmi interfaces and snmp which most PDUs support. The REST interface is supported. Building infrastructure data is collected via BACNet/TCP. New plugins can be easily added via generator scripts and stubs.

Many plugins are for in band data so they are deployed on compute nodes to read the sensors. This generates some overhead on the compute nodes. The runtime overhead has been measured against High Performance Linpack on Intel SkyLake and Intel Knight's Landing processors. How much overhead the data collection causes is of course dependent on the sampling frequency and the number of sensors. Many different choices can be made. For a realistic sampling configuration that one might want to use in a production setup the overhead measured on the SkyLake cluster was less than 1%. On the KNL cluster with very poor single thread performance, at very high number of sensors (10000), the overhead proved to be higher.

Querying data from the command line can be done by dcdbquery, which produces CSV output files that can be imported into Excel etc. This dcdbquery has integrated conversion of units and some arithmetic operations like delta, integral and derivative. There is also a REST API, that can be used with curl from bash scripts, and a wrapper around libdcdb for python.

Virtual sensors can be used to combine real sensor data to see the bigger picture. For example, sensor data can be aggregated to see data per rack or to see computed values, KPIs like the PUE. Virtual sensors can do arbitrary length arithmetic operations on raw sensors or other virtual sensors. Grafana does not integrate directly with Cassandra so LRZ defined their own plugin for it to use libdcdb. As a benefit you get a hierarchical view to the database. For thousands of sensors this hierarchical view is useful.

With REST API data can be analysed on the fly. SLURM integration is coming with nodelist information per job, to enable drill down views for Grafana to see the measurements for individual nodes on the job.

OpenDCIM (Data Centre Infrastructure Management)

Luca Bacchetta, CSCS

The CSCS machine room relocation in 2012 brought to the surface a need to manage machine room hardware during and after the move. CSCS evaluated six commercial software candidates for this purpose in 2010. The result of the evaluation was that none of these applications were entirely appropriate for an HPC computer centre. Most of the evaluated applications were only for network and office structures. They were also very expensive proprietary software and had high maintenance costs. Nonetheless, CSCS chose one of the evaluated applications and used it for four years.

Things changed when the CSCS team met with Scott Milliken of the ORNL facility management team. Scott Milliken had developed, as a university degree work, a DCIM software package specifically tailored for the needs of an HPC centre. CSCS's experiences with the first DCIM software releases were not completely satisfactory. There was only a partial match with what CSCS was looking for. CSCS was looking for software that could feasibly be supported and extended within CSCS and externally for a longer period of time. An open source project with a strong supporting community would have been ideal. CSCS was also looking for a system that offered the possibility of importing or integrating old databases. DCIM had evolved into the open source project OpenDCIM, which CSCS started to use OpenDCIM in the new datacentre in Lugano. In the old datacentre, each system had its own specific hardware records.

OpenDCIM has three developers: Scott Milliken, Wilbur Longwisch and Jose Miguel Gomez. This software is released under a GPLv3 license. OpenDCIM source code is public and can be modified and shared with others. A web-based client has support for multiple languages.

CSCS had the following requirements for the DCIM application:

- Tool for hardware inventory management;
- Load and weight balance management for the machine room, for islands or racks;
- Overview of the availability of space or electrical power for future installations;
- Overview and control of power supply to systems;
- List contact person for each system;
- A workflow for requesting and hosting a new installation via the tool;
- Multiple levels of user access rights.

Luca Bacchetta's presentation documented that the required overviews and features are implemented in nice uncluttered screens and are reachable by means of a well-organised navigation system with ample screenshots of the user interface. Details on maps, such as sensor values, device names, types, etc. are easily displayed by intuitive mouse pointing. In addition, switch ports, statuses, and path to console connection and power outlet can be seen per system. Figure 18 shows an example of the OpenDCIM user interface and gives an overall view of the heterogeneous and detailed information stored in the system. Figure 19 shows an example of a more "zoomed out" overview.

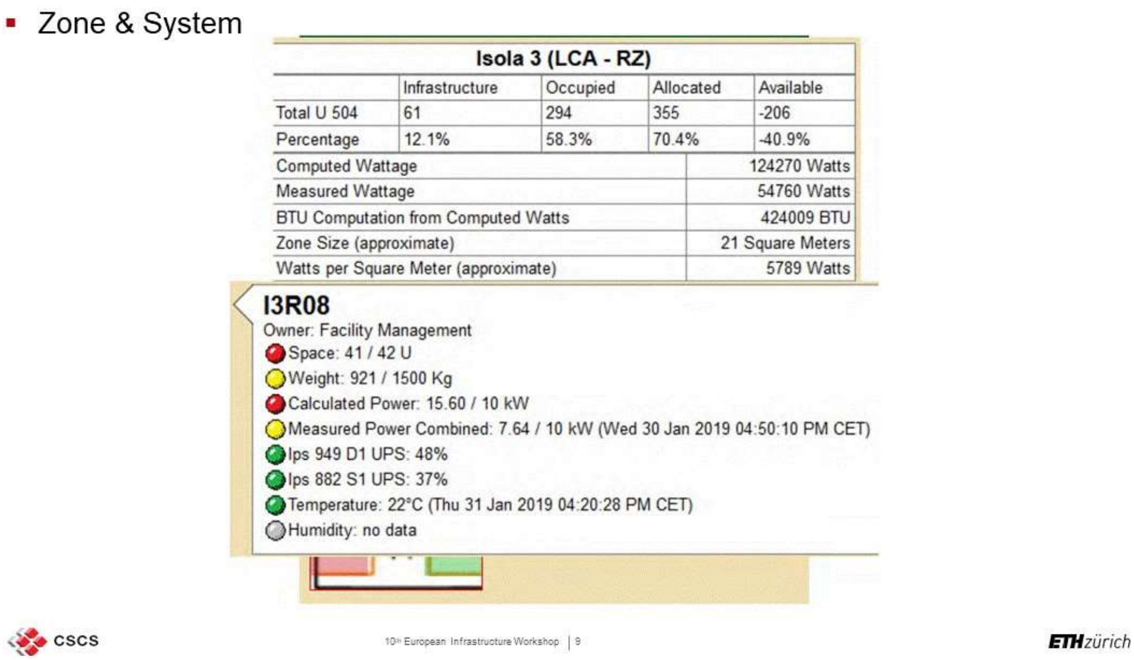

Figure 18: Zone and system-level details of island 3 in the computer room.

The starting page of OpenDCIM displays the total used space, the space labelled for future use, as well as the power used and calculated. Colour codes are consistently used to show the status of datacentre space: red denotes full, yellow denotes nearly full, and green denotes free. Bulk moves and bulk data entry can be done by means of input via an excel file.

CSCS has implemented an efficient and orderly workflow via OpenDCIM in which the datacentre team receives room allocation requests from other teams via the tool and responds by giving back, specifying in the system, the location and connection information.

In addition to the features that CSCS originally required, OpenDCIM has quite a few other features that proved useful for the CSCS datacentre team:

- Fault simulations to see affected systems of a PDU failure and impact simulation of a panel or source feed outage;
- Image mapping with a custom image for creating clickable zones for each cabinet;
- Overlay layers on maps for Power, Space, Temperature, and Weight capacity;
- Mapping of power connections from device to power strip, to panel, to source feed;
- Mapping of network connections to any device classified as a switch;
- Reporting on hosting costs, based on a cost per unit and cost per Watt formula;

- Reporting on fault tolerance status for devices;
- Support of APIs;
- Management of warranty expirations.

Figure 19: Higher-level overview of zones and racks

At present, OpenDCIM meets the needs of the CSCS facility management group, though there is still room for improvement in several areas. For instance, management dashboards, with simple overviews of some key information could be supported in a better and easier way. Currently, they are only available via reports that are created by additional software that uses an API to talk to OpenDCIM. However, better support for dashboards is already on the wish list for OpenDCIM, and so is the support for Grafana.

The CSCS facility management group is also content with the pace at which the software evolves. Important functionalities are regularly added. Though CSCS is not using the cable management and overview of virtual machines features of OpenDCIM, these features were not present in older versions but have now been successfully integrated. CSCS actively participates in the development and propose changes to the code via the GitHub repository where the latest version can be downloaded. There is also a mailing list for the discussion with developers and others and a demo site to play with the software. Documentation is available in Wikipedia and in a YouTube channel.

Reference links

- https://www.opendcim.org/
- https://github.com/samilliken/openDCIM
- https://wiki.opendcim.org/wiki/index.php/Main_Page
- https://repository.opendcim.org/
- https://www.youtube.com/channel/UCdDKR8jKgL_3C9YbH-cwb8Q

EuroHPC hosting entities selection for precursors to exascale and petascale supercomputers

Oscar Diez and Evangelos Floros, European Commission

One of the major issues at stake that the EuroHPC Joint Undertaking (JU) tries to address is the fact that the European funding gap for HPC systems has increased compared to USA, Japan and China. Furthermore, the EU has no top-ranked supercomputers and depends very much on non-EU technology for many of its most capable systems. There is only weak integration of EU technology in HPC machines. The EuroHPC Joint Undertaking is co-investing into a world-class European HPC, Big Data and Cloud Ecosystem for our scientists, industry and the public sector and supports the development of technologies and applications across a wide range of fields.

The EuroHPC Joint Undertaking has 30 participants: 29 participating states and the European Commission (EC). Its budget for 2019-2020 is around one billion Euro. The JU was established in November 2018 and is expected to operate at least until 2026. Decision-making takes place in the governing board in which the 29 participating states and EC are represented. There are two advisory groups: the Infrastructure Advisory Group (INFRAG) and the Research & Innovation Advisory Group (RIAG), which together form the EuroHPC JU Industrial and Scientific Advisory Board. Their mandate is to provide independent advice to the Governing Board on the strategic research and innovation agenda and on the acquisition and operation of the supercomputers owned by the Joint Undertaking.

The overall strategic goal is to develop a thriving European HPC ecosystem. In terms of infrastructure, the capacity for acquiring leadership-class computers must be improved. With respect to technology, the goal is to secure an independent, European, HPC system supply. For applications, the goal is to excel in HPC applications and to widen HPC use and impact.

Budget

Of the total budget of about one billion Euro, roughly half comes from the EU, and the other half comes from the participating states. The budget is to be used for the acquisition and operation of three precursor-to-exascale systems and acquisition of five petascale systems. The cost of a precursor to exascale system is about 125 million Euro for capital expenditure (CAPEX) and about the same for operational expenditure (OPEX). The EU contribution in both CAPEX and OPEX is at most 50% and at most 250 million Euro.

The range of cost for the petascale systems still has to be decided by the Governing Board. The EU contribution for these systems is maximised at 35% of CAPEX and maximum at 30 million Euro.

Calls for proposals and timeline of the calls

The call for expression of interest for the selection of hosting entities for precursors-to-exascale-supercomputers has been published on 21 January 2019, and for petascale supercomputers on 15 February 2019. Call texts are available on the EuroHPC website[8]. An indicative timeline for the acquisition of pre-exascale systems is shown in Figure 20. A similar timeline for the petascale systems is presented in Figure 21.

The objective of the calls is to select hosting entities for the Joint Undertaking pre-exascale and petascale supercomputers. The contractual outcome includes the hosting agreement and operational grant. The overall philosophy is to have fair, non-discriminatory and transparent procedures. Input comes from working groups on "Hosting & Procurement", EuroHPC INFRAG Multiannual Strategic Agenda and from a survey on the minimum requirements.

Evaluation criteria

The evaluation and selection procedure has three steps. The first step is the evaluation of individual proposals, which is done by independent experts following H2020 rules and based on a preliminary evaluation summary report.

Step two consists of hearings where the questions raised by the evaluation panel are clarified and discussed. The applicants give an oral presentation and respond to the questions.

Step three is the selection procedure. The Executive Director of EuroHPC JU presents the final ranked list. The Executive Director may, however, suggest to the governing body to deviate from the ranked list proposed by the experts with a justification. It is up to the Governing Board to consider such a suggestion and take the final decision.

[8] http://eurohpc-ju.europe.eu/participate.html

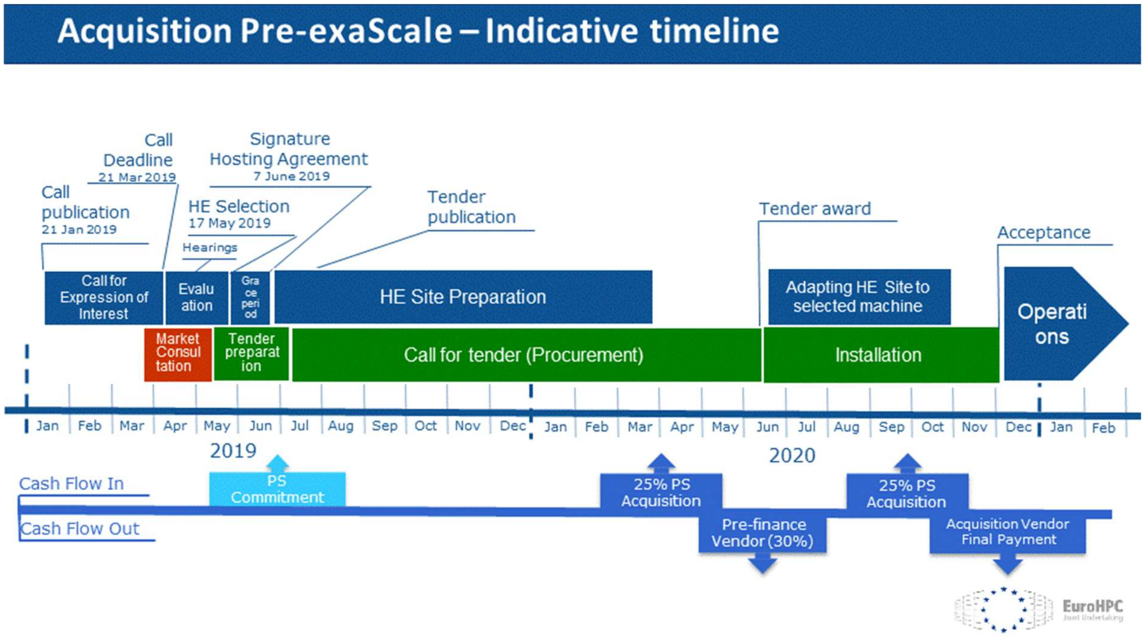

Figure 20: Indicative timeline for the acquisition of exascale precursor systems

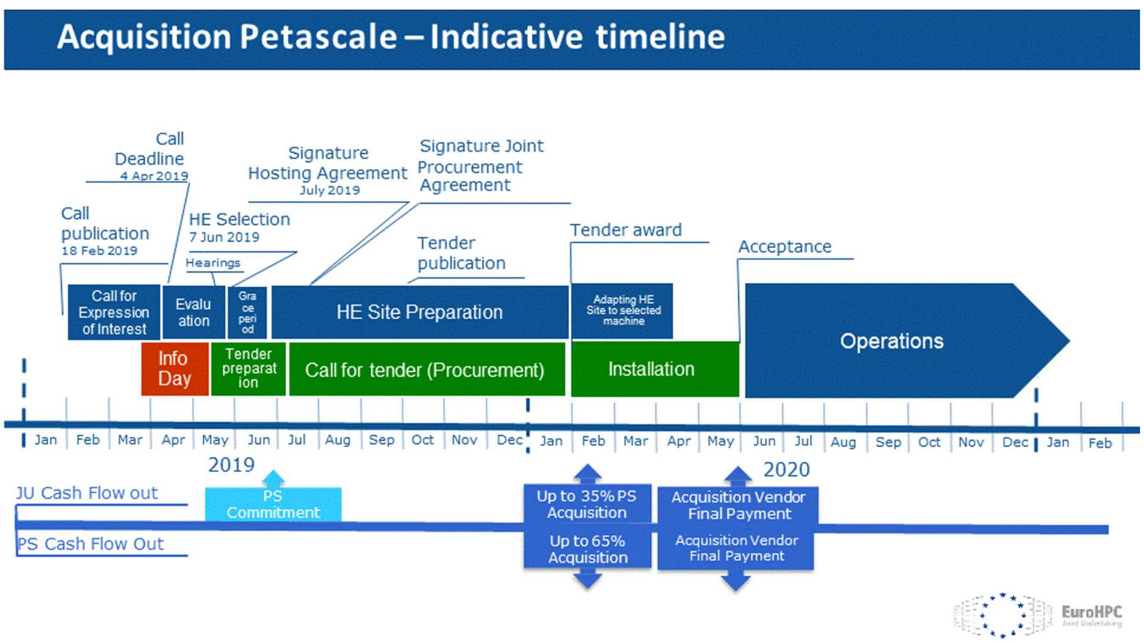

Figure 21: Indicative timeline for the acquisition of petascale systems

There are five evaluation criteria, each worth 20 points:

1. Compliance with the general system specifications defined in the call for expression of interest; (0-20 points);
2. Estimation of the total cost of ownership (TCO) of the supercomputer and methodology to calculate it; (0-20 points);
3. Experience of the hosting entity in installing and operating similar systems; (0-20 points);
4. Quality of the hosting facility's physical and IT infrastructure, its security and its connectivity with the rest of the Union; (0-20 points);

5. Quality of service to the users, namely capability to comply with the service level agreement provided among the documents accompanying the selection procedure; (0-20 points).

There is a minimum threshold of 10 points per criterion area and the total score must be at least 60 points.

General system requirements

The general system specifications for the precursor-to-exascale-systems include that the proposed system must be a capability computing system with an aggregate performance of at least 150 petaflops (sustained performance measured with Linpack). The system must be able to support a wide range of applications like key and grand challenge applications that demonstrably require the capability usage of the supercomputer. The hosting site needs the capability to offer at least 10-15 MW of power for total consumption, at least 700 square meters of contiguous floor space, and at least 100 Gbps connectivity to the GÉANT network.

For petascale systems specifications the required performance level is between 20 and 100 petaflops (using the Linpack benchmark). Hosting sites needs to provide at least 50 Gbps connectivity to the GÉANT network and at least 150 square meters of contiguous floor space.

For both pre-exascale and petascale systems alike, the specifications also require that UPS power covers the critical systems, that there is enough capacity for air and liquid cooling, that the raised floor can cope at least with 2200kg/square meter distributed load. Proper physical access security, fire mitigation equipment/procedures, IT access security, and the ability to perform at least level 1 measurement quality for a Top500 submission, must be in place at the hosting site at the time the system is delivered. An on-call service support teams for IT issues must be available, as well as a dedicated on-call service team for facility issues. The satisfaction of the users with the service must be measured regularly, via a user survey.

The application for a system must describe how the specifications will be met, both for the EuroHPC supercomputer and the site. It must describe:

- The supercomputer architecture and the site that will host it;
- The expected performance of the system;
- The types of nodes and their configuration (e.g. accelerated, CPU, high memory etc.);
- The ratio of different node types within the system (accelerated/CPU, memory size etc.);
- What types of applications will the system be optimised for (computational, big data, AI etc.);
- Other related software/services used, like containers, virtualisation or workflow management;
- Acceptance test and benchmarks to be used for the acceptance of supercomputer.

Total cost of ownership

The estimation of the total cost of ownership (TCO) of the supercomputer that the applicant proposes to host has to include site preparation cost for delivery of the machine in June 2020. Acquisition cost needs to indicate clearly what will be included, how the costs are calculated and who will pay for them. The operation costs specification should also indicate an auditable methodology to calculate and verify the operating costs of the supercomputer. TCO calculation also needs to specify average power usage effectiveness, current electricity price in EUR/kWh, number of system administrators, number of user support staff, the average cost of IT on-call service and depreciation time.

Experience of the hosting site

The hosting entity/consortium for a pre-exascale system has to list its experience with installing and operating a pre-exascale supercomputer. For a petascale system, the experience, know-how, and capability of the intended team, available and in charge of the existing or new hosting entity, has to be described.

Quality of the hosting facility's infrastructure and quality of service to the users

The quality of the hosting facility's infrastructure, security and connections must meet the minimum specifications defined in the call. The hosting entity must provide planning of how and in what timeline the upgrade of the site is intended to be realised. It must also indicate the capability to comply with the service level agreement (described in Model Hosting Agreement).

Session VII – Panel Discussion, chaired by Ladina Gilly

In contrast to previous European HPC Infrastructure Workshop, where the workshop was usually concluded with vendor session and a vendor panel, the 10th European HPC Infrastructure workshop featured a closing panel consisting of experts of EU and US supercomputing sites. This allowed for a more open dialogue, as usually discussions with vendor representatives tend to be constrained by certain non-disclosure agreements.

The general discussion topic of the panel was on "How do different sites prepare their infrastructures for new incoming machines?" and was moderated by Ladina Gilly (CSCS). Six partners represented the panel from six different HPC centres, namely: Herbert Huber (LRZ); Norbert Meyer (PSNC); Jim Rogers (ORNL); Frédéric Souques (CEA); Grant Stewart (LANL); and Gert Svensson (KTH). A number of questions, posed by the moderator, were made available to the panel members in advance.

Question from the moderator: How do you set yourselves up to procure infrastructure work?

ORNL: With calls for the attention on land ownership, as at ORNL the reservation belongs to US Department of Energy (DOE), but the building facility, under a very special agreement, is allowed to become a third party tenant facility, i.e. it belongs to an outside corporation – landlord. The facility upgrades are accomplished by jointly working with the landlord, allowing for direct work with mechanical and electrical engineers for assessing the amount of the work and associated costs. As these engineers are pre-selected, an independent 3rd party assessor is involved for ensuring that the offered work/price ratio within given constraints is competitive.

KTH: KTH puts the system deployment speed to great importance. For that reason, KTH follows framework agreements to ensure the installation speed. These framework procurements are done on a triennial basis. KTH reserves the right on the selection of subcontractors.

CEA: The in-house maintenance team usually accomplishes the minor tasks. For major tasks, as a large-scale HPC system procurement, a specification is written which is then edited by an engineering team (100% CEA internal) and handed over to the administration team. Overall, the planning takes about 9 months.

LRZ: If there is a need to extend or build a new datacentre building, LRZ needs to ask the Bavarian building department for approval, which has framework contracts for planning, engineering, and execution teams. Usually, this planning takes around a year. On the other hand, LRZ is allowed to accomplish HPC system procurements on its own.

LANL: For the current development of the next Crossroads supercomputer, various projects using different methods were selected that were congressionally authorised and expected to work in sequence. There are also many small projects, such as a detailed thermal analysis of underground feeder circuits conducted in a conjunction with a consulting team using the existing indefinite-quantity contract. Overall, the process is very protractive and it takes around five to ten years to build a new supercomputing facility.

PSNC: For building a new data centre facility PSNC needs to organise a public tender. For building facility, due to the lack of specialists, PSNC consults externally before starting the tender. On the contrary, the specifications relating to IT infrastructure are covered solely by PSNC.

Question from the moderator: How do you deal with uncertainties regarding the weight-bearing capacity of their raised floor, electrical & cooling capacity, and cooling temperature/medium required for a future installation whilst planning the infrastructure for a supercomputer still under procurement?

PSNC: PSNC gives an example of a national project being a tender for eight sites in Poland with different requirements as each of these datacentres has its own building infrastructure related peculiarities (e.g. technologies already in place, available capacities, etc.). In such cases, the state of the art for all eight HPC sites is described and the requirements document is developed. It was agreed across eight sites to be as homogeneous as possible in the requirements – a milestone that is difficult to achieve due to already existing differences in the IT supporting building infrastructures of these eight sites.

LANL: LANL mentions several uncertainty examples:

- <u>*Example1:*</u> Will the existing computer have an operating period overlapping with the commissioning of a new system? From the power standpoint, the highest peak of power use is during the initial commissioning and start-up of the supercomputer, which can propagate to a year, implying almost a double power demand during this overlapping period. Provision of this large power demand leads to high operating costs. This is a difficult choice as it is not clear if there is going to be an overlap or not, leading to a 30-40 MW uncertainty in the power demand.

- *Example2:* LANL has an existing facility that is designed for air-cooling, but the HPC system under consideration is warm water-cooled. The question to answer here is whether the machine should be moved to a new building, or the existing one should be modified? LANL provides almost a complete design for either option – for both power and water supplies as well as for the physical space that host the system.

LRZ: LRZ has a number of mandatory criteria in the procurement documents. Criteria like maximum false floor load, maximum power capacity available, etc. are specified in the procurement document. For example, in the case of power consumption, the vendor has to obey the predefined boundaries; otherwise, the vendor will not be selected during the competition. In case of a false floor load, if the provided racks are heavier than 1.5 T/m^2, the vendor has to strengthen the false floor (the corresponding costs are carried by the vendor and not by LRZ). Direct liquid-cooling is a mandatory criteria at LRZ, with the efficiency requirement for warm-water cooling loop being 97%, implying that vendor delivers 100% warm-water cooled system (where also power supplies and network components are directly liquid cooled) or the vendor installs an adsorption chiller(s) allowing for waste heat reuse for the production of chilled water.

CEA: Tries to identify if the reuse of the building is possible. If the reuse is not possible, then due to the modular container solution the amount of work required is drastically reduced. If the reuse of the building is possible then an approach similar to LRZ is taken: specification with certain constraints is created which becomes part of the IT procurement process.

KTH: Follow the procedures that are specified regarding the facility. The vendors are invited to visit the facility. Vendors are then expected to specify the amount of investment needed for fitting their system in. During the evaluation of the bids, KTH then estimates the costs of required adaptations, which is added to the TCO of the system. If adaptations are not feasible, the vendor is removed from competition, as TCO will be high.

Question from the audience: Given that usually the facility is on a longer-term than a single machine, how do you fairly amortise the cost?

CEA: The building was designed for three different machines. Each modification required a substantial amount of work. With a modular approach, the cost is not that high as it would have been for building adaptation/adjustment. For example, if there is a problem with the strength of the concrete used in the floor, then it is relatively expensive to reinforce the ground floor. The reuse of building is difficult, as it yields to be more expensive.

LRZ: When LRZ moved from Munich to Garching (2006), a completely new datacentre was built. In 2011, LRZ had to extend the building. Future outlooks seem to require to extend the building even further for hosting an exascale system. Building a concrete datacentre is way too expensive, as one would usually need a cheap building with good power connection and cooling devices and, not the least, where you can bring compute racks with a truck (personal statement).

ORNL: Usually, ORNL has two systems overlapping in production for at least a year. Thus, there is a need for two separate facilities allowing the built for the new system and the operation for the current system. The building process of a new facility should start well in advance of the deployment of the new supercomputer. Cooling, power, floor load, etc. requirements are provided in the request for proposals (RFP). Once the choice decision of supercomputer is complete, the "inside work" is conducted – the requirements for water distribution, breaker configurations for the switchboards, etc. are finalised. These processes are intentionally separated. Afterwards, the information from the RFP is taken and the constraints are weakened, as the vendors are usually too conservative in their specifications. ORNL also ensures to build flexibility in the large units. For example, during the Summit installation, the cooling plant was built to the maximum, as it would not be possible to reverse and change the pipe - the pipe was built to the largest possible size, and the electrical distribution allowed customisation based on the deployed IT system, as the newly built facility is expected to host three to four machines.

Question from the moderator: How do you deal with the uncertainty related to the final cooling and power connections that a supercomputer still under procurement will require? How do you commission/test new liquid cooling installations without the IT load being installed?

ORNL: Load-banks are brought in and connected to the electrical systems.

KTH: Uses load banks when the facility is newly built. Afterwards, no testing is conducted, as it is not easy during the operation.

CEA: No explicit testing (modular approach).

LRZ: The delivery of the internal direct liquid cooling solution (e.g. pipes, heat exchangers, etc.) is part of the contract. The external cooling solutions are accepted once the building is built. The internal cooling solution is part of the system contract, and the acceptance is together with the supercomputer. No load banks were needed.

LANL: For every machine that is changed out, all the piping for the warm-water system is removed and reinstalled (due to compatibility issues).

PSNC: PSNC extended the warranty time, as there was a situation when DLC was delivered with the building. The process was not in parallel to HPC system deployment, which came later. The warranty time is usually defined for three years (for DLC it was five years). Tender defines the load and how the DLC is going to be tested under the load. How the load is delivered is left to the vendor (as PSNC might not have been able to generate a significant load due to the possible absence of the actual machine). In terms of DLC, there are some problems (e.g. leaks) which are not visible initially, as in the beginning the expected 80%-90% of the final system load is not generated. This requires an extension of the warranty time.

For the current tender, PSNC defines the supplies/entry to the cooling system. The capacity of the cooling system is extended, and the cooling can be tested simultaneously with the machine, as it will be delivered during the same timeframe.

Question from the audience: To what extent do you have a buffer for emergencies and future extensions?

ORNL: Ensures always to have untapped capacity available.

CEA: The facility is typically oversized during the design phase. If the system does not fit, then there is an attempt to find a modular approach, as a quick modification of the facility is not possible.

LRZ: Ensures to install some spare capacity (unused outlets, free capacity concerning power, etc.)

LANL: Ensures to have extra capacity in every part of the system - extra capacity for water, floor, racks, power, etc. LANL assures the flexibility built-in by the design.

PSNC: The PSNC datacentre is designed for a long period of time. Currently, 20% of energy capacity is used. PSNC still has the capacity in terms of space and cooling, but, if required, corresponding updates will be carried out. PSNC states that it is not optimal to invest at the very beginning and also the required budget is not always available. An example would be that back in 2013, when PSNC was starting to document the requirements for building the datacentre (built in 2015), the idea was to have an air-cooled system, which was modified to DLC afterwards, outlining the risks when planning ahead for five to six years.

Question from the moderator: What are the main challenges/surprises faced so far?

LANL: Multiple circuits in a single duct bank heat each other.

LRZ: A closer work with facility constructors is needed, as they do not always recognise the needs of an HPC site. One of the main challenges was how to operate the cooling infrastructure in the most energy-efficient way. For this, there is an imperative need for understanding all the knobs that one can possibly tune. Companies delivering the corresponding infrastructure usually do not cover that requirement.

PSNC: PSNC receives the investment budget on an annual base. The investment decision is sent, usually, in the middle of the year. When starting with complicated tenders (e.g. with a more complicated than an IT tender), one cannot directly start doing the design and do a proper demand and market analysis, as the time is very limited (six to seven months). In addition, the complicated tender law in Poland makes it difficult to go to the court, when necessary.

CEA: Indicates to have a similar to PSNC challenges related to procurement and delays. One surprise was to receive a machine with a weight the hosting facility was not designed to handle. Concrete could not handle it, and for that, the "rack was spread".

KTH: Experienced problems while attaching the air cooling ventilation to the system for heat reuse, as they did not fit due to the differences between the initial drawings. However, the cooling loops were afterwards adapted with minuscular costs.

ORNL: Indicated the unreliability of rotary UPS forcing to move to a battery solution for specific loads.

Question from the audience: What are the challenges when transitioning from an air-cooled to a water-cooled datacentre?

ORNL: Outlines the long-term effectiveness of liquid cooling as compared to air-cooled solution.

LANL: Notes on the increased floor load with liquid cooling, as the system is expected to have a higher density and more weight. One of the surprising challenges LANL faced was with the duct fire/smoke detectors systems, which require a proper calibration (not easy), as they are very sensitive and might lead to many false alarms.

PSNC: Notes on problems related to water leaks and raises the importance of leakage detecting systems. DLC and energy supplies should be separated as much as possible.

LRZ: Suggests a leak detection method for cases when the pipes are already installed: fill the pipes with pressured air and wait overnight – if the pressure drops significantly, then there is a leak, the exact place of which should be determined. It is also suggested not to install air-cooled systems (e.g. storage) together with the liquid-cooled system (e.g. HPC) in the same room, as that would imply either the continuous operation of the air coolers, or the need for two cooling loops – one with chilled water and the other one with warm water.

Question from the audience: Do you prefer a computer room with a raised floor or rather one with a concrete floor?

LRZ: Suggests that there is no need for the traditional raised floor, as the power and cooling can both be brought from the roof. The raised floor is expensive, and the weight of the racks is projected to increase in the future, leading to a problem with a raised floor solution.

ORNL: Agrees with LRZ's viewpoint and outlines the example with the SUMMIT system.

PRACE Session

CSC (Finland): The new Finnish research infrastructure for data management and computing

CSC is a non-profit state organisation with special tasks. The head office is located in Espoo and the datacentre in Kajaani. More than 350 employees are working for CSC. CSC provides a wide range of solutions including, for research, computing and software, data management and analytics, support and training, and administration. CSC is involved in a large number of international collaborations and participates in PRACE since its beginning.

The Kajaani datacentre is installed in an old paper storage warehouse with 10 MW of redundant power capacity and a floor space of 3000 m2, both being easily expandable. The PUE is 1.03 (2015). The current systems installed in Kajaani include:

- A Cray XC40 supercomputer (Sisu-Phase 2) with a performance of 1.7 petaflops (peak) since August 2014. This machine was be decommissioned in July 2019;
- A general-purpose cluster (Taito) for small and medium-size computational workloads but with large memory requirements. Some of its nodes have 1.5 terabytes of memory. This cluster includes:
    - Two partitions based on Intel CPU;
    - One partition with NVidia GPU accelerators.

The next step in terms of computing resources for CSC will be funded in the context of the government-funded "Data and Computing 2021 development programme" (DL2021).

This programme is based on a scientific case that identified key scientific drivers for the new infrastructure. It includes large-scale simulations and also mid-scale simulation, AI, data-intensive computing, data-intensive computing for sensitive data, and internet of things and data streams. The scientific drivers for the new infrastructure are:

- Workflows;
- Convergence of AI and HPC;
- Material science;
- AI workloads;
- Importance of data and storage;
- Rich data environment;
- Support of data streams.

In the context of the DL2021 programme, CSC will put in place in the Kajaani datacentre a set of new systems:

- A computing cluster (Puhti), currently running acceptance tests, with
    - A conventional processors partition (Intel Cascade lake architecture),
    - An AI partition with conventional processors (Intel Cascade lake architecture being also optimised for AI inference workload) and NVidia V100 GPU.
- An Atos BullSequana XH2000 supercomputer (Mahti) with AMD EPYC Rome GPU. The installation of this machine with a peak performance of 6.5 petaflops is planned for the end of 2019;
- A storage service (Allas) for all computing and cloud services.

The supercomputer will be water-cooled while the other systems will be air-cooled.

PSNC (Poland): National distributed HPC infrastructure

PSNC (Poznań Supercomputing and Networking Centre) has a national mission in terms of the network as an operator of the Polish NREN "PIONIER". This network is connected to the pan-European backbone.

PSNC is now also in charge of the coordination of a national initiative in terms of computing and storage called PPRACE-Lab. The goal of this initiative is to set up in Poland a distributed infrastructure with 20+ petaflops (in 4 locations) and 100+ petabytes (in 8 locations) interconnected by multiple 100 Gb/s links. The end-users include industry and SMEs in addition to large international research consortia, HEP/WLCG (CERN), European projects such as PRACE, Centres of Excellence, and EuroHPC communities.

A procurement was launched by PSNC for providing homogeneous IT equipment to the selected sites. The sites have to provide the necessary infrastructure (air-cooling for storage, DLC for compute). However, this procurement was not successful. It will be restarted soon. According to the new schedule, the deployment of the new IT equipment is expected to take place in the first half of 2020.

LRZ (Germany): Update on SuperMUC-NG

LRZ (Leibniz-Rechenzentrum) is located in Garching. It provides a large range of services from general IT services to universities to supercomputing services to scientists from all over Europe. As such, LRZ hosts SuperMUC-NG, one of the German PRACE Tier-0 systems. Provided by Lenovo and based on Intel processors (Skylake) with a mix of thin and fat nodes, the HPL performance is 19.5 petaflops (Top500/Nov. 2018: #8 in the world, #2 in Europe).

The Intel processor of SuperMUC-NG has two operation modes: one mode with a TDP of 205W, one mode with a TDP of 240W. The 205W mode is used for normal production, in this mode; the maximum frequency is lower than in the 240W mode that is used for exceptional cases, including benchmarks. For this processor, as well as for other Intel processors, the measured AVX-512 frequency when all cores are active (2.3 GHz) is lower than the nominal frequency 2.7 GHz) and the peak frequency (3.7 GHz). This means that the peak AVX-512 performance of one node is 3.5 teraflops, which is less than the peak performance calculated using the nominal frequency.

SuperMUC-NG is currently in the system acceptance phase. Most of the acceptance items were reached and the weighted measured benchmark performance is 44.6% higher than contractually committed. System is accessible by regular users starting from August 2019.

LRZ is a pioneer in hot water cooling and reuse of waste heat. This started in 2011 with CoolMUC-1. SuperMUC-NG operates with an inlet temperature of 47°C. Adsorption chillers (Fahrenheit ECOO) perform part of the heat reuse with a total capacity of 600 kW.

In terms of storage, the data science storage serves a set of different services:

- High-performance / high throughput batch processing on LRZs Linux Cluster or SuperMUC-NG;
- External access and sharing via Globus Online;
- High-performance backup and archive of data on LRZs Backup and Archive System;
- Batch and interactive processing on dedicated, hosted HPC Cluster at LRZ;
- Remote visualisation on LRZs visualisation systems;
- Interactive processing on LRZ Compute Cloud.

It is built with the following design focus:

- Usability;
- Unified Access (worldwide);
- Data Sharing;
- Dropbox Like.

CEA-GENCI (France): PPI4HPC: project update and overview of the system procured for the French lot

Within the work programme 2016-2017 of Horizon 2020, the Commission launched the call EINFRA-21-2017 in order to provide support to a public procurement of innovative (PPI) HPC systems. The PPI4HPC project (see, for more details about the PPI4HPC, PRACE 5IP/D5.4[9]) prepared by four PRACE partners (CINECA, BSC, GENCI/CEA and JUELICH) in answer to this call was selected by the European Commission in December 2016 and started its activity in April 2017.

During the project, each partner will procure an innovative IT equipment to be integrated into its computer centre and to be used as a production system. Among the four partners, one (BSC) will procure a storage and computing infrastructure for high-performance data analytics while the others will procure compute equipment. The EC is providing 35% of funding for the IT equipment.

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[9] PRACE 5IP, public deliverable D5.4, "HPC Infrastructures Workshop #9", p. 51
http://www.prace-ri.eu/IMG/pdf/D5.4_5ip.pdf

The procurement is organised as a competitive dialogue procedure. The procurement documents include a common part mostly based on a set of topics of common interest and four local parts related to site-specific context and needs. Consequently, it was decided to divide the procurement procedures into two steps: a first step conducted jointly until the selection of candidates for each site; a second step conducted separately until the selection of the winner for each site.

The publication of the contract notice, the formal start of the procurement, occurred in May 2018. Then the four partners performed the qualification of candidates for each lot jointly on 7 August 2018 and the qualified candidates were invited to participate in the dialogue phase.

At the time of the workshop, among the four partners, only one partner (France, GENCI-CEA), has completed the procurement procedure. The three others are expected to do so before the end of 2019 or at the latest in early 2020.

The system procured by GENCI-CEA is based on the Bull Sequana XH2000 architecture. It includes three partitions: one x86 partition with bi-socket AMD Rome nodes, one pre-post HPDA/AI partition with four NVidia V100 GPU per node, one ARM partition with bi-socket Marvell THX3 nodes. The total performance will exceed 13 petaflops (peak). The key drivers for choosing this system were innovation and TCO (see, for more details about the TCO approach, PRACE 5IP/D5.4[10]).

Regarding innovation, mandatory criterion for all lots procured within the PPI4HPC project, the main items are the following:

- HPC/HPDA/AI workloads through Heterogeneous technologies in a shared common infrastructure on BullSequana XH2000 (Compute and interconnect);
- Support Capability to cool the extremely high CPU TDP while maintaining a high density;
- ARM ThunderX-3 to prepare the path to EPI transition and exascale;
- High bandwidth, scalable and less costly DragonFly+;
- Energy efficiency – All PRACE-3IP/PCP results implemented;
- NVMEoF Smart burst flash on the fly, integrated with Slurm.

Regarding TCO, the goal is to get the highest throughput, which is driving lowest TCOb (CAPEX + five years OPEX including electricity/cooling, maintenance). For this call, a new TCOb based on heterogeneous nodes and mixed HPC/AI workloads was designed with 13 real applications including one single node AI test.

The installation of the new system started in September 2019. Grand challenges will get access to the system in December 2019 and the full production is expected to start in January 2020 with a share of 60% to PRACE.

CINES (France)

CINES (Centre Informatique National de l'Enseignement Supérieur - National Computing Centre for Higher Education) is the French national computing centre for higher education and universities. It is located in Montpellier with three national strategic missions:

- High-performance computing;
- Long term digital preservation;
- National hosting computer platforms.

The HPC resources installed at CINES include:

- In the production environment: the OCCIGEN supercomputer (3.5 petaflops) with DLC cooling (hot water around 32°C) that provides also visualisation and pre/post-processing services;
- In the prototype environment: the FRIOUL cluster (coming from the PRACE-3IP/PCP) and several other small systems for testing new technologies (Intel Optane, NVidia V100, BeeGFS storage).

The work conducted at CINES in terms of energy-efficiency capitalises on what has been done within PRACE-PCP (see PRACE-5IP/D5.4 for more details[11]). Therefore, several tools developed by ATOS/Bull in this project are being deployed on the OCCIGEN supercomputer. This includes BEO (Bull Energy optimiser) and BDPO (Bull Dynamic Power optimiser). This operation needed to upgrade Slurm to 17.02 and SCS5 to r2.

[10] Ibid., p. 23

[11] Ibid., p. 15

For BEO, several improvements were implemented by ATOS/Bull and this product is already installed on OCCIGEN. Its key features include the possibility to get the consumed energy for a job from the post-PSU equipment, and possibility to implement power capping. After the first tests of BEO on OCCIGEN several issues need more investigations, including idle power and huge differences between 2 jobs running on the same number of nodes.

For BDPO a new version is available but has not been installed so far.

In addition to the usage of the tools derived from the PRACE-3IP/PCP, CINES is currently deploying an infrastructure in order to measure power usage from the facility side. This requires to deploy a large number of sensors at the level of the breakers (around 3000), to enhance the software (developed in house) to be able to deal with sensor data, and to consider implementing a GUI for monitoring and to improve reporting features.

The goals are the following:

- To analyse the efficiency of the equipment;
- To compare observed behaviour versus a previous state, and thus make every change noticeable;
- To detect bad behaviour/failures.

This approached made already possible to detect balancing issues and the detection of a current too large in neutral.

The future work regarding the whole power supply chain at CINES includes the collection and analyse of many different data sources that are already available in order to:

- Detect defective sensors or enhance precision;
- Detect defective apparatus and cables;
- Monitor behaviour of the supply chain;
- Use available information: ex. Harmonics, temperatures, etc.;
- Monitor behaviour and efficiency of equipment: UPS, chillers, adiabatic groups.

NSC-LiU (Sweden)

NSC-LiU (National Supercomputer Centre-Linköping University) procured recently five different clusters in two different public procurements. ClusterVision BV (Based in Amsterdam - Netherlands) was selected for providing these clusters:

- Tetralith, and Sigma, for academic research, were installed in the second half of 2018;
- Cirrus, Stratus, and Nebula, for weather prediction, were installed at the end of 2018.

NSC-LiU learnt in February 2019, by a headline of HPCwire that ClusterVision was in bankruptcy. Fortunately, the procurement requirements included an economic part: any bidder had to demonstrate that they had the financial muscle to complete the installation. ClusterVision partnered with UK based distributor Hammer (now Exertis Hammer) for both hardware distribution and financial muscle. This included that both were jointly responsible for the contract (including installation, service, and support) even if ClusterVision was the outward face for the deal.

For an older system installed in 2014 and provided by ClusterVision (Bifrost) the situation is more complicated. A support contract was agreed upon with ClusterVision but cancelled after the bankruptcy.

The lessons learnt are the following:

- Financial requirements in procurements do work;
- Handling all system software internally frees you from provider dependency;
- Having spare parts on-site for hardware replacements gives some breathing room to sort out who is actually going to support the system going forward.

In addition, some recent infrastructure “surprises” were mentioned. These occurred during a planned power maintenance 2019-05-15 during the spring-cleaning in the substation that included dusting transformers and cutting the power to the building.

It was discovered that:

- One UPS of the five clustered turned out to be non-working;
- Kill switches covering 60% of the machines in the DC were not functional;
- Pump bearings should be replaced every other year.

CEA (France)

CEA is a French organisation involved in research and development. The computer complex of CEA, installed in the site of Bruyères-le-Châtel, close to Paris, is divided into two parts: the TERA part, for internal use, the TGCC part, open to external users.

Since winter 2018/2019, a heat reuse system is connected to the new Tera-1000 DLC supercomputer and provides heating for the CEA site of Bruyères-le-Châtel (more than 2000 employees – 18 GWh/year) (see PRACE 5IP/D5.3[12] for more details about the project).

The heat provided by Tera-1000 (outlet water temperature = 44°C) replaces geothermal heating (water temperature = 35°C). For the first winter, Tera-1000 provided 57% of the heat while gas-fired heating provided the remaining part. In 2021, it is expected that the balance will be 90% heating by supercomputers, 10% by gas.

When not used for heating purposes, the heat produced by Tera-1000 is rejected by 6 cooling tower without the use of any chiller.

With the heat reuse in place, the Tera datacentre performance KPI (DCp) is 1.04 which translates into class B, the second-best class.

Main Findings

The presentations that were given during the 10th European Workshop on HPC Infrastructures and the plenary discussions following these presentations revealed some important trends in developments of technologies for cooling, power provisioning and power management, and tooling for integral datacentre management.

Trends with respect to cooling

Air-cooled solutions for compute part of the current state of the art HPC systems is generally deemed infeasible. Direct liquid cooling solutions are predominant. Some centres even make direct liquid cooling mandatory in their RFPs for new HPC machines. Immersion cooling has been around for a number of years as well but has not achieved comparable popularity. The presentations held at this workshop, however, show that the newer immersion cooling solutions have evolved into containers that are much more serviceable and maintainable than the ones that early adopters had to cope with. Reluctance to use such a system in part comes from the limited number of equipment vendors that certify that their equipment remains fully functional for the normal lifespan when fully submerged in a particular coolant. In addition, there is some reluctance about the more extensive use of floor space, the lower density per square meter, resulting from racks being lower and ‘horizontal’ rather than ‘vertical’.

Trends with respect to power

Despite the progress that has been made in terms of flops per Watt in modern CPUs and GPUs, most centres envisage that they need more power in the coming years to supply HPC capacity that meets demands. Since the larger centres have a power draw of several megawatts, or even tens of megawatts, the possibly large impact of machines on the regional electricity grids, still figures prominently on the agenda. In some cases, the HPC datacentre figures as the potential cause of instability on the grid. The worry is not so much about the large quantities of power, but rather about the potentially large and rapid fluctuation in power drawn by the site. This comes from the quest for energy-efficiency that often leads to a variation of the processor frequency. If this is applied in large jobs in which all tasks are orchestrated, this can result in steep rises and falls in the power draw of the machine. Large fluctuations in a short time interval can result in voltage drops that have a destabilising effect on the power grid. Maximising energy-efficiency may be constrained by the need to operate in a more grid-friendly way, or measures must be taken to improve “grid-stiffness”.

There may be financial benefits in scheduling in a more predictable grid friendly way. In last year’s workshop, it was already concluded that the pricing of electricity is often such that it is cost-optimal to strive for a predictable power draw that has fluctuation between a predetermined lower and upper bound. In this year’s workshop, it was demonstrated that sites, with the help of their monitoring and subsequent analyses of application runs, can predict the power usage of the applications that are sitting in the queue, waiting to be scheduled, and can take this into

[12] PRACE 5IP, public deliverable D5.3, “HPC Infrastructures Workshop #8”, p. 39
http://www.prace-ri.eu/IMG/pdf/D5.3_5ip-1.pdf

account in their scheduling policies. Thus, they can actively schedule to stay in the ‘safe’ area of power usage between the upper and lower bound.

With the introduction of more power coming from sun and wind sources in power grids, more fluctuations in the amount of power supplied by the grid is to be expected, independent of what datacentres do. This workshop showed developments in UPS technology and in the organisation of the electricity market, that could enable datacentres to become part of the solution to stabilise the grid rather than to have a destabilising effect.

Monitoring and control

The predominance of warm water-cooled high density systems has led to areas of tighter coupling of facility management proper and management of the HPC system. Most facility management teams have come to the conclusion that broad instrumentation of all components of the datacentre and the HPC system and its operating system and job scheduling software is a basic requirement for improving energy-efficiency. This, however, leads to fairly large data streams from multiple sources that must somehow be integrated and aggregated into meaningful and manageable overviews. The many sensors involved must all be carefully calibrated to avoid getting the wrong information, and quality control measures must be devised to check regularly whether the sensor data are still to be trusted.

The predominance of warm water-cooled high-density systems has led to areas of tighter coupling of facility management proper and management of the HPC system. Monitoring and control of the numerous data sources from the facility, as well as from the HPC system hardware and software, must be integrated and aggregated into meaningful and manageable overviews.

Many sites have taken the path to invest in tooling that they can customise to their datacentre and HPC system. There is no out of the box commercial product available. Most centres build their own integrated datacentre management tool, relying heavily on open source projects – such Apache Kafka, Apache Cassandra, Grafana, OpenDCIM - for providing core blocks of functionality.

Sites are also trying to go beyond mere monitoring. Broad instrumentation and integrated highly frequent data capturing and analyses open prospects of automating control, of feeding back decisions into facility control systems, and/or the job scheduling environment, that are based on such analyses.

Conclusions

The 10^{th} Workshop on HPC Infrastructures has been very successful in bringing together experts from various disciplines and in various stakeholder roles working on HPC site infrastructures. Figure 22 shows that the annual workshop, which is attended upon invitation only, has become an institution that is capable of consistently attracting a stable number of experts in the field.

The format of ‘lightning talks’, new on the agenda, proved suitable for the presentation of a number of ideas and will probably return in the programme of the next edition of the workshop, which will be hosted by LRZ, and is planned to take place in Garching, in May 2020.

The workshop is important for sharing best practices and contributes to sustaining a high level of expertise and to the spread of advanced technologies in European HPC centres. The programmes of the EuroHPC Joint Untertaking aim to foster a more autarchic European HPC ecosystem. The workshop confirms that HPC centres in Europe are able to host and operate large supercomputers in a reliable and energy-efficient way. The workshop activities are important for making sure that EuroHPC can indeed deploy large systems in Europe, and for identifying key technologies that may benefit from research and infrastructure funded by EuroHPC.

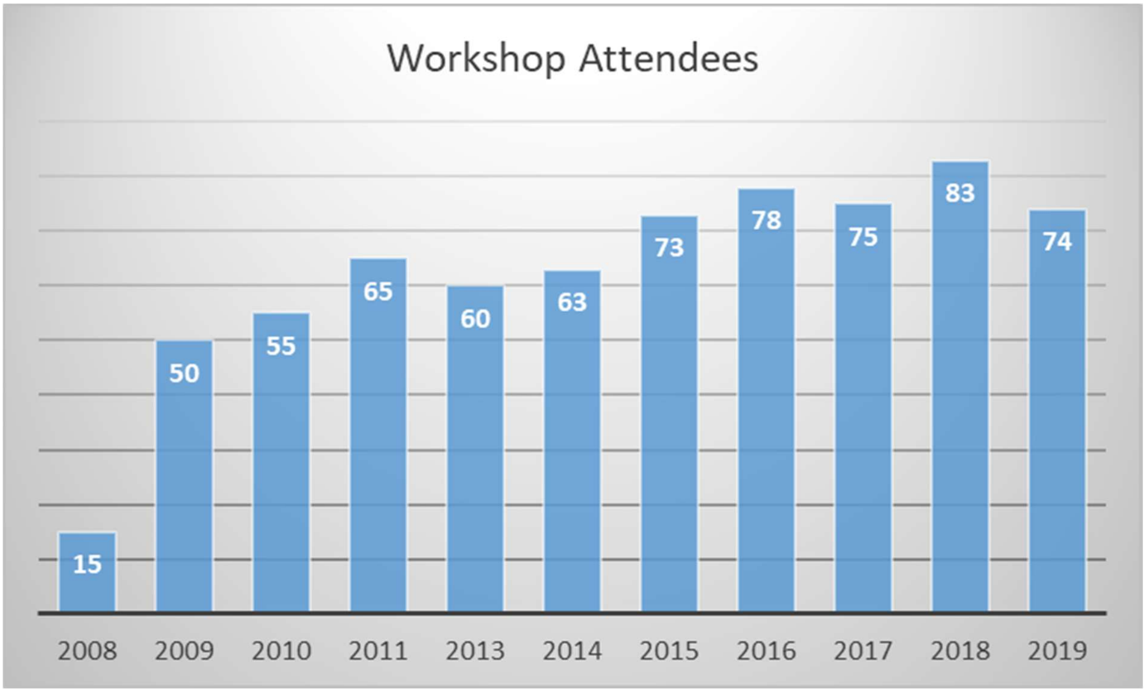

Figure 22: Number of Workshop on HPC Infrastructures attendees in a historical perspective

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