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Abstract. Access and exploitation of large scale computing resources, such as those offered by general purpose HPC centres, is one important measure for ATLAS and the other Large Hadron Collider experiments in order to meet the challenge posed by the full exploitation of the future data within the constraints of flat budgets. We report on the effort of moving the Swiss WLCG T2 computing, serving ATLAS, CMS and LHCb, from a dedicated cluster to the large Cray systems at the Swiss National Supercomputing Centre CSCS. These systems do not only offer very efficient hardware, cooling and highly competent operators, but also have large backfill potentials due to size and multidisciplinary usage and potential gains due to economy at scale. Technical solutions, performance, expected return and future plans are discussed.

1. Introduction
The challenges posed by the High Luminosity LHC (beyond 2020) to the LHC computing are substantial and cannot be met by means of a purely evolutionary approach. Estimates show that already in the first year of the HL-LHC (2027), compared to 2016, we can expect requirements on disk and CPU to be up to one order of magnitude higher than what we can expect from technology improvement, considering a flat level of funding. Efforts are ongoing worldwide to find solutions that will help to meet the demand. It is clear that a single simple solution cannot be expected, and optimisation must occur in several realms: from computing models to software performance in the experiments; from infrastructure evolution and optimisation to efficient use of manpower.

As of September 2016, the Worldwide LHC Computing Grid (WLCG) consists of 167 sites, providing 310 PB of disk, 390 PB of tape storage and 3.8 M hepspec06, mainly provisioned via dedicated Linux clusters. Switzerland contributes with 4% of the ATLAS [1] Tier-2 CPU capacity with four standard Linux clusters operated at three sites. A consolidation of the LHC computing to fewer but bigger sites should result in significant operational cost savings. We investigate the use of academic cloud resources [2] and HPC centres for ATLAS computing for potential cost savings, or obtain more computing for the same money. General purpose HPC centres seem a good alternative to dedicated clusters: typically featuring high-end hardware, efficient operational models, and the perspective of profiting from economy of scales when procuring hardware. We report on the efforts in integrating high-end Cray systems in WLCG.

2. HPC Integration Challenges
The Swiss National Supercomputing Centre (CSCS) hosts the Piz Daint supercomputer, a Cray system, which, at the time of writing, ranks 8th worldwide and 1st in Europe according to the
TOP500 list [3]. The HPCs are generally restricted and self-contained environments, subject to tight access rules. Consequently, their integration in a distributed computing environment poses challenges. Further challenges are posed by the general nature of these systems. For example, the processor architecture and/or the OS might not always be suitable. The application provisioning itself is not trivial, considering that a single ATLAS release is about 20 GB in size and the release cycles are very short and unpredictable. Furthermore, the integration with the experiment factories requires generally running middleware services at the site as superuser, in addition to outbound IP connectivity, both of which are not generally allowed at HPC centres. For real data processing, the data exchange systems should be able to cope with rates of about 0.2 MB/sec per core for input and about half of that for output, continuously.

In order to address these challenges, we have obtained access to test Cray systems at CSCS. The complex integration process has been studied first. In a second phase, the experiment specific workload integration has been addressed, including the problem of co-existence of the different and often orthogonal computing ecosystems of the experiments. Performance tests are foreseen for several ATLAS workloads in order to produce a detailed cost study, with the view of a possible future migration of the Tier-2 resources operated at the site for ATLAS and other LHC experiments from a dedicated Linux cluster to the flagship shared Cray system Piz Daint.

3. Cray Grid Integration
In 2014/15 we performed a first integration study on the Cray XK7 Tödi, a former integration system featuring a CPU/GPU hybrid architecture with AMD Opteron CPUs, running Cray Linux Environment 5 and the SLURM LRMS. We adopted a non-invasive approach centred around the Advanced Resource Connector Compute Element (ARC CE) [4]. A remote ARC CE instantiated as a VM at the University of Bern and integrated with the ATLAS production system mounts via sshfs a shared file system of the Cray at CSCS, holding the job directories. Wrapper scripts to the ARC CE SLURM back-end were used for remote job submission and monitoring via ssh [5]. We were able to run unmodified binaries out of the CVMFS repositories, tested scalability up to 100 16-core concurrent jobs and ran real production ATLAS simulation workloads for several months until the Cray Tödi was decommissioned. The integration scheme can be seen in Fig. 1, and a detailed account of the exercise can be found in [6].

Figure 1. Cray integration into the Grid with a remote ARC CE as a frontend. Clouds denote connections made over the network.
4. The LHConCray Project

In 2016, the LHConCray project has been setup between CSCS and the HEP partners in Switzerland (ATLAS, CMS and LHCb) [1,7,8] with the goal of studying the feasibility and possible cost-advantages of migrating all the WLCG Tier-2 workloads from the dedicated Tier-2 Linux cluster Phoenix to the flagship Cray Piz Daint at CSCS. In addition, the integration of the Grid Storage Element within the central storage infrastructure at CSCS is considered for the future. We have been granted access to the Cray Brisi, the Test Development System (TDS) for Piz Daint. The system is a Cray XC40 featuring Broadwell (Intel Xeon E5-2695 v4 @2.10GHz) CPUs with 64 HT-cores, 128 GB RAM and a hepspec06 [9] rating of 13.4/core. The nodes are diskless, run the latest version of the Cray Linux Environment 6 (which is based on SUSE 12), the interconnect is Cray Aries and the LRMS is SLURM.

Since CSCS has officially endorsed the effort, some of the integration challenges have been automatically addressed, so that we could better concentrate on performance and scalability. However, several adaptations were needed for the CSCS infrastructure (mainly network). These have required a fair amount of work, constituting the first stage of the project, the feasibility study. With the second phase, which has just been concluded, we have concentrated on moving to a stage somewhere in between proof-of-concept and pre-production. The work has focussed on integrating as many workloads as possible by the three experiments, address the application software provisioning and the fair-share complexities. Some preliminary performance studies have been conducted for ATLAS. In a future phase, evaluation at scale is foreseen. This should provide detailed performance metrics to feed back to the cost study. The integration scheme can be seen in Fig. 2.

![Figure 2. LHConCray current shared architecture.](image)

4.1. Technical Solutions

We have seen earlier what the main challenges for integrating a Cray into the WLCG Grid are. During the integration phase we have addressed all of them to some level. The solutions adopted are listed below. Some of them will require testing at scale in order to be validated or further tuned for performance.

4.1.1. Processor architecture and OS, memory management. The processor architecture of the Piz Daint Cray is what the WLCG environment expects. However, the Operating System
is not. While it is true that the latest version of the Cray Linux Environment abandons many proprietary solutions and makes the Cray a more Linux-like system, thus facilitating the integration process, it cannot be expected that all type of workloads could run unmodified on it. In order to address this, jobs run within Shifter containers. The container is a CentOS 6.8 full image with the same packages as in the dedicated WLCG Tier-2 cluster and configured accordingly. The main challenge of this approach has been reducing the memory overhead caused by the container itself. This is crucial, since the memory specification of the Cray nodes is quite tight at 2 GB/core and no swap. In addition, the memory requirements and memory management strategies of each experiment are completely different between each other, which means that an optimal sharing of the system between the three of them is particularly challenging. In SLURM, jobs are allowed to be not node-exclusive (a departure from the typical HPC model), so that running single or low-core count jobs would not result in part of the resources being left idle. This also means that memory limits must be carefully considered and enforced in order to ensure a smooth running of the system. This introduces further complications in the fair-share settings and management, which is essentially the core of the HPC vs. HTC scheduling challenge.

4.1.2. Compliance with tight access rules. As the policies have been relaxed for this specific use case, we no longer need to restrict all access to occur via ssh under a single user. The pool accounts needed for the integration with the experiment frameworks have been granted and we have been able to integrate the ARC CE services directly inside the Cray high speed network.

4.1.3. Application provisioning. The integration of the middleware services goes further to allow the root fuse mount required on the compute nodes in order to use CVMFS as software repository for the three experiments. However, the nodes are diskless, so the local CVMFS cache cannot be deployed simply. After trying a few different approaches, including pre-loading the entire CVMFS stratum-0 repository contents on to the Cray shared file system, the approach chosen is currently to deploy the cache as a single xfs file system per node. The file system itself consists in turn of a single sparse xfs file that can be located anywhere on the internal network. This has the advantage of reducing drastically the number of meta-data operations involved and also provides the flexibility of moving the caches to more performant or even ad-hoc file systems, should the need arise (in terms of performance). This solution still needs testing at a scale and perhaps consequent optimisation.

4.1.4. Workload management integration. The ARC CE integrates by design with the ATLAS factories, furthermore its integration with CMS and LHCb has been relatively recently established in production by the experiments. The ARC CE thus ensures the main layer of integration for the Cray resources. Lack of outbound IP connectivity can be worked around by the ARC CE itself. However, CMS and LHCb can not readily benefit from it because of the late binding of their workloads. Consequently the restricted outbound IP connectivity policy has been lifted, and the Cray nodes have now even public IPs with standard Linux IP packet forwarding. The internal network infrastructure has been adapted in order to ensure that all the security policies are met by the setup.

4.1.5. Data input, processing and retrieval. For ATLAS, we leverage the ARC CE technology that provides its own Data Delivery services. These are demonstrated to be sufficiently performant at scale. Since the ARC CE is integrated in the Cray high speed network and full IP connectivity is ensured, both functionality and performance at scale should be ensured. CMS and LHCb make use of the tools built in their pilot frameworks, thus also benefiting
from the node full IP connectivity. It should be noted that with diskless nodes, the shared file systems serving the Cray become central to the performance of the system. These are normally not tuned for the I/O patterns of several WLCG workloads. Sustained tests at the scale of several thousand cores are needed in order to evaluate properly the impact on the performance of the chaotic mix of workloads from the experiments running concurrently. This can have direct implications on the effective costs of the system, should a significant performance degradation result from such tests. This is still an open question that we need to address.

5. Preliminary Performance
Some preliminary performance tests have been carried out running ATLAS detector simulation workloads on the Cray Brisi and the Tier-2 Linux cluster Phoenix. The workloads run and their input files were identical for the two systems, thus the results are directly comparable. The tests have been performed at a scale of up to about 500 cores and are reproducible between the systems and at different points in time. We have therefore chosen to run continuously multiple copies of the same identical job on both systems for fixed period of times (24h or 48h) and measured the mean WallClock registered on both systems for the job. The tests have been repeated for single core and 8-core jobs and fixed number of events per job. Since the considered simulation is a CPU bound workload, which in normal circumstances is up to 99% efficient in terms of CPU/WallClock, the mean WallClock can be directly compared to the hepspec06 ratings of the two systems. From this test we have found that while the hepspec06 rating of the Cray is 18% better compared to that of the Phoenix Tier-2 nodes, the Cray WallClock performance per job is 22% to 25% better than that of the Phoenix Tier-2 nodes. If we consider the hepspec06 the base performance unit and normalise the results to it, this translates into a net performance gain of up to 5% with the Cray. The test results are summarised in Table 1.

Table 1. Compared performance with CPU-bound workload. 24h and 48h tests.

| System       | Hours | OK Jobs | Fail Jobs | OK Rate | CPU/WC  | HS06 | Mean WC  |
|--------------|-------|---------|-----------|---------|---------|------|----------|
| Cray 1-core  | 24    | 4316    | 56        | 98.8    | 0.97    | 13.39| 10386    |
| Phoenix 1-core| 24    | 2117    | 0         | 100     | 0.99    | 11.46| 13450    |
| Cray 8-core  | 48    | 340     | 12        | 96.6    | 0.97    | 13.39| 17978    |
| Phoenix 8-core| 48    | 75      | 0         | 100     | 0.98    | 11.46| 23029    |

6. Conclusions
We have investigated the suitability of HPC systems for integration in the WLCG computing environment, with the aim of identifying cost effective computing solutions for the next decade. Cray systems at CSCS have been used to perform the related studies: feasibility, integration, performance. We have developed a set of technical solutions allowing us to perform ATLAS and LHC computations on such systems. These solve a number of technical challenges, with changes required on the resource centre side, mainly due to the intrinsic nature of these centres and the involved systems. First performance tests for ATLAS with CPU bound workloads (identical on the two systems) show a few percent performance gain at the same hepspec06 level. While this is not very significant, it should be noted that these tests have been performed before any optimisation on the system has been carried out. They should be repeated on the optimised system and in parallel performance tests for I/O intensive workloads should be carried out,
including stress tests with a production-like mix of experiment workloads at the scale of several thousand cores.

Given the number of complexities we had to deal with, this study has not been in the position yet to show that a HPC is necessarily a cost effective solution for the future of LHC computing. More investigations are needed and the studies are ongoing.

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