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Extending ATLAS Computing to Commercial Clouds and Supercomputers

Paul Nilsson[1]
University of Texas at Arlington
Physics Dept., 502 Yates St., Room 108 Science Hall, Arlington, Texas 76019, United States
E-mail: `Paul.Nilsson@cern.ch`

Kaushik De[2], **Andrej Filipcic**[3], **Alexei Klimentov**[4], **Tadashi Maeno**[4], **Danila Oleynik**[1], **Sergey Panitkin**[3], **Torre Wenaus**[3], **Wenjing Wu**[4] on behalf of the ATLAS Collaboration
[2]*University of Texas at Arlington (US),* [3]*Jozef Stefan Institute (SI),* [4]*Brookhaven National Laboratory (US),* [5]*Institute of High Energy Physics (CN)*

Abstract

The Large Hadron Collider will resume data collection in 2015 with substantially increased computing requirements relative to its first 2009-2013 run. A near doubling of the energy and the data rate, high level of event pile-up, and detector upgrades will mean the number and complexity of events to be analyzed will increase dramatically. A naive extrapolation of the Run 1 experience would suggest that a 5-6 fold increase in computing resources are needed - impossible within the anticipated flat computing budgets in the near future. Consequently ATLAS is engaged in an ambitious program to expand its computing to all available resources, notably including opportunistic use of commercial clouds and supercomputers. Such resources present new challenges in managing heterogeneity, supporting data flows, parallelizing workflows, provisioning software, and other aspects of distributed computing, all while minimizing operational load. We will present the ATLAS experience to date with clouds, supercomputers and Volunteer Computing, and describe efforts underway to automate and scale the utilization of such resources. In particular, we will describe the successful use of these resources through the ATLAS workload management system, PanDA, and future development plans.

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1. Introduction

The computing model of the ATLAS Experiment [1,2] at the Large Hadron Collider (LHC) was originally based on the grid paradigm [3] with hierarchically distributed computing and storage resources. During Run-1 (2009-2013) at the LHC, ATLAS produced and processed over 130 PB of data. The computing model was proven to be very successful. However, a naive extrapolation of the Run 1 experience indicates that the computing resources needs in Run-2 (2015-2018) might increase by a factor 5-6, which will be impossible to manage with the current computing and storage resources within the anticipated flat computing budgets in the near future. Furthermore, while ATLAS currently uses more than 100,000 cores at well over 100 grid sites with a peak performance of 0.3 petaFLOPS, Run-2 data processing will require more resources than grid computing can possibly provide. The Worldwide LHC Computing Grid (WLCG) infrastructure will be sufficient for the planned analysis and data processing, but it will be insufficient for Monte Carlo (MC) production and any extra activities. Additional computing and storage resources are therefore required.

To alleviate these challenges, ATLAS is engaged in an ambitious program to expand the current computing model to include additional resources such as the opportunistic use of supercomputers at Leadership Computing Facilities (LCF) as well as commercial and volunteer clouds.

2. Supercomputing in High Energy Physics

The Production and Distributed Analysis (PanDA) system [4] was designed to meet ATLAS requirements for a data-driven workload management system for production and distributed analysis processing capable of operating at the LHC data processing scale. It has been used in the ATLAS experiment since 2005 and is now expanding into a BigPanDA [5] project to extend PanDA as a meta application, providing location transparency of processing and data management, for High Energy Physics (HEP) and other data-intensive sciences, and a wider exascale community. BigPanDA aims to extend the ATLAS Computing Model beyond the grid into the domains of LCFs and further advance the usage of commercial and volunteer clouds.

Modern High Performance Computing (HPC) involves a very large number of cores connected through a high-speed network. The multi-core CPUs have high speed interconnects that can be complemented or essentially replaced by ultrafast and massively parallel GPUs. On an HPC, a typical job is highly parallel and each core calculates a small part of the problem and coordinates the activity via the processor interconnects. While this is different from the HEP paradigm it still shares common features such as the use of parallelization. It is not a requirement that HPCs are able to run any possible task, nor is it relevant how many kinds of job types can be run. What matters is the total number of cycles that can be offloaded from the grid.

The most suitable task for HPCs in HEP is event generation. Event generators are mostly computational, stand-alone code, with few input requirements. There is no need to stage-in much data. The event generation in ATLAS corresponds to 10-15% of all jobs on the grid. A less suitable and more difficult task for HPCs, but highly useful, is detector simulation. Simulation tasks tend to be tied to the framework of a particular simulation and often require database access for geometry and relevant run conditions. However, there is a lot to be gained since simulation tasks correspond to 2/3 of the grid capacity.

2.1 HPC Challenges

Unlike grids and clouds, HPCs are built to execute parallel payload as fast as possible. Standard ATLAS workflow is not well adapted for HPCs due to several complications such as fixed worker node setups, no outbound network connections, no local disks, limited memory, specialized operating systems and non-Scientific Linux (SL6) environments, binary incompatibilities with ATLAS software releases, etc. A reorganization of the standard workflow is therefore needed. The following is a non-exhaustive list of some of the known problems with suggested solutions.

- Problem: Communication with PanDA server is not possible on the worker node level. Solution: The payload must be fully defined in advance, and all communications with the PanDA server will be done from the HPC front-end node (where network connections are allowed).
- Problem: The central software repository is not always accessible from within the HPC. Solution: Synchronize the central software repository to a shared file system instead.
- Problem: The database service cannot be accessed from the worker node due to the network restriction. Solution: Use a local copy of database release file.
- Problem: Network throughput to and from the HPC is limited which makes jobs with large input/output unsuitable. Solution: Use CPU intensive event generation and Monte Carlo simulations since they are ideal tasks for HPCs.
- Problem: HPCs typically do not provide a Storage Element (SE). Solution: Use the SE from a close Tier-1/2 for stage-in and stage-out.

2.2 Event Generation on ALCF Intrepid

A demonstration for running ATLAS jobs on an HPC was performed at the Argonne National Laboratory Leadership Computing Facility (ALCF). The ALPGEN Monte Carlo [6] event generator was used to generate 81M physics events. Jobs defined in PanDA were executed on the Intrepid supercomputer. The Intrepid IBM Blue Gene/P system consists of 163,840 850 MHz CPU cores and is as of March 2014 ranked as the 67th fastest supercomputer in the world (Top 500 Supercomputer Sites, http://top500.org). The following components were used in this project and are further described in [7].

- Data Stager: an intermediary data staging and message queuing system between PanDA, the Open Science Grid (OSG) and ALCF.
- Balsam Service: a service that periodically queries the Data Stager for available jobs.

- Balsam Daemon: a daemon that receives input data, manages payload execution and stages-out output data.

2.3 PanDA on OLCF

The current number two (number one from November 2012 until June 2013) on the Top 500 list is located at the Oak Ridge Leadership Computing Facility (OLCF) in Oak Ridge National Laboratory, US. The supercomputer, called Titan, was the first large-scale system to use a hybrid architecture that utilizes both AMD 16-core Opteron 6274 CPUs and NVIDIA Tesla K20 GPU accelerators.

Development on Titan is the current focus for BigPanDA developers. The project aims to integrate Titan with the PanDA system using an updated PanDA Pilot [8] that runs on the front-end node and submits ATLAS payloads to the worker nodes using the local batch system (PBS) [Fig. 1] via the SAGA (Simple API for Grid Applications, http://saga-project.github.io) interface. This solves several complications of running on HPC worker nodes, including the lack of connectivity to the PanDA server. The pilot can communicate with the PanDA server from the front-end machine. The interactive front-end machines and the worker nodes use a shared file system which makes it easy for the pilot to stage-in any input files that are required by the payload and stage-out the produced output files after the payload has finished at the end of the job. A close Tier-1/2 SE will be used for the storage.

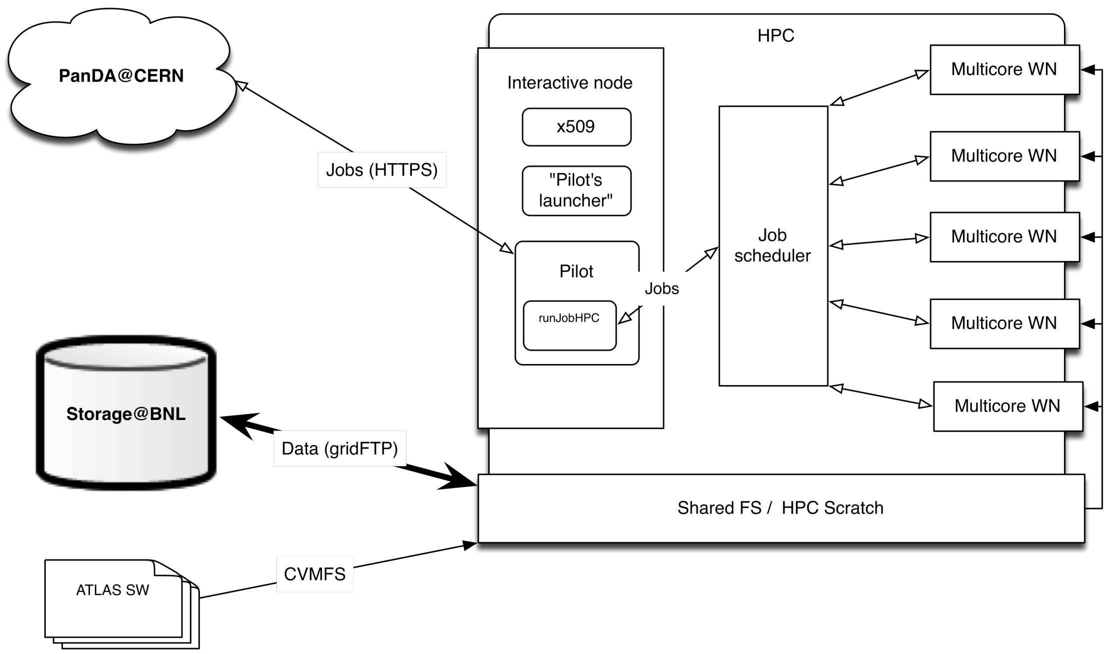

Figure 1. The proposed pilot based PanDA workflow on Titan. ATLAS payloads are downloaded from the PanDA server by the PanDA Pilot and submitted into Titan. The pilot itself is launched by a pilot factory (APF), which is also running on the front-end machine.

The BigPanDA project has been allocated 0.5M core hours on Titan, as well as 1.1M core hours on the supercomputers at the National Energy Research Scientific Computing Center (NERSC).

2.4 HPC Resources in ATLAS Production

Several less restricted HPCs (i.e. HPCs where e.g. the PanDA Pilot can be executed without modification) are already being used in ATLAS production on Nordugrid using the ARC Control Tower (aCT) [9] as an intermediary service between the HPC and PanDA.

- The C2PAP (Computing Center for Particle and Astrophysics) HPC at LRZ in Germany consists of 128 nodes with 2048 Intel SB-EP cores and has been used in ATLAS production since Autumn 2013.
- Abel at University of Oslo, Norway, has 10,080 Intel Xeon E5-2670 cores and has been running ATLAS jobs since beginning of 2013. Abel is currently number 240 in the top 500 list.
- Abisko at Umeå University, Sweden, consists of 15,456 AMD Opteron 6238 cores. Abisko has been used in ATLAS since early 2013. It is currently number 398 in the top 500 list.

An additional Swedish HPC, Triolith at the National Supercomputer Centre in Linköping (79th in top 500), is in the commissioning phase. Several other HPC centers have expressed interest in running ATLAS jobs, including Hydra (RZG Munich, Germany), IT4i (Ostrava, Czech Republic) and Piz Daint (6th in top 500, Zurich, Switzerland).

2.5 HPC Backfill

HPC nodes are geared towards large-scale jobs by design. About 10% of capacity on a typical HPC machine is unused due to mismatches between job sizes and available resources. Time allocation on an HPC is competitive and large projects are often preferred. On the Titan supercomputer, an estimated 300M core hours per year are unused. This offers a great possibility for ATLAS to instrument PanDA to harvest the opportunistic resources on Titan and use a similar mechanism on other HPCs.

Functionality has been added to the PanDA Pilot to collect information about available resources on especially Titan, which in effect serves as a test bed for the development on how to best incorporate the more restrictive HPCs into the PanDA workflow. The aim is to develop a general solution that can be used on several HPCs. The backfill algorithm works as follows:

- The pilot queries the MOAB scheduler about unused transient resources.
- The scheduler returns information about available resources, including the number of currently unscheduled nodes and period of availability.

- The pilot chooses the largest available block of free nodes and generates appropriate job submission parameters taking into account Titan's scheduling policy limitations.

3. Cloud Computing and ATLAS

ATLAS has evaluated distributed cloud computing systems especially for running Monte Carlo simulation jobs. Cloud systems provide virtualization which shields the applications from changing technologies and reduces the need for systems personnel to have knowledge about the user application, which in turn allows resource centers that do not have expertise in ATLAS software or distributed computing to still make a contribution.

An ATLAS Cloud Computing project was set up a few years ago to exploit virtualization and clouds with a goal to utilize public and private clouds as extra computing resources and as an additional mechanism to cope with peak loads on the grid [10, 11]. The project has performed studies and incorporated several cloud services into the PanDA system and has shown excellent progress. Both commercial and private clouds have been studied for use in production and will be described in the following sections.

3.1 Workflow

The PanDA system is using pilot jobs to execute the ATLAS payloads on the worker nodes. The pilot itself is launched on the worker node by a wrapper script that on a normal grid site is sent to the worker node from a pilot factory via the local batch system. On a cloud system an additional layer is needed since the pilot and the payload will be executed in a virtual machine (VM), which first needs to be started. The chosen approach is to use Cloud Scheduler [12] for managing the VMs and HTCondor (http://research.cs.wisc.edu/htcondor) for scheduling the jobs [Fig. 2].

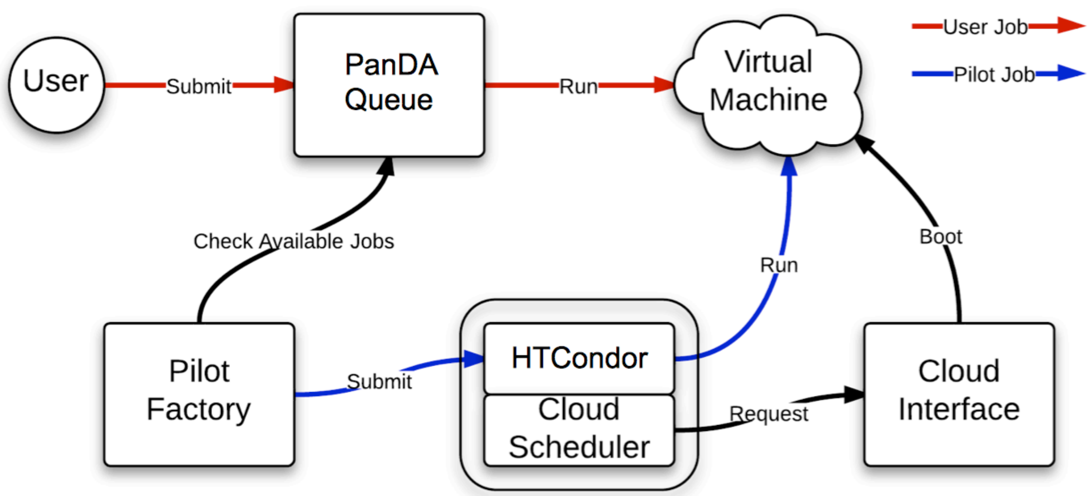

Figure 2. Job workflow in the cloud.

3.2 Academic Clouds

The distributed cloud computing system uses academic Infrastructure-as-a-Service (IaaS) clouds located at CERN, Canada (Victoria, Edmonton, Quebec and Ottawa), the United States (FutureGrid clouds in San Diego and Chicago), Australia (Melbourne and Queensland) and the United Kingdom. The Victoria and FutureGrid clouds use Nimbus (http://www.nimbusproject.org) while the other clouds use OpenStack (http://www.openstack.org). Since April 2012, the cloud system has completed over 1,100,000 ATLAS jobs running up to 1,000 jobs concurrently [Fig. 3].

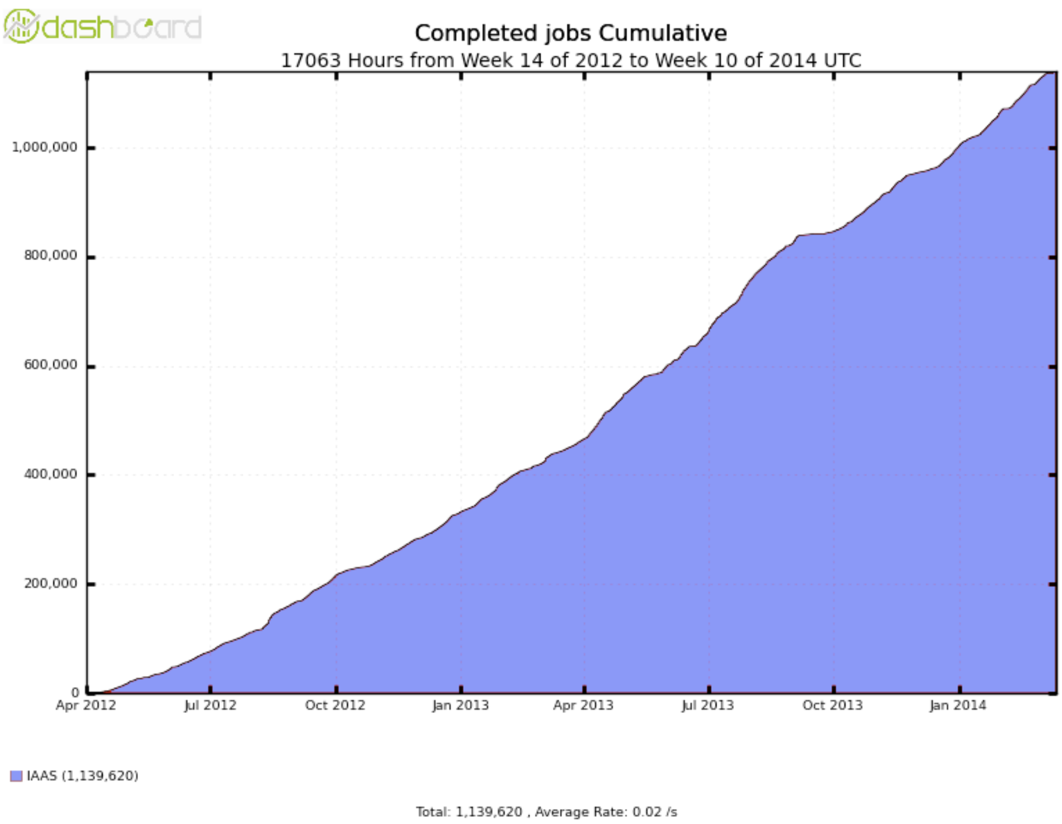

Figure 3. The total number of completed ATLAS jobs running in clouds since April 2012.

3.3 Google Compute Engine Project

ATLAS was invited to participate in the closed preview of the Google Compute Engine (GCE) Project (https://cloud.google.com/products/compute-engine) in August 2012. After an initial preparations period of several months, Google allocated 5M core hours on 4,000 cores to ATLAS for two months in March-April, 2013. The goal of the project was to test long term stability while running on a cloud cluster similar in size to a Tier-2 grid site in ATLAS. Resources were organized as an HTCondor based PanDA queue and was transparently included in the ATLAS computational grid.

CPU intensive workloads, such as physics event generators, fast detector simulations as well as full detector simulations were run in GCE over a period of eight weeks. Some 458,000 jobs were completed [Fig. 4] that generated and processed about 214M events. All output data was transferred automatically to ATLAS grid storage. The project was overall very successful with stable running on the GCE side. The overall failure rate was about 6% where most of the problems were on the ATLAS side and not related to the cloud.

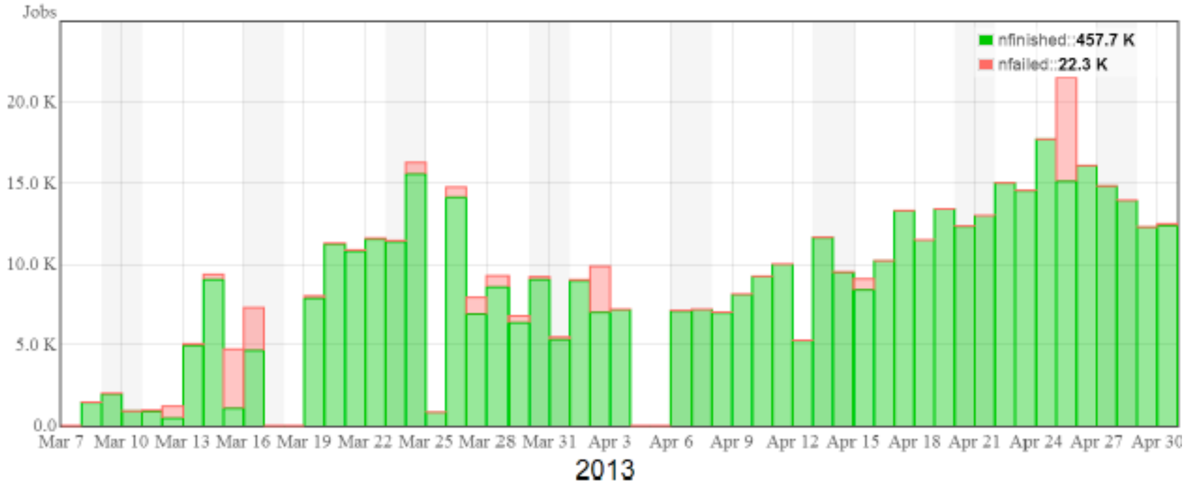

Figure 4. ATLAS jobs running in GCE.

3.4 Amazon Elastic Compute Cloud

The Amazon Elastic Compute Cloud (EC2, http://aws.amazon.com/ec2) spot market offers an interesting alternative to otherwise expensive commercial clouds. The EC2 spot pricing, which trades a willingness to accept abrupt VM terminations for a significantly reduced cost, has turned IaaS into an economical alternative to site-based dedicated resources.

The RHIC and ATLAS Computing Facility (RACF) group at Brookhaven National Laboratory (BNL) received a grant allocation from Amazon EC2 in 2013. A hybrid cloud was setup that included resources from the BNL Tier-1 and the "elastic" part of the cloud on Amazon EC2, spanning geographically distributed EC2 sites (US-East, US-West1 and US-West2 zones).

Standard ATLAS production simulation jobs, with high CPU and low I/O usage, were run on 5,000 VMs in the large virtual cluster for nearly three weeks. The paid spot price was 0.007 USD per core hour (as of August 23, 2013) for an "m1.small" type of instance corresponding to a worker node with a 1.2 GHz Xeon CPU, 1.7 GB RAM, 160 GB disk and low network I/O. The total cost was 13,000 USD with only 750 USD for the data transfers. Since the pricing is dynamic (it is also region based) the applied strategy was to declare a maximum acceptable price (chosen to three times the baseline cost, 0.021 USD per core hour) but pay the current variable spot price until it reached the maximum acceptable price. At that point the VMs, and thus the jobs, were terminated. Operations on the EC2 platform were found to be very reliable but the job efficiency was poor due to long running jobs.

3.5 Commercial Clouds Conclusions

On average, clouds are more expensive than private computing centers. However, for varying resource demands with big but short-term spikes followed by low activity, clouds are more attractive than private computing centers. In ATLAS, clouds are used only when there are special needs. A study performed at RACF in 2013 showed that the cost of computing per core at dedicated data centers compared favorably with cloud costs [13]. The cost of computing at a US Tier-1 (BNL) was estimated to 0.04 USD per core hour as compared to the EC2 spot price range 0.007 USD (m1.small) – 0.12 USD (on demand, m1.medium) per core hours. As indicated in the previous section, the cheapest cloud option on EC2 is only useful for short running jobs.

3.6 Volunteer Computing

Volunteer computing (VC) can potentially supply more computing power to science than any other type of computing due to the huge number of computers in the world. It also encourages public interest in science and offers a way for practically anyone who owns a computer to participate in scientific computing. ATLAS is currently developing a project called ATLAS@Home, with the goal of running simulation jobs on volunteer computers using the BOINC platform [14]. BOINC has around 50 VC projects ranging from biology and environmental science to physics and cosmology. There are some 490,000 active volunteer computers providing a real time computing power of 7.2 petaFLOPS.

Since standard ATLAS software is required for ATLAS@Home, the volunteer computers need to be virtualized. ATLAS@Home uses a CernVM [15] image and the CernVM File System (CVMFS) pre-packaged with all the necessary software. The volunteer cloud should be integrated into PanDA, i.e. all the volunteer computers should appear as a site, with jobs being created by PanDA. In order to avoid placing credentials on the volunteer hosts, the ARC Compute Element (ARC CE) [11] is introduced in the architecture together with the BOINC platform. The ARC CE, which includes the aCT, is a front-end on top of the computing resources and is placed as an intermediary layer between the host and the PanDA server.

ATLAS@Home was successfully demonstrated in February 2014 in which a client running on a volunteer computer downloaded simulation jobs (real production jobs) from PanDA via the aCT. The PanDA Pilot running on the host inside the VM executed the payload. At the end of the job, the results were uploaded to the aCT, which transferred the output files to the proper Storage Element and updated the PanDA Server with the final job status. All the ATLAS@home resources currently appear as a Tier-2 site (ND.ARC_T2) in the PanDA system.

Since VC benefits from the existing infrastructures developed for grid and cloud computing it will not carry a heavy development cost. The cost is estimated to 1 FTE in manpower for operation, communication and outreach. There will also be some additional costs for the central services, i.e. the BOINC servers and maintenance.

The project is near completion and is expected to be formally released to the BOINC community and the general public soon.

4. Summary

The ATLAS Experiment is currently preparing for the massive computing challenges posed by Run-2 at the LHC. With a doubling of the beam energy and luminosity as well as an increased need for simulated data, a large increase in the computing resources is also needed. Storing and processing Run-2 data is a challenge that cannot be resolved with the currently existing computing resources in ATLAS. To resolve this challenge, ATLAS is turning to commercial as well as academic Cloud services, Volunteer Computing and HPCs via the PanDA system. Tests have been performed on several Cloud services including Amazon EC2, Google Compute Element, and many others, and are already routinely being used in ATLAS production. The development of integrating HPCs with the ATLAS Computing Model is progressing rapidly, with several HPCs already added to the PanDA workflow.

References

[1] The ATLAS Collaboration, G Aad et al., "The ATLAS Experiment at the CERN Large Hadron Collider," Journal of Instrumentation, Vol. 3, S08003, 2008.

[2] D. Adams, D. Barberis, C. Bee, R. Hawkings, S. Jarp, R. Jones, D. Malon, L. Poggioli, G. Poulard, D. Quarrie, T. Wenaus, "The ATLAS computing model" Tech. rep. CERN CERN-LHCC-2004-037/G-085, 2005.

[3] I. Foster and C. Kesselman (eds), "The Grid: Blueprint for a New Computing Infrastructure" (Morgan-Kaufmann), 1998.

[4] T. Maeno on behalf of the PanDA team and ATLAS collaboration, "PanDA: Distributed Production and Distributed Analysis System for ATLAS", J. Phys.: Conf. Ser. Vol. 119, 062036, 2008.

[5] T. Maeno on behalf of the PanDA team and ATLAS collaboration, "Evolution of the ATLAS PanDA Workload Management System for Exascale Computational Science", to be published in CHEP 2013 Proceedings.

[6] M. L. Mangano, M. Moretti, F. Piccinini, R. Pittau, A. D. Polosa, "ALPGEN, a generator for hard multiparton processes in hadronic collisions", JHEP 0307 (2003) 001.

[7] D. Benjamin, A. Filipcic, A. Klimentov, T. LeCompte, D. Oleynik, S. Panitkin, T. Uram, "Extending ATLAS Distributed Computing on Leadership and High-Performance Class Computers", submitted to International Supercomputing Conference ISC 2014, Leipzig

[8] P. Nilsson on behalf of the PanDA team and ATLAS collaboration, "Next Generation PanDA Pilot for ATLAS and Other Experiments", to be published in CHEP 2013 Proceedings.

[9] M. Ellert et al., "Advanced Resource Connector middleware for lightweight computational Grids", 446 Future Generation Computer Systems 23 (2007) 219-240.

[10] F. Barreiro Megino et al. for the ATLAS collaboration, "Exploring Virtualization and Cloud Computing in ATLAS", J. Phys.: Conf. Ser. Vol. 396, 032011, 2012.

[11] S. Panitkin et al. for the ATLAS Collaboration, "ATLAS Cloud Computing R&D project", to be published in CHEP 2013 Proceedings.

[12] P. Armstrong et al., "Cloud Scheduler: a resource manager for a distributed compute cloud", arXiv:1007.0050v1 [cs.DC]

[13] T. Wong et al., "Operating Dedicated Data Centers – Is it Cost-Effective? ", to be published in CHEP 2013 Proceedings.

[14] D. P. Anderson, "BOINC: A system for public-resource computing and storage", Grid Computing 2004 Proceedings Fifth IEEEACM International Workshop (R. Buyya, ed.), pp. 4-10, IEEE Computer Soc, 2004.

[15] P. Buncic et al., "CernVM - a virtual appliance for LHC applications". Proceedings of the XII. International Workshop on Advanced Computing and Analysis Techniques in Physics Research (ACAT08), Erice, 2008 PoS(ACAT08)012