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Integration of PanDA workload management system with Titan supercomputer at OLCF

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Abstract.
The PanDA (Production and Distributed Analysis) workload management system (WMS) was developed to meet the scale and complexity of LHC distributed computing for the ATLAS experiment. While PanDA currently distributes jobs to more than 100,000 cores at well over 100 Grid sites, the future LHC data taking runs will require more resources than Grid computing can possibly provide. 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.

We will describe a project aimed at integration of PanDA WMS with Titan supercomputer at Oak Ridge Leadership Computing Facility (OLCF). The current approach utilizes a modified PanDA pilot framework for job submission to Titan's batch queues and local data management, with light-weight MPI wrappers to run single threaded workloads in parallel on Titan's multi-core worker nodes. It also gives PanDA new capability to collect, in real time, information about unused worker nodes on Titan, which allows precise definition of the size and duration of jobs submitted to Titan according to available free resources. This capability significantly reduces PanDA job wait time while improving Titan's utilization efficiency. This implementation was tested with a variety of Monte-Carlo workloads on Titan and is being tested on several other supercomputing platforms.

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1. Introduction

The ATLAS experiment [1] at the Large Hadron Collider (LHC) is designed to explore fundamental properties of matter at the highest energy ever achieved in a laboratory. Since the LHC became operational six years ago, the experiment has produced and distributed more than 150 petabytes of data worldwide. Thousands of ATLAS physicists are engaged in daily analysis of this data.

Modern research in high-energy physics is practically impossible without massive computing infrastructure. ATLAS currently uses more than 100,000 CPU cores deployed in a hierarchical Grid [2, 3], spanning well over 100 computing centers. But the next LHC runs will require more resources than this Grid can possibly provide to sustain the pace of the proposed research. The Grid infrastructure will be sufficient for the planned analysis and data processing, but it will fall short of the requirements for the large-scale Monte Carlo simulations as well as any extra activities. Additional computing and storage resources are therefore required. To meet these challenges, ATLAS is engaged in an ambitious program to expand the current computing model to incorporate additional resources, including supercomputers and high-performance computing clusters.

In this paper we will describe a project aimed at integration of PanDA Workload Management System (WMS) [4] with Titan supercomputer at Oak Ridge Leadership Computing Facility (OLCF).

2. PanDA workload management system

ATLAS utilizes the PanDA WMS for distributed data processing and analysis. Acronym PanDA stands for Production and Distributed Analysis. The system has been developed to meet the growing ATLAS production and analysis requirements for a data-driven workload management system capable of operating at LHC data processing scale.

PanDA has a highly scalable architecture. Scalability has been demonstrated in ATLAS through the rapid increase in usage over the past several years of operations, and is expected to meet the continuously growing number of jobs over the next decade. Currently, as of 2015, PanDA WMS manages processing of over one million jobs per day on the ATLAS Grid. PanDA was designed to have the flexibility to adapt to emerging computing technologies in processing, storage, networking as well as the underlying software stack (middle-ware). This flexibility has also been successfully demonstrated through the past six years of evolving technologies adapted by computing centers in ATLAS, which span many continents and yet are seamlessly integrated into PanDA.

PanDA is a pilot [5] based WMS. In the PanDA job lifecycle, pilot jobs (Python scripts that organize workload processing on a worker node) are submitted to compute sites. When these pilot jobs start on a worker node they contact a central server to retrieve a real payload (i.e., an end-user job) and execute it. Using these pilot-based workflows helps to improve job reliability, optimize resource utilization, allows for opportunistic resources usage, and mitigates many of the problems associated with the inhomogeneities found on the Grid.

3. HPC platforms and PanDA

The High Performance Computing (HPC) platforms encompass a broad spectrum of computing facilities, ranging from small-scale interconnected clusters to the largest supercomputers in the world. They are rich sources of CPUs some claiming more cores than the entire ATLAS Grid. The HPC machines are built to execute large scale parallel, computationally intensive, workloads with high efficiency. They provide high-speed interconnects between worker nodes and facilities for low latency inter-node communications. In this environment, significant limitations can exist: typically the worker node setup is fixed, with no outbound network connections, the amount of RAM per core can be quite limited, and in many cases a customized operating system is used along with a specialized software stack. All of these factors pose significant challenge for the integration with PanDA WMS that was initially designed to be used on Grid resources.

4. Titan at OLCF

The Titan supercomputer [6], current number two (number one until June 2013) on the Top 500 list [7] is located at the Oak Ridge Leadership Computing Facility. in Oak Ridge National Laboratory, USA. It has theoretical peak performance of 29 petaFLOPS. Titan, was the first large-scale system to use a hybrid architecture that utilizes worker nodes with both AMD 16-core Opteron 6274 CPUs and NVIDIA Tesla K20 GPU accelerators. It has 18,688 worker nodes with a total of 299,008 CPU cores. Each node has 32 GB of RAM and no local disk storage, though a RAM disk can be set up if needed, with a maximum capacity of 16 GB. Worker nodes use Cray's Gemini interconnect for inter-node MPI messaging but have no network connection to the outside world. Titan is served by the shared Lustre filesystem that has 32 PB of disk storage and by the HPSS tape storage that has 29 PB capacity. Titan's worker nodes run Compute Node Linux which is a run time environment based on the Linux kernel derived from SUSE Linux Enterprise Server.

5. PanDA integration with Titan

The project aims to integrate Titan with the PanDA system. Taking advantage of its modular and extensible design, the PanDA pilot code and logic has been enhanced with tools and methods relevant for HPC. The pilot runs on Titan's front-end nodes which allows it to communicate with the PanDA server, since front end nodes have connectivity to the Internet. The interactive front-end machines and the worker nodes use a shared file system which makes it possible for the pilot to stage-in input files that are required by the payload and stage-out the produced output files at the end of the job. The ATLAS Tier 1 computing center at Brookhaven National Lab is currently used for data transfer to and from Titan, but in principle that can be any Grid site. The pilot submits ATLAS payloads to the worker nodes using the local batch system (PBS) via the SAGA (Simple API for Grid Applications) interface [8]. It also uses the SAGA facilities for monitoring and management of PanDA jobs running on Titan's worker nodes. Figure 1 shows the schematic diagram of PanDA components on Titan. We will describe relevant parts of the system in more details in subsequent sections.

5.1. MPI wrappers

The majority of experimental high energy physics workloads do not use Message Passing Interface (MPI). They are designed around event level parallelism and thus are executed on the Grid independently. Typically, detector simulation workloads can run on a single compute node using multiprocessing. A notable exception is ATLAS Event Service (ES) [9] workload that was specifically designed for opportunistic resources like HPC and Cloud Computing. In particular the implementation for HPC [10] ES utilizes MPI natively for event distribution to worker nodes. For running "ordinary" - non ES compatible - workloads on Titan we developed an MPI wrapper that allows us to launch multiple instances of single node workloads simultaneously. MPI wrappers are typically workload specific since they are responsible for set up of workload specific environment, organization of per-rank worker directories, rank specific data management, input parameters modification when necessary and cleanup on exit. The wrapper scripts is what pilot actually submits to a batch queue to run on Titan. The pilot reserves the necessary number of worker nodes at submission time and at run time a corresponding number of copies of the wrapper script will be activated on Titan. Each copy will know its MPI rank (an index that runs from zero to a maximum number of nodes or script copies) as well as the total number of ranks in the current submission . When activated on worker nodes each copy of the wrapper script, after completing the necessary preparations, will start the actual payload as a subprocess and will wait until its completion. In other words the MPI wrapper serves as a "container" for non-MPI workloads and allows us to efficiently run unmodified Grid-centric workloads on a parallel computational platforms, like Titan.

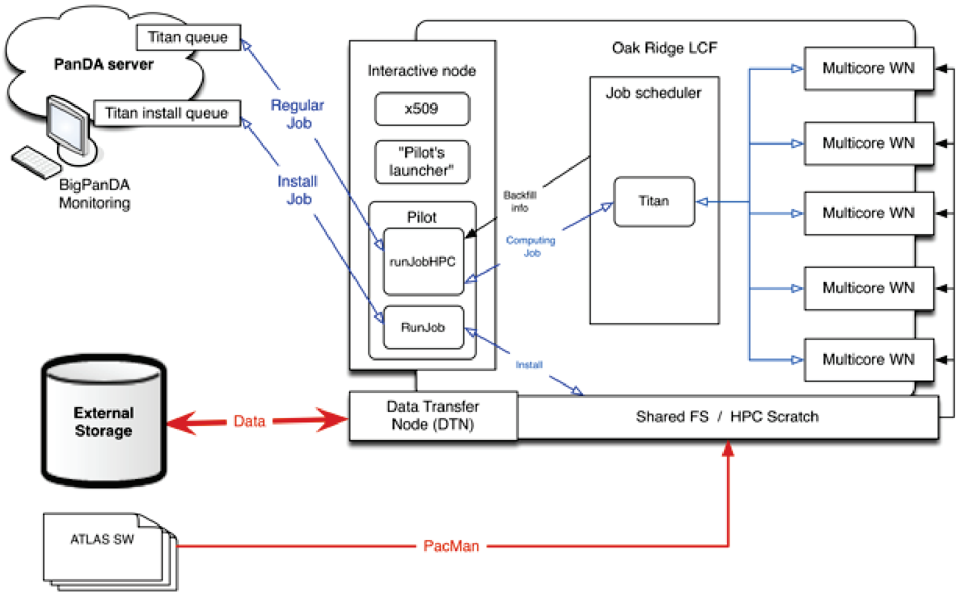

Figure 1. Schematic view of PanDA interface with Titan

5.2. Backfill: Capturing free resources on Titan

Leadership Computing Facilities (LCF), like Titan, are geared towards large scale jobs by design. Time allocation on an LCF machines is very competitive and large scale projects are often preferred. This is especially true for Titan at OLCF which was designed to be the most powerful machine in the world, capable of running extreme scale computational projects. As a consequence, on average, about 10% of capacity on Titan is unused due to mismatches between job sizes and available resources. The worker nodes sit idle because there are not enough of them to handle a large scale computing job. On Titan, these 10% correspond to estimated 300M core hours per year. Hence, a system that can occupy those temporarily free nodes would be very valuable. It would allow to deliver more CPU cycles for scientific research while simultaneously improving resource utilization efficiency on Titan. This offers a great possibility for PanDA to harvest these opportunistic resources on Titan. Functionality has been added to the PanDA pilot to interact with Titan's scheduler and collect information about available unused worker nodes on Titan. This allows the PanDA pilot to define precisely size and duration of jobs submitted to Titan according to available free resources. One additional benefit of this implementation is very short wait times before the jobs execution on Titan. Since PanDA submitted jobs match currently available free resources exactly or at least very closely, they present, in majority of cases, the best solution for Titan's job scheduler to achieve maximum resource utilization, resulting in short wait times for these jobs. The first tests of the system were quite successful and showed great promise of increasing the resource utilization on Titan. We demonstrated increased system utilization levels by ≈3% of total capacity (≈14.3% of free cycles) during the performance period of this test, as well as provided short wait times (≈70 seconds) to jobs submitted to Titan via PanDA; all with no negative impact on OLCFs ability to schedule large scale jobs. These results were obtained with single stream of pilots. Multiple pilot streams will improve backfill utilization.

5.3. Workloads and ATLAS software deployment model for Titan

Typically, installation on Titan of stand alone HEP physics software packages, like event generators, Root, etc, consists of a straightforward compilation and build from source code. In order to run ATLAS production workloads, we need to install and maintain official software releases and corresponding databases on Titan. The ATLAS software releases have been distributed using the pacman [11] package manager. Usage of native CVMFS [12] was not possible because the FUSE [13] module was missing on the Titan kernel modules, while CVMFS and Parrot [14] proved not to be a stable installation.

During the course of the project, we ported to Titan a number of HEP workloads ranging from Monte-Carlo event generators to full Geant4 [15] detector simulation chains. We installed ATLAS software releases on Titan and ran several types of calculations for ATLAS physics analyses, concentrating on those which can not be effectively simulated on the Grid.

In collaboration with a group of ATLAS physicists from NYU and Manhattan College we calculated the Vector Boson Fusion channel for Higgs productions and delivered more than 15 million simulated events. Figure 2 shows distributions in invariant mass of Z-bosons in the process of Higgs creation with no or just one accompanying jet (pp→0J1JX2→ZZ→4l), for a hypothetical spin 2 Higgs (X2). This distribution was obtained from calculations with MadGraph5 [16] performed on Titan. Also we studied the jet distributions in the process of gluon fusion pp→JJH for the Higgs boson production and delivered more than 15 million simulated events performing simulations with PowhegBox/HJJ model+MINLO [17, 18]. These studies are important for the determination of the Higgs boson properties and experimental searches for the process of vector boson fusion with H→4l decay.

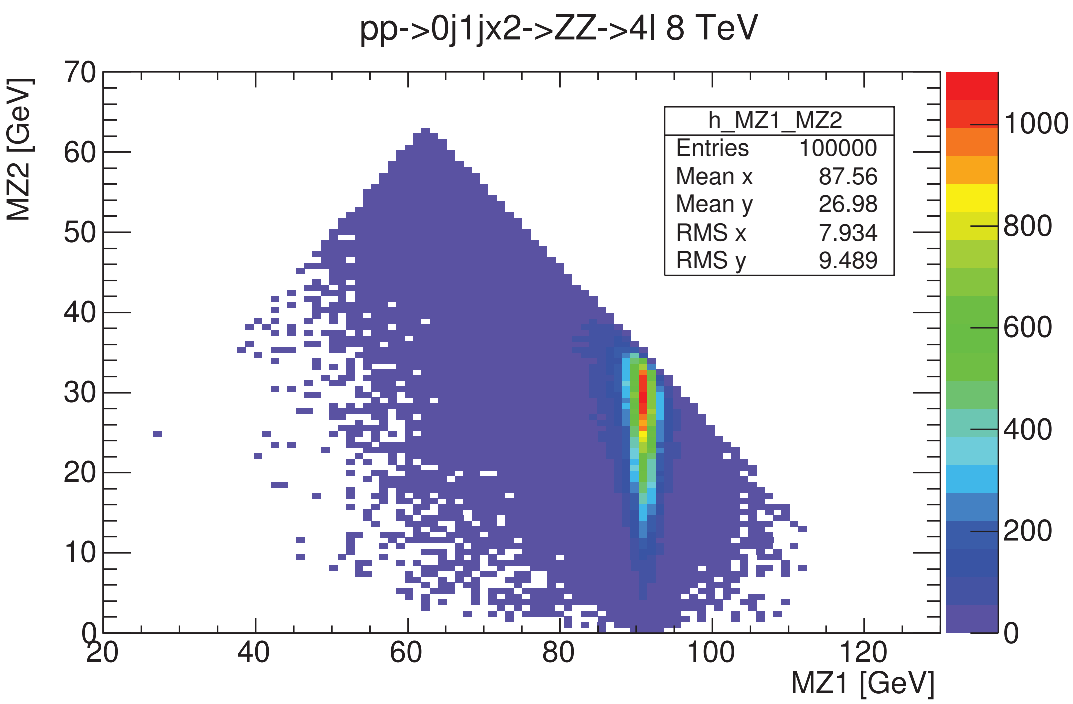

Figure 2. Invariant mass distribution of Z-bosons in the pp→H→ZZ→4l process.See description in the text.

We also implemented the integration with the new ATLAS production system (ProdSys 2) developed for management of ATLAS Monte-Carlo production during LHC run 2. The production task can be defined for Titan by the ATLAS production manager and PanDA jobs will be directed to Titan along with coordinated movement of input and output data from and to ATLAS Grid. At the time of writing a validation sample of ATLAS production Geant simulation is being generated on Titan. Figure 3 shows a monitoring plot with a number of completed ATLAS jobs on Titan since May 1, 2015. More than a hundred thousand ATLAS jobs were completed on Titan since the integration with PanDA was completed, delivering more than a million core-hours to the experiment.

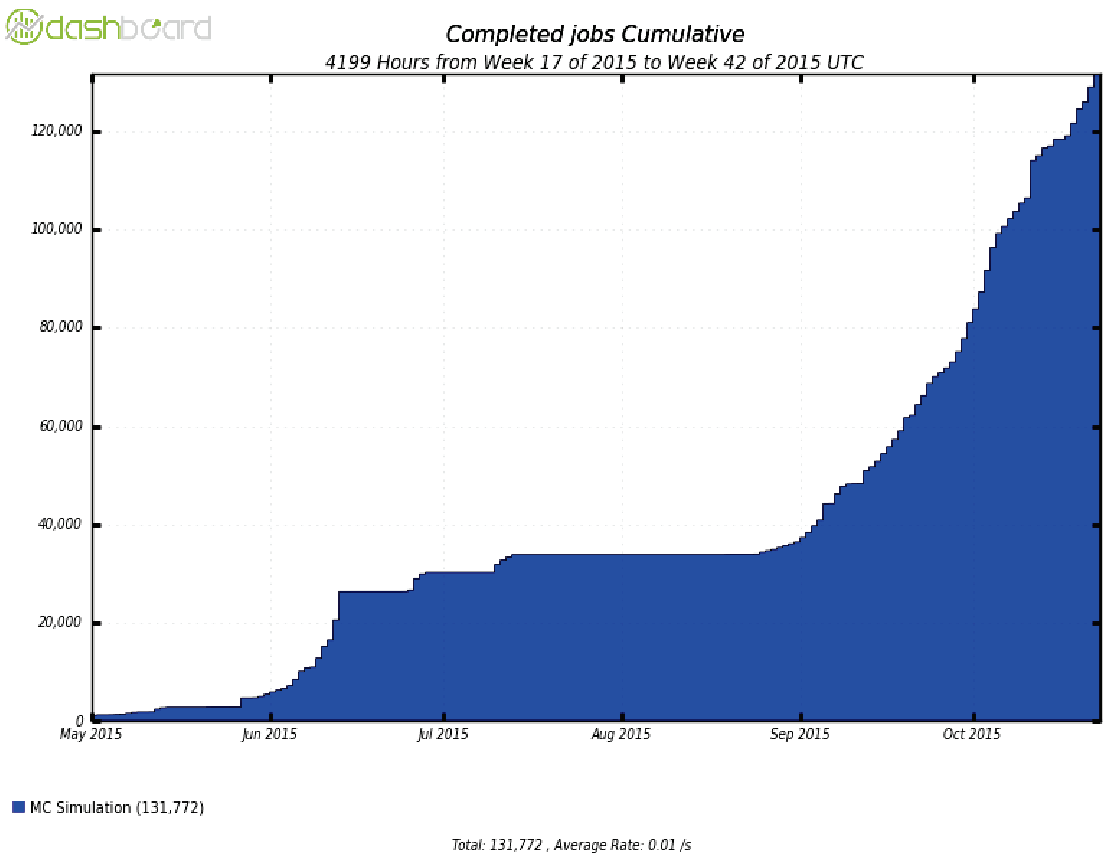

Figure 3. Cumulative plot of the number of completed ATLAS production jobs on Titan. See description in the text.

6. Extentions beyond ATLAS and Titan

It was important to demonstrate that new PanDA capabilities developed for Titan can be used by scientific communities outside of ATLAS as well as at other HPC facilities.

In collaboration with physicists from the Electron Ion Collider (EIC) project at BNL, we ported FairRoot [19] and EICRoot software frameworks to Titan and performed an initial validation of the code.

With colleagues from the ALICE experiment [20] at the LHC we prepared and ran Geant-based Monte Carlo simulations of the ALICE detector, which included runs with multi-threaded version of Geant4. For these tests ALICE specific MPI wrapper were developed and jobs were submitted to Titan, by ALICE scientists, via PanDA server deployed on Amazon EC2 cloud.

We also demonstrated that the technology developed for Titan can be used at other supercomputing platforms. The setup was deployed on supercomputers at NERSC at LBNL and Anselm at IT4I in Ostrava, Czech Republic, both sites are used by the ATLAS Collaboration.

7. Conclusion

The LHC run 2 will pose massive computing challenges for ATLAS. With a doubling of the beam energy and luminosity as well as an increased need for simulated data, the data volume is expected to increase by a factor 5-6 or more. Storing and processing this amount of data is a challenge that cannot be resolved with the currently existing computing resources in ATLAS. To resolve this challenge, ATLAS is exploring use of supercomputers and HPC clusters via the PanDA system. In this paper we described a project aimed at integration of PanDA WMS with Titan supercomputer at Oak Ridge Leadership Computing Facility. The current approach utilizes modified PanDA pilot framework for job submission to Titan's batch queues and local data management, with light-weight MPI wrappers to run single threaded workloads in parallel on Titan's multi-core worker nodes. It also gives PanDA new capability to collect, in real time, information about unused worker nodes on Titan, which allows us to precisely define the size and duration of jobs submitted to Titan according to available free resources. This capability significantly reduces PanDA job wait time while improving Titan's utilization efficiency. Also the work underway is enabling the use of PanDA by new scientific collaborations and communities as a means of leveraging extreme scale computing resources with a low barrier of entry. The technology base provided by the PanDA system will enhance the usage of a variety of high-performance computing resources available to basic research.

8. Acknowledgment

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