Beyond ATLAS: A Scalable Workload Management System For Data Intensive Science

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On behalf of ATLAS Collaboration

March 28, 2014
ISGC 2014 talks

- T.Maeno : PanDA’s Role in ATLAS Computing Evolution (Thu Mar 27th; Physics & Engineering Applications(I))
- K.De : Integrating Network Awareness in ATLAS Distributed Computing (Fri Mar 28th; Physics & Engineering Applications(III))
- J.Schovancova : The New Generation of the ATLAS PanDA Monitoring System (Fri Mar 28th; Physics & Engineering Applications(III))
- P.Nilsson : Extending ATLAS Computing to Commercial Clouds and Supercomputers (Fri Mar 28th; Highly Distributed Computing Systems (II))

PanDA Beyond ATLAS : A Scalable Workload Management System For Data Intensive Science
Enter a New Era in Fundamental Science

The Large Hadron Collider (LHC), one of the largest and truly global scientific projects ever built, is the most exciting turning point in particle physics.

Exploration of a new energy frontier
Proton-proton and Heavy Ion collisions at $E_{CM}$ up to 14 TeV
Proton-Proton Collisions at the LHC

LHC delivered billions of collision events to the experiments from proton-proton and proton-lead collisions in the Run 1 period (2009-2013)

→ collisions every 50 ns
  = 20 MHz crossing rate

- $1.6 \times 10^{11}$ protons per bunch
  at $L_{pk} \sim 0.8 \times 10^{34}/cm^2/s$
  $\approx 35$ pp interactions per crossing – pile-up
→ $\approx 10^9$ pp interactions per second !!!

- in each collision
  $\approx 1600$ charged particles produced

**enormous challenge for the detectors and for data collection/storage/analysis**

Raw data rate from LHC detector : 1PB/s
This translates to Petabytes of data recorded world-wide (Grid)

The challenge how to process and analyze the data and produce timely physics results was substantial, but at the end resulted in a great success
Our Task

We use experiments to inquire about what “reality” (nature) does.

The goal is to understand in the most general; that’s usually also the simplest.

- A. Eddington

ATLAS Physics Goals

- Explore high energy frontier of particle physics
- Search for new physics
  - Higgs boson and its properties
  - Physics beyond Standard Model – SUSY, Dark Matter, extra dimensions, Dark Energy, etc
- Precision measurements of Standard Model parameters
ATLAS Experiment at CERN

- A Thoroidal LHC Apparatus is one of the six particle detectors experiments at Large Hadron Collider (LHC) at CERN
- One of two multi-purpose detectors
- The project involves more than 3000 scientists and engineers from 38 countries
- ATLAS has 44 meters long and 25 meters in diameter, weighs about 7,000 tons. It is about half as big as the Notre Dame Cathedral in Paris and weighs the same as the Eiffel Tower or a hundred 747 jets
Introduction

- ATLAS computational resources are managed by PanDA Workload Management System (WMS)
- PanDA project was started in fall of 2005 by BNL and UTA groups
  - Production and Data Analysis system
  - An automated yet flexible workload management system which can optimally make distributed resources accessible to all users
- Through PanDA, physicists see a single computing facility that is used to run all data processing for the experiment, even though data centers are physically scattered all over the world.
  - PanDA is flexible
    - Insulates physicists from hardware, middleware and complexities of underlying systems
    - In adapting to evolving hardware and network configuration
- Major groups of PanDA jobs
  - Central computing tasks are automatically scheduled and executed
  - Physics groups production tasks, carried out by group of physicists of varying size are also processed by PanDA
  - User analysis tasks
- Now successfully manages $O(10^2)$ sites, $O(10^5)$ cores, $O(10^8)$ jobs per year, $O(10^3)$ users
Up to 12M jobs completed every month
Running at 100,000 cores worldwide
Consuming at peak ~0.2 petaflops
Available resources are fully used.

Completed jobs
217 Weeks from Week 00 of 2010 to Week 08 of 2014

Analysis
MC
Physics Groups
Data (re)Processing

User Analysis
Others
MC Simulation
MC Simulation (XP)
MC Reconstruction
Group Production
Unknown
T0 Processing
Validation
MC Production

Maximum: 12,070,624, Minimum: 0.00, Average: 8,071,938, Current: 651,245

3/28/14
ISGC 2014

8
ATLAS Computing Challenges

- **A lot of data in a highly distributed environment.**
  - Petabytes of data to be treated and analyzed
  - ATLAS Detector generates about 1PB of raw data per second – most filtered out in real time by the trigger system
  - Interesting events are recorded for further reconstruction and analysis
  - As of 2013 ATLAS manages ~140 PB of data, distributed world-wide to O(100) computing centers and analyzed by O(1000) physicists
  - Expected rate of data influx into ATLAS Grid ~40 PB of data per year in 2015

- **Very large international collaboration**
  - 174 Institutes and Universities from 38 countries
  - Thousands of physicists analyze the data

ATLAS uses grid computing paradigm to organize distributed resources
A few years ago ATLAS started Cloud Computing RnD project to explore virtualization and clouds
  - Experience with different cloud platforms: Commercial (Amazon, Google), Academic, National
Now we are evaluating how high-performance and super-computers can be used for data processing and analysis
150 million sensors deliver data ...
ATLAS is Truly BigData Science

Business e-mails sent per year
3000 PBytes

Current ATLAS managed data volume: 140 PB
1M files transferred per day
Annual data volume ~30PB

Big Data in 2013

Content Uploaded to Facebook each year.
182 PBytes

Library of congress

Climate

LHC Annual
15 PBytes

Google search index
98 PBytes

Nasdaq

US census

Youtube
15 PBytes

Health Records
30 PBytes

http://www.wired.com/magazine/2013/04/bigdata
PanDA’s Success in ATLAS

- PanDA proved highly scalable and successful for ATLAS. The system was able to cope with increasing LHC luminosity and data taking rate. Adapted to evolution in ATLAS computing model.
  - Success in ATLAS has sparked interest among other communities
  - Any organization with large data volumes, distributed resources and a large user base can benefit from PanDA WMS

PanDA was cited in the document titled “Fact sheet: Big Data across the Federal Government” prepared by the Executive Office of the President of the United States as an example of successful technology already in place at the time of the “Big Data Research and Development Initiative” announcement

During past year new PanDA collaborators, and new sources of funding have led to the question – what is the future of PanDA?
Evolving PanDA for Advanced Scientific Computing

- Proposal titled “Next Generation Workload Management and Analysis System for BigData” – Big PanDA was submitted to ASCR DoE in April 2012.
- DoE ASCR and HEP funded project started in Sep 2012.
  - Generalization of PanDA as meta application, providing location transparency of processing and data management, for HEP and other data-intensive sciences, and a wider exascale community.
    - Other efforts
      - PanDA: US ATLAS funded project
      - Networking: Advance Network Services

- There are three dimensions to evolution of PanDA
  - Making PanDA available beyond ATLAS and High Energy Physics
  - Extending beyond Grid (Leadership Computing Facilities, Clouds, University clusters)
  - Integration of network as a resource in workload management
BigPanDA work plan

• **Factorizing the code**
  – Factorizing the core components of PanDA to enable adoption by a wide range of exascale scientific communities

• **Extending the scope**
  – Evolving PanDA to support extreme scale computing clouds and Leadership Computing Facilities

• **Leveraging intelligent networks**
  – Integrating network services and real-time data access to the PanDA workflow

• **3 years plan**
  – Year 1. Setting the collaboration, define algorithms and metrics
  – **Year 2.** Prototyping and implementation
  – Year 3. Production and operations
BigPanDA : factorizing the Core

- **PanDA server.**
  - Tarball made from SVN branch. VO specific modules are in the same package
    - Planned
      - Tag + RPM
      - Split core and experiment specific packages

- **PanDA pilot.**
  - Core pilot has refactored to a generic (VO independent) version;
  - VO specifics are handled as plug-ins

- **Database backend**
  - Oracle database backend (ATLAS, AMS)
  - mySQL (running on EC2 PanDA server) – LSST, NICA

- **PanDA monitoring.**
  - Refactored to ensure modularity. RPMs

- **New SVN structure**
  - Pilot
  - Monitoring

- **RPMs**
  - Need to standardize for the components of a PanDA instance
    - Using python distutils
      - Currently manual build and SVN tagging
Compute Engine (GCE) preview project

- Google allocated additional resources for ATLAS for free
  - ~5M cpu hours, 4000 cores for about 2 month, (original preview allocation 1k cores)
- Resources are organized as HTCondor based PanDA queue
  - Centos 6 based custom built images, with SL5 compatibility libraries to run ATLAS software
  - Condor head node, proxies are at BNL
  - Output exported to BNL SE
- Work on capturing the GCE setup in Puppet
  - Transparent inclusion of cloud resources into ATLAS Grid
  - The idea was to test long term stability while running a cloud cluster similar in size to Tier 2 site in ATLAS
  - Intended for CPU intensive Monte-Carlo simulation workloads
  - Planned as a production type of run. Delivered to ATLAS as a resource and not as an R&D platform.
- We also tested high performance PROOF based analysis cluster
Running PanDA on Google Compute Engine

- We ran for about 8 weeks (2 weeks were planned for scaling up)
- Very stable running on the Cloud side. GCE was rock solid.
- Most problems that we had were on the ATLAS side.
- We ran computationally intensive jobs
  - Physics event generators, Fast detector simulation, Full detector simulation
- Completed 458,000 jobs, generated and processed about 214 M

Failed and Finished Jobs reached throughput of 15K jobs per day
most of job failures occurred during start up and scale up phase
• Expanding PanDA from Grid to Leadership Class Facilities (LCF) will require significant changes in our system

• Each LCF is unique
  – Unique architecture and hardware
  – Specialized OS, “weak” worker nodes, limited memory per WN
  – Code cross-compilation is typically required
  – Unique job submission systems
  – Unique security environment

• Pilot submission to a worker node is typically not feasible

• Pilot/agent per supercomputer or queue model

• Initial tests on BlueGene at BNL and ANL. Geant4 port to BG/P

• BigPanDA project at Oak Ridge National Laboratory LCF Titan
## Leadership Computing Facilities. Titan

### Titan System (Cray XK7)

<table>
<thead>
<tr>
<th>Feature</th>
<th>Specification</th>
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<tr>
<td>Peak Performance</td>
<td>27.1 PF, 18,688 compute nodes</td>
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<tr>
<td>System memory</td>
<td>710 TB total memory</td>
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<tr>
<td>Interconnect</td>
<td>Gemini High Speed Interconnect, 3D Torus</td>
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<td>Storage</td>
<td>Lustre Filesystem, 32 PB</td>
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<td>Archive</td>
<td>High-Performance Storage System (HPSS), 29 PB</td>
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<tr>
<td>I/O Nodes</td>
<td>512 Service and I/O nodes</td>
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Slide from Ken Read
BigPanDA at ORNL LCF (Titan). Motivation

PanDA Backfill

- PanDA has potential to generate 300 M Titan hours in 2014 and again in 2015. Estimated to represent between $10 M to $15 M per year worth of computing.
- Jobs are naturally parallel (no longer embarrassed!) and can be short. Can backfill arbitrary amount of Titan queue.
- Exploring whether PanDA pilot can receive more extensive information concerning schedule than available via “qstat”.
- Multiple “payloads” now at varying stages of functionality. “Payloads” need VALIDATION of performance and correctness.
- Testing possibility of remotely-compiled binaries running with associated shared libraries provided by CERN Virtual Machine Filesystem (CVMFS), presumably only appropriate for backfill jobs. This can greatly reduce the effort for validation. Need to check possible performance penalties and scaling.
- Question: ATLAS code validation? Timescale?

From Ken Read

3/28/14
• Full PanDA workflow has been implemented on Titan
• Native PanDA pilot runs on Titan interactive nodes
  – Pilot collects information about available resources for backfill
  – SAGA framework is used as a local interface to Titan batch system
• Opportunistic job backfill on Titan has been implemented
  – Pilot queries jobs scheduling and management system about unused resources MOAB)
  – MOAB returns a number of unscheduled nodes and validity interval
  – Pilot chooses the largest available block and submits jobs, taking into account Titan’s scheduling policy limitations
Initial backfill runs on Titan

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<th>Walltime limit</th>
<th>Runtime</th>
<th>State</th>
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<td>96</td>
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Indefinitely available nodes

Nodes available for backfill on Titan (unlimited)

Nodes available for backfill on Titan (limited)

Availability time estimate
Adding Network Awareness to PanDA

- **Goal for PanDA**
  - Direct integration of networking with PanDA workflow – never attempted before for large scale automated WMS systems

- **Why PanDA and networking**
  - PanDA is a distributed computing workload management system
  - Data transfer/access is done asynchronously: by DQ2 in ATLAS, PhEDEx in CMS, pandamover/FAX for special cases…
    - Data transfer/access systems can provide first level of network optimizations – PanDA will use these enhancements as available
  - PanDA relies on networking for workload data transfer/access
    - Can integrate network at high level – directly in workflow management
    - Networking is assumed in PanDA – not integrated in workflow

- **Main PanDA use cases**
  - Use network information for cloud selection
  - Use network information for job assignment
  - Use network information for site selection
Adding Network Awareness to PanDA

- LHC Computing model for a decade was based on MONARC model
  - Assumes poor networking
    - Connections are seen as not sufficient or reliable
      - Data needs to be preplaced. Data comes from specific places
  - Hierarchy of functionality and capability
    - Sites have specific functions
    - Nothing can happen utilizing remote resources on the time of running job
  - Canonical HEP strategy: “Jobs go to data”
    - Data are partitioned between sites
      - Some sites are more important (get more important data) than others
      - Planned replicas
        - A dataset (collection of files produced under the same conditions and the same SW) is a unit of replication
    - Data and replica catalogs are needed to broker jobs
    - Analysis job requires data from several sites triggers data replication and consolidation at one site or job splitting on several jobs running on all sites
      - A data analysis job must wait for all its data to be present at the site
    - The situation can easily degrade into a complex n-to-m matching problem
  - There was no need to consider network as a resource in WMS in static data distribution scenario

- New networking capabilities and initiatives in the last 2 years (like LHCONE)
  - Extensive standardized monitoring from network performance monitoring
  - Traffic engineering capabilities
    - Rerouting of high impact flows onto separate infrastructure

...and dramatic changes in computing models
  - From strict hierarchy of connections becomes more of a mesh
  - Data access over wide area
  - “no division” in functionality between sites

We would like to benefit from new networking capabilities and to integrate networking services with PanDA. We start to consider network as a resource on similar way as for CPUs and data storage
Intelligent Network Services and PanDA

- In BigPanDA we will use information on how much bandwidth is available and can be reserved before data movement will be initiated.

- In Task Definition user will specify data volume to be transferred and deadline by which task should be completed. The calculations of (i) how much bandwidth to reserve, (ii) when to reserve, and (iii) along what path to reserve will be carried out by Virtual Network On Demand (VNOD).

Measurement sources:
- Sonar
- PerfSonar
- XRootD

Site Status Board:
- Raw data, historical data

Grid Information System:
- Averaged network data for atlas sites

SchedConfigDB:
- Averaged network data for panda sites

Brokerage:
- Site selection module

PanDA
### Site Status Board: Data Injection and Monitoring

**Show** 200 entries

<table>
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<tr>
<th>Site Name</th>
<th>SrcSite</th>
<th>SrcCloud</th>
<th>SrcTier</th>
<th>DstSite</th>
<th>DstCloud</th>
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*Image by Alexei Klimentov, BNL/PAS*
# Network Performance Measurements

## DDM Sonar

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<th>AvgBRS (MB/s)</th>
<th>EvS</th>
<th>AvgERM (MB/s)</th>
<th>EvM</th>
<th>AvgBRL (MB/s)</th>
<th>EvL</th>
<th>MinThr (MB/s)</th>
<th>AvgThr (MB/s)</th>
<th>MaxThr (MB/s)</th>
<th>MinPL</th>
<th>AvgPL</th>
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| SSB: [http://dashb-atlas-ssb.cern.ch/dashboard/request.py/siteview#currentView=Sonar&highlight=false](http://dashb-atlas-ssb.cern.ch/dashboard/request.py/siteview#currentView=Sonar&highlight=false) |

3/28/2014

ISGC 2014

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The Growing PanDA Ecosystem

- **ATLAS PanDA**
  - US ATLAS, CERN, UK, DE, RF, ND, CA, Dubna, OSG …

- **ASCR BigPanDA**
  - DoE funded project at BNL, UTA – 3 years

- **ANSE PanDA**
  - US NSF funded network project - CalTech, Michigan, Vanderbilt, UTA

- **High-Performance Computing and Cloud PanDA**

- **Taiwan PanDA – not only AMS**

- **LSST PanDA**

- **AliEn PanDA**

- **MegaPanDA**

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AlieEn – ALICE analysis and Production framework
AMS - Alpha-Magnetic Spectrometer experiment
ANSE – Advanced Network Services (for LHC)
ASCR – Advanced Scientific Computing
LSST – Large Survey Synoptic Telescope
OSG – Open Science Grid
BigPanDA is all of the above – it is the evolution of PanDA, not just PanDA for BigData!