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PanDA for ATLAS Distributed Computing in the Next Decade

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Introduction

- PanDA = Production and Distributed Analysis System
  - Designed to meet ATLAS production/analysis requirements for a data-driven workload management system capable of operating at LHC data processing scale
  - Performed well for ATLAS in the last decade including the LHC data taking period
- Many new components and features have been delivered to ATLAS before LHC Run2
  - DEFT, JEDI, Dynamic job definition, event service, new monitoring, and so on
- The system has revealed great improvements in LHC Run2 but still has issues to be addressed

Issues

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- ➢ Inefficiency due to old resource partitioning based on geographical grouping of computing centers
- ➢ Suboptimal usages of non-traditional resources due to job-based workload management
- ➢ Incoherent implementations for various HPC workflows
- ➢ Overstretched architecture of the pilot to support non-traditional resources
- ➢ To leverage prediction capabilities for resource availability actively developed with recent computing technologies like machine learning
- ➢ Operational difficulties with new workflows due to job-centric visualization

System Evolution

Resource Consolidation

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- Old MONARC hierarchical model
  - Tier1 + Tier2 centers: 10 Tier1 centers → 10 partitions
  - Rather static combination between Tier1 and Tier2 centers based on geographical grouping
  - Problematic when small partitions got high priority tasks → Complicated workload brokerage
- New model with no hierarchy
  - A single resource partition
  - Two new concepts
    - Nucleus : destination of output data
    - Satellite : processing jobs to produce output data
  - Formation of sub-partition (nucleus+satellites) based on static configuration and dynamic information on network quality between nuclei and satellites
  - Reliable Tier2 centers as nuclei in addition to Tier1 centers
- Details in CHEP16 talk

  F. H. Barreiro Megino : ATLAS World-cloud and networking in PanDA

Intelligent Brokerage

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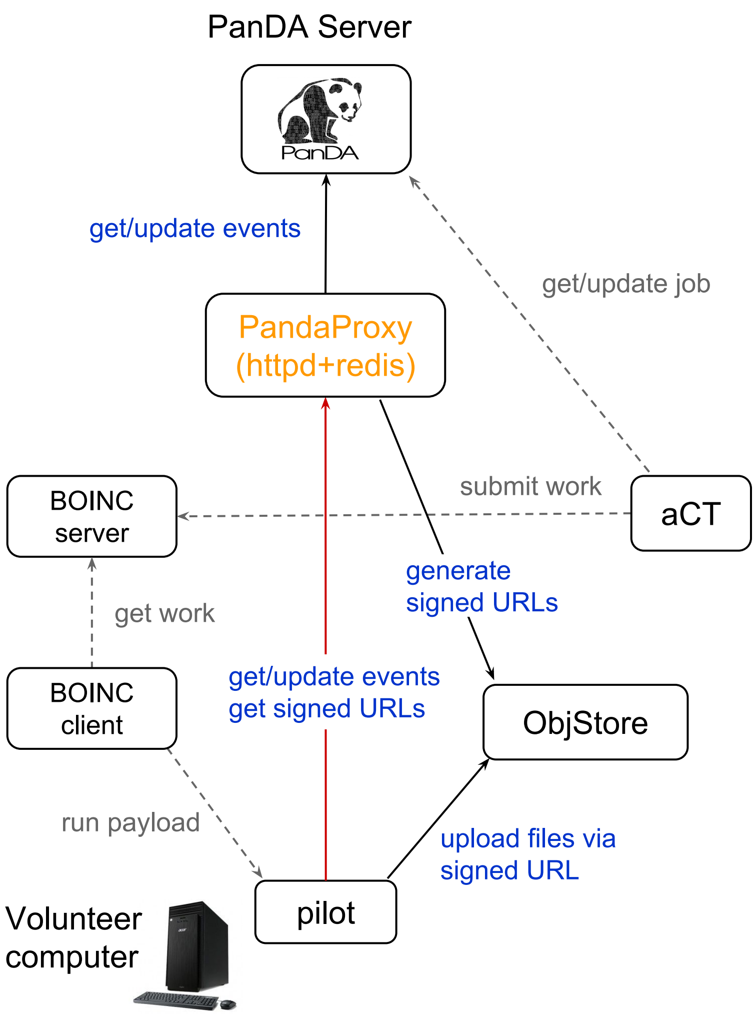
- More intelligence to the brokerage based on
  - Job retry history
  - Network forecast
  - Cache hit rate
- Adding a new capability for workload provisioning
  - Passive workload assignment
    - Assigning jobs to resources once they become active
    - Good for traditional resources as a steady number of CPUs is usually available there except short disruptions
    - Latency too high for non-traditional resources like the ATLAS HLT farm as the number of available CPUs tends to ramp up and down immediately
  - Proactive workload assignment
    - Assigning jobs just before resources become available
    - Removing jobs just after resources become unavailable
    - Based on (quasi) real-time resource information
  - Workload assignment could trigger input data transfers
    - Should be smart enough for proactive assignment to minimize redundant data transfers

In-House Security

- To authenticate requests from the pilot running on special environment where standard X509-based auth is unavailable and/or suboptimal



- Using an internal secret token
  - Generated by the PanDA server per job or pilot scheduler to be kept in redis
  - Propagated to the pilot via job specification or VM contextualization
  - Sent to PandaProxy together with normal pilot requests for verification
- Use-cases
  - Volunteer computing
  - Off-grid
  - Commercial clouds with rapid spin-up

PanDA at HPC Centers

- Titan at OLCF
  - 18,688 nodes: 16 CPU cores
  - MPI jobs with multiple PanDA jobs
  - Data transfers with the DTN scheduler or pilot movers
  - Steady operations for continuous PanDA production job submission in backfill mode
    - 10k jobs per day on average (18k at peak)
  - Details in CHEP16 talk

    S. Panitkin : Integration of the Titan supercomputer at OLCF with the ATLAS Production System

- SuperMUC at LRZ
  - 3072 nodes: 28 CPU cores
  - MPI jobs with Event Service + ARC CE
  - Data transfers with ARC
  - Changed from short jobs to Event Service jobs due to frequent preemption

NERSC

- Edison/Cori at NERSC
  - 9,304 nodes: 68 CPU cores
  - MPI jobs with Event Service
  - Data transfers with 3rd party service or pilot movers
  - Low CPU efficiency to be addressed
  - Commonalities for coming Theta and Aurora at ALCF

- HPC2 at NRC-KI
  - 2560 nodes: 4 CPU cores
  - non-HEP : Next Generation Genome Sequencing (NGS)
  - No data transfers
  - Details in CHEP16 talk

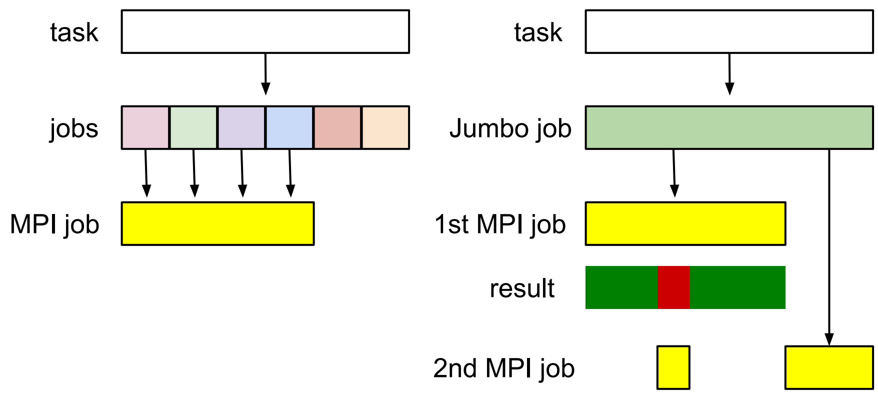
    A. Klimentov, R. Mashinistov : Using HEP Computing Tools, Grid and Supercomputers for Genome Sequencing Studies

- Many other HPCs ...

Enhancement of Event Service

- Fine grained (event-level) workload partitioning
  - Allowing jobs to be revoked in the middle of processing with minimized losses
- The old implementation assumed a modest number of events per job (~1k)
  - Good for preemptable resources
    - Dynamic fragmentation of jobs
  - Not good for large HPC resources
    - Preference for a large number of events in one go
    - Combination of multiple jobs to a single MPI job
      → Complicated workload management and bookkeeping

- New feature : Jumbo jobs allowing workloads to be tailored to any sizes of MPI jobs
- CHEP16 talk for Event Service
  T. Wenaus, V. Tsulaia : Production Experience with the ATLAS Event Service



Monitoring Evolution

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- Rise of data visualization such as plots, histograms, and task chain diagrams
- Adding predictive analytics for the expected task completion time and comparison with actual task computation progress
- Intensive use of Redis cache and page preloading to improve user experiences
- Quick access to the data in external monitoring systems: Kibana, Agis, Rucio, dashboard
- Current development activities
  - Oracle side data aggregation
    - Supports for free search queries is mandatory in monitoring
    - On-demand data aggregation triggered by a typical query takes minutes to process 6 months historical data with 2M jobs per day
    - Data aggregation on Oracle server side with an advanced data layout strategy successfully demonstrated to reduce the query processing time from ~1 min (30k jobs limit, last 12 hours jobs) to ~10 sec (without limit, for last 12 hours = ~800k jobs)
  - SSO, VOMS, IGTF authentication
    - To introduce an information access control layer
    - Ability to execute commands directly from monitoring pages
    - Future implementation of user-centric contents

Pilot 2.0

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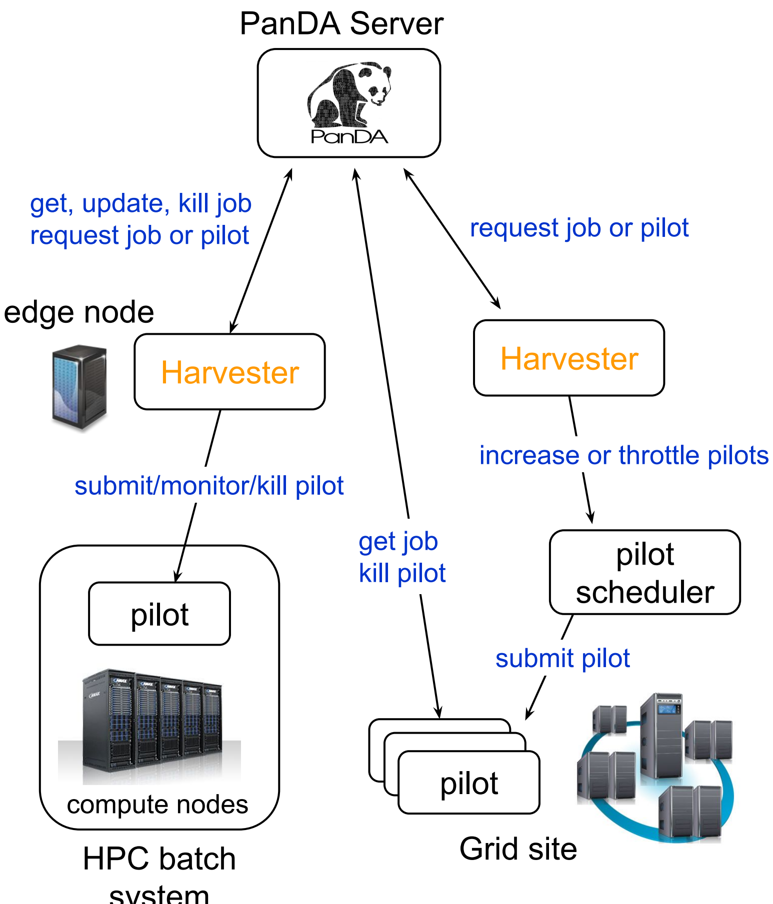
- New PanDA Pilot Project launched in April 2016
  - Maintenance difficulties of aged PanDA Pilot
  - Overstretched architecture due to new features and workflows
  - Long-term project to span the next couple of years
  - An almost complete rewrite except some recent developments
  - Involvement of developers both within core PanDA and BigPanDA teams as well as from external teams
- Currently the project is in the design stage
  - Development for a MiniPilot system
    - A fully working pilot script for developers to test new components
    - Future evolution into a SimplePilot to new PanDA users for a rapid introduction
  - Git-based testing framework
    - A pull request into the Pilot Git repository to trigger a verification sequence including unit tests
  - Test implementations of the component model being evaluated with all workflows

Harvester

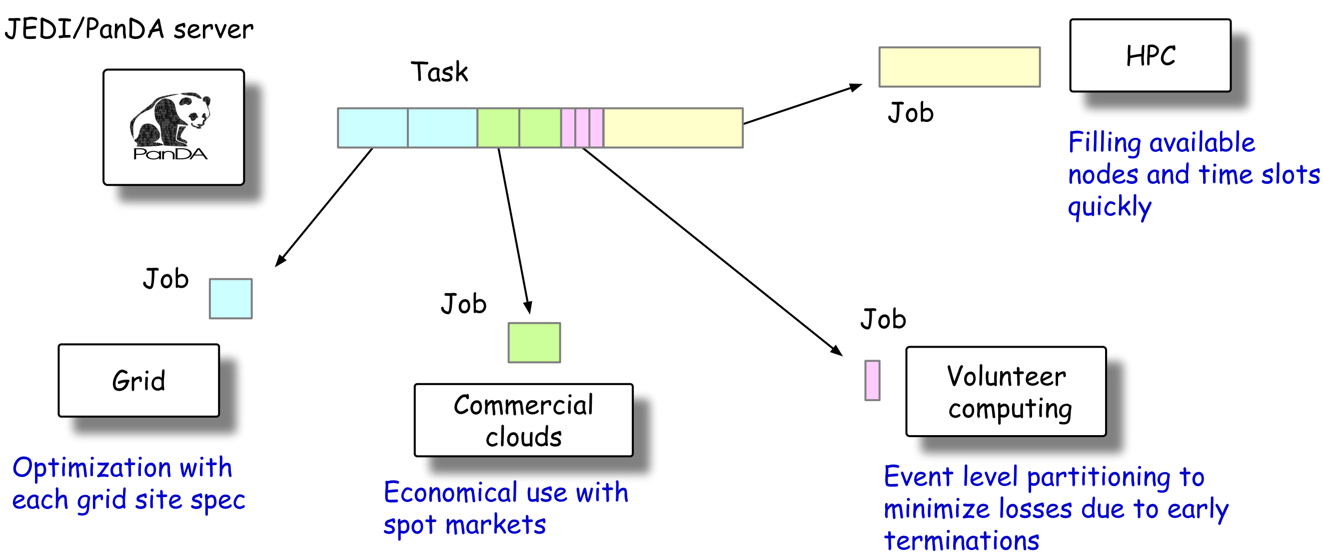
- A resource-facing service between PanDA server and collection of pilots
  - Propagating information or requests between PanDA server and resource managers such as batch systems and pilot schedulers



- Objectives
  - To add a capability for timely optimization of CPU allocation among various resource types
  - To provide a commonality layer in bringing coherence to HPC implementations
  - To have better integration between PanDA system and resources for new workflows
- Developments actively in progress with wider collaboration
  - First prototype for NERSC/Titan after CHEP

Future Plans

- Proactive control of the network to optimize workflows and dataflows
- New components in production
- Automation of the system based on prediction for resource availability and the expected completion time for each task
- More efficient and economical use of traditional and new computing resources



Summary

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- PanDA has performed well for ATLAS in the last decade including the LHC Run 1 and Run2 data taking periods
- New components and features have been delivered to ATLAS
- Many developments and challenges to come while steadily running for LHC Run 2

Highlights

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- PanDA has performed well for ATLAS in the last decade including the LHC Run 1 and Run2 data taking periods
- New components and features have been delivered to ATLAS
  - Resource consolidation
  - Intelligent brokerage
  - In-House security
  - PanDA on HPCs
  - Enhancement of event service
  - Monitoring evolution
- Many developments and challenges to come while steadily running for LHC Run 2
  - Pilot 2.0
  - Harvester
  - Network provisioning
  - Automation based on prediction capabilities
  - More optimal use of computing resources