Integration of PanDA workload management system with Titan supercomputer at OLCF

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Outline

- Introduction and motivation
- PanDA workload management system (WMS)
- PanDA architecture for Titan
- PanDA Pilot with backfill capability
- MPI wrapper
- Workloads
- Summary

ATLAS and Supercomputers

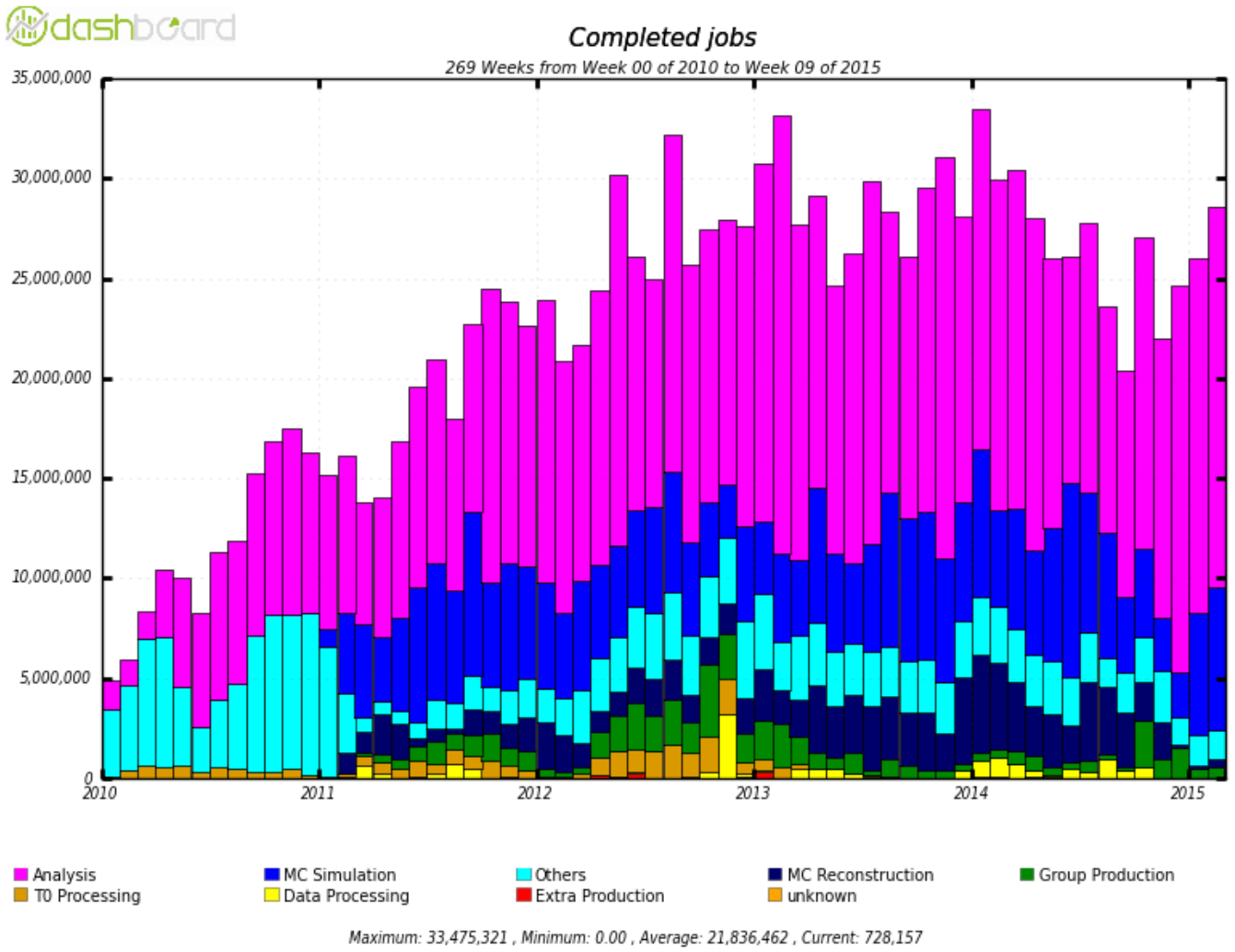
- Current pace of research and discovery is limited by ability of the ATLAS computing Grid to generate Monte-Carlo events - ”Grid luminosity limit”
  - Currently O(100k) cores available to ATLAS worldwide, ¾ dedicated to MC production.
  - Still not enough CPU power !
  - Many physics simulation requests have to wait for many months
- Supercomputers are rich source of CPUs
- ATLAS initiated R&D project aimed at integration of supercomputing and HPC resources into ATLAS distributed computing
- DOE ASCR supported project aimed at integration of PanDA WMS with Titan supercomputer at OLCF is part of this effort

PanDA in ATLAS

- ATLAS uses PanDA Workload Management System (WMS) to run jobs on WLCG
- PanDA - **P**roduction **an**d **D**ata **A**nalysis WMS

- Goal: An automated yet flexible WMS which can optimally make distributed resources accessible to all users
  - Adopted as the ATLAS wide WMS in 2008 (first LHC data in 2009) for all computing applications
  - Currently PanDA successfully manages O(10E2) sites, O(10E5) cores, O(10E8) jobs per year, serving O(10E3) users per year
  - PanDA is exascale now: 1.2 Exabytes of data processed by PanDA in 2013

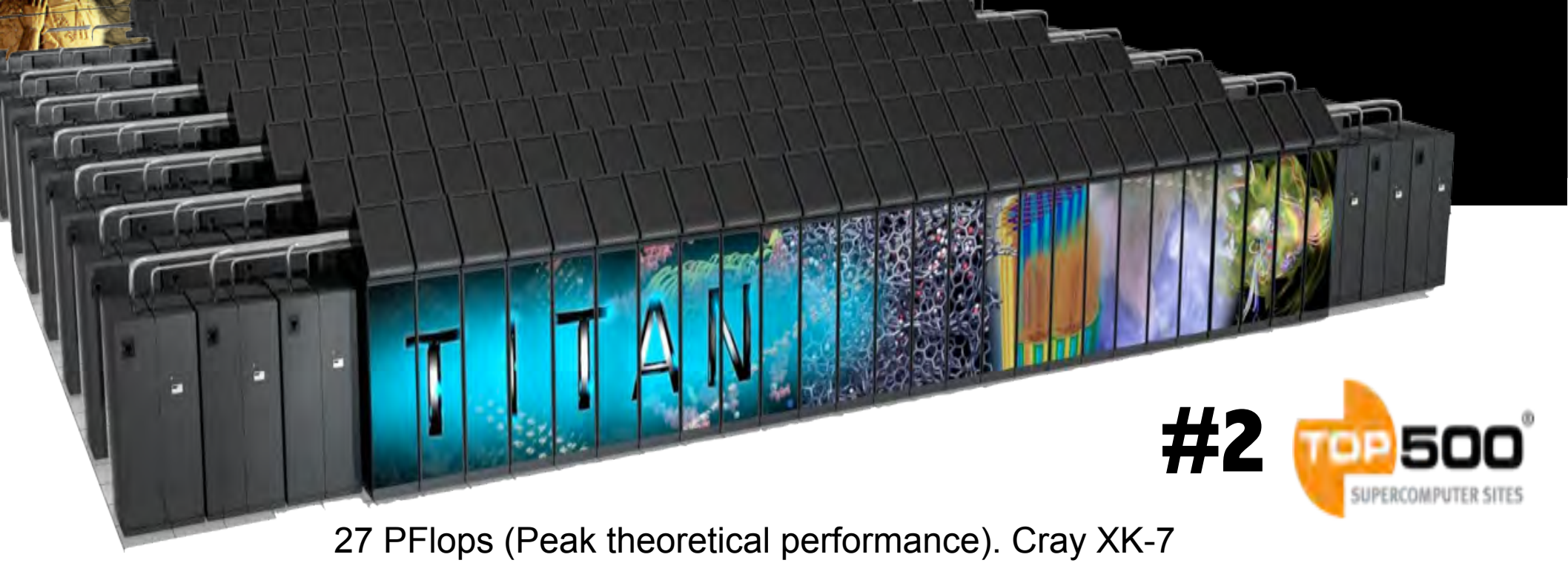
PanDA Performance



Current scale – 25M jobs completed every month at more than a hundred of sites

Key Features of PanDA

- Pilot based job execution system
  - Pilot manages job execution on local resources, as well as data movement for the job
  - Payload is sent only after pilot execution begins on CE
  - Minimize latency, reduce error rates
- Modular design
- Central job queue
  - Unified treatment of distributed resources
  - SQL DB keeps state - critical component
- Automatic error handling and recovery
- Extensive monitoring
- HTTP/S RESTful communications
- GSI authentication
- Use of Open Source components
- Workflow is maximally asynchronous



#2 TOP500 SUPERCOMPUTER SITES

27 PFlops (Peak theoretical performance). Cray XK-7
18,688 compute nodes with GPUs

299,008 CPU cores

AMD Opteron 6200 @2.2 GHz (16 cores per node)

32 GB RAM per node

NVidia TESLA K20x GPU per node

32 PB disk storage (center-wide Luster file system)

>1TB/s aggregate FS throughput

29 PB HPSS tape archive

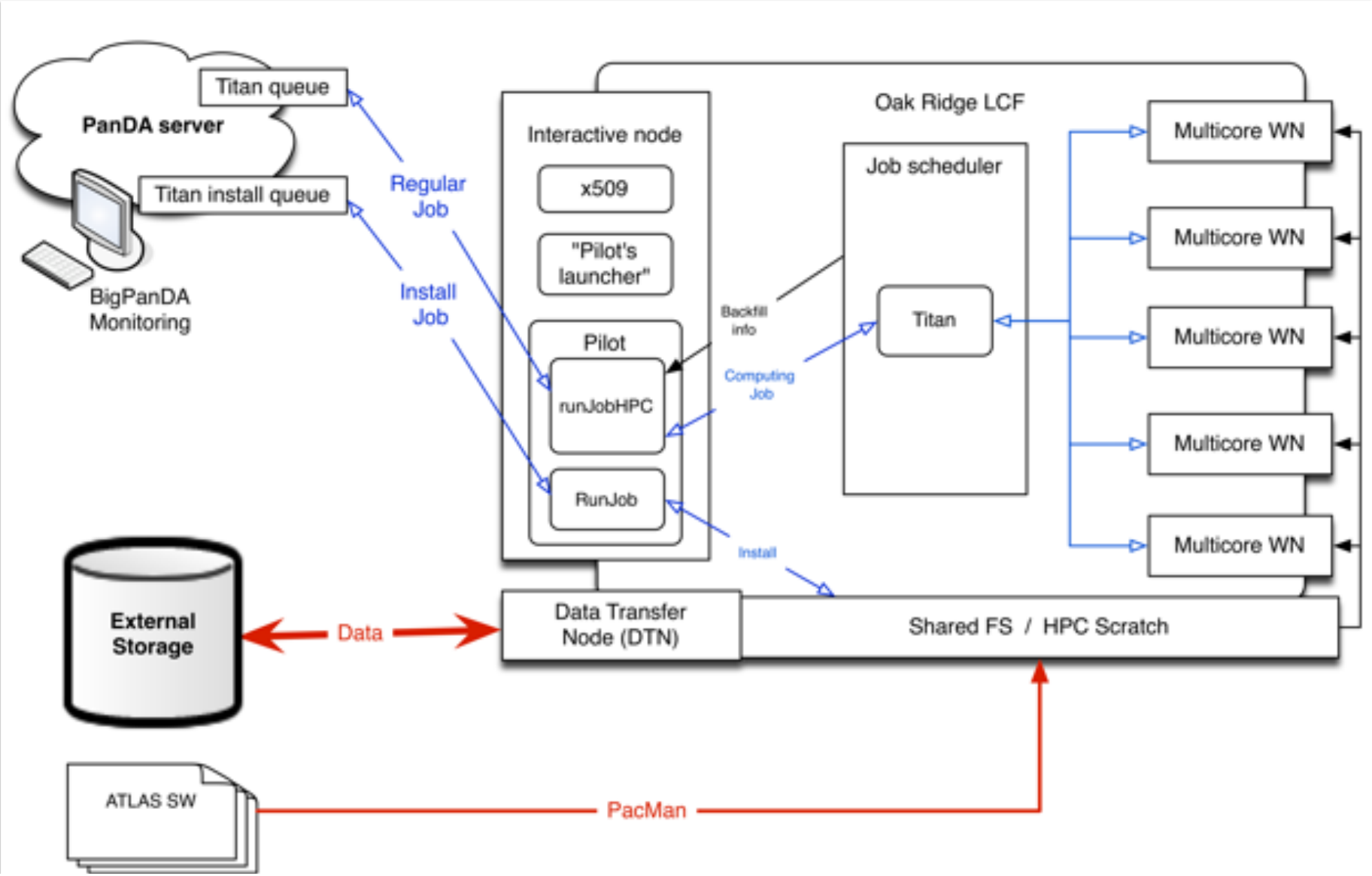
Some Titan features that affect integration with PanDA

- Highly restricted access. One-time password interactive authentication
  - No portals, gatekeepers, VO boxes. Pilot needs to run on Titan's login nodes
- No network connectivity from worker nodes to the outside world
  - Pilot can not run on worker nodes, needs a new mechanism for batch workload management
- Limit on number of submitted jobs in batch queue per user and limit on number of running jobs per user
  - Sequential submissions of single node jobs is not an option
  - Have to use MPI in some form!
- Specialized OS (SUSE based CNL) and software stack
- Highly competitive time allocation. Geared toward leadership class projects and very big jobs
  - Creates opportunity for backfill

PanDA setup on Titan

- Main idea - try to reuse existing PanDA components and workflow logic as much as possible
- Modified PanDA pilot runs on Titan's front end nodes, in user space
- All connections to PanDA servers at CERN or EC2 are initiated from the front end nodes by PanDA Pilot over HTTPS
- For local HPC batch interface use SAGA-Python (Simple API for Grid Applications) framework by Rutgers U. group
  - http://saga-project.github.io/saga-python/
  - http://www.ogf.org/documents/GFD.90.pdf
- Custom light-weight Python MPI wrapper scripts for running (single node) workloads in parallel on multiple multi-core WN
- Pilot instrumented to utilize information about free nodes on Titan
- Software is installed/ported in advance on Titan shared file system

PanDA setup on Titan



MPI wrapper for workloads

- In order to use Titan efficiently we have to use MPI
- We utilize light-weight Python MPI wrapper, specific to each workload type
- Uses mpi4py Python module
- The wrapper is launched on Titan by PanDA Pilot as MPI job of arbitrary size
- Then each wrapper instance knows its MPI rank and serves as “mini-Pilot”
  - Sets up Titan specific environment – like loading appropriate modules, environment, etc
  - Sets up workload specific environment
  - Creates working directory, copies necessary files to $PWD, creates symlinks, etc
  - Manipulates necessary input files for each rank to ensure uniqueness of every job output (random seeds, input file lists, etc)
  - Launches actual workload as sub-process and waits until it finishes
  - Performs necessary clean up of working directory or post-processing, if needed
- The wrapper allows to run simultaneously, arbitrary single-threaded or multi-threaded, non-MPI workloads on multiple multi-core worker nodes on Titan

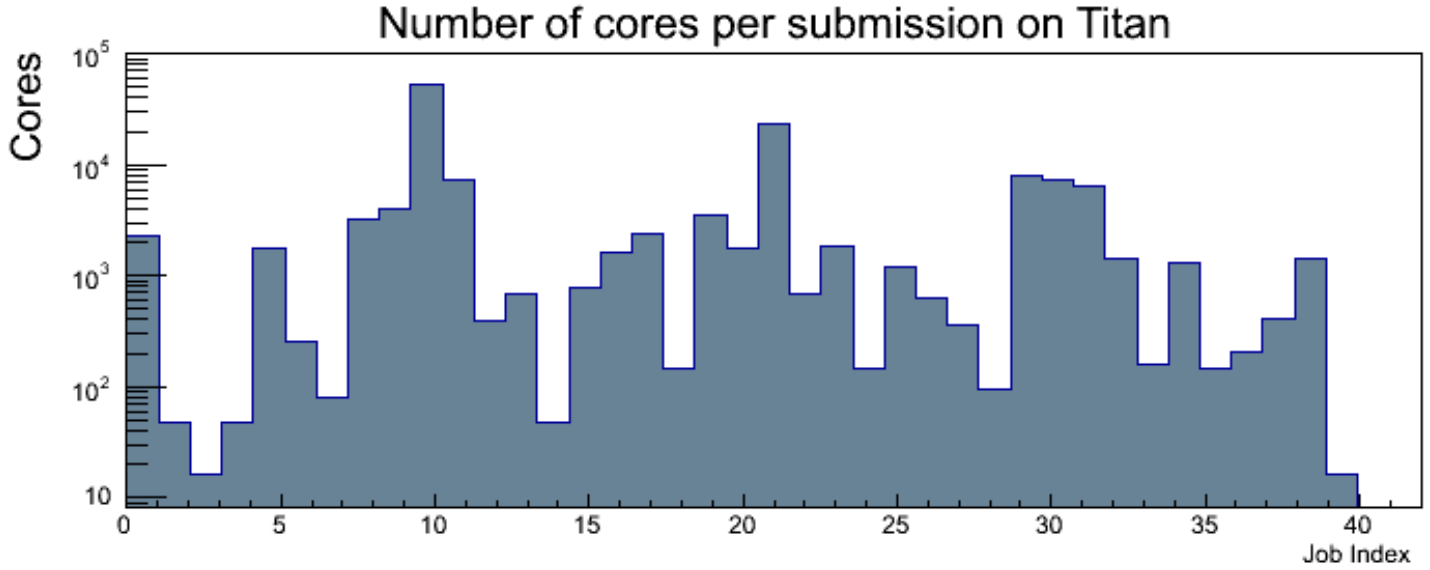
Backfill Enabled Pilot

- Typical LCF facility is ran on average at ~90% occupancy
  - On a machine of the scale of Titan that translates into ~300M unused core hours per year
- Anything that helps to improve this number is very useful
- We added to PanDA Pilot a capability to collect, in near real time, information about current free resources on Titan
  - Both number of free worker nodes and time of their availability
- Based on that information Pilot can define job submission parameters when forming PBS script for Titan, thus tailoring the submission to the available resource.
  - Takes into account Titan's scheduling policies
  - Can also take into account other limitations, such as workload output size, etc
  - Modular architecture, adaptable to other HPC facilities

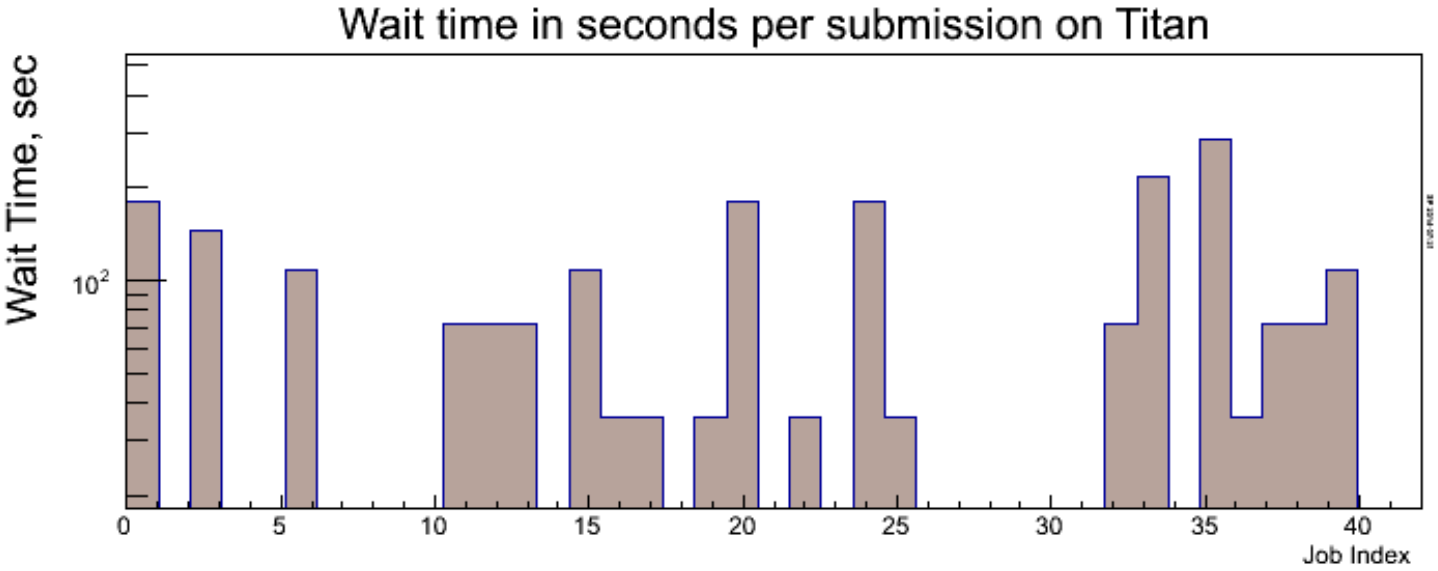
Titan Backfill tests

- We ran multiple continuous job submission tests with PanDA on Titan
- Goals for the tests
  - Test job submission chain and all system components
  - See what works, what breaks, what can be improved
  - Demonstrate that current approach provides tangible improvement in Titan's utilization.
- Through improvements in Pilot's job submission algorithm we have shown that we are able to capture significant CPU resources on Titan even with a single stream of pilots
  - In one of the tests we were able to collect ~200K core hours in 10 hours
  - Max number of nodes per job was 5835 (93360 cores)
    - Close to the entire ATLAS Grid in size!
  - Consistently short wait times for PanDA jobs. (~1min vs several hours)
  - **Used ~2.3% of all Titan core hours or ~14.4% of free core hours**

Example of PanDA test on Titan



- Backfill enabled pilot
- MPI wrapper



Average wait time
70 seconds !

Workloads on Titan

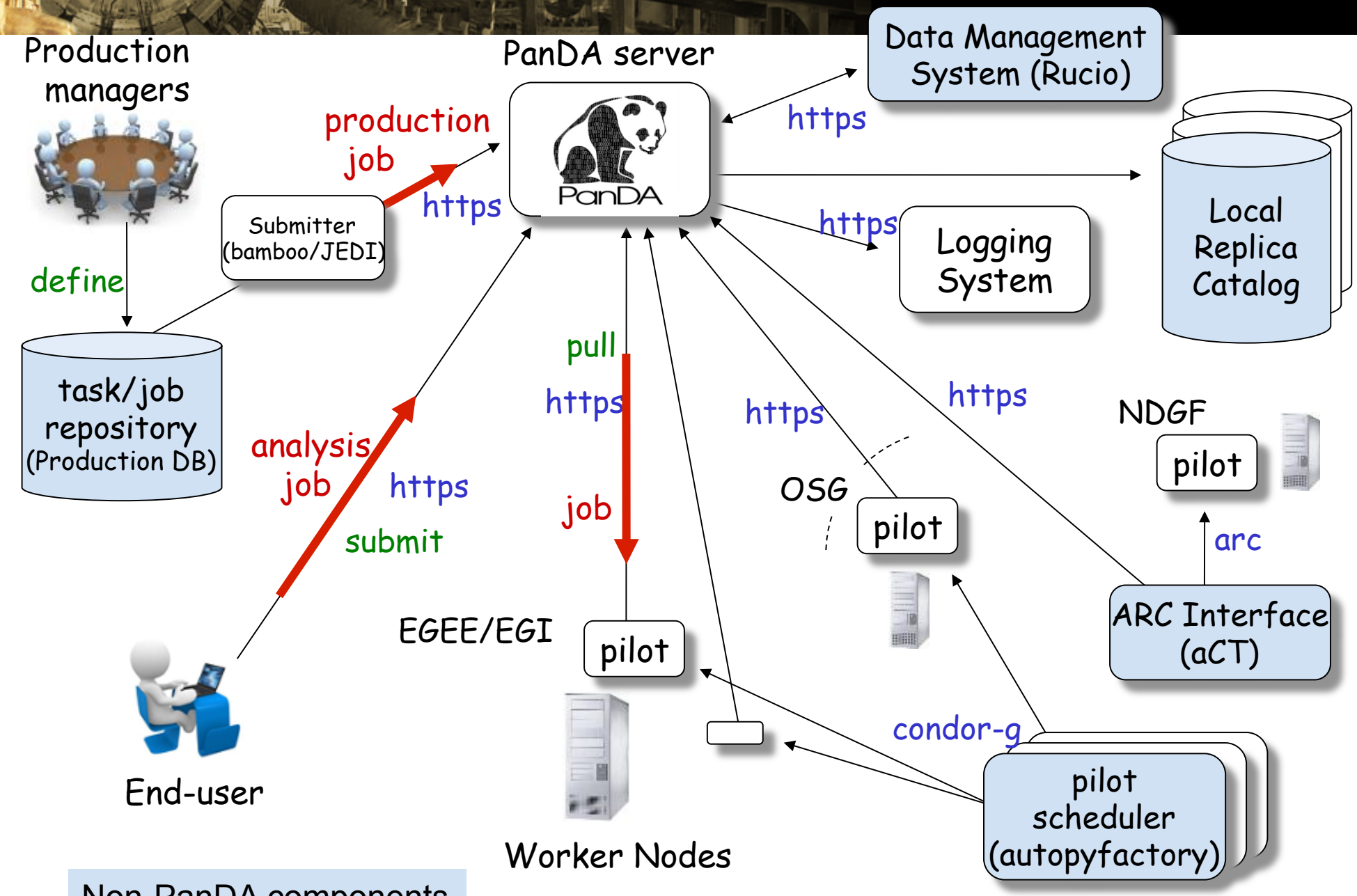
- Many physics packages were ported to Titan
  - Event Generators – SHERPA, MADGRAPH, ALPGEN, POWHEG, PYTHIA
  - Root
  - FairRoot and EICRoot frameworks
  - Geant4, including multithreaded v10
- ATLAS workloads
  - Several ATLAS software releases installed on Titan
  - Event Generation, Geant4 Simulation and Reconstruction chains were ran for several ATLAS physics scenarios
  - Already delivered several million simulated events to ATLAS physicists
  - Integration with the new ATLAS production system (ProdSys II) is in progress

Summary

- Work on integration of Titan with PanDA is well advanced
- PanDA pilot now uses information about free worker nodes on Cray machines for job submission.
- MPI wrappers developed to run unmodified single node workflows as multi-node MPI ensembles
- Ran continuous PanDA job submission tests in backfill mode on Titan
  - Stable operations, Short wait times
  - Demonstrated significant resource collection capability, and improvement in Titan utilization
- Work on ATLAS workloads is in progress
  - Already delivered several million simulated events to ATLAS physicists
  - Integration with ATLAS production system (ProdSys II) is in progress
- Collaboration with multiple groups and experiments
  - ALICE, nEDM, LSST, EIC,…
- Successful functional tests of the setup developed for Titan at NERSC and at IT4I in Ostrava, CZ
- Our project was showcased at SC14 Conference in November, 2014 as part of the US DOE Science Data Pilot Projects

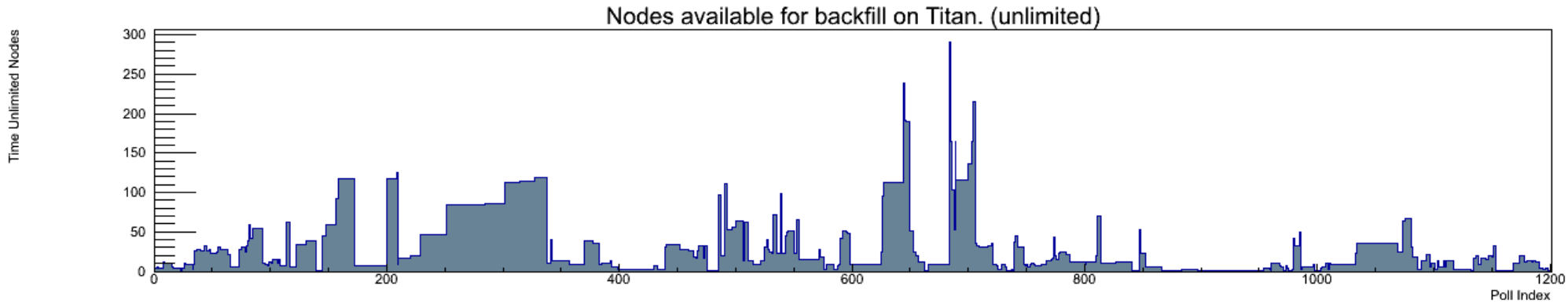
Backup Slides

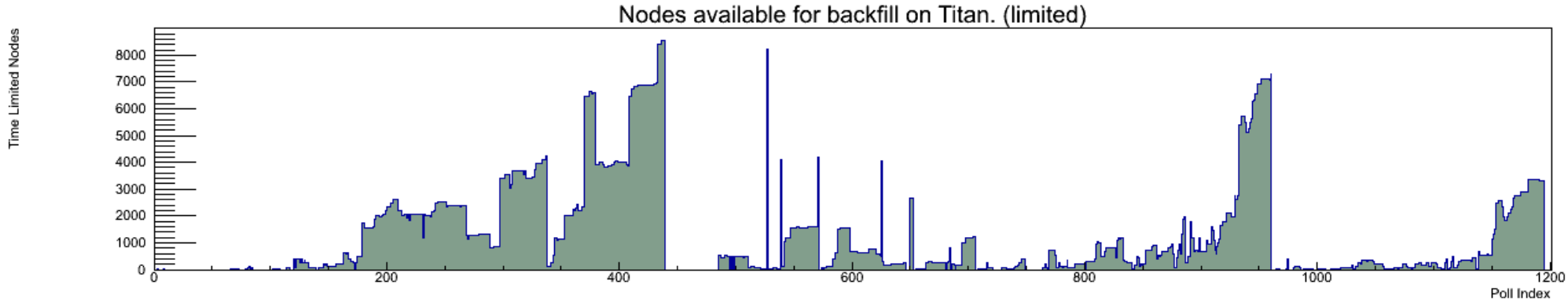
PanDA Workload Management System

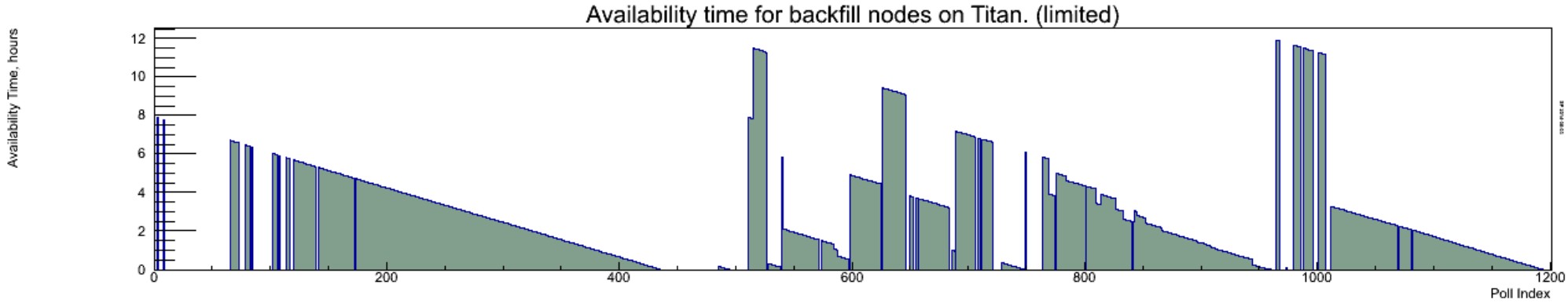


Non-PanDA components

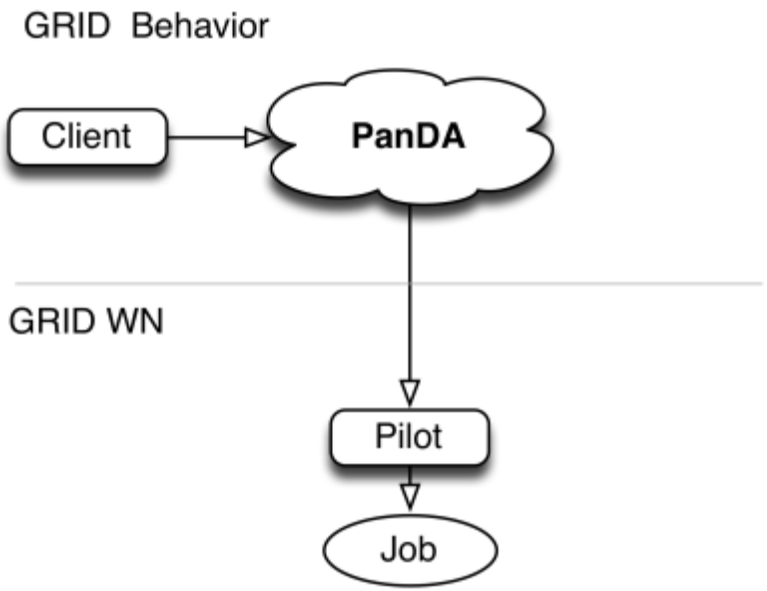
Typical Titan free resource availability pattern

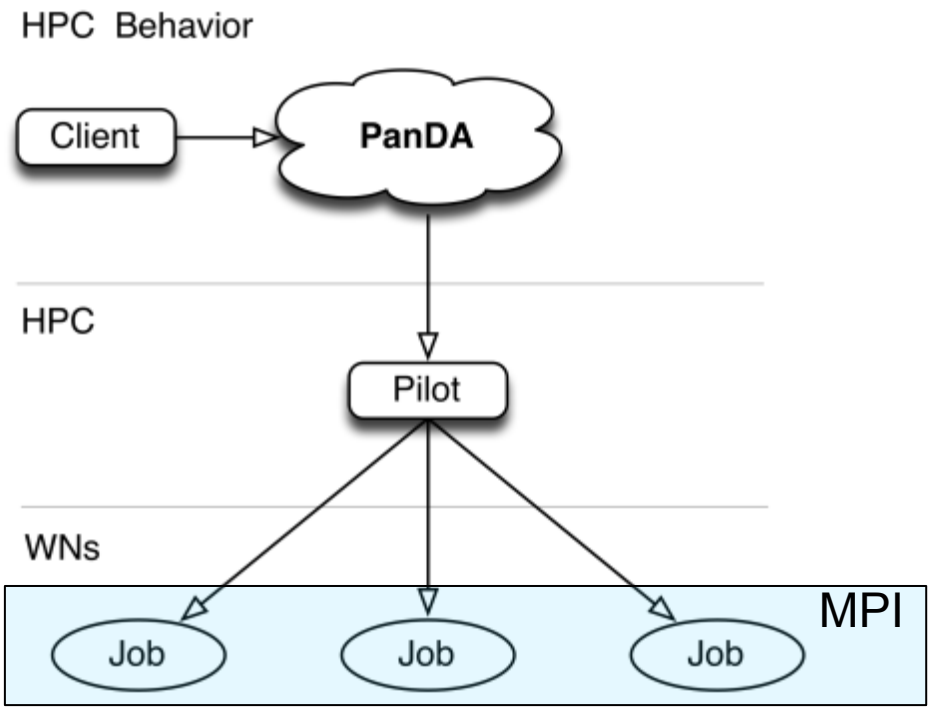






Pilot on HPC with MPI wrapper





"One to One"

"One to Many"