Evolution of the ATLAS PanDA Workload Management System for Exascale Computational Science

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Outline

- Introduction
- Overview of the BigPanDA project
- Current status and plans
- Conclusions

Introduction

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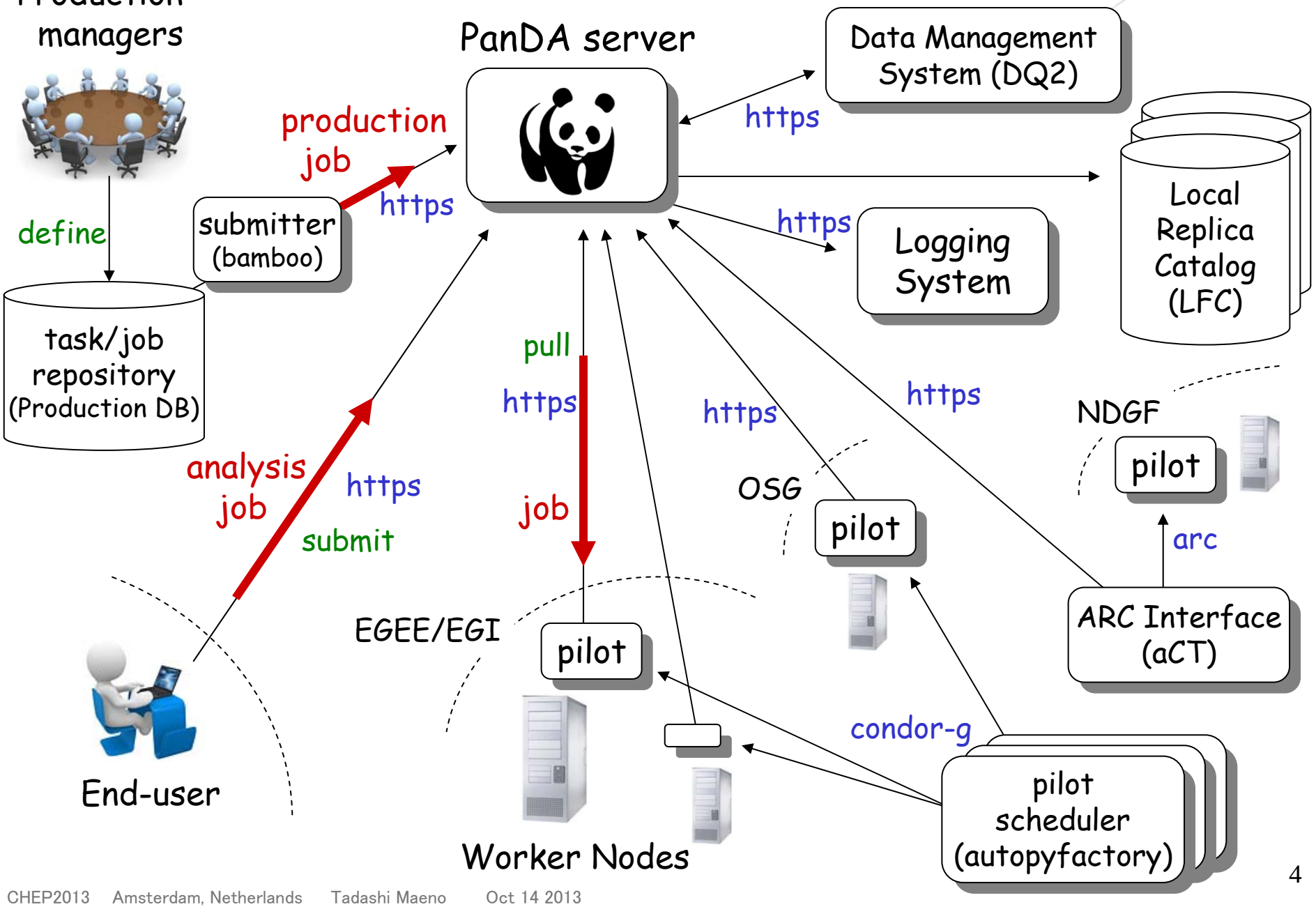
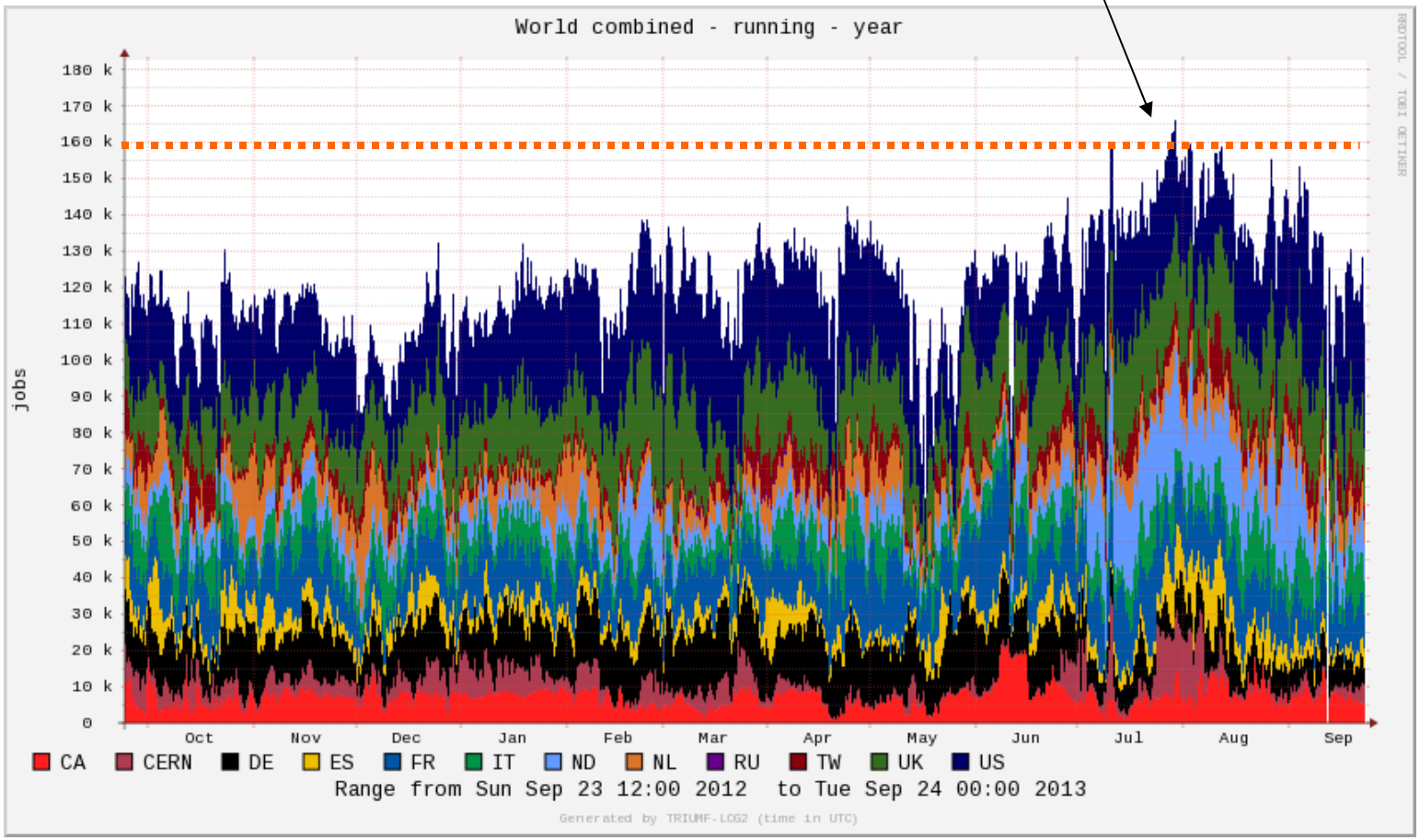
- PanDA = Production and Distributed Analysis Sytem
  - Designed to meet ATLAS production/analysis requirements for a data-driven workload management system capable of operating at LHC data processing scale
- Highly automated, low operational manpower, integrated monitoring system
- History
  - Aug 2005: Project started, Sep 2005: The first prototype, Dec 2005: Production in US ATLAS,
    2008: Adopted as the workload management system for the entire ATLAS collaboration, Recent: AMS and CMS have deployed own PanDA instances
- Performed well during LHC Run 1 for data processing, simulation and analysis, while actively evolving to meet rapidly changing physics needs
  - Successfully managing more than 100 sites, about 5 million jobs per week, and about 1500 users

PanDA System



ATLAS Jobs Concurrently Running ’12 –’13

~ 160 k running jobs at peak



Overview of BigPanDA project

BigPanDA project

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Evolving PanDA for Advanced Scientific Computing

- The interest in PanDA by other big data sciences provided the primary motivation to generalize the PanDA system
- A project to extend PanDA as meta application, providing location transparency of processing and data management, for HEP and other data-intensive sciences, and a wider exascale community
- 3 FTE for 3 years from 2012
- Three dimensions to evolution
  - Making PanDA available beyond ATLAS and High Energy Physics
  - Extending beyond Grid (Leadership Computing Facilities, Clouds, University clusters)
  - Integrating network as a resource in workload management

Work Plan

- 3 year plan
  - Year 1. Setting the collaboration, define algorithms and metrics
    - Hiring process was completed in June 2013
    - Development team is formed (3 FTE)
  - Year 2. Prototyping and implementation
  - Year 3. Production and operations
- 4 work packages
  - WP1 : Factorizing the core
  - WP2 : Extending the scope
  - WP3 : Leveraging intelligent networks
  - WP4 : Usability and monitoring

Work Packages 1/4

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- WP1 (Factorizing the core)
  - Factorizing the core components of PanDA to enable adoption by a wide range of exascale scientific communities
  - To take the core components of PanDA and package them in an experiment neutral package
    - General components + customizable layers
    - The experiment specific layers as plug-ins + configuration files
  - Advanced features will have sensible defaults and can be turned on for demanding applications

Work Packages 2/4

- WP2 (Extending the scope)
  - Evolving PanDA to support extreme scale computing clouds and Leadership Computing Facilities
    - Historically HEP community used the Grid infrastructure for large scale production
      - E.g., Leadership Computing Facilities were not used very extensively
  - Adding extra resources
  - Further expansion of the potential user community and the resources available to them

Work Packages 3/4

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- WP3 (Leveraging intelligent networks)
  - Many of the research efforts into dynamic network provisioning, quality of service and traffic management
  - Integrating network services and real-time data access to the PanDA workflow
    - Integrating these services within existing and evolving infrastructures
      - E.g., PanDA currently does not interface with any of the advanced network provisioning technologies available
    - Automating the discovery and use of such services transparently to the scientists
      - E.g., instead of exposing intelligent network services directly to scientists, PanDA could be updated to directly interface with them without any involvement of scientists

Work Packages 4/4

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- WP4 (Usability and monitoring)
  - The PanDA monitoring has been identified to require a special effort for factorization and generalization
    - Each experiment has own workflow and visualization needs
  - To design a generic PanDA monitor browser view and skeleton from which experiment (ATLAS and other) browser views are derived customizations
  - To provide generic components and APIs for user communities to easily implement and customize their monitoring views and workflow visualizations

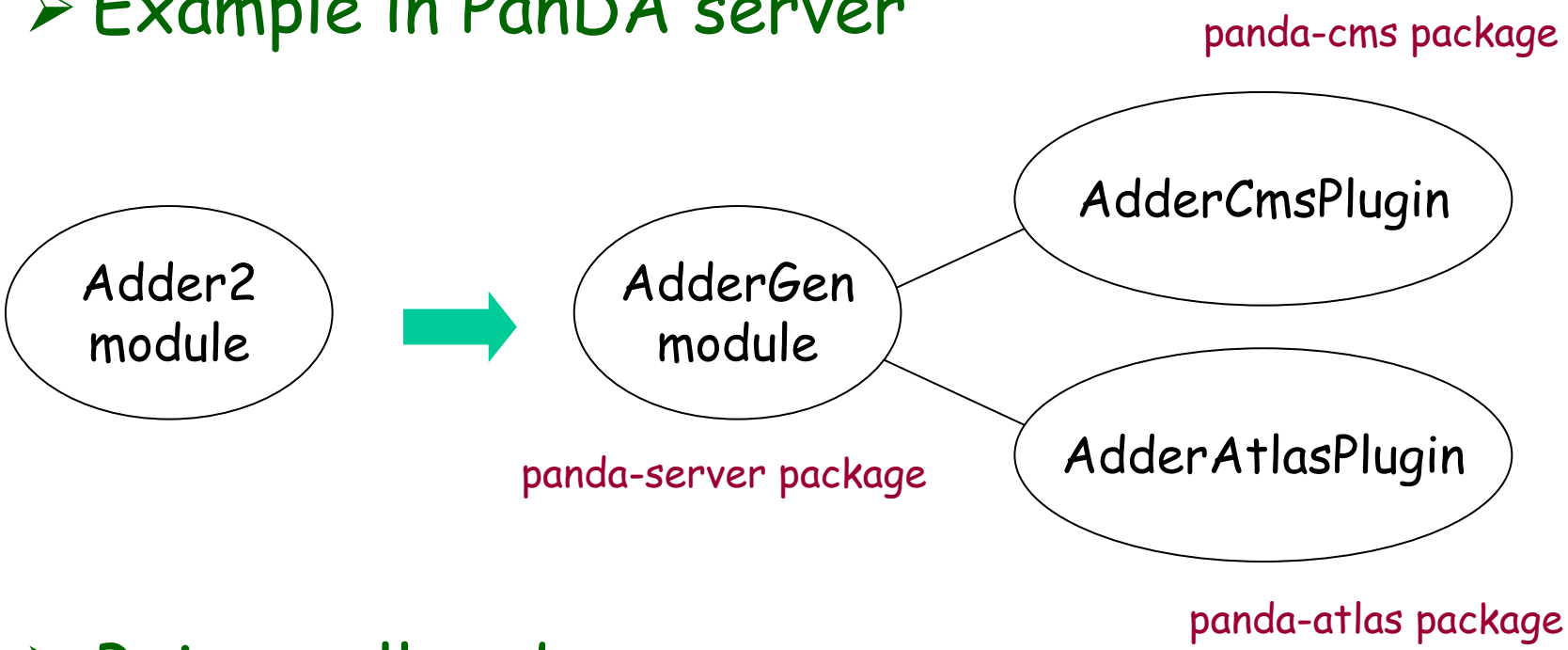
BigPanDA and ATLAS

- ATLAS remains the largest user community and provides the primary focus to PanDA development although PanDA is not only for ATLAS any longer
- Working very close with ATLAS PanDA developers
- One set of software packages for all experiments including ATLAS
  - Core packages + experiment-specific plug-ins
- The effort has to be incremental and coherent with many challenging developments for ATLAS

Current Status and Plans

Factorization of Core Components

- Example in PanDA server



- Being well underway
  - Decomposition of experimental code to plug-ins & separate packaging
  - See Paul Nilsson's poster as well

    Nilsson P., *Next Generation PanDA Pilot for ATLAS and Other Experiments*

VO-independent PanDA Server

- PanDA server with MySQL database backend
  - Multiple backend support
    - Oracle or MySQL can be selected in config file
    - Code is being merged to the main branch
- PanDA server @ Amazon EC2
  - Serves experiments which don't want to maintain own PanDA server
  - MySQL backend

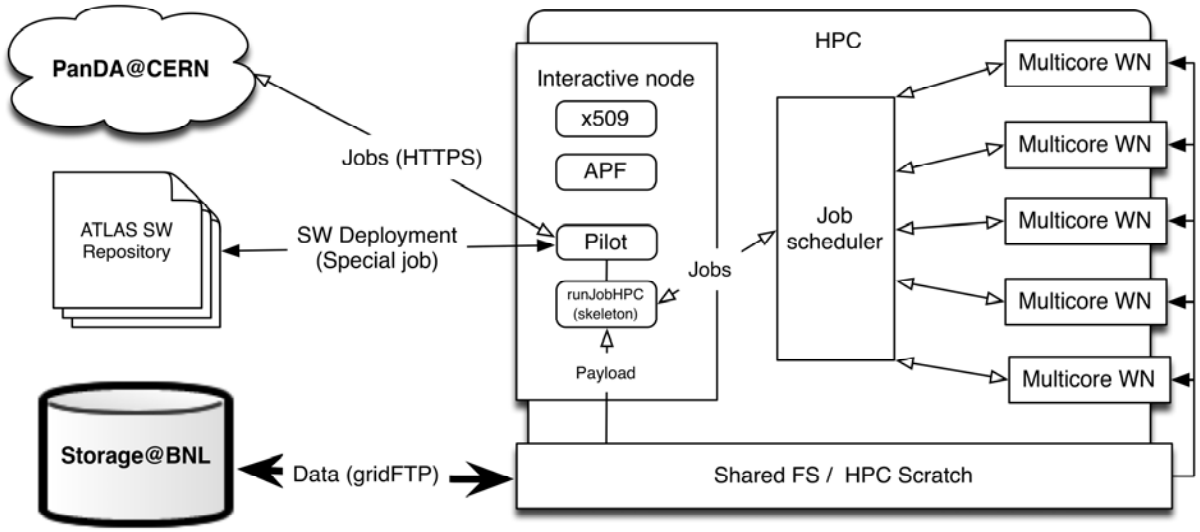
Google Compute Engine (GCE) preview project

- Google allocated resources for ATLAS for free
  - ~5M cpu hours, 4000 cores for ~2 months
- Transparent inclusion of cloud resources into ATLAS grid
  - Resources were organized as HTCondor-based PanDA queue
- Delivered to ATLAS as a production resource and not as an R&D platform
- See Sergey Panitkin's talk for details

  Panitkin S., *ATLAS Cloud Computing R&D*

PanDA + HPC

- In collaboration with ORNL Leadership Computing Facility
  - Get experience with all relevant aspects of the platform and workload
    - job submission, security, storage, monitoring, etc
  - Developing appropriate pilot/agent model for Titan



Leveraging Network

- Synchronized with two other efforts
  - Integration of FAX (Federated Xrootd for ATLAS) with PanDA
  - ANSE project
- Three layered software architecture
  - Collector
    - Collecting network performance information from various sources such as perfsonar, Grid sites status board, FAX, etc
  - AGIS (ATLAS Grid Information System)
    - Information pool
  - Calculator
    - Calculating weights which the brokerage take into account for site selection
- The site selection algorithm in the PanDA brokerage has been improved to consider cost metrics of FAX

Conclusions

- The PanDA system played a key role during LHC Run 1 data processing, simulation and analysis with great success, while actively evolving to meet rapidly changing physics needs
- The interest in PanDA by other big data sciences provided the primary motivation to generalize the PanDA system
- The BigPanDA project gives us a great opportunity to evolve PanDA beyond ATLAS and HEP
- Progress in many areas : networking, VO independent PanDA instance, cloud computing, HPC
- Strong interest in the project from several experiments and scientific centers to have a collaborative project