Integrating HPC and HTC at BNL – A Year Later

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Background

• Scientific Data & Computing Center (SDCC) formed in 2016 to leverage existing HTC expertise in the RACF to kickstart support for HPC activities
• Acquired Institutional Cluster (IC) and KNL-based cluster for HPC-based projects
• IC and KNL in stable production configuration
• Available to approved users
Expanded responsibilities...

• Traditional areas (HTC)
  • HEP and NP
    • RHIC/eRHIC
    • ATLAS
    • Belle-2
  • Intensity Frontier
    • DUNE
    • Daya Bay
  • Cosmic Frontier
    • LSST
    • Legacy projects

• New areas (HPC)
  • LQCD
  • Photon Science
  • Others
...but limited resources

• Manpower shortage
  • Hired one person in April
  • Multiple openings still unfilled
• Resource shortage
  • Current resources fully utilized
  • RHIC experiments falling behind in processing campaigns
• Encouraged to seek resources on shared clusters at BNL and elsewhere
Fully Utilized ATLAS Farm
Existing Resources

• Dedicated
  • Custom workloads whose rigid constraints make it difficult for others to use productively
  • Legacy RHIC/ATLAS clusters
• Shared
  • HPC clusters (IC, KNL and others)
  • Recently purchased RHIC/ATLAS resources
  • New general-purpose cluster in 2018
Enabling Resource Sharing

• Integration of cyber infrastructure
  • Discussions on single sign-on to integrate distinct user bases
  • Cross-mounting of disk storage instances
  • Plan to offer access to tape storage via BNLBox
• Rethink HTCondor policy to increase productivity of RHIC/ATLAS clusters. Possibilities are:
  • Collapse multiple HTCondor pools into a single pool and expand usage of hierarchical group quota model deployed on ATLAS Tier 1
  • Increase flocking among multiple Condor pools in existing model
• HTC workloads on HPC clusters
  • Direct access for HPC-adapted workloads
  • Mechanism to submit HTCondor jobs to Slurm at BNL
Current HTCondor configuration
Possibility #1

Access to other resources (flocking, job routing, etc...)

Shared Pool

CRS

STAR

Analysis

PHENIX

Analysis

Others...

Anatrain

PHENIX

CRS
Possibility #2

Shared Pool

Analysis
- STAR

Anatrain
- PHENIX

CRS

Access to other resources (flocking, job routing, etc…)

Others…
Institutional Cluster (IC)

- In production since January 2017
- Original cluster with 108 nodes
  - Two Xeon E5-2695v4 (Broadwell) cpu’s (36 physical cores)
  - Two Nvidia K80 gpu’s
  - 256 GB RAM and ~2 TB SAS disk drive
  - Non-blocking Infiniband EDR fabric
  - 1 PB of GPFS storage with up to 24 GB/s bandwidth via EDR
- Expansion underway
  - Nvidia P100 instead of K80 gpu’s
  - First batch of 18 nodes in production since September
  - Another 36 machines purchased in October
  - Full expansion by Spring 2018
- Available to HPC and HTC users
KNL Cluster

- Entered production in June 2017
- 144 nodes
  - One Xeon Phi 7230 cpu (1.3 GHz) with 64 physical cores and 16 GB RAM on chip
  - 2 x 512 GB high-performance SSD drives and 192 GB RAM
  - Dual-rail Intel Omni-Path interconnect fabric with 400 Gbps (nominal) peak aggregate, bi-directional bandwidth
  - Access to IC GPFS storage via custom gateway server and available to users via NFS
- Cluster in useful state, but not optimized
  - Optimization delayed for the sake of stability and availability
  - KNL heavily used by LQCD community
  - Used by ATLAS on an opportunistic basis
Titan @ ORNL

- 18,688 compute nodes (299,008 logical cores) with GPU’s (Cray Xk-7)
- AMD Opteron 6200 @ 2 GHz
- 32 GB RAM per node
- Nvidia K20x
- 32 PB Luster-based disk storage (1 TB/s aggregate throughput)
- 29 PB HPSS-based tape storage
- 27 Pflops peak theoretical performance

Slide kindly provided by Sergey Panitkin (BNL)
• Job sizes shaped to backfill opportunistically via PanDA
• Used 129M core-hours from July 2016 to June 2017
• ~2.5% of total available time on Titan
• ~10% of all US-ATLAS computing
What’s Next?

- Plans to buy another cluster to be shared between HPC and HTC
  - Likely based on Skylake for ATLAS Tier-1 at BNL
    - Standard dual-socket worker node configuration
    - Add IB EDR interconnect fabric for HPC requirements
  - Available to users in early 2018
- Implement HTCondor changes to increase current RHIC/ATLAS cluster productivity
- Continue to facilitate usage of non-traditional clusters
  - Increase HTC access to HPC resources
  - Employ HPC clusters as jumping point to Leadership Class Facilities
Likely Future Direction

• Broad effort to encourage use of LCF’s to meet computing needs
  • ALCF
  • NERSC
  • ORNL
• Alternative (and possibly) complementary solutions
  • Commercial providers (still in touch with Amazon and Google)
  • Academic clouds