Joint USATLAS-USCMS HPC/Cloud Workshop Summary

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LHCOPN-LHCONE meeting, 25 Oct 2022, CERN

Based on summary slides prepared by Dirk Hufnagel and Lincoln Bryant

Overview

Why did we do this?

- US LHC Operations Program review (Feb 2022) recommendation
  - Blueprint document about Cloud/HPC usage and evolution in U.S. ATLAS and U.S. CMS
    - Internal document deadline: Dec 2022

Workshop

- Organized workshop as part of the process, held Sept 26-28 (3 half days)
  - https://indico.cern.ch/event/1183995
- Hybrid format: meeting room at UChicago, but majority of people connected remote
- Good attendance, about 30-40 participants across CMS, ATLAS, OSG-LHC and WLCG
- Deliberately light on presentations and heavy on discussions
- Few invited contributions: HPC facilities, ESNet, CERN, Vera Rubin

Discussions about HPC

HPC Landscape in US

- User Facilities (NERSC, ACCESS, Frontera)
- Leadership Class Facilities (LCF), more restricted, but also (much) larger

Integration

- Integration frequently depending on HPC architecture/restrictions
- Streaming or intermediate storage within HPC
- Raises network/storage requirements at associated sites
- Large(r) storage allocations at LCF should be explored (incl. full DM integration)
  - Also potentially at User Facilities, but streaming is easy there, so no pressing need

Workflows

- Currently do what is easiest considering storage integration
  - ATLAS: Simulation
  - CMS: almost all MC production through StepChains
- Workflow “specialization” doesn’t help on the pledging discussion (more on this later)

Discussions about HPC

Cost

- Computing resources no direct cost to experiment
  - Indirect effects at the funding agency levels about replacing our own resources with HPC were outside the scope of the blueprint process (but we had a short discussion about it during the BSC presentation)
- Cost at personpower level
  - Proposals time and effort consuming
  - Commissioning and support costs (have to provide interface between experiment and HPC)
  - Software porting to new architectures/accelerators outside the scope of the blueprint process

Proposals

- Planning horizon mismatch between allocation process and LHC experiments
- LCF proposals currently require selling our use cases, not very interested in generic T2 production activities

Discussions about HPC

Edge Services

- Many HPC seem to experiment with platforms for edge services (often Kubernetes based)
  - No overall (visible) coordination in this area
- Can we take advantage?

CVMFS

- Less of a worry these days: *cvmfsexec* works on any modern kernel/OS
- Needs edge service squid (which so far seems to be possible everywhere, even LCF)

General comments about our HPC usage

- We are not treating HPCs for what they were designed (e.g. MPI, GPUs)
- We use HPCs like another T2 and we are an average user for HPCs (vs e.g. LatticeQCD)
- Community needs to make jump to GPU or become legacy computing and accept limitations

Discussions about Cloud

Cloud Landscape

- Considering mostly global, large providers (Google, Amazon, Azure)
- Briefly discussed Lancium
  - Low cost due to use of cheap renewable energy, but also limited features

Integration

- Site extension vs. standalone cloud site
- Storage integration done, but policy to use only for transient replicas (no custodial data)

Workflows

- No technical restrictions. In principle we can run everything
  - However some workflows can be more interesting from cost perspective
- Interactive analysis setups

Elasticity

- Allows evaluation of “exotic” types of hardware (ARM, GPU, FPGA) in a cost effective way
- Allows using (and paying for) capacity as needed
  - “Scheduling for peak”: possibility of high intensity / short runs vs. spreading out use over time on fixed resources

Discussions about Cloud

Cost

- Main discussion topic for cloud
- Cost comparison for CMS Reconstruction Scale Tests ~5 years ago
- ATLAS Cost Simulation
  - Plugs in publicly available numbers for on-demand vs. pre-commitment, spot vs. regular, AWS vs. Google Cloud
  - Allows to estimate costs for various combinations of compute, storage and egress
- ATLAS Google Cloud Subscription
  - Fixed price for certain amount of resources for a certain time period (15 months here)
  - Negotiated by each customer
  - Flexible resource use is still possibly (could use the total compute in subscription in first month in principle)
  - Keeps a running total of “charges” using list prices, but everything is included in subscription (also egress)
- Facilities also looking at this
  - Programs can buy Cloud cycles directly or T1/T2 sites could decide to replace on-prem with Cloud cycles
- Outlook
  - Prices have dropped over the years, should be ready to use them once the cost becomes attractive
  - Cloud providers want to make money, but they are also in competition with each other
  - Cloud providers have economies of scale we cannot achieve on our own

Discussions about Networking

Invited talk from ESnet

- DOE HPC
  - ESnet6 built physical network into each DOE national lab
  - Site infrastructure (border routers, security stuff, storage) will be a more limiting factor than WAN
    - Wide disparity in HPC support for data-centric workflows
- NSF HPC
  - Some very well connected, others not so much, depending on where they are
- Cloud providers
  - Multiple 100Gbit interconnects
  - Enables capabilities, doesn't help with egress costs
- LHCONE
  - Participation in LHCONE defacto based on IP address, effectively excludes HPC/Cloud traffic
  - Possible workaround is to keep traffic partitioned (Global LHC <-> US LHC <-> US HPC/Cloud)
    - Puts more load on US sites and also means less flexibility in using HPC/Cloud

Discussions about Pledging

- Current HPC/Cloud use is opportunistic / “beyond pledge”
  - One view point: can just keep doing this and not care about pledging / getting credit
  - Resources can’t really be considered for planning purposes
  - Problematic if HPC/Cloud use increases a lot
- Current MoU policies require pledging a fixed #cores
  - Incompatible with US HPC resource provisioning policies
    - Just a customer, we get in the queue with all other users and our jobs run ‘eventually’
  - Would need a change to allow time integrated pledge (kWh vs kW)
- Pledges currently are for universally usable resources
  - How restrictive can we be with workflow selection for them to be eligible as pledges?
- How to pledge GPU resources? (not just a HPC/Cloud problem)

- Indication to resolve the technical questions (benchmarking, accounting) will open up the discussion on more flexible policies

Discussions about Benchmarking/Accounting

Benchmarking

- Invited talk from CERN about HEP benchmarking on HPC
  - One conclusion is that increased heterogeneity affects benchmarking
    - Not just one number anymore to describe performance, at minimum CPU vs. GPU
    - Lots of variations in GPU architectures, how to compare them among each other?
    - Even more complex once more use cases like AI/ML get added

Accounting

- Need to make sure HPC/Cloud use gets reported (via APEL)
  - U.S. ATLAS doesn't do this currently
  - U.S. CMS spent some effort last year on this, some HPC still not correct
- Only talking about traditional CPU accounting here
- Have nothing for GPU accounting (not just an HPC/Cloud problem)

Discussions about R&D

AI/ML

- Question whether this is a large enough use-case to matter
  - Hyperparameter optimizations potentially very expensive
    - Invited talk from CERN about training and hypertuning on HPC
  - Continuous training models were mentioned
  - Could matter, depending on where we go with AI/ML

Other R&D topics

- Unique cloud offerings (special accelerators, FPGA etc)
- LCF integration work (to bring operational costs down)
  - This includes work on how to use the edge service platforms
- Full-chain: minimizing output egress by running all steps in the cloud
- Function-as-a-service (funcX, parsl)
  - Primarily Cloud, but potentially also applicable to HPC
  - Not much usage now, will have to see how this evolves
  - Analysis is a very different resource scheduling problem vs. production
- External inference servers on GPU (SONIC)