Conclusions from the PRACE/CERN Workshop

Geneva, 26 October 2018

On 22 October 2018, representatives from CERN and PRACE met to discuss activities and opportunities at PRACE (Partnership for Advanced Computing in Europe) and possibilities for collaboration and joint activities. The link is available at https://indico.cern.ch/event/760705/
The morning focused on PRACE mission, structure of support and opportunities for training, and current PRACE interactions with science projects. The afternoon concentrated on the LHC and SPS experiments, the CERN-IT experience with HPC and plans for the future as well as specific requirements for Machine Learning workflows at the LHC on HPC infrastructures.

The meeting was productive, highlighting a strong willingness to collaborate on all sides. The meeting had an ambitious list of goals, most of which were met.

- Learn how PRACE works and how we can interact together
- Understand mechanisms for resource allocation, scheduling, I/O and data serving , authentication and authorization, and firewalls
- Understand the interactions of PRACE with other EU HPC initiatives
- Understand PRACE plans for the next generation of hardware deployments
- Understand how all of these elements impact the scientific use-cases
- Understand how HEP software can be better optimized to run efficiently on HPC resources
- Present the current experience of the experiments on HPC. LHC experiments have successfully utilized a number of European HPC centers, including PRACE sites. Up to now these efforts have been independent experiment initiatives with individual sites and would benefit from cross experiment and cross site coordination.
- Discuss potential/possible changes on the infrastructure and application side to enable more efficient usage of HPC resources

There are significant differences in scheduling, access, and services between the PRACE HPC community and large scientific communities such as the LHC. It is not reasonable to expect that either community will entirely bridge the existing gap. However, it is worth recognizing that improving the scientific applications to be better tuned for HPC environments and evolving the HPC centers to be better suited for data intensive sciences would bring the two communities much closer.

A few interesting challenges were identified.

- LHC and other data intensive sciences like SKA are often open-ended multi-year projects that need predictable computing resources, which cannot be easily accommodated by the PRACE annual proposal-driven allocations.
- Most LHC/HEP applications currently make very little use of communication between data processing instances (running processes) due to the nature of HEP workflows. In

turn, HPC centers typically invest significantly into optimizing the interconnecting links between the worker nodes. Therefore, an expensive component of the infrastructure is not being used at all.

- A common set of interfaces for authorization, resource allocation and data management are needed for HPC centers to reduce the cost of adoption.

None of the challenges was seen as insurmountable and represent interesting R&D opportunities. A few early joint strategic and technical activities were proposed during the workshop wrap-up discussion, some of them being very relevant to SKA as well.
It was also decided to write a two-page note, stating the interest for a three-way collaboration among CERN, SKA and PRACE.

Proposed Activities:

Strategic

1.) Develop a three-way agreement between CERN, SKA and PRACE to explore long-term cooperation to support the LHC and the SKA science programmes.

2.) Survey of current LHC experiment activities using PRACE resources. Document successes and challenges. Develop a list of priorities for a development project to make efficient use of PRACE sites and resources for as many LHC workflows as possible.

3.) Development of services and tools for LHC and SKA workflows. Assessment of e-infrastructures like FENIX.

4.) Develop a software-driven initiative to tackle the LHC and SKA needs in terms of software optimization and performance on HPC resources.

5.) Creation of training programmes tailored to the LHC experiments' adoption of HPC architectures and performance optimization of high-end accelerators such as GPUs and FPGAs.

Technical

1.) Definition and execution of a pilot project for an HTCondor overlay for HPC resources in PRACE based on similar work at CERN. HPC resource allocation could then be performed generically for the LHC community via a HTCondor pool.

2.) Definition and execution of a data federation demonstrator: the goal is to demonstrate data delivery at run-time through the HPC firewalls at an incoming rate sufficient to efficiently operate at scale HPC processing resources for data intensive workflows.

3.) Definition of a programme to demonstrate that local storage at HPC sites can record data at production scale from high-output workflows (reconstruction and simulation). This demonstrator should also verify that export from the HPC facilities to remote custodial storage can be sustained at a level which permits continuous operations.