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HIGH PERFORMANCE COMPUTING SYSTEM IN THE FRAMEWORK OF THE HIGGS BOSON STUDIES AT ATLAS

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Higgs boson physics is one of the most important and promising fields of study in modern high energy physics. To perform precision measurements of the Higgs boson properties, the use of fast and efficient instruments of Monte Carlo event simulation is required. Due to the increasing amount of data and to the growing complexity of the simulation software tools, the computing resources currently available for Monte Carlo simulation on the Large Hadron Collider (LHC) Grid are not sufficient. One of the possibilities to address this shortfall of computing resources is the usage of institutes' computer clusters, commercial computing resources and supercomputers. In this paper, a brief description of the Higgs boson physics, Monte Carlo generation and event simulation techniques are presented. A description of modern high performance computing systems and tests of their performance are also discussed. These studies have been performed on the Worldwide LHC Computing Grid and Kurchatov Institute Data Processing Center, including Tier-1 WLCG sites and the OLCF Titan supercomputer. Monte Carlo simulated events produced with the Titan supercomputer were used in the Higgs boson analysis and the results have been published by the ATLAS collaboration.

Keywords: high performance computing, ATLAS, Higgs, CERN, supercomputers, data, LHC, physics, reconstruction, GRID, cloud computing, WLCG, Tier-1, Titan

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1. High performance computing in high energy physics

The observation of a new particle compatible with the Standard Model (SM) Higgs boson by the ATLAS and the CMS experiments [1, 2] has been an important step towards the validation of our understanding of nature. This observation is based on the information from the Large Hadron Collider (LHC). Experimental data was obtained during the first LHC data taking period (Run 1) in 2011-2012. Other impressive discoveries based on the LHC data include the pentaquark observation [3] and the observation of CP violation in rare baryon decays [4], both by the LHCb experiment.

To perform more detailed studies in these areas and to probe the new physics beyond the Standard Model (BSM), theoretical predictions for the physics processes under consideration must be obtained. The most convenient way to obtain such predictions is to use Monte Carlo (MC)-generated events. MC simulations are based on concrete theoretical models, which describe the processes under consideration.

MC simulations usually require a large amount of computing resources. Generally, there are two reasons for that. First, modern particle physics theories become more and more complex: they are based on non-trivial mathematics and calculations required by these theories are resource-intensive. Second, as far as measurements in particle physics are performed by the particle detectors, the detector effects must be also taken into account. The ATLAS detector [5] consists of millions of structural elements (more than 150M sensors). The response of each of them must be modelled and taken into account. For the physics analyses, it is necessary to perform so-called Full Simulation of the detector, which takes into account all the detector effects [6].

The resource intensity of MC tasks can be illustrated in terms of statistics. Figure 1 shows the fraction of CPU time consumption of all jobs submitted to Worldwide LHC Computing Grid (WLCG) by all its users during the first 35 weeks of 2017. The jobs were categorized according to their type: Data processing, Validation, Testing, MC Simulation, MC Simulation Full, MC Simulation Fast, MC Event Generation, MC Reconstruction, Group Production and Others. This plot shows that MC-related jobs take more than 85% of all CPU time provided by the WLCG.

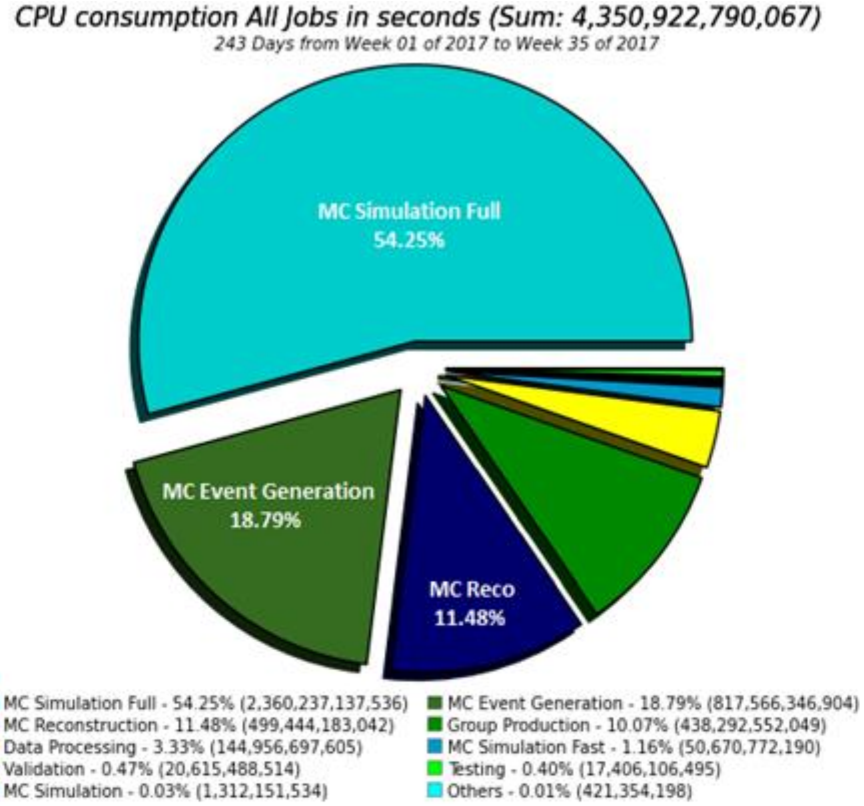

Figure 1. Consumption of CPU time for all WLCG jobs in seconds, obtained with the ATLAS Dashboard [7].

2. Higgs boson physics

Higgs boson physics is one of the most promising fields of study in modern particle physics. However, this topic is not only promising, but also complex. The most intensive channel of the Higgs boson production at the LHC in high energy proton-proton collisions is the gluon-fusion production (ggF). The Feynman diagram of such a process at the leading order (LO, first-order terms of Lagrangian in the Perturbation theory of Quantum Chromodynamics [8]) is shown in Figure 2.

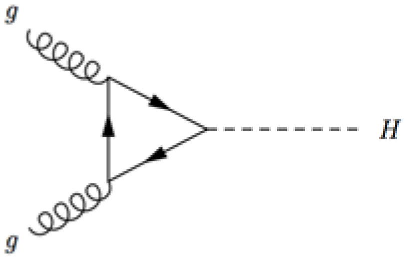

Figure 2. Feynman diagram of the LO ggF Higgs boson production. Two gluons, emitted by protons, interact and then produce the Higgs boson through the loop of t- or b-quarks [9].

When the center-of-mass energy of two protons is about 10 teraelectronvolts (TeV) or higher, more than 90% of all Higgs bosons are produced by the ggF mechanism. The process shown in Figure 2 is relatively simple, because there are no outcoming particles except the Higgs boson and there are no hadron jets (so-called 0-jet final state).

Considering second-order terms of the Lagrangian (Next-to-leading order corrections, NLO), the situation becomes more complex. Figure 3 presents some of the Feynman diagrams of ggF Higgs boson productions in the NLO.

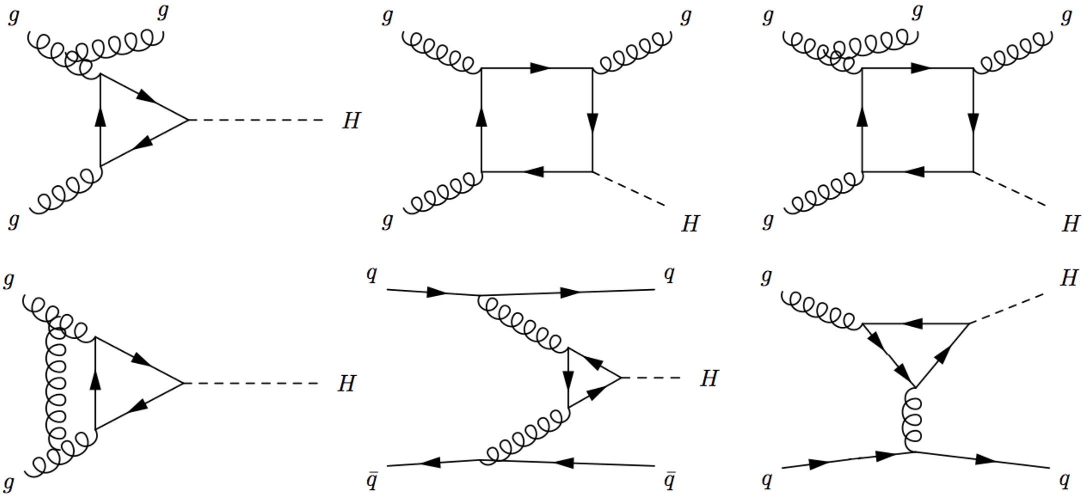

Figure 3. Feynman diagrams of the NLO ggF Higgs boson production. Higgs boson is still being produced from t- or b-quark loops, but now the final state might contain one or two additional hadron jets [9].

The complexity of NLO calculations is directly correlated with the number of jets. In NLO case, 0-jet category consists of 29 Feynman diagrams. The generation time of 100k events at CERN on LXPLUS machines [10] is about 10 minutes. The 1-jet category consists of 1050 diagrams and the calculation time increases up to about 2 hours. The 2-jet category consists of 21510 diagrams and the calculation time increases even more, up to about 24 hours. For the ggF Higgs boson production NLO corrections can contribute up to 45% to the cross sections and thus must be taken into account.

3. Role of High Performance Computers' in HEP

High Performance Computers (HPC) are presently the most valuable instruments for CPU-intensive tasks, such as Higgs boson production simulation with NLO corrections. One of the most impressive realizations of supercomputer-based HPC system for science tasks, including high energy physics, is the OLCF Titan, launched in 2012 by Oak Ridge National Laboratory, the performance of which is higher than the computing power of all the ATLAS resources in WLCG [10]. Some technical characteristics of the Titan supercomputer are listed below [11]:

- 27 PFLOPS (Peak theoretical performance);
- Cray XK-7 18,688 compute nodes with GPUs;
- 299,008 CPU cores AMD Opteron 6274 @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);
- More than 1TB/s aggregate FS throughput;
- 29 PB HPSS tape archive;

The Titan supercomputer was used to perform the simulation of the Higgs boson production associated with two hadron jets at NLO level with consequent decay of the Higgs boson to four leptons: $pp \to Hjj \to 4\ell jj$. Some technical parameters of this simulation are listed in Table 1, namely: *nFiles* is the number of files in the input dataset; *nEventsPerInputFile* is the number of events per input file and *nEventsPerJob* is the number of events per job. Expected CPU time is estimated by internal GRID benchmarks based on previous information about the occupancy of the particular GRID resource [12].

It is important to note, that while with CERN LXPLUS machines the generation event rate is about 2.5k events/hour, with the Titan it is about 650k/hour.

nEventsPerInputFile	nEventsPerJob	nFiles	CPU Time, HS06 seconds [13]	
			Expected	Total
2000	100	3000	72048000000	2284598809

Table 1. Parameters of MC Full Simulation of the Higgs boson production with Titan.

The datasets produced with the Titan supercomputer were subsequently used by the ATLAS collaboration for physics analysis, with the results of this study presented in the public note [14]. The main purpose was to probe the separation power of BDT discriminants to distinguish ggf and vector boson fusion (VBF) signals. As an example of obtained results, Figure 4 shows the distribution of the Boosted Decision Tree (BDT) discriminant for a possible detector layout for the ATLAS HL-LHC upgrade. The separation between the red and blue distributions visualises the ggf-VBF separation.

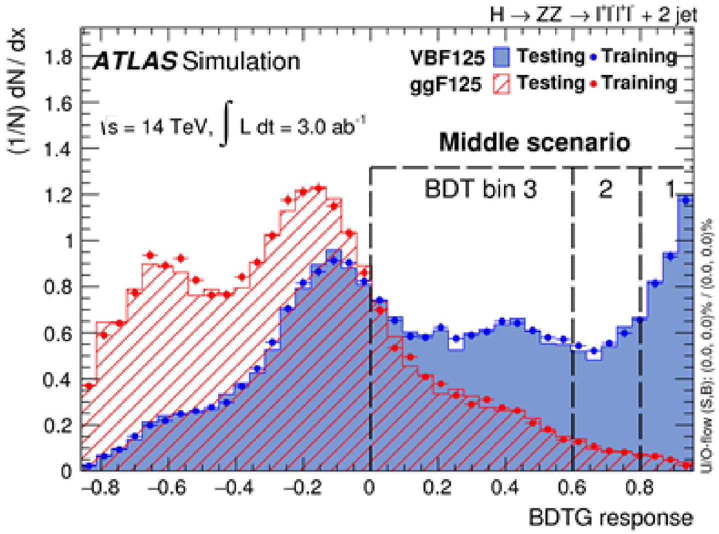

Figure 4. BDT classifier distributions for one of possible detector layouts [14].

4. Cloud computing at Tier-1 clusters

The resource-intensive tasks can be handled not only by supercomputers, but also by WLCG computing facilities and cloud computing. WLCG is made up of four layers, or "tiers"; 0, 1, 2 and 3. Each tier provides a specific set of services:

- Tier 0 corresponds to the CERN Data Centre, which is located in Geneva, Switzerland and also at the Wigner Research Centre for Physics in Budapest, Hungary. The two sites are connected by two dedicated 100 Gbit/s data links. All data from the LHC passes through the central CERN hub, but CERN provides less than 20% of the total computer capacity. Tier 0 is responsible for the safe-keeping of the raw data (first copy), first pass reconstruction, distribution of raw data and reconstruction output to the Tier 1s, and reprocessing of data during LHC down-times.
- Tier 1 corresponds to thirteen large computer centres with sufficient storage capacity and with round-the-clock support for the Grid. They are responsible for the safe-keeping of a proportional share of raw and reconstructed data, large-scale reprocessing and safe-keeping of corresponding output, distribution of data to Tier 2s and safe-keeping of a share of simulated data produced at these Tier 2s.
- Tier 2 are typically universities and other scientific institutes, which can store sufficient data and provide adequate computing power for specific analysis tasks. They handle analysis requirements and proportional share of simulated event production and reconstruction. There are currently around 160 Tier 2 sites covering most of the globe.
- Tier 3 corresponds to computing resources, which can consist of local clusters in a University Department or even just an individual PC. There is no formal engagement between WLCG and Tier 3 resources.

The most effective systems here are Tier-1 clusters, which are represented by well-organized and powerful computing systems of participating national organizations and countries. In order to test the performance of National Research Center "Kurchatov Institute" Tier-1 cluster (ANALY_RRC-KI-T1) and compare it with other WLCG sites, 50k of 2-jet ggF Higgs boson production events were generated with aMC_NLO Monte Carlo generator [15]. The results of this simulation are indicated in Table 2.

WLCG Site	nEventsPerJob	nFiles	CPU Time, HS06 seconds	
			Expected	Total
ANALY_RRC-KI-T1	5000	10	28500000	17197806
ANALY_DESY-HH	5000	10	19550000	11357616
ANALY_INFN-LECCE	5000	10	17648874	10350000
ANALY_GLASGOW_SL6	5000	10	15050000	9020417
ANALY_IN2P3-CC	5000	10	15250000	4677853
ANALY_TOKYO_ARC	5000	10	14000000	9457170

Table 2. Parameters of 2-jet ggF Higgs boson Monte Carlo production at several WLCG sites.

The results of performance tests can vary depending on the condition of each individual machine, its occupancy and some other parameters. However, the performance of considered GRID sites are close to each other. Similar expected times mean that clusters offer similar compute power as estimated by their specifications and certain benchmarks, while similar total times means that the ratio of actual to expected performance is similar across all clusters.

5. Conclusion

High performance computing systems are now an integral part of the high energy physics landscape. One of the main physics fields where HPC has a major impact are the Higgs boson studies. Increasing precision of measurements in particle physics leads to a complexity of subsidiary calculations and HPC is a great resource to work with. It is also important to notice that some analyses require even more precision. They have to use next-to-next-to-leading order corrections (NNLO). Thus, the complexity of calculations will continue to increase in the near future.

In this paper, a brief overview of the high performance computing systems was presented. An overview of the Titan supercomputer was provided, and its capabilities for the Higgs boson physics was demonstrated. Performance of NRC-KI Computing cluster was studied and comparison with other ATLAS GRID sites was shown. This comparison demonstrates that NRC-KI Computing cluster is capable of handling tasks in high energy physics computing on par with other ATLAS GRID sites.

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