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Hannes.Bartosik@cern.ch

Performance of space charge simulations using High Performance Computing (HPC) cluster

H. Bartosik, G. Rumolo

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Summary

In 2016 a collaboration agreement between CERN and *Istituto Nazionale di Fisica Nucleare* (INFN) through its *Centro Nazionale Analisi Fotogrammi* (CNAF, Bologna) was signed [1], which foresaw the purchase and installation of a cluster of 20 nodes with 32 cores each, connected with InfiniBand, at CNAF for the use of CERN members to develop parallelized codes as well as conduct massive simulation campaigns with the already available parallelized tools. As outlined in [1], after the installation and the set up of the first 12 nodes, the green light to proceed with the procurement and installation of the next 8 nodes can be given only after successfully passing an acceptance test based on two specific benchmark runs. This condition is necessary to consider the first batch of the cluster operational and complying with the desired performance specifications.
In this brief note, we report the results of the above mentioned acceptance tests.

1 Introduction

In May 2016, a common project was undertaken by CERN and the *Istituto Nazionale di Fisica Nucleare* (INFN), through its *Centro Nazionale Analisi Fotogrammi* (CNAF, Bologna), to provide the infrastructure enabling advanced calculation in the framework of the High-Luminosity LHC (HL-LHC) and LHC Injectors Upgrade (LIU) projects. In particular, the project was aimed at setting up the computing environment to allow:

- Beam dynamics simulations using parallelized codes;
- Optimization of the existing codes to improve their performance with the IT resources of INFN-CNAF;
- Development of codes for cutting-edge High Performance Computing platforms.

The hardware involved, to be physically located at CNAF, consists of a cluster of 20 nodes with 32 Intel 2683-v4 cores each, with InfiniBand connection, to be used by CERN users in the execution of the project. The project is planned to unfold through the following phases:

- Purchase, installation and configuration of the first 12 nodes;
- Successful completion of benchmark runs with the performance described in Fig.1 (i.e. the acceptance test);
- Purchase, installation and configuration of the remaining 8 nodes;
- Four year operation period (estimated lifetime of the cluster) during which the cluster is fully exploited under the CNAF maintenance and support within the limits specified in [1].

Parameters	PSB	PS
Length	157 m	628 m
# macro-particles [10^3]	500	250
# turns/job	1000 to 5000	500
# space-charge nodes	~200	~70
Space-charge calculation method	Direct	Direct + indirect
Physical model (machine lattice)	Linear (+ space charge)	Non-linear (+ space charge)
Maximum required wall clock time for the simulation	<2 s/turn	<20 s/turn

Figure 1: Extract of the Annex 1 of [1]. The first part of the cluster with 12 nodes will be deemed operational after the successful completion of the benchmark runs with the PyORBIT code provided by CERN with the parameters and desired duration of the simulations outlined in the table above.

2 The execution of the acceptance test

First of all, the PyORBIT code [2], which is widely used at CERN for beam dynamics simulations under strong space charge mainly in the LHC injectors, was successfully compiled on the cluster. After installing all the required packages, the existing MPI version of the code could also be run correctly both interactively and by submitting the jobs to the existing LSF queues. The simulation cases of the PSB and of the PS shown in Fig. 1 were run with an increasing number of cores. The main findings are:

- Excellent scalability with number of cores thanks to the InfiniBand connection between nodes (see Fig. 2);
- The acceptance criteria mentioned in [1] are met when running with 64 physical cores for the PSB case and with 32 physical cores for the PS case. In particular, the execution of a single turn of the simulation setup for the PSB case described in Fig.1 takes about 100 s with a single CPU, while with 64 physical cores (requesting 128 at job submission with HyperThreading) it takes about 1.9 s. For the PS, the run with a single CPU takes about 500 s per turn while with 32 physical cores it takes about 20 s.

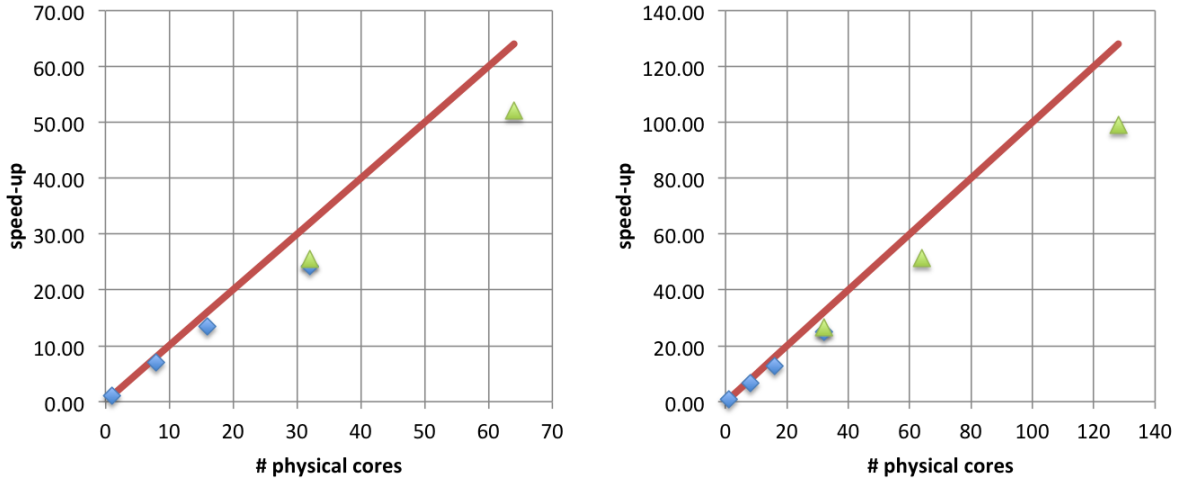

Figure 2: Speed-up factor as a function of the number of physical cores for the PSB (left) and PS (right) benchmark runs. For the cases indicated by the green markers the number of cores requested at job submission was double compared to the number of physical cores actually used in the simulation due to HyperThreading.

Therefore, the acceptance test can be declared successfully passed and the second phase of the project can be launched.

References

[1] Collaboration agreement Contract nr. KE3108/BE "Related to the development of computing resources for beam dynamics simulations relevant for the upgrade of LHC and its injectors"

[2] PyORBIT code, https://github.com/PyORBIT-Collaboration/