INFN Computing interests for Particle and Astroparticle Physics

T. Boccali[1], G. Carlino[2], L. Dell'Agnello[3], C. Grandi[4], D. Lucchesi[5], G. Maron[3], D. Menasce[6], L. Perini[7], D. Salomoni[3], P.Vicini[8], A. Zoccoli[9]
[1] INFN Sezione di Pisa
[2] INFN Sezione di Napoli
[3]CNAF Bologna
[4] INFN Sezione di Bologna
[5] University and INFN Padova
[6] INFN Sezione di Milano
[7] University and INFN Milano
[8] INFN Sezione di Roma
[9] University and INFN Bologna

Abstract

The INFN sees two major areas of application for high energy physics computing in the time scale relevant for the Snowmass process: the exploitation of high performance computing (HPC) and the use of Quantum Computing. The first one can be realized within a few years, with high energy physics experiments becoming major users of HPC. Quantum computing is still at the level of research and development, but it can be the new disruptive technology changing the computing horizon. A possible exploitation of the former and the research and development of the latter are described in the document.

The path toward HEP High Performance Computing

Scientific and technological context

The computing for HEP relies today heavily on in-house custom-built computing farms, glued by the GRID middleware as developed in the previous decades, referred to as High Throughput Computing (HTC). Experiments' Computing Models are constantly evolving, with a slow but steady transition towards a smaller list of requirements, helped, in this process, by recent technologies allowing resource virtualization. As of today, even if not predominant, Cloud access is already a reality for all medium-large size experiments, while not in the initial Computing Models.

At the same time, mostly due to concerns about the sustainability of the HEP-specific infrastructure and of its middleware, larger experiments have prototyped the utilization of HPC systems. This comes from a variety of factors:

- The availability of large sized research grants from HPC centers for HEP use cases. A typical PRACE HPC [1] system deploys computing resources comparable to the current full HEP scale.
- The push by funding agencies and countries gouvernements to avoid the deployment of two parallel HPC and HTC infrastructures. While the former is seen as strategic beyond science purposes (for technological and industrial leadership), the latter has a smaller overall strategic impact, and thus is felt as less important at continental and national scale.

An efficient use of HPC systems by High Energy Physics experiments is not trivial, since these systems are custom-built having in mind use cases largely different from the HEP ones. Such science-related use cases range from Lattice QCD to astrophysical simulations, material sciences, simulations of nuclear systems.

While the PRACE long term roadmap beyond 2020 is still not completely clear, the EuroHPC JU initiative will be active up to 2023 to fund three EU level pre-exascale[2] systems (one in Italy), followed shortly by actual Exascale systems. Technologies are not finalized yet, but at least for pre-exascale deployments this will involve the utilization of system accelerators, like GPGPU or FPGA.

In the next future, the European HPC arena will be enriched by a number of initiatives focusing on the development of European based technology and its adoption in future HPC systems:

- The FET-HPC EU funded projects are working on the evaluation of selected technologies to implement a) low-power, high granularity, scalable systems and b) configurable, high performance computing

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[1] See CINECA Marconi as an example, http://www.hpc.cineca.it/hardware/marconi

[2] https://www.etp4hpc.eu/euexascale.html

acceleration based on FPGA. Prototypes will soon be available and open to scientific communities;
- The outputs of R&D projects will be the enabling technologies for HPC ExaScale systems to be funded in the next decade in the framework of EuroHPC JU initiative.
- The just launched European Processor Initiative (EPI), aims to define and prototype a low power high performance CPU and a computing task acceleration architecture leveraging previous design experiences and technologies know-how from academic, research and industrial European partners.

Objectives

The panorama is quite complex. There are differences between the computing approaches in HEP and in HPC that need to be overcome. The political environment is evolving quickly towards directions that may not be suited for HEP. The major objectives that INFN believes are to be pursued are the following:

- the adaptation of current and future experiments software to tap into the enormous computing power EuroHPC JU funded systems will deploy in the next decade in Europe;
- a world wide collaboration between HPC providers and HEP experiments to define a common path for the use of HPC resources;
- the contribution of HEP experiments to European/Worldwide efforts for the development of HPC systems and infrastructures.

Quantum Technologies for HEP

Scientific and technological contest

Quantum Technologies are emerging in research and in industry: it's important now to identify generic systems in which the peculiar characteristics of quantum systems can be used to perform measurements which are not possible in classical systems.

At least 3 different aspects of quantum technologies can be relevant for HEP:

1. Quantum sensing, in which detectors use the peculiarities of quantum states in order to perform measurements on a physical system;they are outside the scope of this letter;
2. Quantum simulators, which use a quantum system to simulate other quantum systems; they can be used to simulate, on controlled systems the behavior, of particles subject to specific interactions;
3. Quantum computers, which use the peculiar capability of quantum systems to perform "parallel" computations, ideally outside the possibilities of classical computers ("quantum supremacy").

The roadmap towards an available quantum computer competitive for general utilization is not clear yet. Even though several vendors (Microsoft, IBM, Google, Amazon, Rigetti, ...) are providing access to small quantum machines or emulators via Cloud-like interfaces; these systems are useful for initial R&D, but too small for practical HEP applications at the moment.

The European Commission has launched the Quantum Flagship Program[3] with the ambition to drive the quantum revolution in Europe, and large programs exist in the US. A strict collaboration is essential, in particular when approaching the QC for HEP usage; this should include theoretical and applications level studies (see for example[4,5]) and a partnership for accessing quantum machines and emulators. A very good example of collaboration, albeit on more technical aspects, has been announced between multiple US institutions and INFN[6,7].

It seems realistic to assume that Quantum Technologies will have in the future a large impact on our computing, while being outside the scope of the next decade. Still, it is important for the field to start explorations and studies in order to speed-up the technology, and to be ready for its adoption whenever possible.

Objectives, Methodology and Challenges

The objective we feel worthwhile to pursue is to involve HEP groups in the relevant research, in a way to make sure the capabilities and the performances of the systems are understood from the theoretical point of view. At the same time, we consider it important to test use cases and problems on the available emulators and small systems, in order to

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[3] https://qt.eu/

[4] https://www.nature.com/articles/nature24047

[5] https://arxiv.org/abs/2004.13747

[6] https://news.fnal.gov/2020/08/fermilab-to-lead-115-million-national-quantum-initiative-center-to-build-revolutionary-quantum-computer-with-rigetti-computing-northwestern-university-ames-laboratory-nasa-infn-and-additional-par/

[7] LoI "INFN interests in Quantum Science and Technology for Particle and Astroparticle Physics" at Snowmass 2021

gain experience in case a major technological breakthrough happens and new workable systems appear on the market. In this approach the economic investment is rather moderate, but the return is, potentially, huge in case the technology panorama makes progress more quicker than expected today.

One clear use case of quantum simulator for HEP would be the realization of simulators of the particle interactions, as done today via algorithmic code (Pythia, Madgraph, Herwig, Sherpa, Alpgen, …).

While in principle the generation process, via such tools, does not necessarily scale with the luminosity of accelerator experiments, in practice the precision measurements planned in the next 10 years will need more accurate simulations, with generators precise up to higher order in the resummation and perturbative orders. These are known to require larger and larger processing times on classical computing systems, and can represent, for example, a non-negligible fraction of all the HL-LHC computing resources. A quantum simulator of specific standard model processes (QCD, EM, even single diagrams) is in principle exact, and does not need the utilization of perturbations or such. While far from being possible today, it could effectively replace a part of the generation process when interfaced to standard computing resources.

As of today, the use of quantum computers in HEP can be at the level or R&D. Such computers have their strength in the simultaneous application of an algorithm of many states in parallel, in principle being very well suited for applications which show an explosion in the number of possible combinations. In addition, the capability to probe large portions of the accessible phase space even in multidimensional functions, theoretically allows one to use quantum computers as “generic minimizers”. Such minimization capabilities offer a clear link towards another major area of Computing: Machine Learning, with expected applications important for the HEP experiments in fields like the Reconstruction, the Simulation of the interaction between particles and the detector materials, and the final user analysis. Indeed, in the presence of a very high dimension minimizer, Machine Learning could easily become the easiest application to port to Quantum Computing, and as such pave the way for its adoption in the field.

There are many aspects specific to HEP which need more technological understanding, like the quite peculiar need by HEP algorithms to be fed with large amounts of data, an I/O problem of unclarified applicability at the moment.

Since quantum computing requires a general and complete rethinking of the way HEP algorithms are written, beyond the typical experience of HEP scientists, a program of training on quantum computer utilization and programming (being it in Cirq, Q#, QISKit or any other available or future language, or even simply via interfacing to Tensorflow for Machine Learning training) is absolutely necessary and should be properly fostered. At the same time, a close collaboration with the experts in the field of algorithm translation / porting / design should be established, in order to have guidance on the best practices and training about the best ways to use quantum computing.