Supporting advanced HPC/HTC scientific workloads with QCG services

All researchers agree that efficiency, flexibility and ease of execution of scientific computation workloads were always key requirements of in-silico experiments. Nowadays, when the computational facilities reach exascale and the complexity of applications increases, the situation hasn't changed. There are still the same questions and unresolved practical problems how to perform computations easily and effectively.

Trying to address the growing needs of science, the QCG services and tools have been developed and offered to the various research communities, e.g. fusion[1], biomedicine[2], hydrology[3] or quantum chemistry[4]. Basically, QCG is a comprehensive environment for execution of complex workloads on distributed HPC/HTC resources. It supports and simplifies execution of different application scenarios, starting from regular parallel (MPI/OpenMP) jobs, through parameter sweep, distributed workflows and finishing on multi-scale assets. For its users, QCG offers generic client-tools (command line, web, desktop) that can be easily adjusted to specific needs and preferences of more specific use-cases[5]. Additionally, in order to enhance flexibility and efficiency of more demanding application scenarios, QCG delivers a lightweight pilot job implementation.

The presentation will include both a description of the basic functionality of QCG as well as a discussion about the applicability of QCG solutions for diverse scenarios, from simple ones to highly-demanding.

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