Leverage large-scale HPC machines with QCG-PilotJob

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Effectively executing a huge number of conceptually different tasks on large-scale computing resources, as current multi-peta flop machines and emerging exa-scale ones, is challenging in many aspects. One of the main technical problems is the fact that basic mechanisms available on HPC infrastructures promote large tasks over many small tasks. Thus, when the execution scenarios require running a large set of replicas or ensembles, such as in the case of Uncertainty Quantification, the standard mechanisms are no longer sufficient.

This issue may be addressed in different ways. Our proposition is QCG-PilotJob - a lightweight, fully user-space software that brings an additional level of scheduling over the regular mechanisms available on HPC machines or clusters. With this concept, only a single QCG-PilotJob task is submitted for the execution, but once it is started, it plays a role of a user's personal queuing system. New tasks can be easily added to the running QCG-PilotJob instance by a user, or programmatically, while the service will take care of its proper execution. What is exceptional, QCG-PilotJob, in contrast to the other similar software, can be installed by a regular user, without any intervention of administrators.

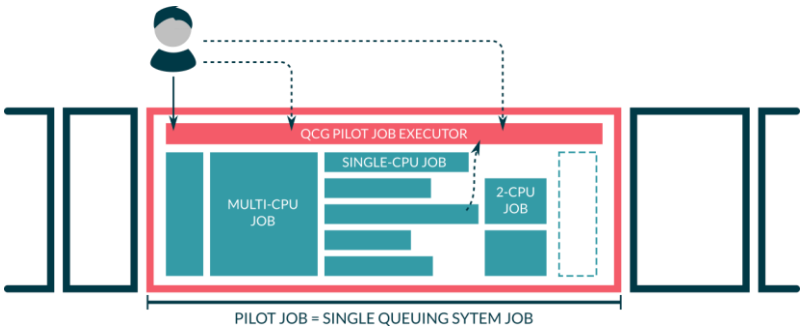

Figure 1 *QCG-PilotJob is a user-level service that supervises tasks run within an allocation. It can be started in batch mode, but also accessed dynamically with Python API or remote interface*

The key importance when designing and developing QCG-PilotJob was to ensure good efficiency and scalability of the software. Although we are still in the process of enhancing the tool's capabilities in this matter, the scalability tests performed recently on several large-scale resources, including Archer2 in UK, Carthesius at SurfSARA, SuperMuc-NG at LRZ and Altair at PSNC, confirmed the readiness of its current version for the application for real-world demanding use-cases. It is worth mentioning that QCG-PilotJob has been already used by several groups of scientists from different domains, including Nuclear Fusion, Materials, Air Pollution as well as Medicine.