

QosCosGrid – new middleware for new communities

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The QosCosGrid (QCG) middleware is an integrated system offering advanced job and resource management capabilities to deliver to end-users supercomputer-like performance and structure. By connecting many distributed computing resources together, QCG offers highly efficient mapping, execution and monitoring capabilities for variety of applications, such as parameter sweep, workflows, MPI or hybrid MPI-OpenMP. Thanks to QosCosGrid, large-scale applications, multi-scale or complex computing models written in Fortran, C, C++ or Java can be automatically distributed over a network of computing resources with guaranteed QoS. The middleware provides also a set of unique features, such as advance reservation and co-allocation of distributed computing resources.

The QosCosGrid middleware consists of two logical layers: Grid and local one. The Grid-level QCG-Broker (metascheduler) that controls, schedules and generally supervises the execution of tasks that are spread between independent administrative domains. QCG-Broker is based on dynamic resource selection, mapping and advanced scheduling methodology, combined with feedback control architecture, deals with dynamic Grid environment and resource management challenges, e.g. load-balancing among clusters, remote job control or file staging support. The QCG-Broker metascheduling service in QCG is in tight cooperation with administrative domain-level component: the QCG-Computing service, which provides comprehensive dynamic information about the current cluster status. The QCG-Computing service, deployed on access nodes of the batch systems like Torque, PBS Pro or SLURM, is able to provide secure and efficient remote job management capabilities over standardized OGSA-BES interface. The other important component of the QosCosGrid stack is the QCG-Notification service, which serves as the main message bus between the services, applications and the end-user. It is capable of sending notifications using variety of transport mechanism, including SOAP, SMTP and, what is a unique feature, the XMPP protocol.

The QosCosGrid middleware was deployed within the Polish National Grid Initiative (PL-Grid)[3] where it provides a unified interface for computing and storage resources offered by leading HPC centers in Poland. We have managed to successfully integrate many new services and tools to build a new multilayered e-Infrastructure to make it deal efficiently with computationally intensive large-scale simulations, including parameter sweep, workflows and more importantly large parallel applications. QosCosGrid is used on daily basis by many researchers in Poland coming from various research domains such as quantum chemistry, nanotechnology, metallurgy, astrophysics and bioinformatics and its currently the first middleware in PL-Grid counting the cpu hours consumed by its users.

From the end-user point of view QosCosGrid offers two main user tools: a command line QCG-Broker client called QCG-SimpleClient and a GUI application called QCG-Icon. The QCG-SimpleClient application is a set of command line tools, inspired by the simplicity of batch system commands, that allow user to submit, control and monitor large number of grid batch jobs. The learning effort needed to start using QCG-SimpleClient is relatively small as the job description file is a plain BASH script file only annotated with #QCG directives.

QCG-Icon is a desktop application written specifically for the Windows platform, but with Linux and Mac OSX distribution available also. It was designed to enable the selected applications installed on the computing resources of the PL-Grid infrastructure, and available through the QosCosGrid services. While developing QCG-Icon special emphasis was put on the following fact: using an application installed in the grid environment should be as intuitive as using a locally installed application. At the moment, the QCG-Icon support large portfolio of applications, including MATLAB, R, NAMD, Gaussian (integrated also with GaussView), GAMESS, Molpro, LAMMPS, Quantum ESPRESSO, GROMACS. Any other application can be also run as soon as a proper BASH script is provided.

In October 2012 a memorandum of understanding was signed between EGI.eu and Poznan Supercomputing and Networking Center. This document was an official step toward sustainable deployment of the QosCosGrid stack into the European grid ecosystem. The collaboration will focus both on integrating the contributed software components into the operational infrastructure, i.e., monitoring, accounting, information, support services and conducting joint dissemination activities.

Moreover the QosCosGrid middleware has been recently extended to support authorization mechanism based on Virtual Organization Management Support (VOMS) infrastructure. This new capability facilitates adoption of the QosCosGrid stack by existing Virtual Organizations and resource providers.

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