



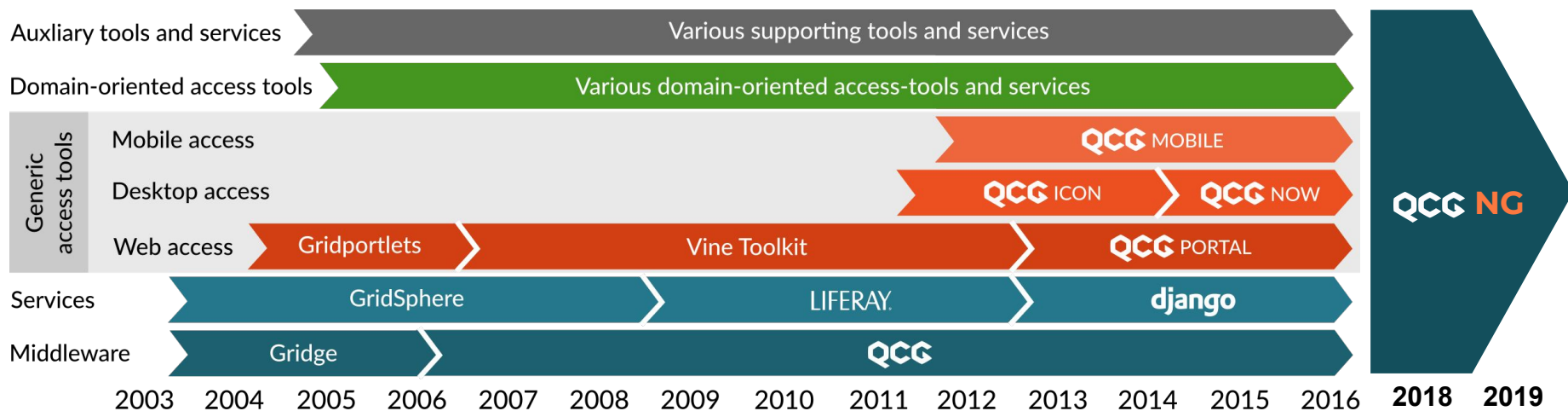
Supporting advanced HPC/HTC scientific workloads with QCG services



Bartosz Bosak, Piotr Kopta, Tomasz Piontek
{bbosak, pkopta, piontek}@man.poznan.pl
Poznan Supercomputing and Networking Center

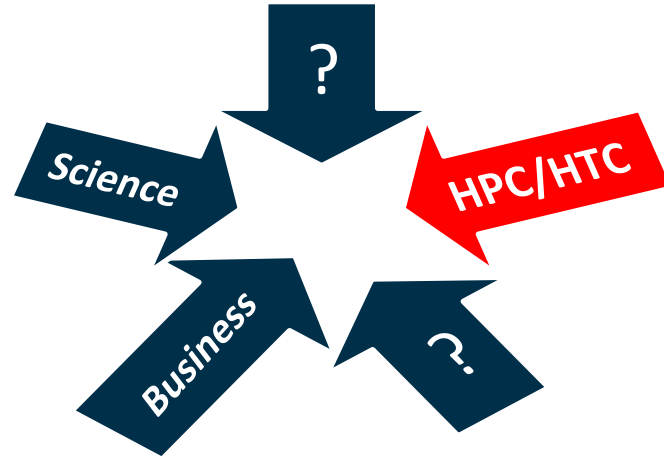
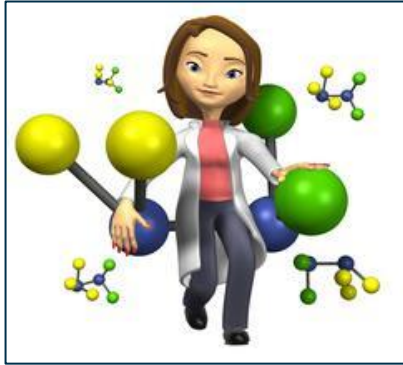


A bit of history



Our motivation

It is not enough to give scientist access to resources. They need tools and support.



The world has changed... We cannot ignore this fact

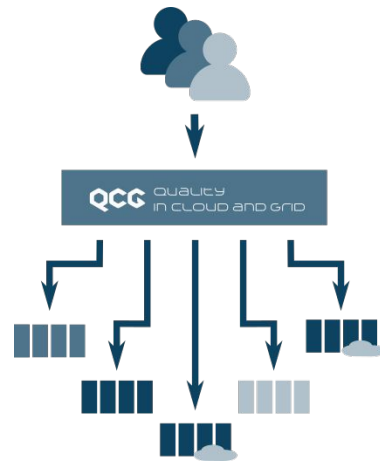


Most of the new users need easy and intuitive tools to overcome the initial barrier in accessing the infrastructure



The idea

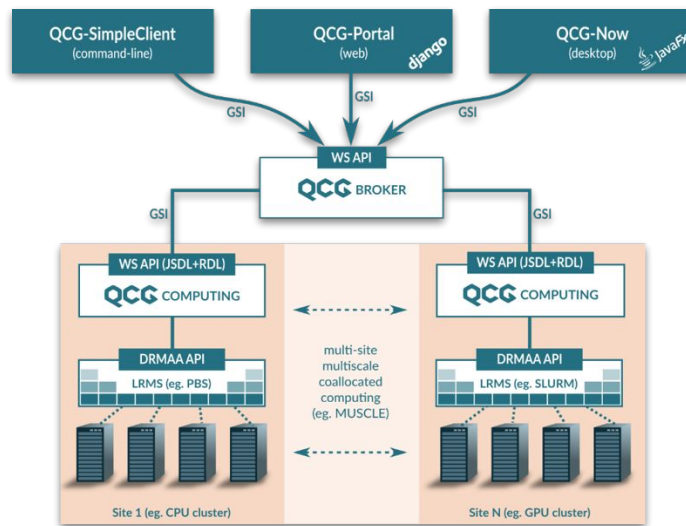
- > QCG is a set of services, tools and libraries providing uniform and efficient access to HPC/HTC resources.
- > Integrates many computing resources, but preserves simplicity of execution on a single machine.
- > Provides highly efficient mapping for a variety of applications, such as parameter sweep, workflows, MPI or hybrid MPI-OpenMP, GPGPU, and multiscale.
- > **Useful and applicable for both experienced and novice users.**



<http://www.qoscosgrid.org>



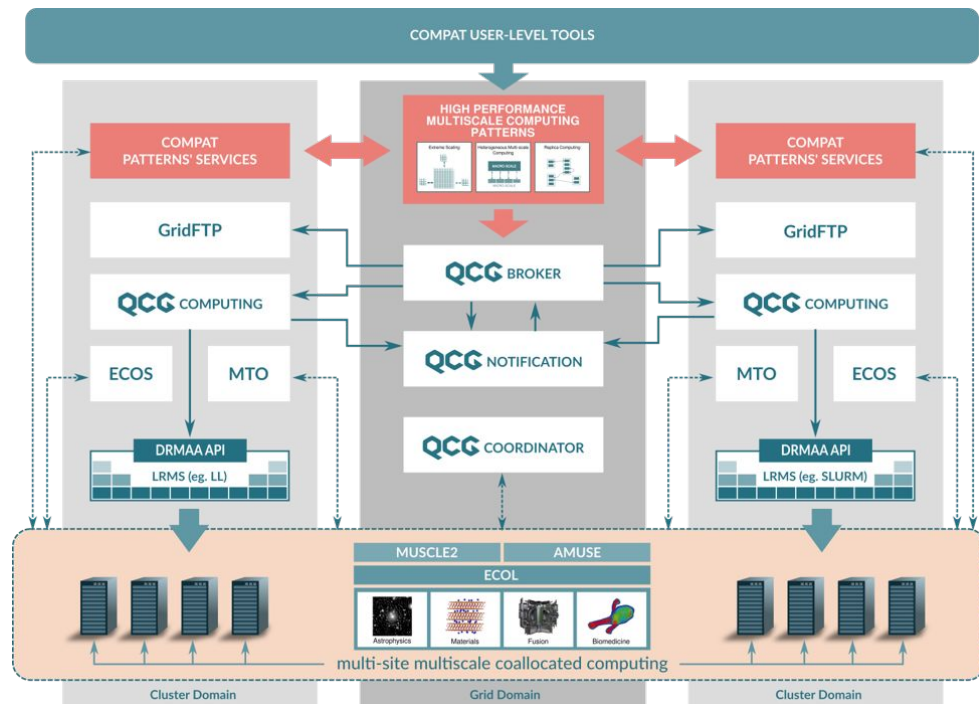
Architecture



- > QCG consists of three basic layers:
 - Client tools
 - High-level services (common)
 - Cluster-level services



Architecture (2)





Basic services: QCG-Computing

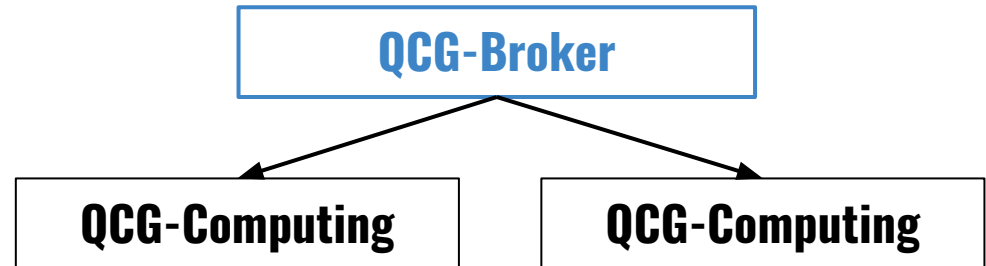
- > Deployed on access nodes of the batch systems (Slurm, SGE, Slurm, torque/maui, LoadLeveler, PBS Pro, Condor, Apple Xgrid)
- > Provides remote access to task submission and advance reservation capabilities of LRMS via DRMAA interface (the own DRMAA implementations)
- > Compatible with the OGF HPC Basic Profile specification (JSDL and BES)

QCG-Computing
Queueing system
Resource



Basic services: QCG-Broker

- > Offers capabilities for scheduling and brokering of jobs
- > supports multi criteria approaches taking into consideration many criteria like energy and resources consumption as well as time-to-finish
- > Controls the execution of whole experiments (including workflows and parameter sweep tasks)
- > Provides requested QoS and co-allocates resources
- > Stages in/out files and directories (the main transport mechanism based on gridFTP)





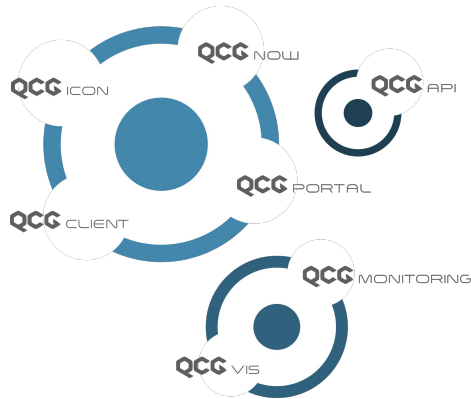
Basic services: QCG-Notification

- > Supports the topic-based publish/subscribe pattern for asynchronous message exchange
- > Serves as the main message bus between the services, applications and the end-user
- > Is capable of sending notifications using variety of transport mechanism, including SOAP, SMTP and XMPP (notifications for users)
- > All major QCG clients indirectly use QCG-Notification to support tracking of statuses and progress of executed application (mail, XMPP, QCG-Monitoring)





Client tools & libs



Users are interested in
tools not services ...

- > Scientists have different preferences in accessing the infrastructure what results in the necessity to provide them with various tools tailored to their habits and expectations. (Swiss army knife approach often fails).
- > Users very often can accept the fact that their jobs need long time to be finished but they would like to know when they finish.
- > For long running simulations users need a possibility to see partial results and to control the execution.



Client tools: QCG-Client

- > Set of commands modelled on queuing system tools
- > QCG-Simple, JSDL, QCG-XML description dialects
- > Detailed information about running and historical tasks
- > Support for interactive tasks
- > Automatic staging in/out files with gridFTP
- > Single access point to all resources

```
#QCG note=NAMD apoa1
#QCG host=hydra.icm.edu.pl

#QCG walltime=PT10M
#QCG queue=plgrid
#QCG nodes=1:12:12
#QCG output=apoa1.output
#QCG error=apoa1.error
#QCG application=NAMD
#QCG argument=apoa1/apoa1.namd
#QCG stage-in-file=apoa1.zip
#QCG preprocess=unzip apoa1.zip
#QCG stage-out-dir=. -> results
#QCG notify=xmpp:tomasz.piontek@plgrid.pl
#QCG watch-output=mailto:tp@mail,20,ENERGY
```



Client tools: QCG-Client (2)

- > Submission and control of tasks:
 - **qcg-cancel** - cancel task(s)
 - **qcg-clean** - clean the working directories of given tasks
 - **qcg-connect** - establish interactive session to the task
 - **qcg-info** - display detailed information about the given tasks
 - **qcg-list** - list tasks in the system
 - **qcg-peek** - display ending of (stdout, stderr) streams
 - **qcg-refetch** - retry/repeat the transfer of output files/directories
 - **qcg-sub** - submit batch or interactive tasks to be processes by QCG
- > Reservation and control of resources:
 - **qcg-rcancel** - cancel reservation(s)
 - **qcg-reserve** - reserve resources
 - **qcg-rinfo** - display information about the given reservation(s)
 - **qcg-rlist** - list reservation in the system
- > Information about resources:
 - **qcg-offer** - provides detailed information about all managed resources, e.g. list of available applications, list of available modules, current load



Client tools: QCG-Portal

- > A web client to QCG, based on the Django framework
- > Offers functionality needed to submit, monitor and manage jobs over QCG middleware
- > Authentication/authorization based on OpenID
- > Includes built-in support for the gridFTP protocol
- > Support for job templates
- > In principle easily extendable and adaptable to certain needs
- > Several ready application / domain based solutions built on top of QCG-Portal



Client tools: QCG-Portal (2)

QosCosGrid Portal Jobs Submit job GridFTP Maciej Tronowski

Jobs list

Search term

Selected filters: **Finished** **Hydra** **Moss** **Zeus** Clear all filters

< 1 > of 1

	Description	Submission	Start	End	Status	Host	
	opisowy opis	03/18/2016 3:05 p.m.	03/18/2016 3:05 p.m.	03/18/2016 3:29 p.m.	FINISHED	hydra	more
		03/18/2016 4:02 p.m.	03/18/2016 4:02 p.m.	03/18/2016 4:28 p.m.	FINISHED	moss	more
	python script	01/25/2016 1:37 p.m.	01/25/2016 1:37 p.m.	01/25/2016 1:38 p.m.	FINISHED	zeus	more
		01/25/2016 1:35 p.m.	01/25/2016 1:35 p.m.	01/25/2016 1:36 p.m.	FINISHED	zeus	more
	basic task	01/19/2016 2:29 p.m.	01/19/2016 2:29 p.m.	01/19/2016 2:30 p.m.	FINISHED	hydra	more
	basic task	01/19/2016 2:15 p.m.	01/19/2016 2:15 p.m.	01/19/2016 2:15 p.m.	FINISHED	hydra	more
	basic task	01/19/2016 2:11 p.m.	01/19/2016 2:11 p.m.	01/19/2016 2:11 p.m.	FINISHED	hydra	more
	basic task	01/19/2016 2:07 p.m.	01/19/2016 2:07 p.m.	01/19/2016 2:07 p.m.	FINISHED	hydra	more

1 of 1

QosCosGrid Portal Jobs Submit job GridFTP Maciej Tronowski

Submit job

Save as template

Basic Resources Files Environment Monitoring Others

Host

Queue

Properties

Modules

Processes

Nodes topology

Wait time Seconds

Memory (MB)

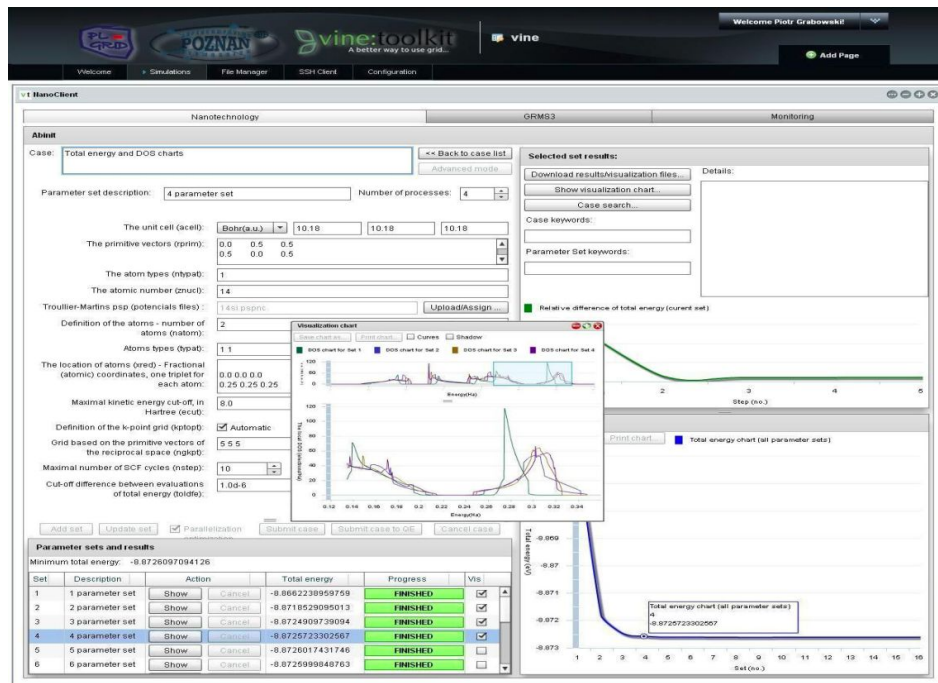
Memory per process (MB)

Reservation



Client tools: QCG-Science-Gateways

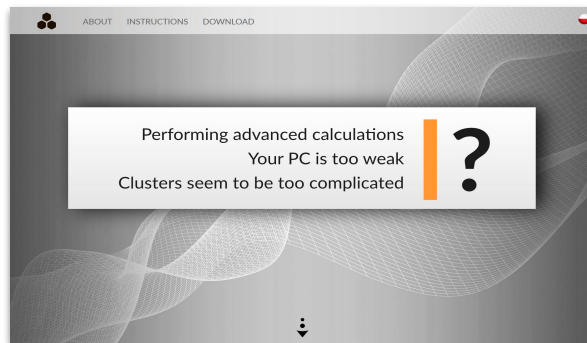
- Domain or problem oriented, highly specialized portal solutions





Client tools:
QCG-Now

- > A desktop (GUI) tool for submission of jobs to computing resources made available with QCG middleware.
- > Available as an installable package for Windows, Linux and OS X.
- > Integrated support for data transfer and application monitoring.
- > Support for job templates and command-line submission (easy integration with other applications).

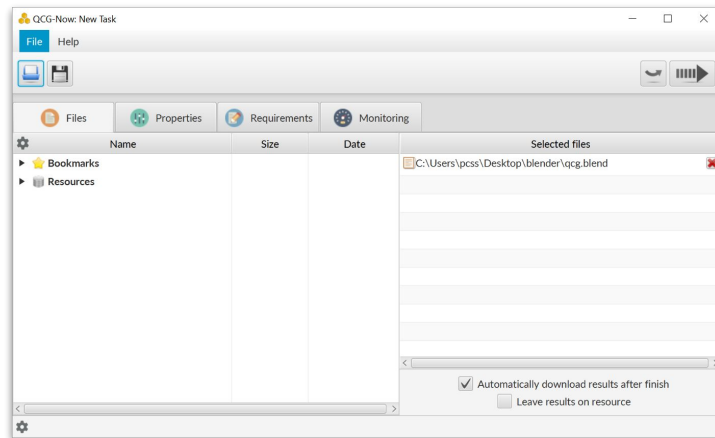


<http://www.qoscosgrid.org/qcg-now>

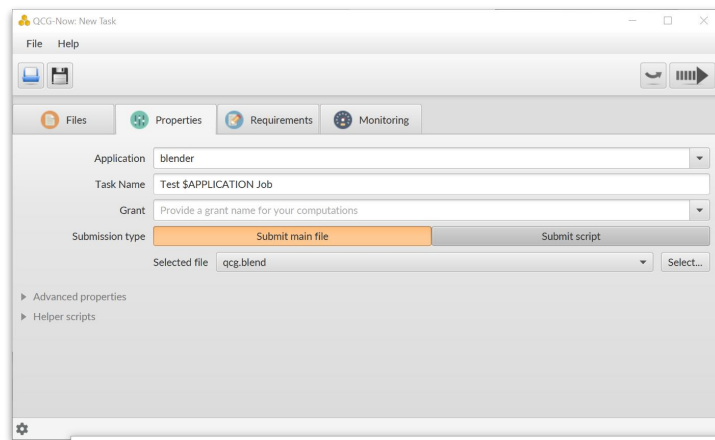


Client tools: QCG-Now (2)

Task definition view - files



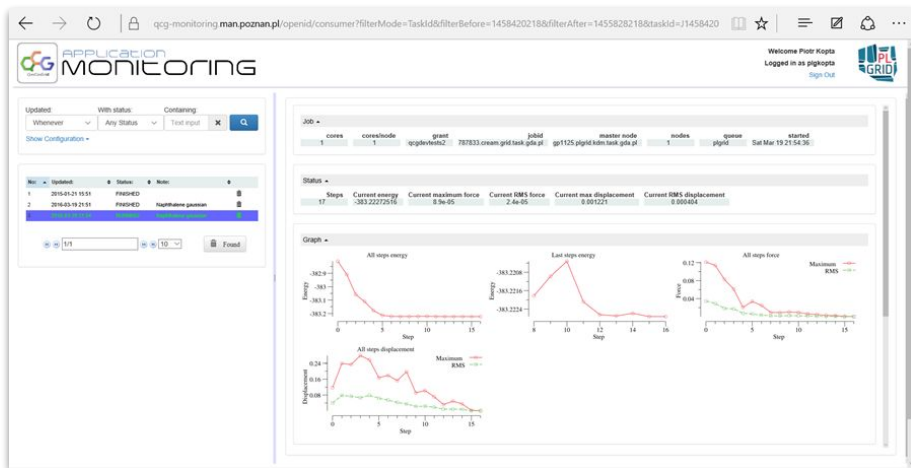
Task definition view - properties





Client tools: QCG-Monitoring

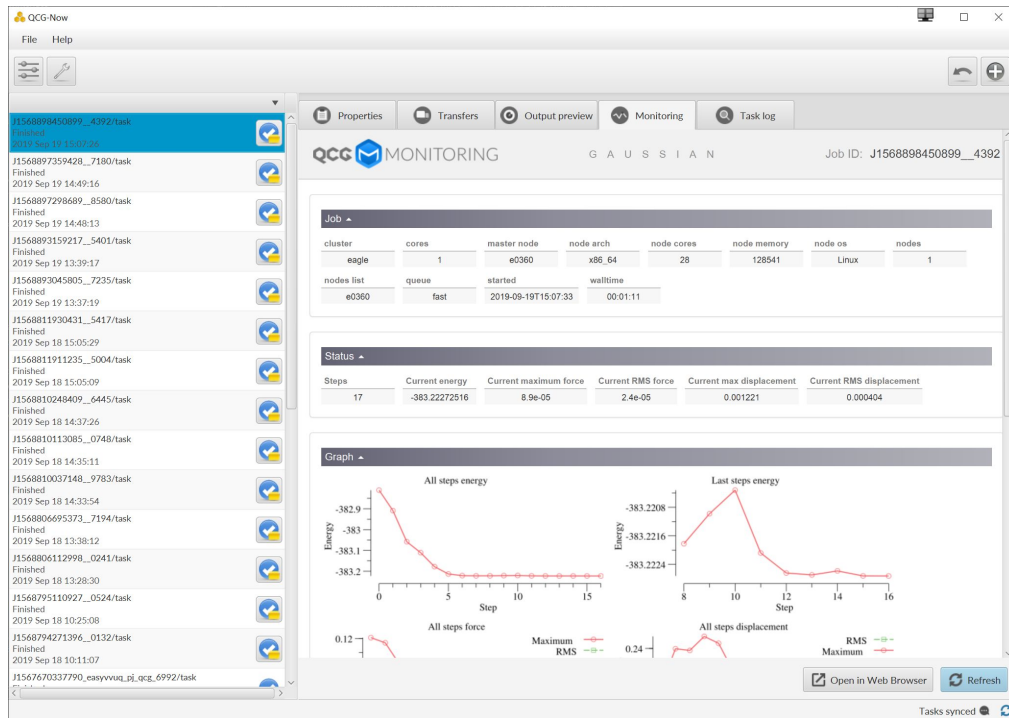
- Monitoring progress of long-lasting jobs
- Cyclic scanning of output files
- Current status presented with text messages, tables, graphs and pictures
- Predefined schemes for different types of applications (e.g. Gaussian)
- Integrated with QCG-Client, QCG-Portal and QCG-Now



QCG-Monitoring

An example monitoring scheme in QCG-Now

- Integration of QCG-Monitoring with QCG-Now (in the testing phase)

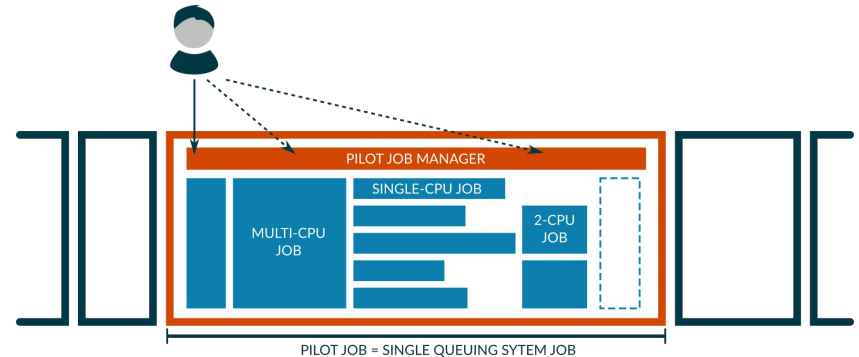




QCG-PilotJob Manager

HTC scenarios are also important ...

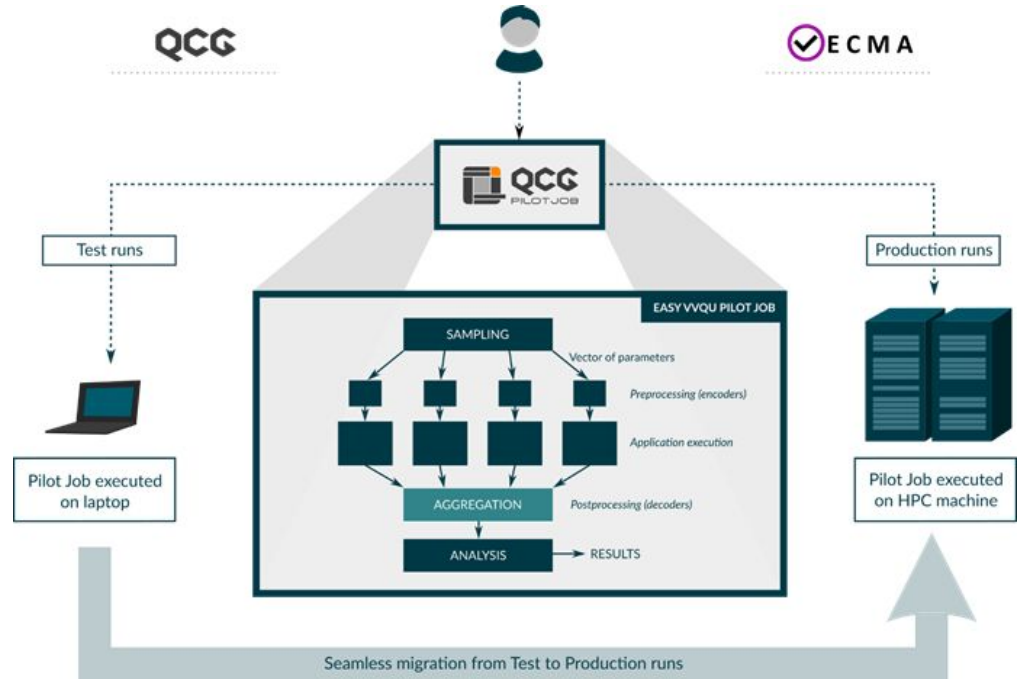
- > Schedules and manages a set of tasks on already allocated resources:
 - to eliminate waiting of every single task in a queue
 - to better utilize resources (better resource granularity)
 - to „overcome“ local administrative policies
- > Can read requests from various sources: file or network socket (static vs dynamic scenario)
- > Contains API (Python) for communication with user programs





QCG-PilotJob Manager

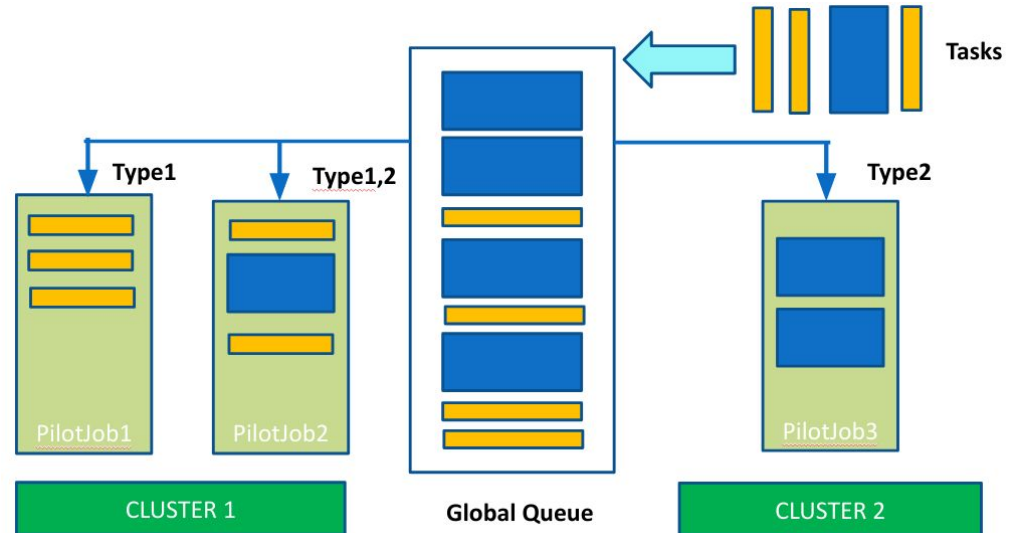
- > Integration of QCG-PJM with EasyVVUQ for uncertainty quantification in the VECMA project





QCG-PilotJob Manager (future plans)

- > Ongoing work on introducing the concept of a global queue
 - to use resources of many clusters
 - to adjust the amount of resources to the current need of the application by adding new allocations when needed
 - to support exascale examples
- > Integration with the QCG-Monitoring system (almost done)





QCG-Comp-NG

QCG Next Generation services

Transition to new technologies

- > Micro-services approach for HA
- > Unified interface on cluster and 'grid' levels
- > Implemented in Python with modular approach
- > REST interfaces
- > New authentication and authorization
- > First version deployed and validated at PSNC as a part of external commercial system



kubernetes



{ REST }





QCG-Comp-NG

QCG Next Generation Tools - Portal

QCG admin Portal Tasks

Filters

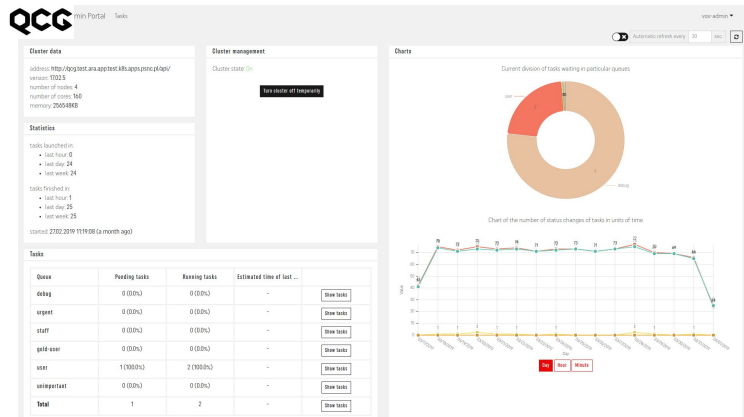
Modify columns

Automatic refresh every 30 sec

Result count: 907

ID	ID	Commissioner	Commissioner role	Arrangement Ident...	Snapshot version	State	Queue	Thumbnail	Commission time relative time	Last modified relative time	Actions
commissioner											
commissioner role											
adviser											
user-role											
arrangement identifier											
snapshot version											
states											
FINISHED	9431										
REJECTED	622										
SUBMITTED	22										
PENDING	1										
COMPLETED	1										
REJECTED	1										
PROCESSING	0										
queue											
user	898										
debug	89										
default-queue	33										
staff	26										
unimportant	2										
gold-user	1										
important	1										
urgent	1										
commission time											

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Success stories



QCG is the primary middleware in Poland



Success stories





Project web page

QCG

QUALITY
IN CLOUD AND GRID

Log in

Preferences

Help

About This Site

Q

About

News

End-user

Application Developer

Components

Installation

Community

Publications

Contact

Strona początkowa Indeks Historia

Last modified 4 message ago

QCG - Quality in Cloud and Grid

The QCG middleware (previously known as QosCosGrid) 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 QCG, 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.

QCG Middleware

QCG provides:

• the most efficient remote access to computational resources in a single cluster or many clusters in Poland and Europe,

• automatic steering of various types of complex computing experiments ranging from multi-parameter sweep studies to cross-cluster executions of parallel applications,

• fully transparent integration with parallel programming and execution environments like OpenMPI and ProActive located on many computing clusters,

• support for Quality of Service (e.g. start time) based on advance reservation mechanisms,

• shorter waiting times and improved resource utilization by hierarchical grid- and local-level job scheduling.

News

QCG-Now 1.2 (3 January 2019)

The refreshed version of QCG-Now has been released and it is available for download from the tool's webpage. The new version introduces a few new features, and improves the general stability of the program.

UMD 4.5.0 (9-August 2017)

New versions of QCG-Broker and QCG-Broker Client has been published as part of UMD 4.5.0. The newly released packages has been marked with version number 4.2.0 and provide a support for execution of Array Jobs and possibility to get instant information about resources with the qcg-resources command.

QCG-Now 1.0 beta (22 December 2016)

QCG-Now - a new multipatform desktop client for QCG - is already available for testing, it may be downloaded from the [product's webpage](#) and easily installed on Windows, OS X or Linux. We encourage, especially the QCG-fans, users to [play with a new software](#) and [give us feedback](#).

<http://www.qoscosgrid.org>

INNOVATION DRIVEN EFFICIENT COMPUTING

The Innovation Computing initiative has been launched by Poznan Supercomputing and Networking Center in 2019 after almost two decades of the involvement in many international and national R&D projects related to resource management in distributed computing environments, including Grids, HPC, Cloud and Edge. It consists of a set of high quality software, infrastructure and hardware components integrated into a consistent PaaS solution which can be provided on request to any computing infrastructure.

HPC

EDGE COMPUTING

CLOUD

BIG DATA

DEEP LEARNING

FDG COMPUTING

<http://www.computing-innovations.org>



Thank you!

Contact:

piontek@man.poznan.pl