

POZNAŃ SUPERCOMPUTING AND NETWORKING CENTER



QosCosGrid

QosCosGrid Middleware

Tools and Services for Advanced Job Management, Advance
Reservation and Co-allocation of Computing Resources

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Outline

- QCG general information
- QCG Architecture & Components
- Tools for end-users
- Success stories
- Integration with EGI
- Documentation & Repositories
- Contact
- Questions



QosCosGrid middleware

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.



QCG functionality

Automatic steering of various types of complex computing experiments:

- Simple tasks
- DAG Workflows with recursive conditions and dependencies on any task status
- Multi-Dimensional parameter sweep tasks
- Single cluster Parallel tasks (MPI/OpenMP)
- Cross-Cluster Parallel tasks

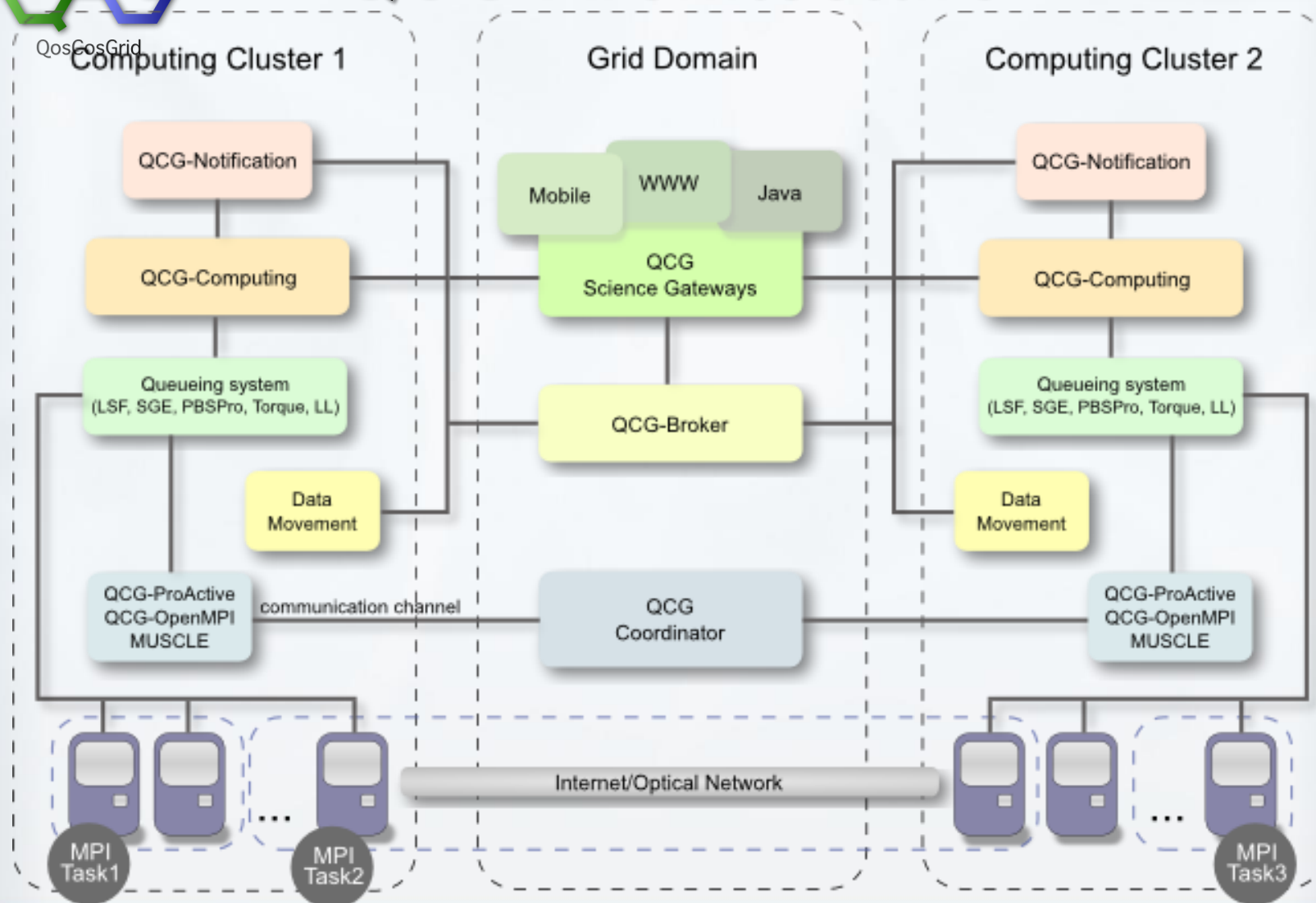


QCG Functionality

- Advance reservation capabilities
 - Quality of Service
 - Co-allocation of resources and cross-cluster
- Support for interactive tasks
- Possibility to connect to running task with interactive session
- Task status and progress notifications



QCG Architecture





QCG-Computing

- Deployed on access nodes of the batch systems (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
- Compatible with the OGF HPC Basic Profile specification (JSDL and BES)
- Offers basic file transfer mechanisms



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, what is a unique feature, the XMPP protocol



QCG-Broker

- Offers scheduling and brokering of jobs capabilities
- Controls the whole experiments execution (including workflows and parameter sweep tasks)
- Provides requested QoS and co-allocates resources
- Stages in/out files and directories



QCG Tools & Clients

- QCG-SimpleClient (command line)
- QCG-Icon (GUI)
- QCG-Science-Gateways (web)
- QCG-QoS-Access (web)
- QCG-Monitoring (web)

- QCG-Data (clone of iDrop, under development)
- QCG-Icon2 (under development)



QCG-SimpleClient

- Set of commands patterned on queuing system tools
- JSDL, QCG-Simple, QCG-XML description dialects
- Support for interactive tasks
- Automatic staging in/out files
- Notifications about statuses and progress of application (mail, xmpp, QCG-Monitor)



QCG-SimpleClient

Submission and controlling 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-proxy** - create user proxy certificate
- **qcg-refetch** - retry/repeat the transfer of output files/directories
- **qcg-refresh_proxy** - refresh user proxy certificate for given tasks
- **qcg-sub** - submit batch or interactive tasks to be processes by QCG

Resources reservation and control:

- **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



qcg-offer command

```
[plgpiontek@qcg ~]$ qcg-offer
```

HYDRA:

Summary:

Metric Name	nodes/cores	share	
Total Resources:	282/5340	100%/100%	
Up Resources:	250/4668	88%/87%	
Used Resources:	114/1710	40%/32%	
Free Resources:	129/2628	45%/49%	(FreeNodes=87x12,17x16,18x48,7x64)
PartFree Resources:	142/2810	50%/52%	(AvgFreeCoresPerNode=19)
Reserved Resources:	2/24	0%/00%	(Utilization=0%)

GALERA:

Summary:

Metric Name	nodes/cores	share	
Total Resources:	195/2700	100%/100%	
Up Resources:	191/2652	97%/98%	
Used Resources:	139/1426	71%/52%	
Free Resources:	38/456	19%/16%	(FreeNodes=38x12)
PartFree Resources:	73/698	37%/25%	(AvgFreeCoresPerNode=9)
Reserved Resources:	9/468	4%/17%	(Utilization=0%)

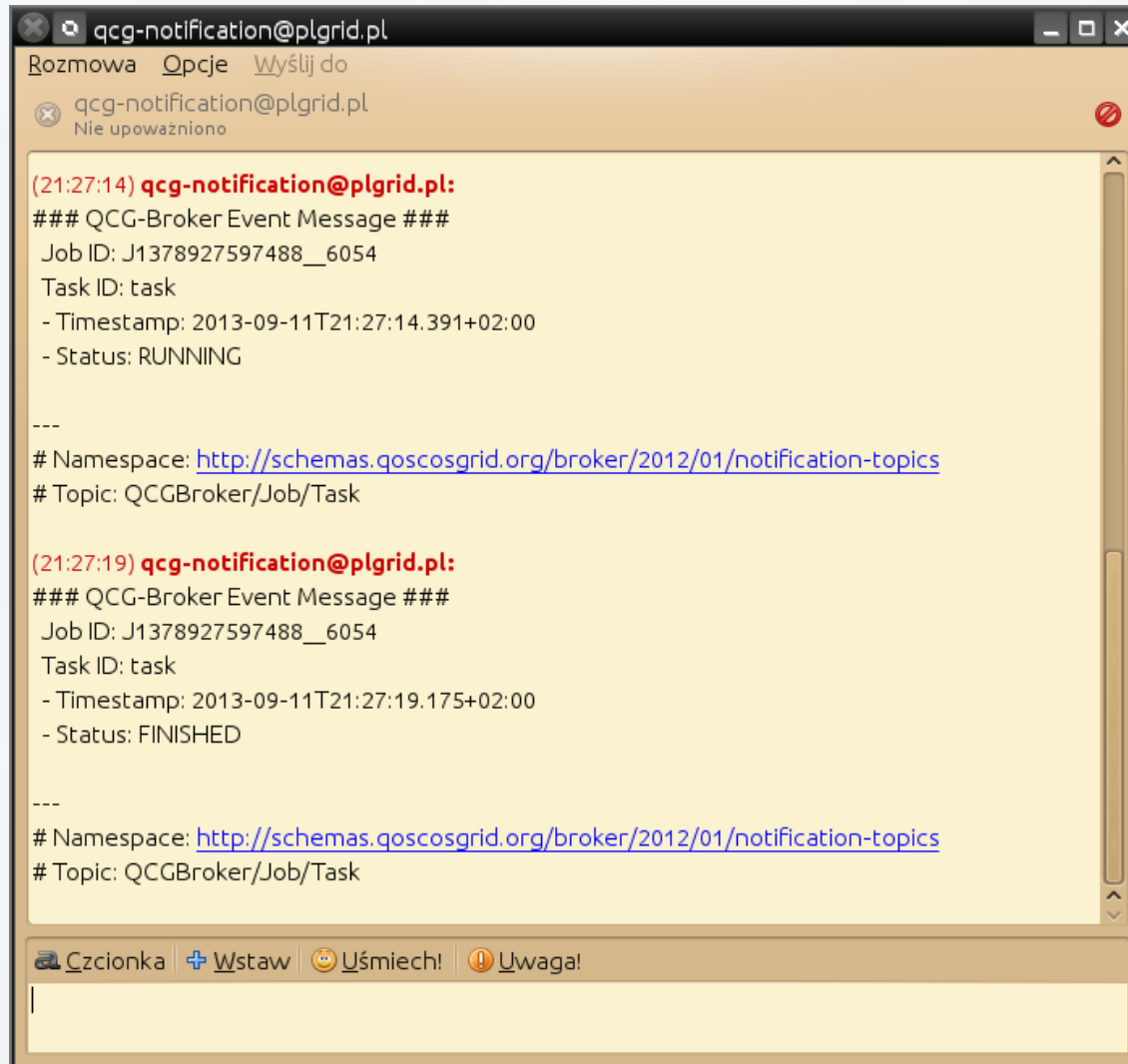


QCG-Simple Description

```
#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
```



XMPP Status Notification





QCG-Icon

- lightweight intuitive application for Windows, MAC OSX and Linux platforms,
- provides transparent, unified access to applications installed on Grid resources and available via QosCosGrid services.
- automatically transfers input / output files between Grid and user-side.
- gives to the user impression of local work



QosCosGrid

QCG-Icon

The screenshot displays the QCG-Icon application interface. The main window shows a list of tasks with columns for Name, Main File, Task Status, Working Directory, Resource, Execution Time, and Sweep Index. A task named 'Rysunki (poprawione)' is selected. A dialog box titled 'Zlecanie zadania...' is open, showing the preparation of the task 'C:\work\matlab\simplePlot.m'. The task list includes various files and their sizes. A file explorer window shows the contents of the 'C:\Documents and Settings\konczak\Pulpit\testing\zsz_2011_12' directory, including files like 'zcg-icon-outputs.zip' and 'matlab.out.txt'. A 'Wczytaj certyfikat PKCS12' dialog box is also visible, showing the file 'nents and Settings\()-(Pulpit\plggestm01.p12' and a password field. A status bar at the bottom indicates 'Zadanie zakończone!' (Task completed!).

Nazwa	Główny plik	Stan zadania	Katalog roboczy	Zasób	Czas zlecenia	Sweep Idx
Rysunki	rysunki.m	Zakończono błędem	C:\Documents and Settings\konczak\Reef (PCSS)			
Rysunki (poprawione)	rysunki.m					
Rysunki (poprawione)	rysunki.m					
Rysunki (poprawione)	rysunki.m					

Nazwa	Wielkość
2011_05_30_14_04_49	
2011_05_30_14_07_22	
2011_05_30_15_04_26	
2011_06_03_13_17_15	
2011_06_03_13_17_45	
garchi.m	712 B
kupiec1.m	266 B
matlab.out	453 B
rysunki_2011_11_08_17_28_13_1	
rysunki_2011_11_08_17_28_14_3	
rysunki_2011_11_08_17_30_33_1	
rysunki_2011_11_08_17_30_33_2	
rysunki_2011_11_15_14_48_03	

Resource: Reef (PCSS)
Limit czasu: 00:20:00
Parameter sweep: ☒
Nazwa zmiennej środowiskowej: QCG_STEP_INDEX
Rozpocznij od: 1
Zwiększaj o: 2
Zakończ po: 5

Wczytaj certyfikat PKCS12
Plik .p12: nents and Settings\()-(Pulpit\plggestm01.p12
Hasło:

Zadanie zakończone!
C:\work\matlab\simplePlot.m osiągnął stan Zakończono



QosCosGrid

QCG Science Gateways

The screenshot displays the 'vine' toolkit interface within the QCG Science Gateways. The interface is divided into several sections:

- Header:** Includes the 'vine' logo and a 'Welcome, Puck CovalentLab' message.
- Navigation:** Tabs for 'Home', 'Solutions', 'File Manager', 'Data Bank', and 'Configuration'.
- Main Panel:**
 - Task:** 'Total energy and QCG charts'.
 - Parameter set description:** '4 parameter set'.
 - Number of processes:** '4'.
 - File set (path):** 'JUBJALL'.
 - Primitive vectors (pm):** '0.0 0.0 0.0'.
 - Atom types (label):** '1'.
 - Atom number (label):** '1.0'.
 - Truettner-Hoppe (potential label):** 'Morse'.
 - Definition of the atom: number of atoms (label):** '2'.
 - Atom's label (label):** '1 1'.
 - The location of atoms (pm): - Fractional (label):** '0.0 0.0 0.0'.
 - Radical kinetic energy (label):** '0.0'.
 - Definition of the k-point grid (label):** 'Automatic'.
 - Definition of the primitive vectors of the reciprocal space (label):** '0.0 0.0 0.0'.
 - Radical number of k-point (label):** '1.0'.
 - Out of difference between evaluations of total energy (label):** '1.0e-8'.
- Results:**
 - Selected set results:** Includes buttons for 'Download results/evaluation files', 'Show visualization of set', and 'Case search'.
 - Case keywords:** A text input field.
 - Parameter set keywords:** A text input field.
 - Results difference of total energy (label):** '1.0e-8'.
- Parameter set automatic:**
 - Minimum total energy:** '-8.872037264125'.
 - Table:**

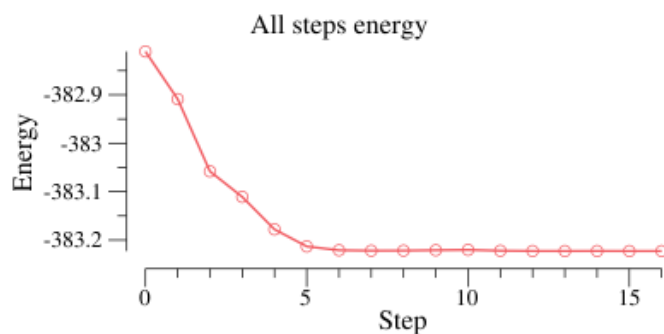
Set	Description	Atom	Total energy	Progress	Vis
1	1 parameter set	Done	-8.864227993780	100%	<input checked="" type="checkbox"/>
2	2 parameter set	Done	-8.871062699033	100%	<input checked="" type="checkbox"/>
3	3 parameter set	Done	-8.872480673808	100%	<input checked="" type="checkbox"/>
4	4 parameter set	Done	-8.872572330267	100%	<input checked="" type="checkbox"/>
5	5 parameter set	Done	-8.872617431740	100%	<input checked="" type="checkbox"/>
6	6 parameter set	Done	-8.872706044783	100%	<input checked="" type="checkbox"/>
- Visualizations:**
 - Wavefunction plot:** A plot showing the wavefunction along the 'Distance' axis.
 - Total energy chart (set parameter sets):** A plot showing the total energy (Etot) versus the 'Set (no.)'.



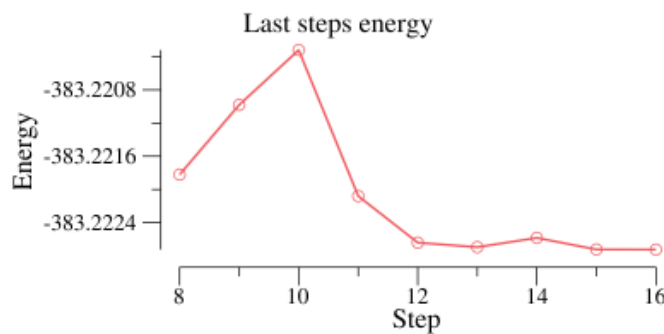
QCG-Monitoring



QCG gaussian job J1368793153691__7065 data



Step	Energy	Difference
0	-382.810458	
1	-382.908823	-0.098365
2	-383.058101	-0.149278
3	-383.110761	-0.052660
4	-383.177936	-0.067175
5	-383.213193	-0.035257
6	-383.221050	-0.007857
7	-383.221981	-0.000932
8	-383.221821	0.000160
9	-383.220981	0.000840
10	-383.220320	0.000661
11	-383.222080	-0.001760
12	-383.222641	-0.000561
13	-383.222695	-0.000054
14	-383.222584	0.000112
15	-383.222723	-0.000140
16	-383.222725	-0.000002





QCG-QoS-Access

QCG-QoS-Access

Count of Reservations on the screen: 5 Reservation range: 0 - 5 Refresh Create Reservation

Reservation ID	Start time	End time	Resource	Status
R1368515738190_RESERVATION_9226	Tue May 14 11:20:00 GMT+0200 2013	Tue May 14 11:22:00 GMT+0200 2013	6	FINISHED
R1368453492238_RESERVATION_9227				FINISHED
R1368452105122_RESERVATION_9228				FINISHED
R1368451751472_RESERVATION_9229				FAILED
R1368451596571_RESERVATION_9230				FAILED

Cancel Selected Reservation

Reservation information:

ID: R1368515738190
Start time: Tue May 14 11:20:00 GMT+0200 2013
End time: Tue May 14 11:22:00 GMT+0200 2013
Status: FINISHED
Slots: 6
Resources:
Host: grass1-dev.ma
Slots: 6
Local ID: R2466
Nodes: 1
Node: grass1 Slots: 6

Create Reservation

Time Window:

Start: 16 : 24 05/15/2013

End: 16 : 24 05/16/2013

Reservation Duration:

Hours: 1 Minutes: 00

Resources:

Cluster:

☒ Reserve Slots: 1

☐ Reserve Nodes: 1 Slots per Node: 1

Create Reservation Close

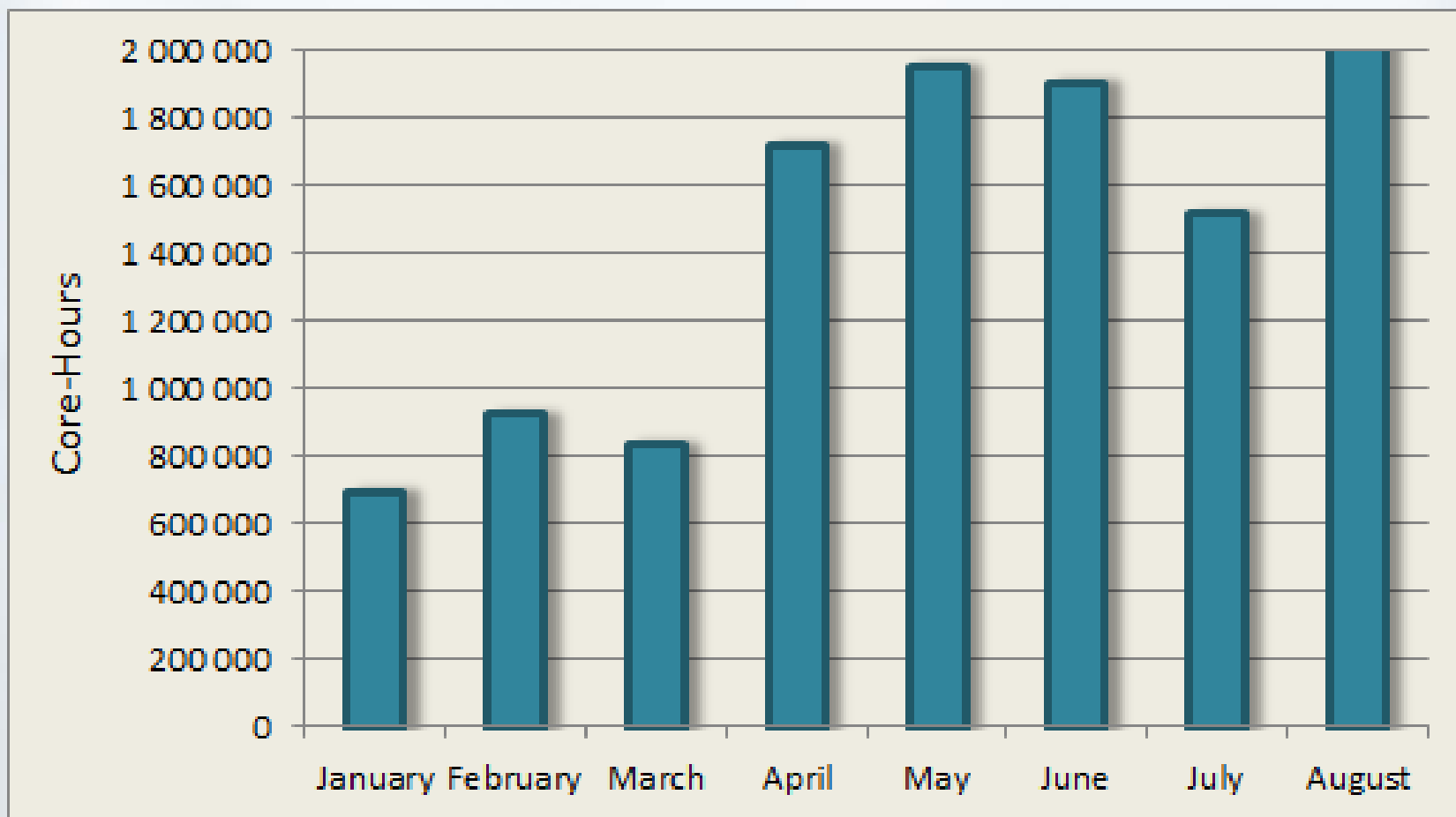


QCG Success Stories

- Infrastructural and research EU and national projects
(PLGridPLUS, pMedicine, AirPROM, MAPPER, ACGT, BEinGRID, PL-GRID, QosCosGrid, BREIN)
- Production deployment on PL-Grid resources (the most popular middleware in Poland)
- EGI & PSNC/QCG MoU (2012)
- BCC-UNG&PSNC/QCG MoU (2013)
- Part of UMD 3.2.0
- Cooperation with PRACE



PLGrid Statistics (2013)





QCG – integration with EGI

- QCG unit support in GGUS
- SAM Nagios probes & Dashboard alerts
- APEL / GRID-SAFE accounting
- Advertising GLUE2 schema information in BDII (in progress)
- Integration with Virtual Organization Management Support (VOMS)
- Part of the UMD 3.2.0 (September 2013)
- QCG-Icon in AppDB



QCG Deployment

- Installation from packages
 - QCG software repository
 - For SL5/SL6 and Debian (QCG-Comp, QCG-Notif)
 - UMD repository
 - SL5 (SL6 in next update with SHA2 support)
- Installation from sources
- Windows/Linux/MacOS QCG-Icon installer



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QosCosGrid

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QosCosGrid

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.

QCG Middleware

QosCosGrid 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

News

QosCosGrid 3.0 [16 July]
A new major release of QCG has been just published! It includes many improvements that will improve the access to application resources, reduce the overhead needed to run a grid environment. Unclassified mechanisms, e.g. of QCG-Client command transfer rate or advanced capabilities, will allow to concentrate even more scientific work.

QCG-Icon 1.4.3 [21 June]
Next version of QCG-Icon is available for download. Since the version 1.4.3 many improvements



Contact

General questions:

contact@qoscosgrid.org

Technical questions:

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**Questions ?
Comments !
Advices ;-)**