





Running Multiscale applications with QosCosGrid



MAPPER 1st Seasonal School

Poznan Supercomputing and Networking Center

The Mapper project receives funding from the EC's Seventh Framework Programme (FP7/2007-2013) under grant agreement n° RI-261507.

Motivations



- Tightly coupled multiscale applications are composed of many single scale models that may have:
 - different hardware requirements (e.g. GPU, MPP, SMP),
 - or different software requirements (e.g. Palabos, CPMD, LAMMPS).
 - These application frequently must be run <u>in parallel</u>, but this is not supported by existing middleware in EGI and PRACE.
 - We have developed new core middleware services, QosCosGrid, which provides these capabilities, and can be deployed on EGI and PRACE resources.

The Tools



- QCG-Computing
 - Basic Execution Service (BES) supports advance reservation.
- QCG-Coordinator
 - Supports QCG-Computing in cross-cluster execution of jobs
- QCG-Notification
 - Notification capabilities based on WS-Notification
- QCG-Broker
 - Resource management and brokering service
- QCG-Client
 - Text-based client for QosCosGrid
- QCG-lcon
 - Lightweight desktop client for QosCosGrid
- QCG-Tools
 - Various elements extending the QosCosGrid stack
- QCG-Nagios
 - Nagios probes for the QosCosGrid stack





- Running multiscale application in crosscluster environment requires addressing the following issues:
 - <u>co-allocation</u> of heterogeneous resources,
 - coordination of <u>application spawning</u> at multiple sites,
 - enabling <u>connectivity</u> between firewalled resources and between private IP domains.



- Based on Advance Reservation mechanism,
- Process managed by QCG-Broker,
- Reservations can be created on demand (using QCG-Computing) or manually (by an administrator).



Application Spawning



- Problem: Kernels are started independently
- Solution: External service: QCG-Coordinator







- Many clusters use private IP addresses for their backend compute nodes.
- Some sites also restrict outgoing traffic.
- Solution:
 - Use predefined port ranges.
 - Deploy Muscle Transport Overlays (MTOs) userspace daemons on the interactive nodes.

Connectivity - MTO (II)





Application: In-stent Restenosis 3D





Example Run – 1st MAPPER Review





 This demo integrated resources provided by EGI, PRACE and local infrastructures.

QCG-Broker - JobProfile





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G OCG icon File Management New experiment Sweep Id× Nazwa Główny plik Stan zadania Katalog roboczy Zasób Czas zlecenia Menu Default name 01-^ah Upload file: Skopiuj ID zadania Rysunki (poprawione rysunki.m muscle 2010-01-11_13-51-27 with QosCosGrid 2.3.0 / P 🖾 Actions ? 🕌 Zlecanie zadania... C:\work\matlab\simplePlot.m Snippet ID=a1 Otwórz katalog z wynikan Choose File No file chosen tysunki (poprawione) rysunki.m vsunki (poprawioni rysunki.m Podolad # configuration file for a MUSCLE CVA Pobierz ponownie cellOSI.txt abort "this is a configuration file for to be used with the MUSCLE bootstrap utility" if FILE == \$0 Kongresonarie pilbón Pregostonarie darpto vejtelowytóć (workiwatlak)dataln-too Pregostonarie darpto vejtelowytóć (workiwatlak)singležko:n Polistrate darpto veiterpelsinjących Przystonarie do dieternia adatal Wienariche žitekk pilbo opkopodicego /om/luster/rest/shared/na Przystonarie do kanadres pilbo Zleć ponownie zadanie *** # add build for this cxa to system paths (i.e. CLASSPATH) outfirst.txt Zleć ponownie zadanie... m = Muscle.LAST kernel/ m.add classpath "#{ENV['HOME']}/isr3d/build/: Usuń z listy m.add_libpath "#{ENV['HOME']}/isr3d/build/:" loadGeometry Ē Prmygotomanie do Wysyłanie pliku Zlecania zadania Zakończono! Nazwa zadania Rysunki (poprawiope) # configure cxa properties cxa = Cxa.LAST palabosresults/ Nazwa cellslistsecond.txt 2011_05_30__14_04_4 cxa.env["cxa_path"] = File.dimame(__FILE__) 2011_05_30__14_07_22 2011_05_30__15_04_24 111 output.txt # declare kernels 2011_06_03__13_17_1 cellShearpalabos.txt cxa.add_kernel('BF', 'kernel.flow3d.Flow3dController' 2011_06_03__13_17_4 Cxa/ cxa.add kernel('DD', 'kernel.dd.DiffusionController') 712 • kupiec1.m 266 B 😋 Wstecz 🔹 🐑 - 🎓 🔎 Wyszukaj 🌔 Foldery 🛛 🏢 • hs_err_pid28714.log No inputs defined for this snippet. I No outputs def matlab.out 453 B Set executable parameters rYsUnkI_2011_11_08___17_28_13__1 rYsUnkI_2011_11_08___17_28_14__3 rYsUnkI_2011_11_08___17_30_33__1 📧 🚞 C:\Documents and Settings\(konczak\Pulpit\testing\zzz_2011_12 💌 🋃 Przejdź log_send.txt rrast. Executable arguments {SNIPPET}@[MULTI:Sites:([VAR:Name];[VAR:Kernels]; [VAR:Cores];[VAR:Reservation])]@[VAR:Execution du isr3d.postprocess Zadania plików i folderi .qcg-icon-outputs.zip duration ß rYsUnkI 2011 11 08 17 30 33 build/ rYsUnkI_2011_11_15___14_48_03 Utwórz nowy folde Variables build.xml 🚳 Publikuj ten folder w sieci matlab.out.txt Sites Dokument tekstow 1 KB Zasób Reef (PCSS surfacecoordshis_txt Name Kernels Reservation 😂 Udosteonii ten folde Limit czasi 00:20:00 cellslist.txt zeus.cyfror SMC:collect 1 Parameter жер filler geom 1.dat p6012.huyg huygens.sa BF 32 S Wczytaj certyfikat PKCS12 surfacecoords.txt 11 **(**) Nazwa zmiennej środowiskowej: OCG_STEP_INDE: Pik .p12 ments and Settings\(}-{)\Pulpit\pigtestm01.p12 Przeglądaj shearpalabosData.txt Rozpocznij od: 1 ‡ CoorData10.txt Execution duration 2 🗘 Zwiększaj o: Ok Anuluj slice.dat 5 🗘 Zakończ po: Note that the variables will be saved only for the current combination outbis.txt interpreter-executor. When you change any of these elements, the Zleć zadanie Anului 3 Zadanie zakończone! variable values will be lost. C:\work\matlab\simplePlot.m osiagnał stan Zakończone out.txt cellslistfirst.txt 🛃 Start 💦 🔤 Wiersz polec 600 C QCG icon

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- Command line clients (QCG-Client).
- Desktop client (QCG-lcon).

Current executor: C=PL/O=PL-Grid/O=Uzytkownik/O=CYFRONET/CN=Eryk Ciepiela/CN=plgciepiela@OosCosGrid 2.3.0 -

QosCosGrid Executor in GridSpace EW.

User Tools

Experiment Workbench







- Distributed Resource Management Application API version 1.0 (more than 8 implementations),
 - Exploited both by QCG and GridSpace,
- DRMAA 2.0 standard already released (Advance Reservation support),
- HPC-BASH

```
module load openmpi
#pragma hpc-bash parallel for
for ((file_num=$first; file_num<=$last; file_num=$file_num+1))
    do
        cd $BASE_DIR/MODEL$file_num/
        #pragma hpc-bash batch-job walltime(00:30:00)
        $CACTUS_HOME/exe/cactus_SandT_SandTank.par
        done
        cd $BASE_DIR/</pre>
```

QosCosGrid in EGI



October 2012 – PSNC signs Memorandum of Understanding with EGI.eu

European Grid Infrastructure

towards a sustainable infrastructure

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New middleware for new communities

EGI.eu has signed <u>an agreement</u> with the <u>Poznan Supercomputing and</u> <u>Networking Centre</u> (PSNC) to integrate the QosCosGrid middleware stack into the European Grid Infrastructure (EGI).

Based in Poznan, PSNC is responsible for the development and management of the national optical research network, high-performance computing and various e-Science services and applications in Poland.



1 November 2012 Sara Coelho

qcg-offer - Look before you leap



- User: provides detailed view of free resources
- Administrator: helps with cluster diagnostics

HYDRA:			
Summary:			
Metric	Name	nodes/cores	share
Total	Resources:	282/5340	100%/100%
Up	Resources:	256/4744	90%/88%
Free	Resources:	107/2248	37%/42% (FreeNodes=66x12,19x16,16x48,6x64)
PartFree	Resources:	148/2878	52%/53% (AvgFreeCoresPerNode=19)
Reserved	Resources:	2/24	0%/00% (Utilization=0%)
GALERA:			
Summary:			
Metric	Name	nodes/cores	share
Total	Resources:	196/2532	100%/100%
Up	Resources:	167/2184	85%/86%
Free	Resources:	6/72	3%/02% (FreeNodes=6x12)
PartFree	Resources:	8/86	4%/03% (AvgFreeCoresPerNode=10)
Reserved	Resources:	7/264	3%/10% (Utilization=0%)

QCG Comunity Modules



 user-space environment modules providing unified and coherent access to self-installed application among many clusters.

```
$ qcg-module-create -g plggmapper muscle/2.0
Creating module for the group: 'plggmapper'
Using module name: muscle
Using module version: 2.0
...
module-whatis "muscle, 2.0"
#prepend-path LD_LIBRARY_PATH your-lib-path
#prepend-path PATH your-bin-path
...
$ module load muscle/2.0
$ muscle2 --version
```

End Users tools: QCG-Icon



- Java based desktop application
- integrates tightly with the system (systray, context menu)
- Platforms: Windows, Mac OSX and Linux
- demo movies: <u>http://www.qoscosgrid.org/trac/qcg-icon</u>



Further Reading



- QosCosGrid homepage: <u>http://www.qoscosgrid.org/</u>
- MAPPER Seasonal School Hands On: <u>http://www.mapper-project.eu/web/guest/wiki/-/wiki/Main/QosCos</u> <u>Grid+tutorial+for+1st+seasonal+</u> <u>school</u>
- DRMAA && HPC-BASH: <u>http://apps.man.poznan.pl/trac/pbs-drmaa/wiki/</u>
- DRMAA 2.0: <u>http://www.ogf.org/documents/GFD.194.pdf</u>



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