e-infrastructure

CAPACITIES

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),
  - different software requirements (e.g. Palabos, CPMD, LAMMPS)

  and must be run in parallel.

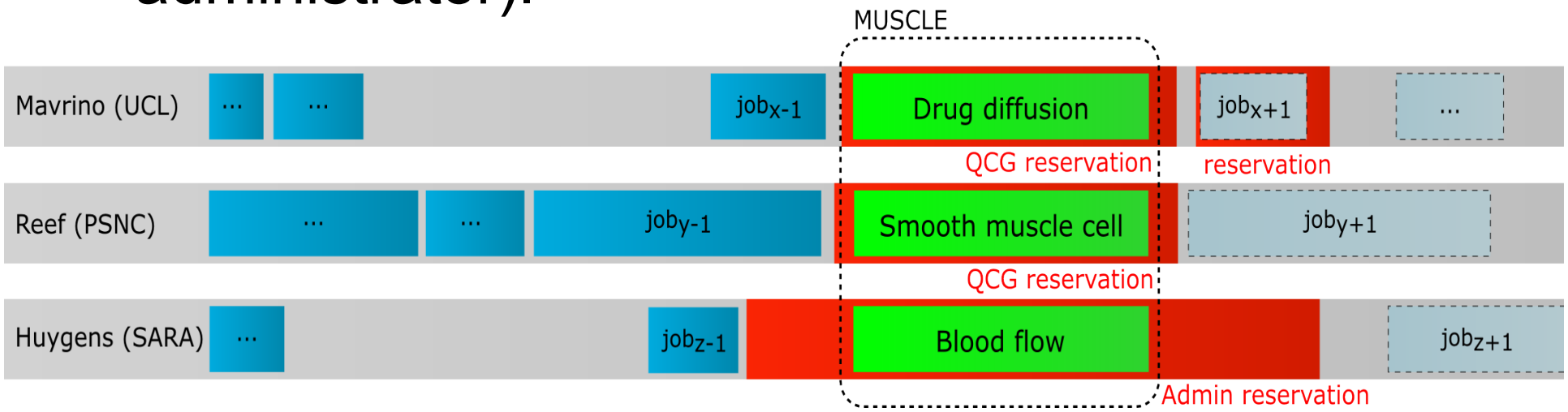
  It is not possible now with existing middleware services available in EGI and PRACE. Therefore, we have developed and deploying now core middleware services - QosCosGrid, extending capabilities available in EGI and PRACE.

Challenges

- Running multiscale application in cross-cluster environment requires addressing the following issues:
  - co-allocation of heterogeneous resources,
  - coordination of application spawning at multiple sites,
  - enabling communication between firewalled and NAT-ed systems.

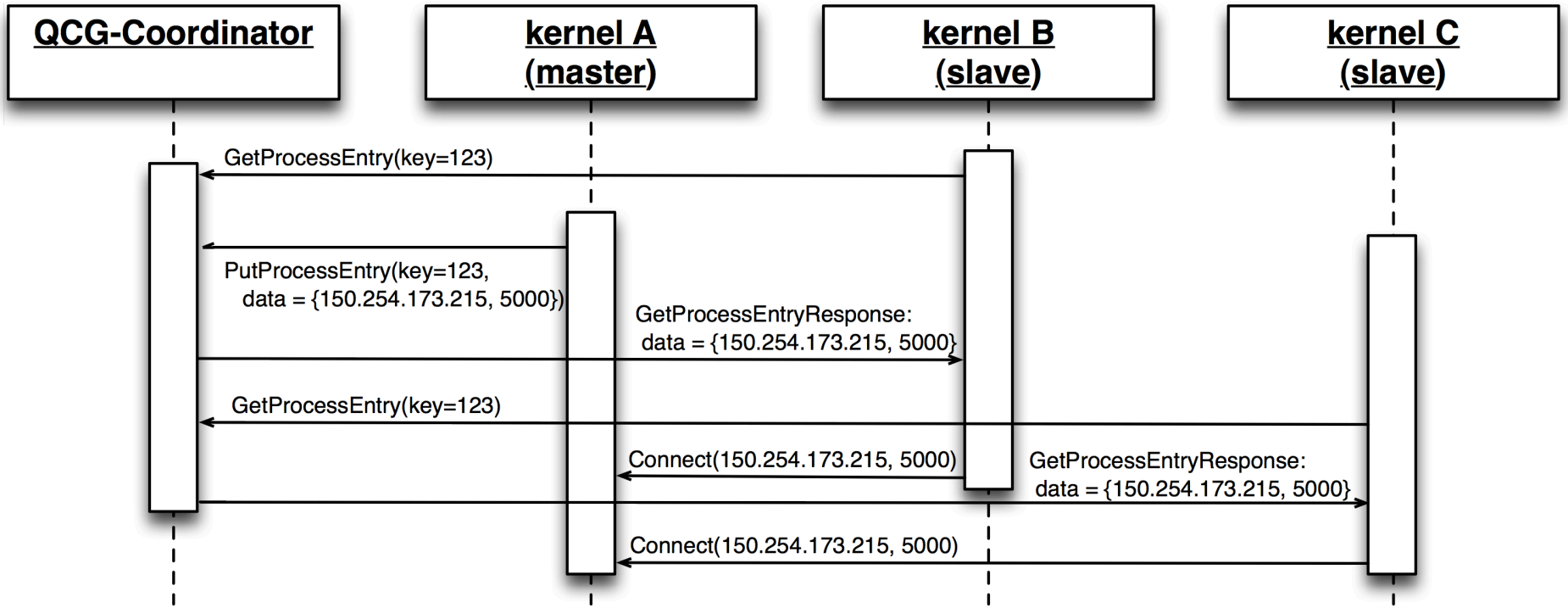
Resources Co-allocation

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



Application Spawning

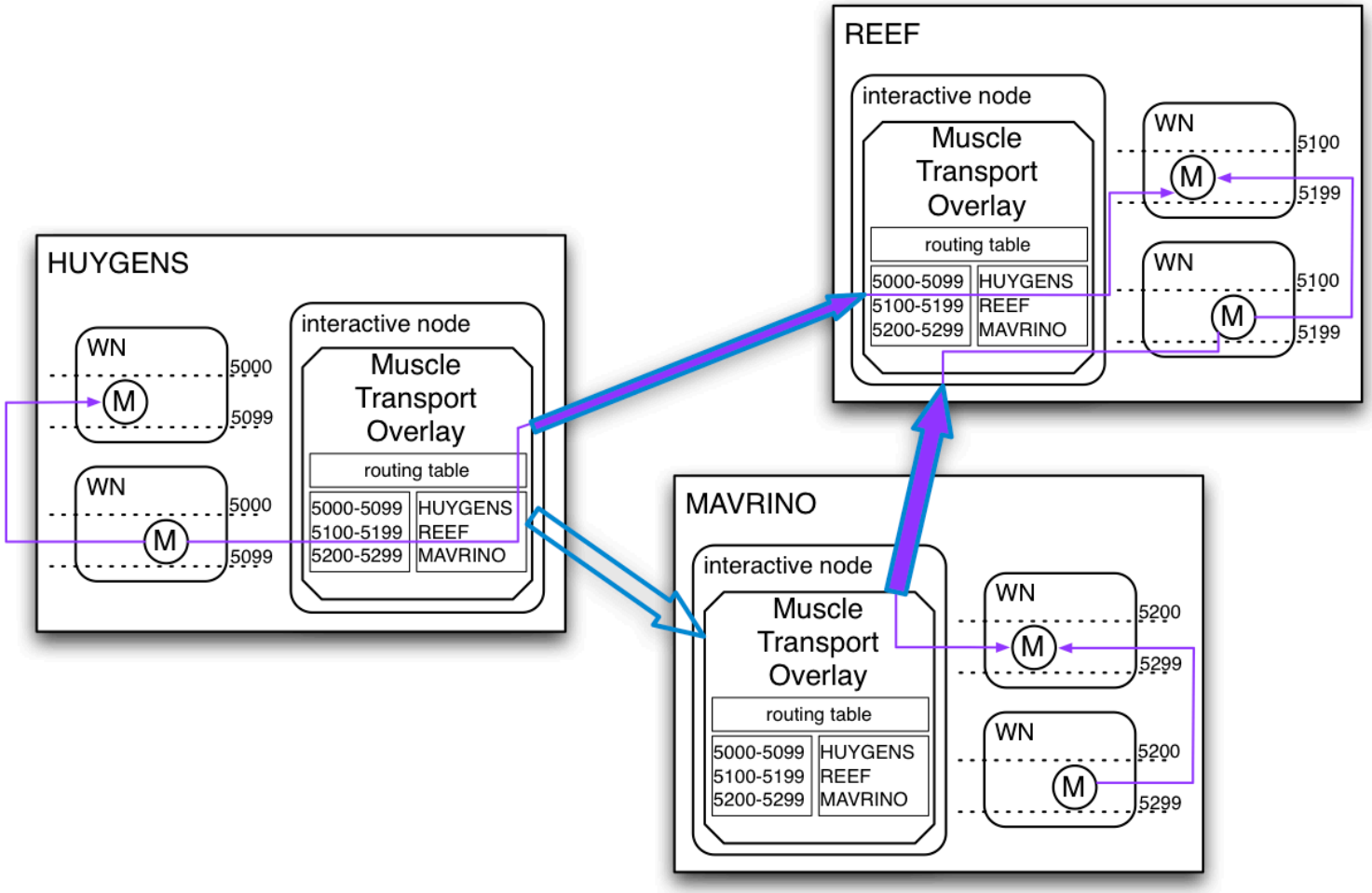
- Problem: Kernels are started independently
- Solution: External service: QCG-Coordinator



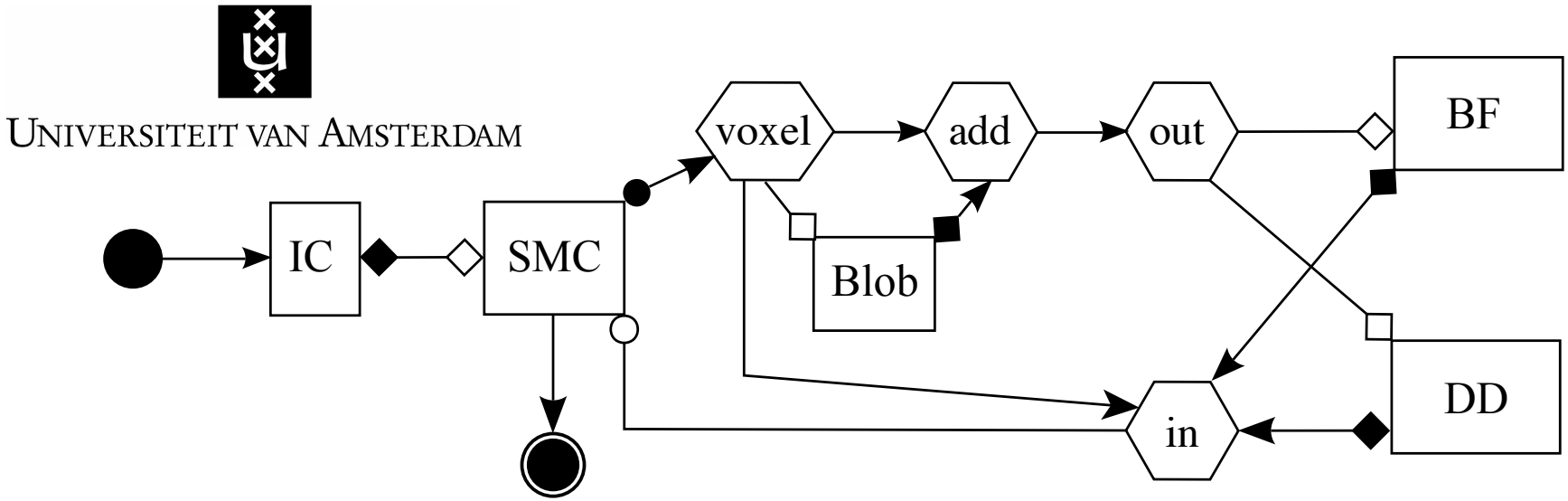
Connectivity (I)

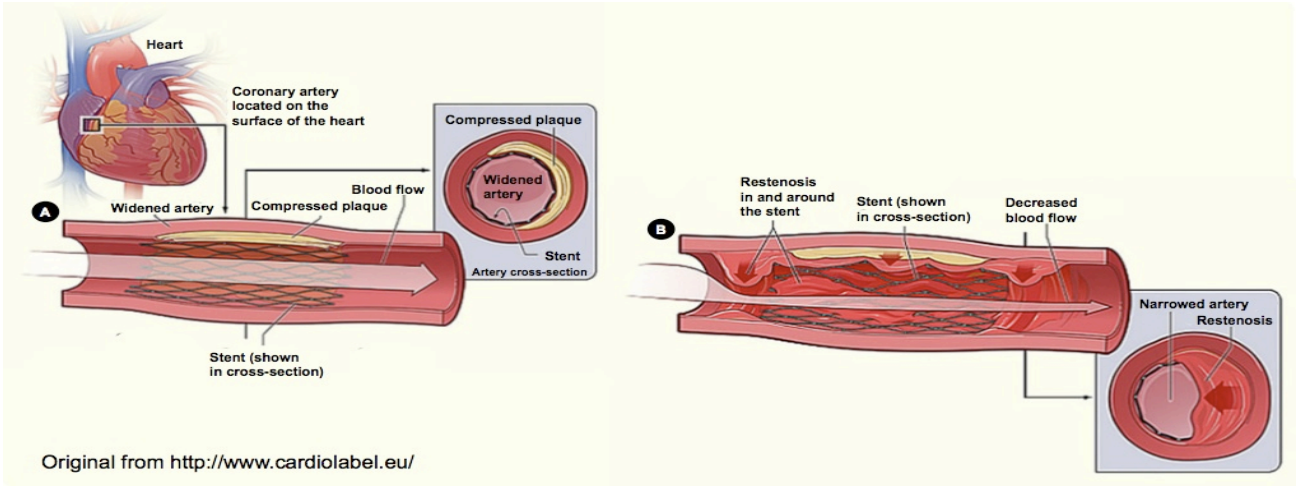
- Majority of clusters use private IP addresses for worker nodes
- Some of sites restrict also outgoing traffic
- Solution:
  - Using predefined port ranges
  - Muscle Transport Overlays (MTOs) user-space daemons deployed on interactive nodes

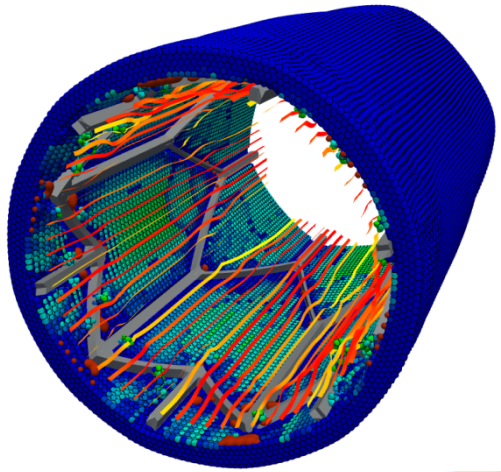
Connectivity - MTO (II)



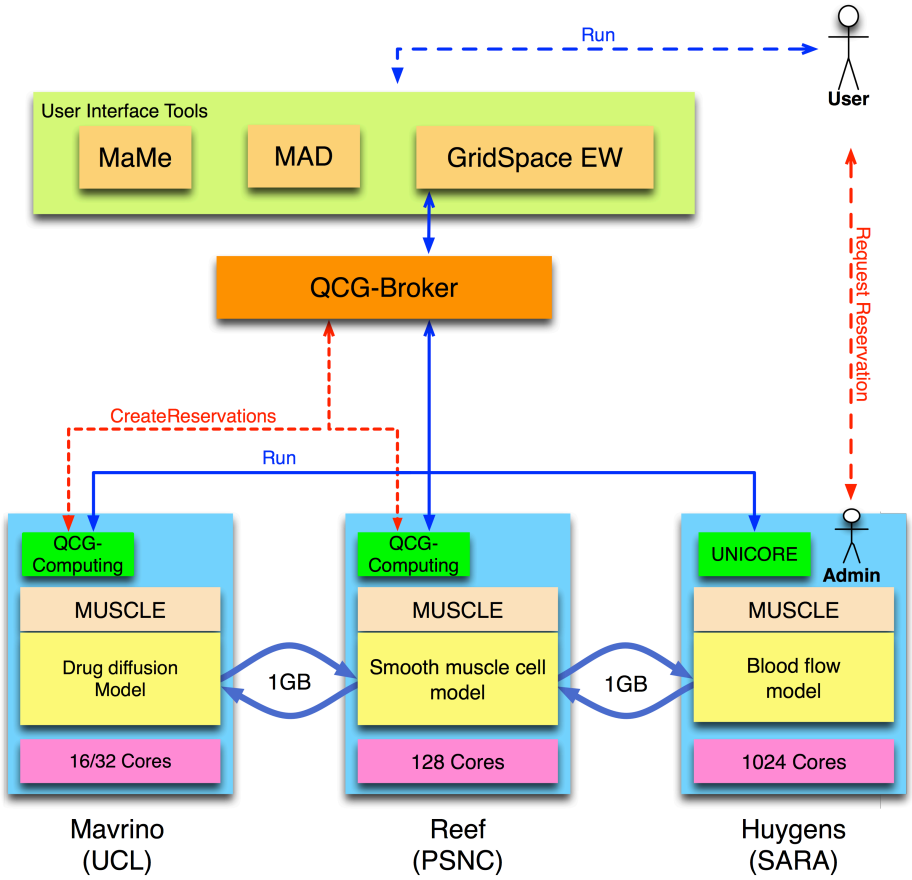
Application: In-stent Restenosis 3D







Example Run – 1st MAPPER Review



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

QCG-Broker - JobProfile


```
<topology>
        <processes processesId="BF">
                <processesCount>
                        <value>64</value>
                </processesCount>
                <candidateHosts>
                        <hostName>huygens.sara.nl</hostName>
                </candidateHosts>
                <reservation type="LOCAL">p6012.huygens.sara.nl.537.r</reservation>
        </processes>
        <processes processesId="SMC:collector:distributor:Blob:voxelizer:thrombusMapper">
                <processesCount>
                        <value>1</value>
                </processesCount>
                <candidateHosts>
                        <hostName>reef.man.poznan.pl</hostName>
                </candidateHosts>
        </processes>
        <processes processesId="DD">
                <processesCount>
                        <value>4</value>
                </processesCount>
                <candidateHosts>
                        <hostName>mavrino.chem.ucl.ac.uk</hostName>
                </candidateHosts>
        </processes>
</topology>
```

Resource Requirements

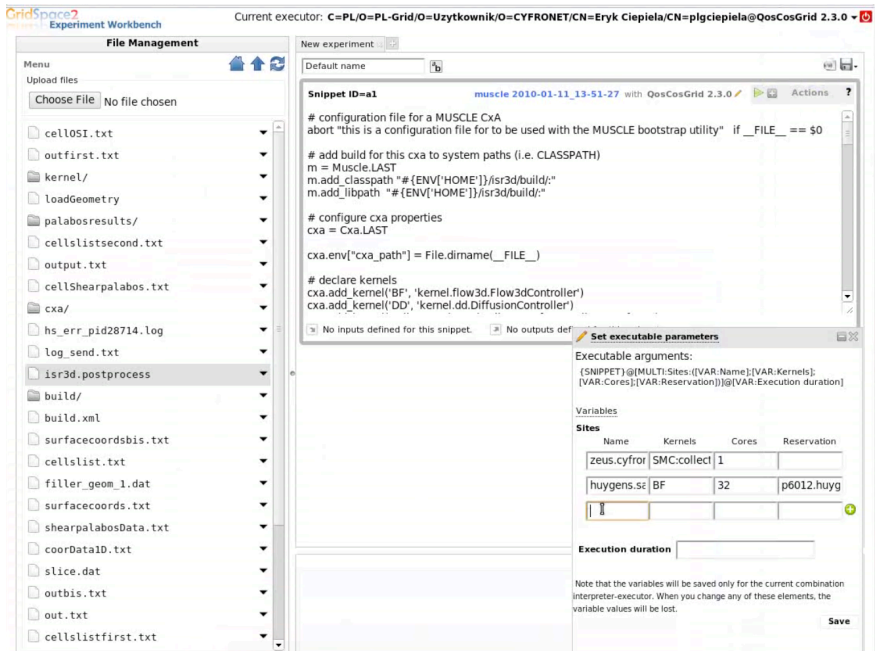
Advance Reservation created by administrator

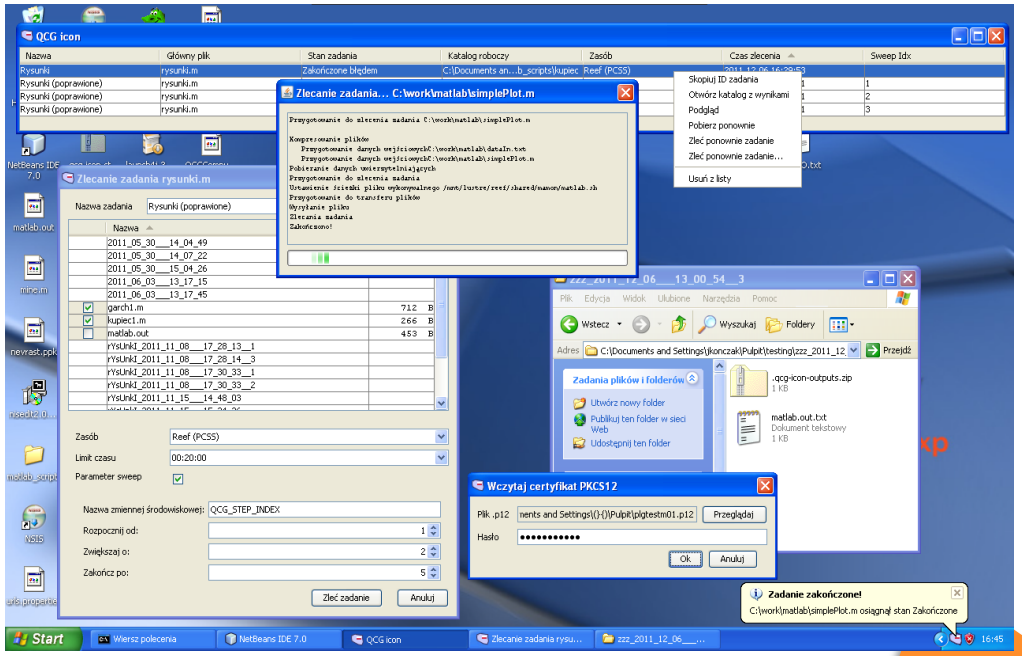
Kernels List

Target System

User Tools

- Command line clients (QCG-Client)
- Desktop client (QCG-Icon)
- QosCosGrid Executor in GridSpace EW





DRMAA

- 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/
```

Further Reading

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

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