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Leiden Grid Infrastructure

for Computational Chemistry

Observed trends in computational chemistry:

- Computers are becoming cheaper and more diverse.
- Computing resources are decentralized and often not owned solely by a single group.
- Chemistry software becomes increasingly harder to compile, install and setup.
- Average group only uses 'at most' five applications.
- Most computational work focuses on results and hardly any time or interest is left to learn about high performance computing.



- Need to have an easy to user-interface for each application.
- Applications should be setup by knowledgeable person on the relevant machines for the group.



LGI is a middle-ware that allows for:

- Easy setup on computers of NCF and your group.
- Easy setup for (chemical) applications.
- Easy to administer for standard UNIX administrators.
- Ease of use and takes care of security.
- Ease of adaptation to various application specific user interfaces.



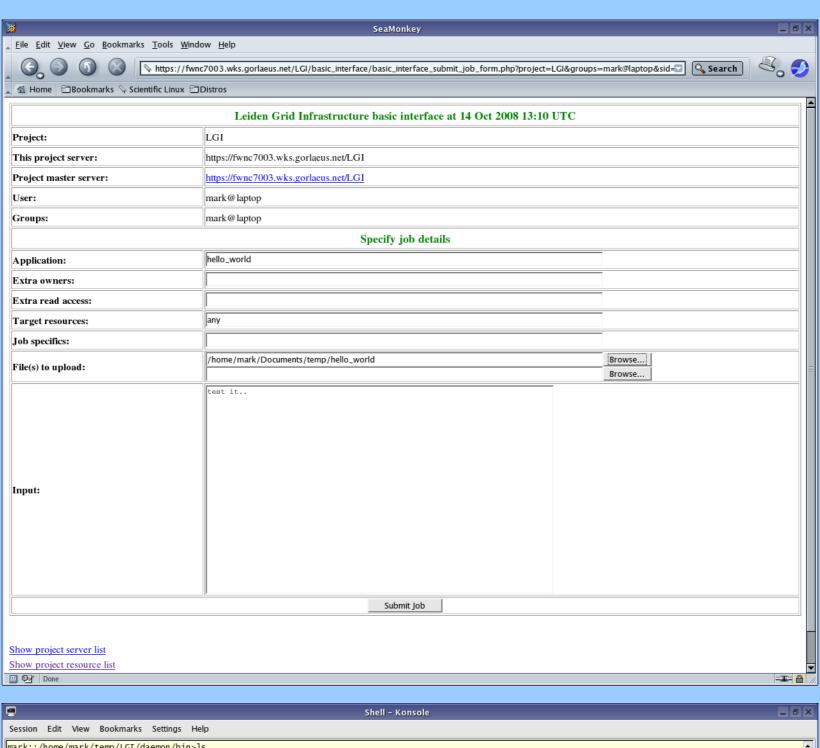
- Computer resources of NCF and individual groups should be bundled into a Grid so they can be shared.



VASP Gaussian ADF SPO-DVR

SA-DVR

Classical



Shell - Konsole	_6X
Session Edit View Bookmarks Settings Help	
mark::/home/mark/temp/LGI/daemon/bin>ls binhex csv hash hexbin LGI_daemon LGI_filetransfer LGI_qdel LGI_qstat LGI_qsub xml mark::/home/mark/temp/LGI/daemon/bin>./L LGI_daemon* LGI_filetransfer* LGI_qdel* LGI_qstat* LGI_qsub* mark::/home/mark/temp/LGI/daemon/bin>./LGI_qstat	_
# job_id state target_resources application time_stam	mp owners
1 341 finished somers@lisa.sara.nl hello_world Tue Oct 14 13:51:39 200 2 342 finished somers@huygens.sara.nl gaussian Tue Oct 14 13:55:13 200 3 343 finished somers@huygens.sara.nl vasp Tue Oct 14 13:55:14 200	08 mark@laptop
Number of jobs listed : 3 This project : LGI This project server : https://fwnc7003.wks.gorlaeus.net/LGI Project master server : https://fwnc7003.wks.gorlaeus.net/LGI mark::/home/mark/temp/LGI/daemon/bin>./LGI_qstat 341	
This project : LGI This project server : https://fwnc7003.wks.gorlaeus.net/LGI Project master server : https://fwnc7003.wks.gorlaeus.net/LGI User : mark@laptop Groups : theor Job id : 341 Job state : finished Job application : hello_world Job specifics : <repository> LGI@fwnc7003.wks.gorlaeus.net:/mnt/sdb1/LGI/trunk/repository/JOB_4410643da6e4c74fd96fe2375c029210 </repository> <repository_url> https://fwnc7003.wks.gorlaeus.net/LGI/repository/JOB_4410643da6e4c74fd96fe2375c029210 </repository_url> Target resources : somers@lisa.sara.nl	
Some Sources Some Sources Some Sources Some Sources Source	
Output : Hello_World from somers@lisa.sara.nl submitted with input: hello input	
Repository content : hash.h, daemon_configclass.h, logger.h, resource_server_api.h, daemon_jobclass.h, interface_server_api.h, daemon_mainclass.h, csv.h, xml.h, binhex.h, dump	
mark::/home/mark/temp/LGI/daemon/bin>	
	_
A ■ Shell	•

Huygens LISA

Laptop
FWNC7003
BOINC
Nocona
Woodcrest
Harpertown