

gLite Porting to the PS3 using ETICS for electronic High Throughput Screening (eHiTS

JAVA_HOME: /usr/java/jdk1.6.0_05

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Since 2003 TCD has invested heavily in middleware porting, constantly engaging with the middleware development groups of the EU DataGrid (EDG), LHC computing Grid (LCG) and EGEE projects. As a result of the accumulated expertise, TCD was invited in 2006 to join a new EGEE-II integration and testing activity (SA3) as the main portability partner for further development in this area, and then for EGEE-III, Trinity College Dublin handled the porting and multi-platform coordination.

The build system has evolved from a primitive python based system to a metadatarich system called ETICS. In 2008, TCD ported gLite to the PS3. TCD produces its own local ETICS builds for the Play Station 3 running Yellow Dog Linux 6.1 (PPC64), Mac OS X 10.5 (Leopard-i386), Debian 4.0/5.0 (x86/AMD64),

CentOS 4.x/5.x (x86/x86_64), openSUSE 11.1 (x86_64), and has previously performed partial ports of the glite-WN/LCG-WN, on AIX 5.3 (PPC), SGI-IRIX (MIPS), Fedora Core 2/4, Mac OS X 10.4, openSUSE 9.3/10.3 (x86) and Solaris 10 (x86).

The images in Figure 1 show the TCD local build results with report tables auto-generated using python scripts wrapping the ETICS client 1.4.9-1.

Two images show that LCG-DM successfully builds to 100% on the PS3 using the locally ported VDT globus and IBM Java 6.0 compiler.

value="--platform sl5_ia32_gcc412 --verbose --ignorelocking --continueonerror --noask" platform="centos5_ia32" />

value="--platform sl5_x86_64_gcc412 --verbose --ignorelocking --continueonerror --noask" platform="centos5_x86_64" />
value="--platform slc4_ia32_gcc346 --verbose --ignorelocking --continueonerror --noask" platform="centos4_ia32" />
value="--platform slc4_x86_64_gcc346 --verbose --ignorelocking --continueonerror --noask" platform="centos4_x86_64" />

value="--platform slc4_x86_64_gcc346 --verbose --ignorelocking --continueonerror --noask" platform="centos4_x86_64" />

<?xml version="1.0" encoding="UTF-8"?>

<bul>drules>

<checkout

<checkout

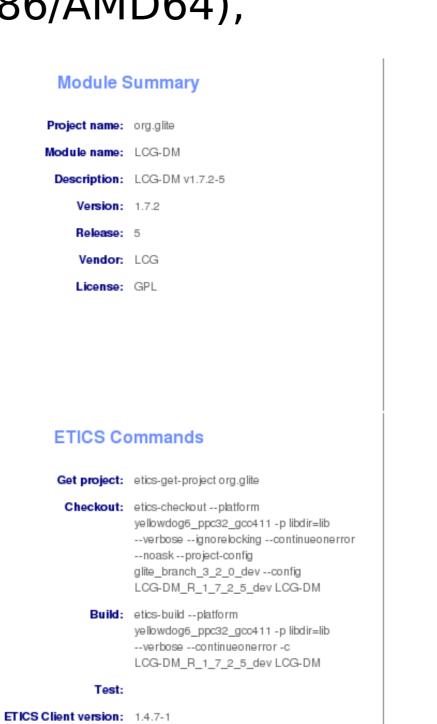


Fig. 1: Local ETICS Infrastructure at TCD **Build/Test Logs etics** glite_branch_3_2_0_dev Configuration: LCG-DM_R_1_7_2_5_dev LCG-DM LCG-DM_R_1_7_2_5_dev Tag: LCG-DM_R_1_7_2_5 VCS Root: :pserver:anonymous@glite.cvs.cern.ch:/cvs Page generated at 20/07/2009 12:28:25 Build host: cell-build.testari **Environment Properties** Configuration Last build time mysql-devel v. 5.0.22-2.2.ydl. alobus v. 4.0.7-VDT-1.10.1-1 GLOBUS LOCATION: /opt/globus vdt_globus_essentials v. 4.0.7-VDT-1.10.1-1 t/commons-lang/commons-lang-2.1.jar:/opt commons-cli/commons-cli-1.0.jar HOME: /home/autobuild/etics/org.glite-workspace PATH: /usr/java/jdk1.6.0_05/bin:/opt/gpt/sbin

org.glite

org.glite

org.glite

Grid-Ireland Local ETICS Build of gLite_branch_3_2_0_dev

Builds using ETICS volatile version: 1.4.9-1

glite-security-voms_R_1_9

glite-security-cgsi-gsoap-2.7_R_1_3_3_1_GL32_cloned

The TCD ETICS wrapper contains many extra pieces of functionality:

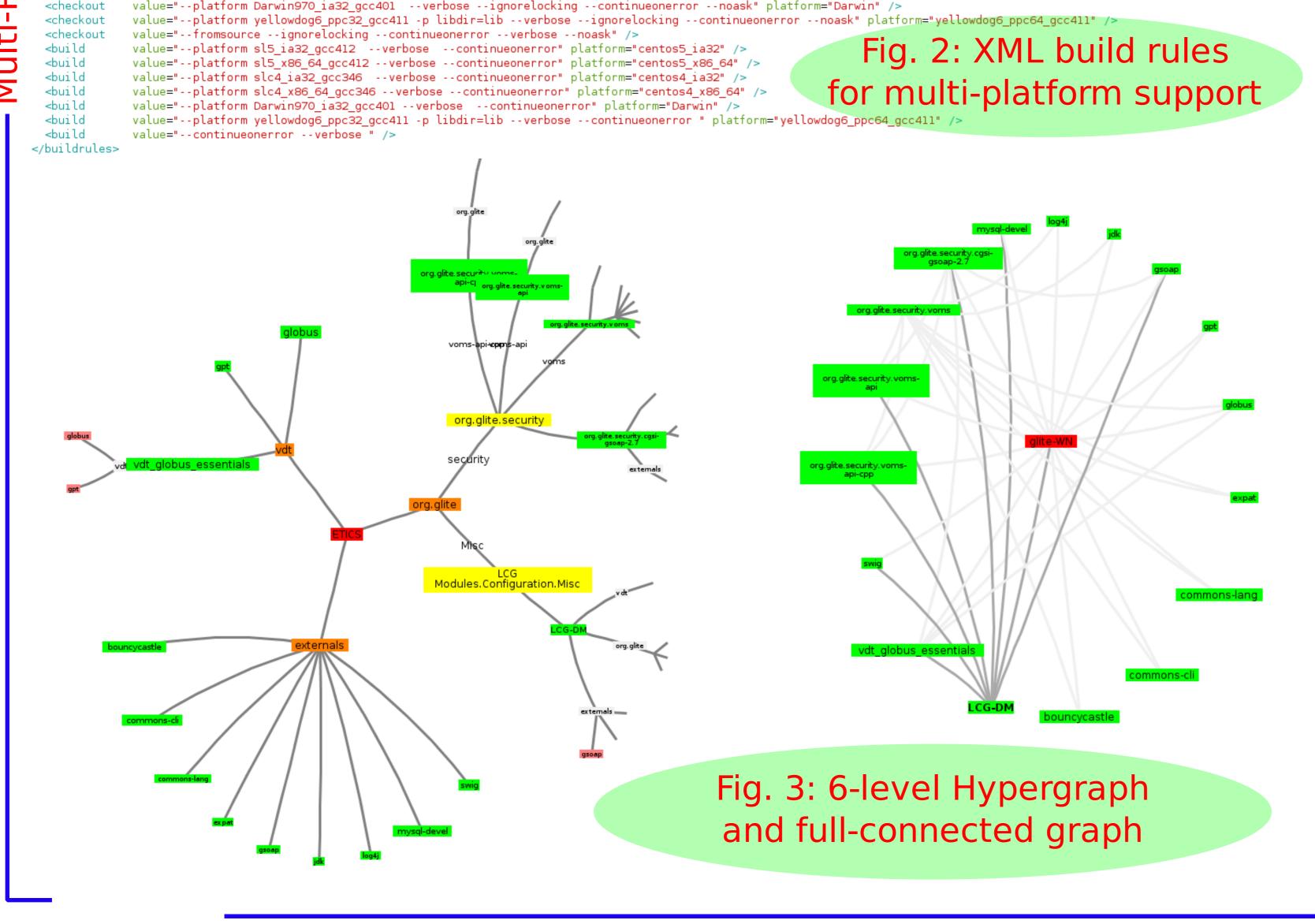
- 1. XML based build descriptions (see Figure 2).
- 2. Per platform patching with XML descriptions.
- 3. Per platform property overrides (in XML).

org.glite.security.cgsi-gsoap-2.7

- 4. Automatic sync and storage of XML/HTML in a directory structure allowing HTML table generation (see Figure 1).
- 5. Hypergraph generation based on the ETICS XML results set (see Figure 3).
- 6. Automatic RPM/deb to tarball generators in a form ready for integration into ETICS.
- 7. A http_proxy patched wrapper for the ETICS client to allow it to work on sites using squid proxy.

 8. Automated GNU patch generation based on fixes to ETIC.
- 8. Automated GNU patch generation based on fixes to ETIC components, timestamped and stored for future patching.9. An intermediate patching system applied between checkout
- and builds to help debug dependent components and keep ahead of the centralised build and test environment.

 Automated timestamped checkouts of ETICS configurations
- 10. Automated timestamped checkouts of ETICS configurations to be patched from the ETICS command-line interface.
- 11. Python scripts used to create wiki tables showing differences between multiple build result files.



The initial gLite port to the PS3 allows job submission, but not data management, however much of the data management code now builds in ETICS. The initial release is a minimal glite-WN containing VDT globus, VOMS, yaim and noarch components.

Jobs are submitted using the following process:

glite-voms-proxy-init --voms <vo_name> glite-wms-job-submit -a -r <ce>:2119/jobmanager-pbs-<queue> -o job.id job.jdl glite-wms-job-output --dir <dir_name> -i job.id

To become a sustainable infrastructure for Grid usage, the PS3 and other platforms must become production ready, centrally distributed nodes of the gLite middleware. In the meantime, TCD has the means to provide a partially maintained experimental minimal workernode.

eHiTS[®] Lightning 2009, is the electronic High Throughput Screening software ported by SimBioSys Inc. (www.simbiosys.ca) for the PS3 to fully utilise the Cell Broadband Engine™ (Cell B./E.).





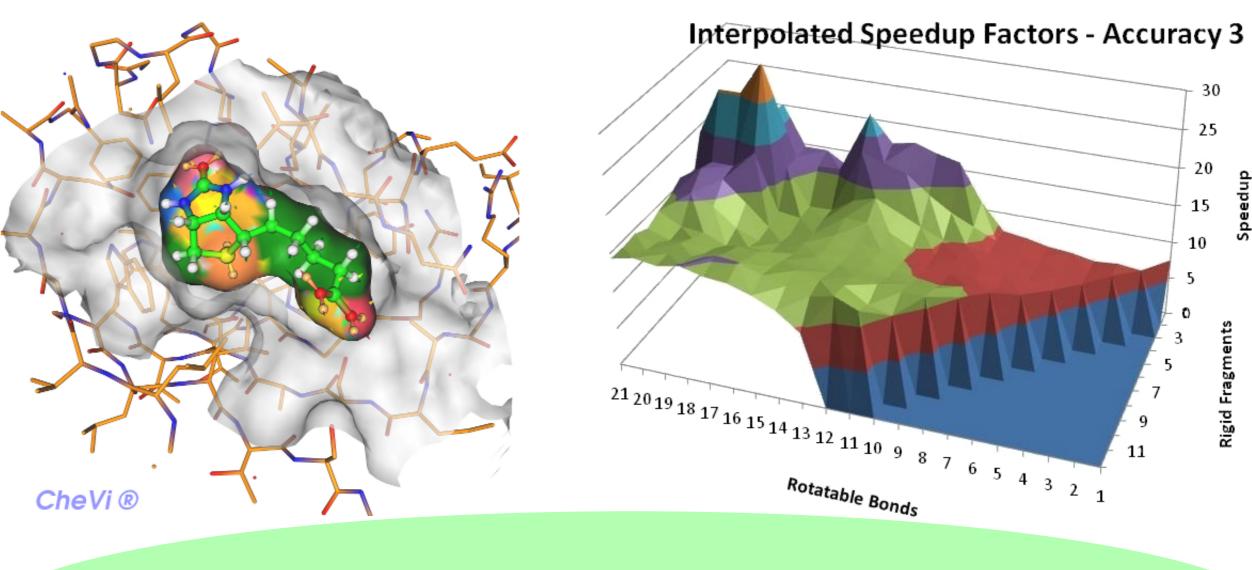


Fig. 4: An example ligand docked with eHiTS, and the docking speedup on the PS3 versus Intel platform

The ported eHiTS[®] software runs natively on the Cell B./E. fully utilizing the vector processing power of the SPEs. The speedup depends on the input data (see Figure 4) generating speedups ranging between 26-fold and 60-fold over Intel based processors.

TCD constructed an 8-node grid-enabled PS3 cluster, to which eHiTS[®] related jobs may be submitted via the EGEE Grid.





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