SCIGRESS Service
Installation Guide
For Job Scheduler

1 About this document

This document describes installation process of SCIGRESS service. It is suitable for job schedulers in computing centers.

2 Architecture

SCIGRESS service is installed to user's home directory in a computing center. Thanks to network files system, installed software is available on all nodes, wherever a given calculation is scheduled to execute.
We call it service, rather than server, because it does not operate permanently. Instead, a single calculation task is submitted to a job scheduler from SCIGRESS client.
Licensing of SCIGRESS service has to be integrated with a job scheduler so that tasks are started only when a sufficient number of license tokens is available. Possible options of integration are described in a separate document titled JobSchedulerIntegration.

3 Software that must be installed

- Java Runtime Environment is integrated in the deployed archive.

- SSH server is needed to access user's home directory and for file transfer.

- If you use a 64-bits version of Linux, 32-bits compatibility libraries need to be installed. In particular, 32-bits glibc and libstdc++.so.6 are needed.

4 Installation procedure

- Untar content of *schedulerServerLin.tar.bz2* into home directory of a selected user. It will create folder */home/your_login/SCIGRESS_server*. This location is fixed because SCIGRESS clients expect it. Copy *license.l4j* file into this folder.

- Try to execute any engine, for example *$HOME/SCIGRESS_server/Plugins/Mechanics/MechanicsManager.exe*, to check for possibly missing dependencies. If all dependencies are present, the executable will keep its process alive. You will need to type Ctrl-C to stop it. If you get a message about missing libstdc++.so.6, you need to install it somehow. If you get another error message, it is likely that you need to install 32-bit compatibility libraries, especially for glibc.

- `qdel.sh`, `qsub.sh` and `qstat.sh` are just stubs that define name and location of actual scripts. User is supposed to select suitable scripts from *scripts* subfolder and overwrite the stubs. The scripts are likely to require some adjustment to the local environment. At the moment, following job schedulers are interfaced: Torque, Open Grid Scheduler and PLGrid.

5 How to start the service

SCIGRESS service is not started manually. SCIGRESS client submits an experiment to a job scheduler. It is the scheduler that starts the service when resources become available. Location of the service must be known to SCIGRESS client. The procedure is described in section 7.

6 Licensing

Since calculations in computing centers are performed on multiple nodes, hardware-based licensing is not suitable in that environment. Instead, online (external) licensing is provided. Obtained *online.l4j* licensing file should be placed directly in *SCIGRESS_server* folder.

7 How to run remote calculations on client

- Open a chemical sample.

- Go to `Experiment -> Run…`

- Click on `Select Server` button. Server data is encrypted with a master password. When you visit this dialog for the first time, you will be asked to setup the password. Next time you visit the dialog, you will be asked to enter the password.

- Click `Add` button and type `queue://login@hostname` substituting real login and real hostname where SCIGRESS server has been installed.

- On successful connection, a list of available engines will be presented.

- Run experiments as on a local machine.

- The next time you visit `Select Server` dialog, you connect to a server by selecting it on the list and clicking `OK` or double-clicking the server name.

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SCIGRESS Server Installation Guide For a Single Node