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SCIGRESS Server Installation Guide For a Single Node

1 About this document

This document describes installation process of the simplest SCIGRESS server. It is suitable for multi-processor, single-node servers. Parallelization is available for selected engines.

2 Architecture

SCIGRESS server for a single node is designed for a standalone, multi-processor computer. It is the simplest one to install and configure, yet offers parallelized calculations up to the number of processor cores. Requires nothing but Java Runtime Environment and SSH access. The latter is present in every Linux distribution by default.

3 Software that must be installed

- Java Runtime Environment is included with the server. There is no need to install one.
- SSH server is needed to access SCIGRESS server 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 *singleNodeServerLin.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, please identify a package for your distribution that contains **32-bit** version of the library and install the package. If you get another error message, it is likely that you need to install 32-bit compatibility libraries, especially for glibc.



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5 How to startup the server

Server can be stopped and started with a maintenance script. Execute `./maintenance start` to start the server. Execute `./maintenance status` to check if it actually started. If it does not start within 10 seconds, review `scigress.out` and `scigress.err` log files. When you execute `./maintenance stop`, new calculations will not be started. However, those already started will continue until completion.

6 Licensing

You can get a hardware-locked license file or an online license key. If you choose the former, you need to collect and email hardware data. The simplest way is to execute `./maintenance start` command. The server will not start but it will generate `hardwareID.txt` file and print additional information into `scigress.err`. Obtained license file, whether `online.l4j` or `license.l4j`, should be placed directly in `SCIGRESS_server` folder.

7 Parallelized MD calculations

SCIGRESS is able to perform parallelized MD calculations. It requires `mpich` library to be installed. Required version is 1.2.7p1 and usually is not available in pre-compiled packages. Its source code can be downloaded from <ftp://ftp.mcs.anl.gov/pub/mpi/mpich-1.2.7p1.tar.gz>. Unpack the downloaded archive, change directory to `mpich-1.2.7p1` and issue the following commands:

```
./configure --prefix=$HOME/mpich --with-arch=LINUX --with-device=ch_shmem
make
make install
```

Path `$HOME/mpich/bin` must be added to `PATH` environmental variable to make `mpirun` available to SCIGRESS. Please note that `$HOME/mpich/bin` is added at the beginning of `PATH` to hide other versions of `mpirun` that might be present in `PATH`:

```
PATH=$HOME/mpich/bin:$PATH
export PATH
```

Finally, you need to replace the default, non-parallelized MD plugin with the parallelized one. Assuming you are in `SCIGRESS_server` folder, following commands should be executed:

```
mv Plugins/MD-ME Plugins/Parallel/MD-ME.serial
mv Plugins/Parallel/MD-ME.shared Plugins/MD-ME
```

Number of MD threads is limited by the number of CPU cores and available MD license tokens.

Another engine MO-G is available in parallelized version. You can switch version with the following commands:

```
mv Plugins/MO-G Plugins/Parallel/MO-G.serial
mv Plugins/Parallel/MO-G.shared Plugins/MO-G
```

7.1 Troubleshooting parallelized MD calculations

Parallelized calculations are more error-prone than other ones. There is a special tool you can use to execute shared-memory MD-ME calculations outside of SCIGRESS server infrastructure. With this tool, you can test correctness of MPICH installation. Output from MPICH is easily accessible and can be used to track down a source of problems.

Follow these steps:

1. Create a temporary folder in any location.
2. Copy `doc/TestShared.tar.bz2` into that folder and unpack with “`tar xjf TestShared.tar.bz2`”.
3. Execute `./runTest`, test sample is included.
4. Test is passed if you can find `MD-ME.sim` file while `MD-ME.err` is empty or missing.
5. In case of failure, the test can be re-executed if you delete all `MD-ME.*` files except for `MD-ME.exp`.

8 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.



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- Click Add button and type `ssh://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.