Pirana

The flexible modeling environment for NONMEM

Quick Guide: Setting up and working with a cluster over SSH on Windows

Version 1.1

Scope

This Pirana Quick Guide explains how to prepare, configure and work with a cluster over SSH, and how to subsequently work with Pirana to execute models on the cluster.

Preparation: SSH access

In order to execute runs on a cluster from a local system with Pirana, SSH access to the cluster from your local computer must be available.

- For Windows, the easiest way to do this is to install Putty. Make sure that you install the complete version of PuTTY, including the command line tool **plink.exe**.
- After installation, make sure Putty is available in the system path, or add the location of the Putty folder to the internal Pirana path via File → Settings → Software integration → 'Add this folder(s) to PATH at Pirana startup'.
- On Linux and Mac OSX, ssh is most likely already installed.

Preparation: Mounting a cluster folder as local drive

A remote folder on the cluster should be mounted as a local drive letter (e.g. R:) on your system. There are several ways to do this, some of which are described below. Please check with your system administrator if you don't manage to mount the cluster as a local drive.

- If the cluster is running Samba, a drive letter may be mounted through My Computer → Extra → Network connections.
- If only SSH (SFTP) access is available, software such as Expandrive may be considered.

Configuring the cluster

If the remote cluster folder can be mounted as drive letter on your system, and you have installed putty, cluster access may now be configured in Pirana.

- Access the settings menu via File → Settings → Clusters. A screen is obtained as depicted in Figure 1.

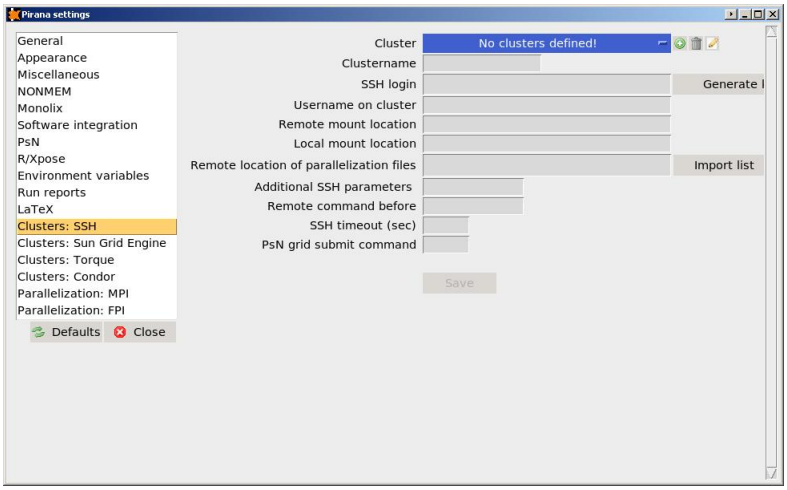

Figure 1: Cluster settings window

- Select the + sign to add a new cluster. Some initial settings are pre-entered in the textboxes of the newly defined cluster (Figure 2), but these have to be updated to match your cluster.

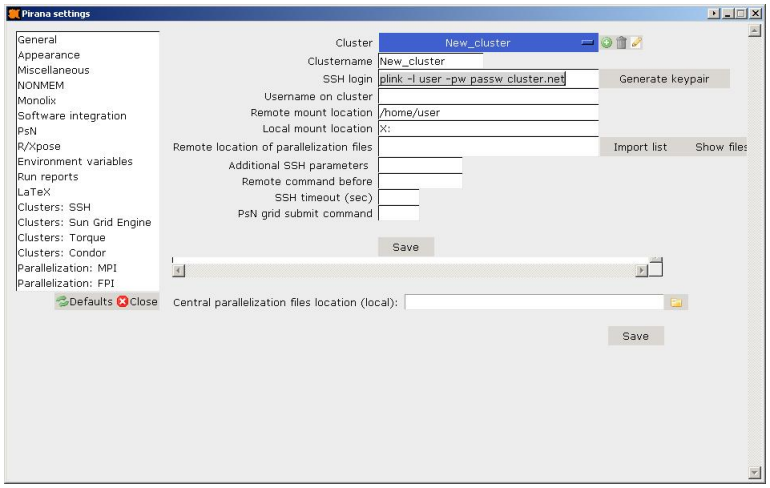

Figure 2: Pre-entered text after adding a new cluster

- In the textbox **Clustername**, define a name for the cluster (can be anything).
- The textbox **SSH login** should contain the command to connect to the cluster. If Putty is used, this command will start with **plink**, followed by the user name, password and name or IP address of the cluster access node, e.g. 'plink -l myname -p mypassw pkpd.server.org'. Passwordless access using a RSA key is also possible.
- The textbox **Remote mount location** refers to a folder on the cluster which you have mounted as local drive.
- The textbox **Local mount location** should contain the drive-letter on the local system which corresponds with the remote cluster path defined in the previous textbox.
- In the following textboxes, **Additional SSH parameters**, and **Remote commands before** connecting to the cluster, and the **PsN grid submit command** may be defined, but these are not required.
- An example of a fully configured cluster is depicted in Figure 3.

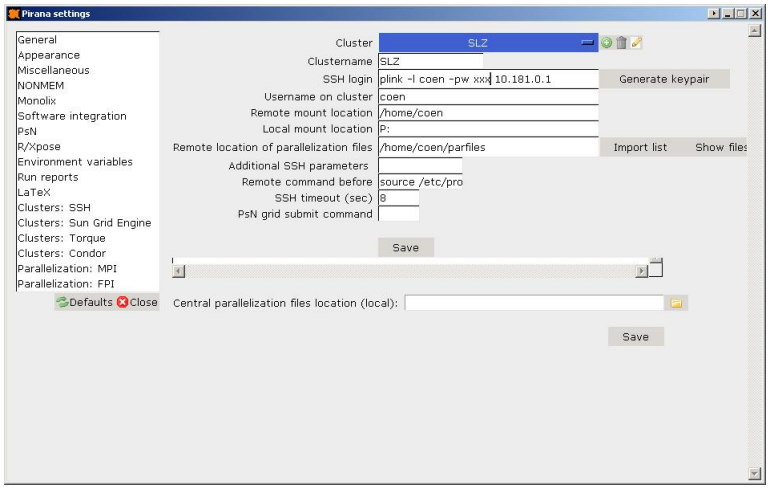

Figure 3: Settings of a fully configured cluster

Working with the cluster

- Any runs which are to be submitted to the cluster should be in a location on the drive which you specified the remote cluster mount location.
- A model can be run on the cluster via either **nmfe** or **PsN**, which are described separately below.

Submitting a run to the cluster via nmfe

- When submitting a run via nmfe, after selecting a model and opening the 'nmfe'-run dialog, select a cluster to connect to (Figure 4, blue quare).

- The option **Submit to [..]** should be selected if the run is to be submitted to a job scheduler. (Figure 4, green square). Currently supported schedulers are Sun Grid Engine (SGE), Torque and Condor.
- Optionally, for NONMEM 7.2, parallalization files may be selected.
- Start the run.

Figure 4: Defining cluster settings for a nmfe run

Submitting a run to the cluster via PsN

- Select a cluster for the PsN run (Figure 5, orange square).
- Add optional arguments to the PsN argument, such as **-run_on_sge**, if the run is submitted to SGE (Figure 5, red square).
- Several PsN arguments are available for other job schedulers such as LSF (Figure 5, blue square). Please note that the configuration of these job schedulers should be done in the psn.conf file on the cluster. Please refer to the PsN manual for more information about this.
- Start the run.

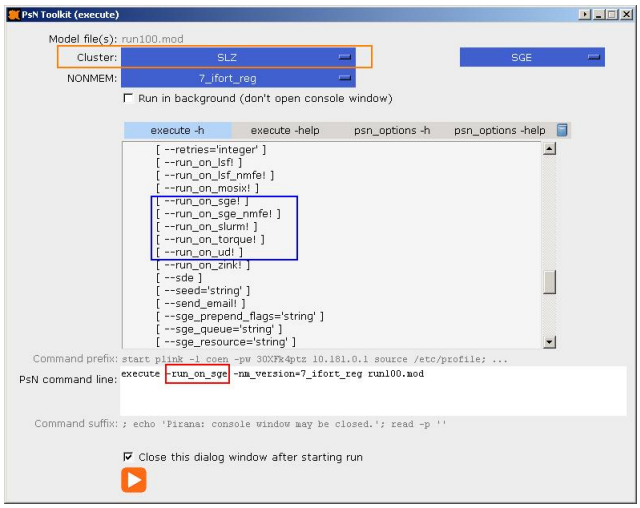

Figure 5: Defining cluster settings for a PsN run

Monitoring jobs on a SGE cluster

- If SGE, Torque or Condor is used as job managment system, the queue may be monitored using the integrated monitor in Pirana.
- This feature may be accessed by clicking the SGE icon in the main Pirana interface (Figure 2, red square).
- In the interface that is opened, an overview will be presented of the jobs that are currently running, scheduled, or have recently been finished. Some information about available nodes in the SGE cluster can also be viewed.
- By right-clicking on a job, you can view more information about it, or kill it. Please note that not only NONMEM jobs are shown here, but any compute job (e.g. MATLAB).

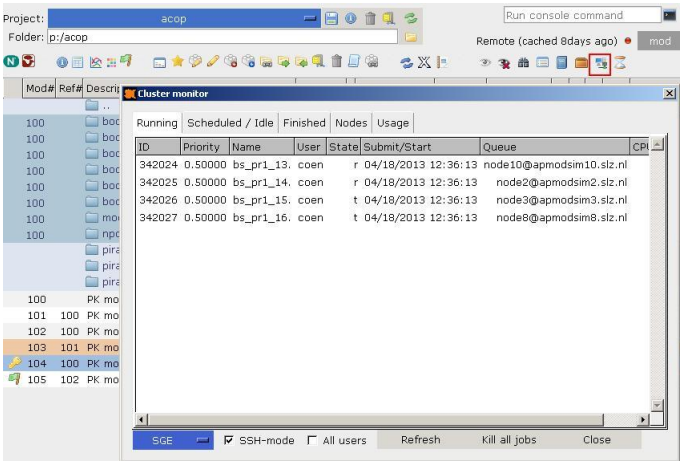

Figure 6: Cluster run window