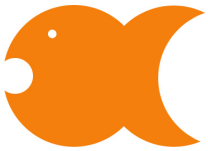
Pirana

The pharmacometrician's workbench



Version $\geq$ 2.9.7
Pirana on Metworx user guide

August 8, 2017

Introduction

Pirana, a modeling interface for NONMEM and PsN, is by default installed on Metworx 3 instances. This document is an overview of how to get started with Pirana on Metworx, as there are a few noteworthy differences compared to running Pirana on your desktop computer. We also provide some additional tips and tricks. A full user manual of Pirana is available at www.pirana-software.com.

This guide will be updated at regular intervals, and is available online from www.pirana-software.com/#docs. This document assumes Pirana 2.9.7 or up, and Metworx version 3.0 or up.

License file

The license file for Pirana is commonly not included on the Metworx instance, and therefore it has to be added by each individual Metworx user. Please note that without a license file, you can still access and use Pirana, but you will see a popup screen come up regularly asking for the license file. If you have a license file for Pirana, you can either upload the file manually to `/data` to activate Pirana, or from within Pirana go to "Help" → "Install license file" and select the file from a location within Metworx. If you do not have a license file yet, please contact `info@pirana-software.com` to obtain one or request further info.

Home folder / settings

Please keep in mind that the Metworx workflow is reprovisioned each time a new workflow is started. This means that all folders that are not in a persistently location – e.g. your home folder – will be wiped when the workflow is destroyed. Your persistent data storage in Metworx is available in the folder `/data`, which will also be used by Pirana to store some preferences.

Note: Pirana normally stores all user settings (such as UI settings, a list of projects, software settings etc) in your home folder, in `~/.pirana` to be specific. To allow you to persist your preferences and projects between Metworx workflows, Pirana will use `/data` to store these settings.

R libraries

A commonly used selection of R libraries is installed by default in Metworx, but other libraries will have to be installed manually. Since obviously we do not want to re-

install the same R libraries each time we start a new Metworx workflow, these libraries should also be installed into the persistent folder, in `/data/R/lib` to be precise. This is the folder that is automatically picked up by both RStudio and Pirana as the default location for custom R libraries. Therefore, when installing a custom R library for use within RStudio or Pirana, use e.g. the command:

```
install.packages("ggplot2", library="/data/R/lib")
```

or, when installing from GitHub:

```
install_github("hadley/ggplot2", library="/data/R/lib")
```

When running R scripts included with Pirana, you might encounter an error that a library was not found (e.g. `xpose4`). When such an error occurs, use the above syntax to install the missing library into the persistent R libraries folder `/data/R/lib`.

Parallelization

Pirana can instruct PsN to run NONMEM models on the Metworx cluster formed by the computational nodes that you started. Keep in mind that there are basically two ways of running in parallel that need to be distinguished:

- *Running a single model in parallel over multiple computational cores (using MPI and SGE)*

  To use this approach, several arguments need to be specified with the `execute` command. These arguments are already built into Pirana for Metworx and the job scheduler is also set by default to SGE. So to run a single model over multiple cores, you only have to select **auto-MPI** and select the number of cores you want to use. You can check in the **Cluster monitor** in Pirana that the model is actually distributed onto the computation server.

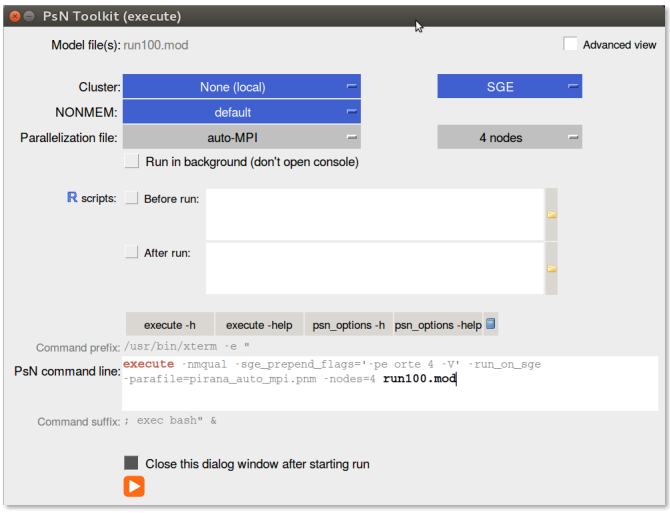


Figure 1: Screenshot 1

- *Running several models in parallel, e.g. bootstrap*

  In this case we usually don't want to use MPI-paralellization, so we set the *parallelization file* to **off**, but keep the *job scheduler* **SGE** selected. This will distribute the runs to the cluster, but won't split single runs over multiple cores. An example is given below.

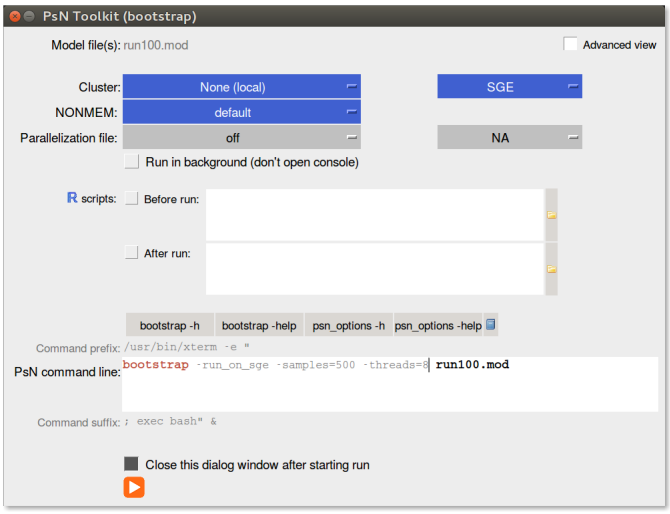


Figure 2: Screenshot 1

Note: Please refer to the manuals for PsN and NONMEM for more information on parallelization with job schedulers (SGE in this case) and MPI.

Anytime you run models using SGE, they will run on the computational node(s) that were started in the Metworx workflow. You should be able to see those runs in the tabs **Runnning**, **Scheduled**, or **Finished** in the cluster monitor within Pirana. See Pirana manual for more details on the cluster monitor.