slotervaartziekenhuis

NKI-AVL

A simple infrastructure and graphical user interface for distributed NONMEM analysis on standard computer networks

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Introduction

PK-PD modeling often demands high processing power, which can be delivered by distributed computing. Several solutions are already available[1,2], but these require investments in hardware, software and/or personnel.

Aim was to develop a cluster infrastructure that would:
- run in a standard network environment
- use spare CPU cycles of network-clients
- be easy to set up and maintain

Alongside, a graphical user interface (GUI, Piraña) was constructed to use the infrastructure and to be used for NONMEM analyses in general.

1. Run selected in Pirana to deploy to cluster
2. Compiled to executable
3. Idle client selected
4. nonmem.exe + auxilliary files copied to shared drive on network
5. Nonmem.exe started by client
6. Run ready. Results copied to shared drive
7. Run results + output available on shared drive
8. Results copied to local PC, evaluated in Piraña

Figure 1. Lifecycle of a NONMEM run deployed to the cluster

Methods

The infrastructure required:
- multiple PCs in a standard network, (that may simultaneously be used by others)
- shared network-drive accessible by all clients
- a cron service installed on every PC: for local execution of runs on the clients
- NONMEM and Piraña installed locally (not on every client): for compilation of model file and to deploy run to cluster

The cluster is easy to set up and maintain. New clients can be added to the cluster easily.

Runs could be deployed to the cluster from the GUI (figures 2-4), both by automated distribution or to specific idle clients.

Conclusion

A NONMEM cluster infrastructure was built using desktop PC's in a standard network environment. The setup could be of particular interest for modeling groups situated in hospital or academic settings.

A GUI, Piraña, was developed to use the infrastructure while also providing some modeling and analysis tools for NONMEM analysis.

Piraña

Aims of Piraña development were:
- Facilitate cluster & local execution
- Provide model management and run evaluation tools

Piraña was developed using Perl, extended with the Tk package, which enables creation of GUIs. Where possible, Piraña uses auxiliary software (such as R and PsN) to perform certain tasks.

Features include:
- Execution of NONMEM runs, on cluster or locally (figure 2)
- Front-end to PsN toolkit
- Automatic installation, compilation and management of multiple NONMEM installations (figure 3)
- Easy creation of goodness-of-fit plots
- HTML run reports from output files (using PsN-core[3], figure 1)
- Manage multiple modeling projects with model-, output- and data-files
- View, explore and convert data files
- Manage and run scripts on models/data
- Quick links to, and integration with auxiliary software

Results

The developed cluster (figure 1) has been used successfully now for over one year by up to five modelers simultaneously.

The infrastructure consisted of approximately 25 clients (standard desktop PCs), and supported multiple distribution to PCs with multi-core CPUs.

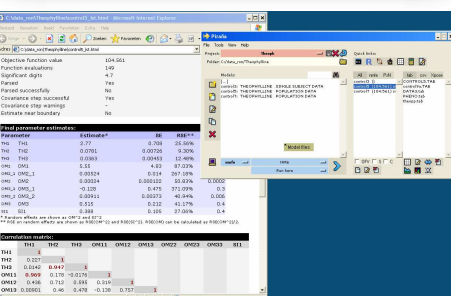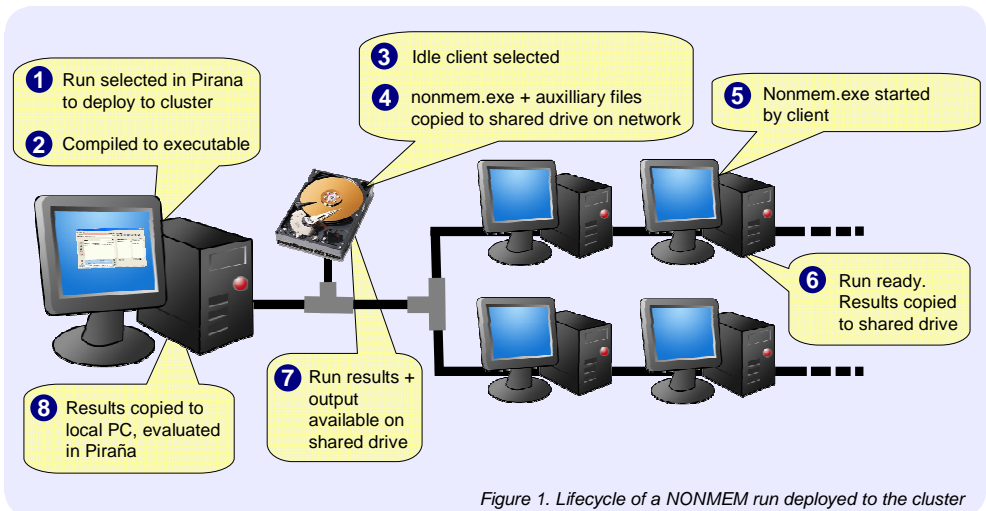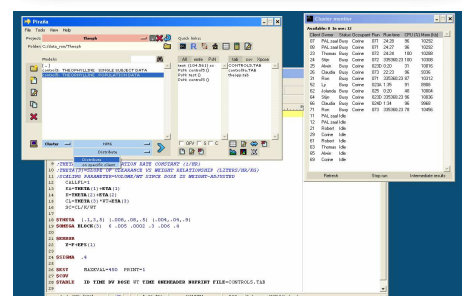The system was time-saving in model-development and high performance tasks, such as bootstrapping.

References

1. Pihlgren P. et al., PAGE 15 (2006) Abstr 1032
2. Lindbom L., PAGE 12 (2003) Abstr 438
3. Lindbom L. et al, Comput Methods Programs Biomed. 2004 Aug;75(2):85-94.

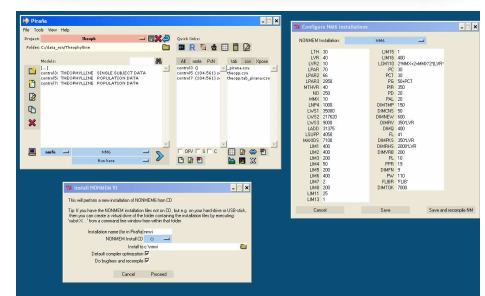*Figure 2. Create HTML report from run output*

Figure 3. Edit models; Monitor cluster

Figure 4. Install and manage NONMEM