Amdahl's law
Master-Worker
posterior state
prior state
system identification
forcing error
Bayesian methods
parameters
CPU
data assimilation
parallel computing
innovation
Message Passing Interface
MMSODA
SODA
Ensemble Kalman Filter
optimization SCEM-UA
walltime

The MMSODA Toolbox for MATLAB

eScience
OpenMPI/GNU
cluster computing
single-objective
model error
multi-objective
objective function
MATLAB
LISA
Jasper A. Vrugt
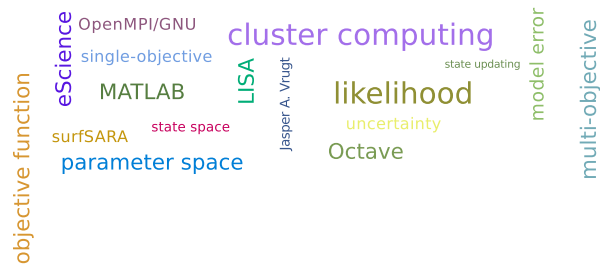likelihood
state updating
surfSARA
state space
uncertainty
parameter space
Octave

UNIVERSITY OF AMSTERDAM

netherlands Science center
by SURF & NWO

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Contents

Chapter 1

Introduction

This document is a manual for learning how to use the LISA cluster computer hosted at SURFsara (https://www.surfsara.nl/systems/lisa) for solving parameter tuning and system identification problems. The manual covers the basic organization of the cluster's hardware, and provides the user with some simple commands you'll need for manipulating the Linux system that LISA is running. The manual further introduces the MMSODA parameter tuning and system identification software that can be run on LISA. While going through this manual, you'll find that most of it is aimed at Windows users, but occasionally there will be brief instructions for Linux users as well (usually in the footnotes). It is assumed that you are proficient in using MATLAB, and that you have a working MATLAB installation on your local machine. Furthermore, it is assumed that you have a basic understanding of some of the general concepts used in optimization.

Chapter 2

Getting started

Effective usage of the LISA system requires that you:

1. have a basic understanding of how the LISA system is organized;

2. know how to copy files from your local machine to LISA and back using SFTP;

3. know how to establish an SSH connection, linking your local machine to the LISA system;

4. have a basic understanding of the Linux commands that are needed to tell the LISA system what it is you want to do.

In the remainder of this Chapter, we cover these items in relevant detail.

2.1 Cluster computing

A *cluster computer* is a system of interconnected computers that work together so that in many respects they can be viewed as a single system. Clusters usually consist of regular off-the-shelf computers such as those you may find in any computer retail shop (see Fig. 2.1). Cluster computers are especially suited for solving a certain class of computational problems, namely those problems that can be divided into smaller, independently solvable tasks. As a trivial example, finding the minimum value in a 2-D array of values (i.e. a map) is such a problem: the map can be split into two parts and sent to two separate machines. After both machines have found the minimum value in the part of the map that they were assigned, the 'global' minimum can be determined by simply comparing the two values. Dividing the task over two or more machines (or actually, *cores*) is called *parallelization*. Parallelization can greatly reduce the *walltime* of a computational task (i.e. the time between starting a task and knowing the solution).

Figure 2.1: Technicians at work on a real cluster computer. Photo from http://en.wikipedia.org/wiki/File:MEGWARE.CLIC.jpg.

2.2 The LISA cluster: hardware

The LISA cluster currently[1] consists of 624 normal computers, which are referred to as *nodes*. In terms of hardware, each node has a Central Processing Unit (CPU), disk storage, and memory. The nodes are interconnected using a Local Area Network (LAN). The LAN has low latency and high bandwidth (Gigabit or Infiniband), meaning that in terms of time it is cheap to send large files (because of the high bandwidth) as well as small files (because of the low latency). Storage space on each node varies a little bit, but at the time of writing is 70–220 GB per node. Most nodes have 8-core CPUs, although some have 12-cores or 16-cores. The clock frequency for individual cores is 1.80–2.26 GHz. In terms of memory, most nodes have 24 GB, but the 16-cores have 32 GB. Furthermore, the bandwidth between memory and CPU varies between 5.86–8.00 GT/s. Finally, all nodes run the Debian Linux AMD64 operating system.

---

[1]LISA's hardware is subject to regular upgrades. For concurrent information, see https://www.surfsara.nl/systems/lisa/description#System_configuration

2.3 Transferring files to and from the LISA cluster

This section documents the necessary steps for connecting to the LISA cluster from a local Windows machine. First, make sure that you have an account for accessing LISA[1]. In order to use the cluster effectively, you need to be able to copy files to and from your user directory on the cluster. The LISA cluster is set up such that it exclusively allows connections that are secure, such as Secure File Transfer Protocol (SFTP) connections or Secure Shell (SSH) connections. There are many programs that can establish secure connections, but we will use WinSCP[2].

▶ 1. Download WinSCP from http://sourceforge.net/projects/winscp/files/WinSCP/4.3.7/winscp437.zip/download[3,4]. Unzip into your local home directory or a USB drive. Double-click on 'WinSCP.exe' to start the WinSCP program. The program will prompt you for some input (see Fig. 2.2). Under 'Host name:', fill in 'lisa.surfsara.nl'. Make sure that the port number is set to '22'. Under 'User name:', fill in your LISA cluster username. You can leave the 'Password' field blank, the program will prompt you later. Make sure 'SFTP' is selected as the file protocol. Click on 'Save...' to store these settings if you like. Then press the 'Login' button to establish the SFTP connection to the LISA cluster. The program will throw a warning about the RSA key fingerprint file. The number shown in the warning dialog should be the same as the number posted at https://www.surfsara.nl/systems/shared/ssh (table at the bottom of the web page). If it is, press 'Yes' and then 'Continue' in the next dialog box. As a final step, fill in your password when prompted. You should now see two panes, one for the local machine on the left and one for the remote machine, i.e. the LISA cluster, on the right (see Fig. 2.3).

▶ 2. Go to https://github.com/NLeSC/esibayes and click the 'Download ZIP' button to download the tutorial files needed when working through this chapter, as well as the files pertaining to the MMSODA Toolbox for MATLAB, which we will use later. Unzip it into your (local) home directory or a USB drive.

---

[1]You can get an account by following the instructions from https://www.surfsara.nl/systems/lisa/account.

[2]If you elect not to use WinSCP, make sure that your alternative program can handle file permissions correctly when transferring between Windows and Linux. Also make sure that line endings are converted properly. Check http://en.wikipedia.org/wiki/Newline for an interesing read on the many ways in which end-of-line characters may cause you trouble. Finally, if you have a text file with Windows-style line endings (CR/LF) and you want to convert it to Linux-style line endings (LF), make sure to check out the free, open-source, Notepad++ editor at http://notepad-plus-plus.org/. This excellent program lets you convert between line endings in just a few mouse clicks.

[3]By the time you read this, there may be a more recent version available—just substitute '4.3.7' and '437' from the address with the version you want. For an overview of available versions, look here: http://sourceforge.net/projects/winscp/files/WinSCP/.

[4]Life is somewhat easier for Linux users. Most Linux distributions come with built-in support for secure connections. Just start up your regular file browser (e.g. PCManFM, Thunar, Nautilus, etc) and type in the address bar sftp://jspaaks@lisa.surfsara.nl/home/jspaaks. Don't forget to substitute your own username. This should automatically establish a connection between your machine and the remote system (i.e. the cluster). Fill in your credentials when prompted.
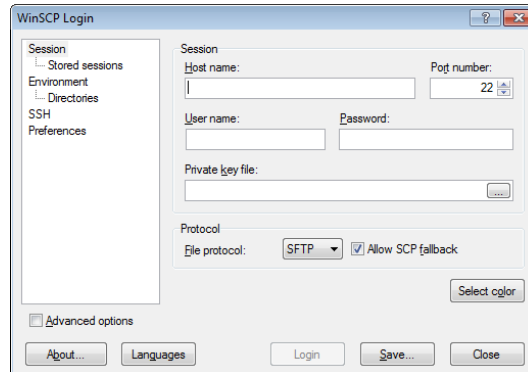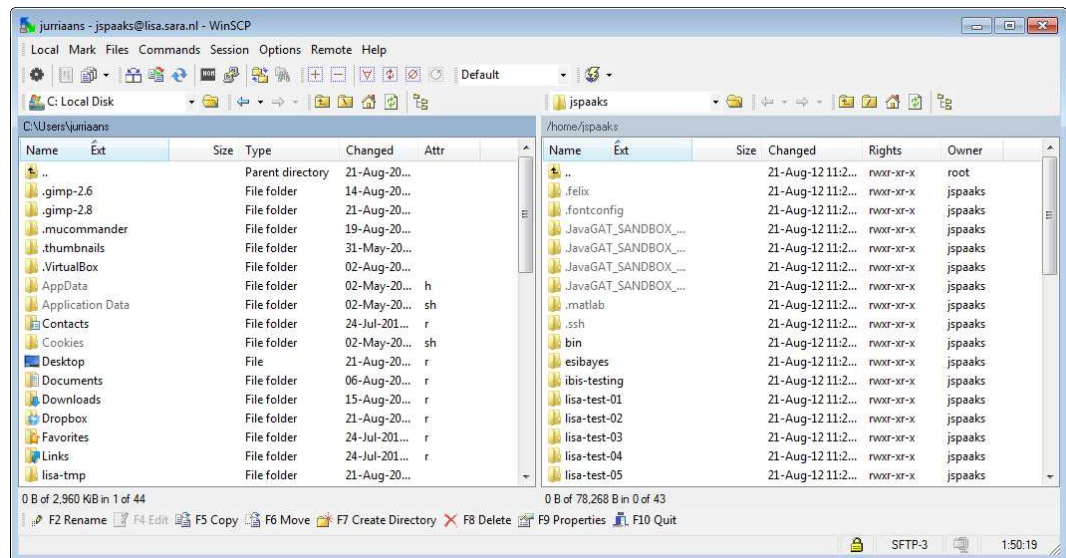
Figure 2.2: WinSCP session dialog box.

Figure 2.3: WinSCP interface. On the left is my local file system, on the right is my home directory on the remote file system. If this is the first time you connect to LISA, the remote file system should be pretty much empty.

▶ 3. In WinSCP, use the left pane to navigate to the directory where you unzipped the files. Change directory into the 'manual' subdirectory. Copy the 'tutorial' directory to the remote directory by selecting it on the left and pressing the F5 button. The tutorial directory should now be present in the right pane as well.

2.4   Issuing commands on the LISA cluster

This section covers how you can issue commands from your local machine, which then get executed by the remote system (LISA). Issuing commands on the LISA cluster can be accomplished through a so-called *terminal emulator* program. A terminal emulator provides you with a prompt at which you can type commands which are then executed on the remote system. It doesn't matter whether the remote system is located just across the street or halfway around the world, you can still operate the remote system through the terminal emulator. However, it is important to note that the LISA cluster, like virtually all clusters[1], runs under the Linux operating system. The commands that you type at the terminal emulator prompt therefore need to be Linux commands, which, as you will see later, are somewhat different from the Windows commands that you may be familiar with.

Let's first download the terminal emulator PuTTY from http://www.chiark.greenend.org.uk/~sgtatham/putty/download.html into your home directory. Double-click the executable to run the program. You should now see the dialog from Fig. 2.4. Under 'Host name (or IP address)', fill in 'lisa.surfsara.nl' and press the 'Open' button. PuTTY first prompts you for your username and then for your password. Fill in your LISA credentials.[2]

You are now remotely logged in to the Linux cluster LISA. Your terminal emulator program should show something like:

```
jspaaks@login2:~$
```

where `jspaaks` is the username and `login2` is the name of the remote machine. There are, in fact, two machines on which you can log in remotely: besides `login2`, there's also `login1`. For our intents and purposes, it doesn't matter whether you are logged in to `login1` or `login2`, but if you want to change from one to the other, you can do so with:

```
jspaaks@login2:~$ ssh login1
```

When you're done with the terminal, you can close the connection using:

```
jspaaks@login2:~$ logout
```

If you want to find out in which directory you are, you can use the `pwd` command ('pwd' is short for present working directory):

```
jspaaks@login2:~$ pwd
```

---

[1]See http://www.top500.org/statistics/ for concurrent statistics on the World's top 500 of supercomputers.

[2]On Linux, bring up a terminal (Ctrl-Alt-t on most distributions) and type in `ssh jspaaks@lisa.surfsara.nl`, substituing your own username in stead of `jspaaks`. Fill in your credentials when prompted.
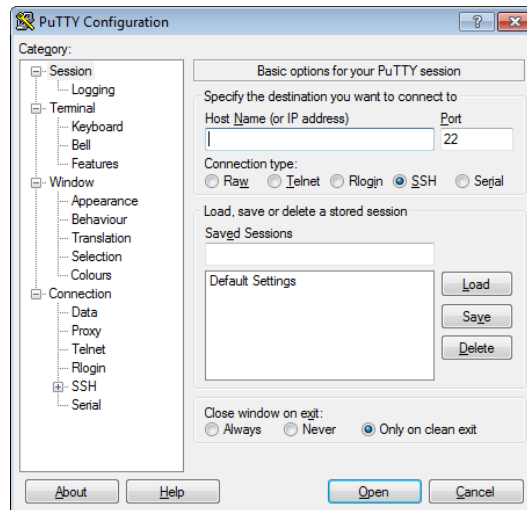
Figure 2.4: PuTTY session dialog box.

which returns:

```
/home/jspaaks
```

It is worth noting that a list of useful commands and terms has been included in the Index section at the back of this document (under 'Linux commands').

So, `pwd` currently returns `/home/jspaaks/`. `/home/jspaaks/` is the user's home directory; it is the Linux equivalent of 'C:\Users\jspaaks' on Windows. Note that on Linux the directory separator is the forward slash '/' sign, whereas Windows uses the backslash '\' sign. You may be wondering why there isn't a 'C:\' in the address returned by `pwd`. The reason is simple: Linux uses '/' instead of 'C:\'. The first forward slash in the address is referred to as the 'file system root'[1]. Under the file system root is a directory 'home', which contains a subdirectory 'jspaaks' in which the user 'jspaaks' keeps all his personal files. As a matter of fact, `/home/jspaaks` is the only place on this file system that user 'jspaaks' is permitted to write anything, meaning that Linux will not allow you to save any files in other users' home directories (although you are allowed to read some of them, depending on how the *permissions* on that directory are set. More about permissions later).

You can view the contents of the current directory using the `ls` (short for 'list') command:

```
jspaaks@login2:~$ ls
```

This should show at least the 'tutorial' folder that we just copied using WinSCP. It is likely that there are a few more files and directories present, but you should leave them as they are.

---

[1]Somewhat confusingly, the account that has Administrator privileges is also referred to as 'root' on Linux systems, but this account has no relation with the root of the file system.

Changing the current working directory works in a similar way as at the Command Prompt on Windows:

```
jspaaks@login2:~$ cd tutorial
jspaaks@login2:~/tutorial$
```

Note that the prompt includes the location of the current directory: '~' (pronounced: 'tilde') represents the home directory ('/home/jspaaks'). Changing from any location on the file system to the user's home directory goes like so:

```
jspaaks@login2:~/tutorial/a/really/deeply/nested/directory$ cd ~
jspaaks@login2:~$
```

or if you want to move just one directory up:

```
jspaaks@login2:~/tutorial/a/really/deeply/nested/directory$ cd ..
jspaaks@login2:~/tutorial/a/really/deeply/nested$
```

make sure to include the space character in between the `cd` and `..` characters though, otherwise it won't work.

A new directory can be created by the `mkdir` command, for example:

```
jspaaks@login2:~$ mkdir anewdir
```

Note that, contrary to Windows file systems, Linux file systems are case-sensitive. For example:

```
jspaaks@login2:~$ mkdir aNewDir
```

will result in an additional directory:

```
jspaaks@login2:~$ ls
anewdir    aNewDir    tutorial
jspaaks@login2:~$
```

The different approaches that Windows and Linux take regarding case-sensitivity of their respective file systems can lead to errors, especially when copying back and forth between Windows and Linux systems. For example, the contents of `anewdir` and `aNewDir` may get merged when they are copied to a Windows system, since Windows regards the folders as being one and the same. To avoid these kinds of errors, the naming convention on Linux is to use only lower caps names for files and folders, so `anewdir` is preferable to `aNewDir`.

Regardless of your native operating system, your code will be more robust and more portable if you stick to these 2 simple rules when naming your files and directories:

1. don't use spaces;

2. limit yourself to the following subset of characters:
   `abcdefghijklmnopqrstuvwxyz_-.0123456789`,
   and, if you must, `ABCDEFGHIJKLMNOPQRSTUVWXYZ` .[1]

Removing a directory goes like this:

```
jspaaks@login2:~$ rmdir aNewDir
```

or like this if you want to remove multiple directories:

---

[1]You'll thank me later!

```
jspaaks@login2:~$ rmdir anewdir aNewDir
```

You can delete a file using the **rm** command:

```
jspaaks@login2:~$ rm the-file-you-want-removed.txt
```

or like this if you want to remove multiple files:

```
jspaaks@login2:~$ rm first-file.txt second-file.zip third-file.m etcetera.exe
```

For many commands, you can specify options. Options to a given command must generally be provided directly after the command itself, i.e. before any other argument such as input or output files. The option argument consists of one dash followed by one (case-sensitive) letter. For example, if you want **ls** to list the contents of the current directory in more detail, you can use the **-l** option (that is the letter l for 'long', not the number 1):

```
jspaaks@login2:~$ ls -l
total 4
drwxrwxr-x 2 jspaaks jspaaks 2 Jun 13 13:07 tutorial
```

which gives you, amongst other things, the *permission bits* (i.e. drwxrwxr-x), the owner of the item (jspaaks), the item's size (2) in bytes and the time when the item was last altered (Jun 13 13:07). Note that, by default, **ls** sorts the items in a directory based on the item's name, so directories and files will appear intermingled. You can easily tell whether an item is one or the other by looking at the permission bits: if the item is a directory, the first character that appears in the permission bits is the letter **d**. For files, the first character in the permission bits is **-**.

Most Linux commands have at least a few optional arguments. If you want to know more about a particular command's usage, you can use the **man** (short for 'manual') command, which lists all the options for a given program including a short description of what each option does. For example, try:

```
jspaaks@login2:~$ man ls
```

(you can scroll down using the 'Up' and 'Down' arrows. Pressing the 'q' key lets you return to the prompt). If you just want to verify that you remember the command right, you can check by:

```
jspaaks@login2:~$ whatis ls
ls (1)                - list directory contents
```

which will give you a short summary of what ls is doing, but without all the technical detail.

In addition to the shorthand notation, some options also have a longer version for improved readibility. The longer version always starts with two dashes instead of one. As an example, the **-h** option makes **ls** list the filesizes in more easily interpretable units such as kB or MB, rather than in bytes:

```
jspaaks@login2:~$ ls -l -h
```

or, combining the shorthand options:

```
jspaaks@login2:~$ ls -lh
```

The longer version of the **-h** option is **--human-readable**, so the complete command becomes:

```
jspaaks@login2:~$ ls -l --human-readable
```

Now that you know a little bit about Linux, let's look at how to manipulate files. **cd** into the 'deeply nested directory' by typing:

```
jspaaks@login2:~$ cd tu
```

if you now press Tab, the *shell* program (i.e. the program that lets you enter commands at the prompt) will automatically complete your command, like so:

```
jspaaks@login2:~$ cd tutorial
```

This autocomplete works because the shell knows that you want to do a `cd`, and since there is only one directory in ~ that starts with `tu`, the shell program knows that you want to `cd` into `tutorial`.

If you `cd` into `a/really/deeply/nested/directory` and list the directory contents, there should be a file called 'with-a-file-in-it.txt'. Because this is an ASCII text file, you can display it in the shell program by using the command `cat`, like so:

```
jspaaks@login2:~/tutorial/a/really/deeply/nested/directory$ cat with-a-file-in-it.txt
```

`cat` is short for 'concatenate', meaning it appends the contents of 'with-a-file-in-it.txt' to whatever is already displayed within the shell. Also note that autocomplete works here as well, but instead of listing any directory names, it will suggest a file from the current directory, since that is the kind of argument that `cat` expects. You will see the following output:

```
jspaaks@login2:~$ cd tutorial/a/really/deeply/nested/directory/
jspaaks@login2:~/tutorial/a/really/deeply/nested/directory$ ls
with-a-file-in-it.txt
jspaaks@login2:~/tutorial/a/really/deeply/nested/directory$ cat with-a-file-in-it.txt
* * * * * * * * * * * * * * * * * * * *
* *                                 * *
* *   hello world, the classic phrase  * *
* *                                 * *
* * * * * * * * * * * * * * * * * * * *
jspaaks@login2:~/tutorial/a/really/deeply/nested/directory$
```

(the lines that start with asterisks are actually the contents of 'with-a-file-in-it.txt'.)

Let's now try to move this file to the top directory in the user's home by using the move command `mv` like so:

```
jspaaks@login2:~/tutorial/a/really/deeply/nested/directory$ mv with-a-file-in-it.txt ~
```

The syntax for this command is the command itself, i.e. `mv`, followed by a space, followed by the first input argument, in this case the name of the file that we want to move, i.e. `with-a-file-in-it.txt`, followed by another space, followed by the name of the directory that we want to move it to ~. Also note that autocomplete works here as well, just type `mv wit` and press Tab to autocomplete.

Let's check that the file really got moved:

```
jspaaks@login2:~/tutorial/a/really/deeply/nested/directory$ cd ~
jspaaks@login2:~$ ls -l
total 6
drwxr-xr-x  4 jspaaks jspaaks    4 Aug 20 11:59 tutorial
-rw-r--r--  1 jspaaks jspaaks  210 Aug 20 15:21 with-a-file-in-it.txt
jspaaks@login2:~$
```

You can also use the `mv` command to rename a file by 'moving' it to a different filename in the same directory like so:

```
jspaaks@login2:~$ ls -l
total 6
drwxr-xr-x  5 jspaaks jspaaks    5 Aug 21 14:45 tutorial
-rw-r--r--  1 jspaaks jspaaks  210 Aug 20 15:21 with-a-file-in-it.txt
jspaaks@login2:~$ mv with-a-file-in-it.txt the-renamed-file.txt
jspaaks@login2:~$ ls -l
total 6
-rw-r--r--  1 jspaaks jspaaks  210 Aug 20 15:21 the-renamed-file.txt
drwxr-xr-x  5 jspaaks jspaaks    5 Aug 21 14:45 tutorial
jspaaks@login2:~$
```

Now suppose we don't want to move a file but we want to copy it. This can be done using

the `cp` command. For example:

```
jspaaks@login2:~$ cp with-a-file-in-it.txt copy-of-the-text-file
```

The copy command `cp` expects the file-to-be-copied as its first argument, and the name of the file-to-copy-to as its second argument. Further note that you don't have to specify extensions such as '.txt' in the filename for the operating system to know that `copy-of-the-text-file` is a text file, as you would normally do on Windows. Nevertheless, including the extension in the file name allows easy identification of the type of file, for example when listing the contents of a directory with `ls`, especially when combined with wildcards such as `*`:

```
jspaaks@login2:~/tutorial/a$ ls -l
total 10
-rw-rw-r-- 1 jspaaks jspaaks 16 Aug 22 10:02 file1.txt
-rw-rw-r-- 1 jspaaks jspaaks 16 Aug 22 10:00 file2.txt
-rw-rw-r-- 1 jspaaks jspaaks 16 Aug 22 10:00 file3.txt
-rw-rw-r-- 1 jspaaks jspaaks 13 Aug 22 10:02 file4.m
-rw-rw-r-- 1 jspaaks jspaaks 13 Aug 22 10:01 file5.m
drwxr-xr-x 3 jspaaks jspaaks  3 Aug 20 11:56 really
jspaaks@login2:~/tutorial/a$ ls -l *.txt
-rw-rw-r-- 1 jspaaks jspaaks 16 Aug 22 10:02 file1.txt
-rw-rw-r-- 1 jspaaks jspaaks 16 Aug 22 10:00 file2.txt
-rw-rw-r-- 1 jspaaks jspaaks 16 Aug 22 10:00 file3.txt
jspaaks@login2:~/tutorial/a$
```

`cp` also lets you copy directories, like so:

```
1   jspaaks@login2:~$ cd tutorial
2   jspaaks@login2:~/tutorial$ ls -l
3   total 5
4   drwxr-xr-x 3 jspaaks jspaaks 3 Aug 20 11:56 a
5   drwxr-xr-x 2 jspaaks jspaaks 5 Aug 20 12:07 simple-jobscript
6   jspaaks@login2:~/tutorial$ mkdir another
7   jspaaks@login2:~/tutorial$ cp -R a/* another
8   jspaaks@login2:~/tutorial$ ls -l
9   total 8
10  drwxr-xr-x 3 jspaaks jspaaks 3 Aug 20 11:56 a
11  drwxrwxr-x 3 jspaaks jspaaks 3 Aug 21 14:46 another
12  drwxr-xr-x 2 jspaaks jspaaks 5 Aug 20 12:07 simple-jobscript
13  jspaaks@login2:~/tutorial$ cd another/really/deeply/nested/directory/
14  jspaaks@login2:~/tutorial/another/really/deeply/nested/directory$
```

Line 1 changes the current directory to `tutorial`, line 2 lists its contents, line 6 creates the directory called 'another'. The actual copying is subsequently done in line 7. The complete command consists of the `cp` command, followed by the `-R` option that makes `cp` copy recursively, followed by the source files and folders `a/*` (i.e. everything under `~/tutorial/a`), followed by the destination directory `another`. Line 8 shows the newly created directory, while lines 13–14 show that the copy operation was indeed recursive.

Besides manipulating files and folders, the shell can do a lot more. For example, you can temporarily turn the shell program into an Octave[1] command window, like so:

```
jspaaks@login2:~$ octave
```

The Octave program welcomes you with its default welcome message, followed by a prompt:

```
GNU Octave, version 3.2.4
Copyright (C) 2009 John W. Eaton and others.
This is free software; see the source code for copying conditions.
There is ABSOLUTELY NO WARRANTY; not even for MERCHANTABILITY or
FITNESS FOR A PARTICULAR PURPOSE.  For details, type `warranty'.
```

---

[1]Octave is a free, open-source clone of MATLAB. See http://www.gnu.org/software/octave/.

```
Octave was configured for "x86_64-pc-linux-gnu".

Additional information about Octave is available at http://www.octave.org.

Please contribute if you find this software useful.
For more information, visit http://www.octave.org/help-wanted.html

Report bugs to <bug@octave.org> (but first, please read
http://www.octave.org/bugs.html to learn how to write a helpful report).

For information about changes from previous versions, type `news'.

octave:1>
```

At the prompt, you can type any Octave command (note that the Octave language is almost completely the same as the MATLAB language). For example:

```
octave:1> for k=1:4, disp(['The value of ''k'' = ',num2str(k)]),end
The value of 'k' = 1
The value of 'k' = 2
The value of 'k' = 3
The value of 'k' = 4
octave:2>
```

If you want to return to the normal shell, just type:

```
octave:2> exit
```

From the example above, you can see that typing everything on the command line can be tricky, even for simple tasks. Wouldn't it be great to have an editor of some kind? You've guessed it, the shell can also be turned into a (very) basic editor, like so[1]:

```
jspaaks@login2:~$ nano
```

You can use the nano program to write a simple Octave script, for example the one in Listing 2.1:

Listing 2.1: Example of a simple Octave script in nano.

```
1    GNU nano 2.2.4                    New Buffer                         Modified
2
3  % This is a simple octave script example written in Nano
4
5  % clear any old variables
6  clear
7
8  for k=1:5
9      str = ['The value of ''k'' is ',num2str(k)];
10     disp(str)
11 end
12
13
14
15
16
17 ^G Get Help    ^O WriteOut    ^R Read File   ^Y Prev Page   ^K Cut Text    ^C Cur Pos
18 ^X Exit        ^J Justify     ^W Where Is    ^V Next Page   ^U UnCut Text  ^T To Spell
```

The first line of Listing 2.1 consists of the name and version of the nano program, followed by either the filename (if you opened an existing file) or the string New Buffer (if the file has

---

[1]For more complicated programs, it can be more convenient to do the editing on your local machine using your own tools, and then upload the file to the remote system using WinSCP.

not been saved yet). The string `Modified` is displayed at the right if the user has made any changes. The bottom two lines list a number of keyboard combinations, where the caret symbol `^` represents the Ctrl key, so `^G` means Ctrl-g. After you've typed your script, you can save it by pressing Ctrl-o, typing the filename that you want your script to have, and pressing Enter. You can exit nano by pressing Ctrl-x. If you happen to press Ctrl-x when your script has not been saved yet, nano will ask you if you want to save it before exiting.

Let's check that the script from Listing 2.1 was written to file:

```
jspaaks@login2:~$ cat simple_octave_script.m
% This is a simple octave script example written in Nano

% clear any old variables
clear

for k=1:5
    str = ['The value of ''k'' is ',num2str(k)];
    disp(str)
end
jspaaks@login2:~$
```

Now we can call the Octave program using the name of the script as an input argument like so:

```
jspaaks@login2:~$ octave simple_octave_script.m
```

This starts the Octave program, runs the script within it as if you had typed 'simple_octave_script' at the Octave prompt, and returns to the shell:

```
jspaaks@login2:~$ octave simple_octave_script.m
GNU Octave, version 3.2.4
Copyright (C) 2009 John W. Eaton and others.
This is free software; see the source code for copying conditions.
There is ABSOLUTELY NO WARRANTY; not even for MERCHANTABILITY or
FITNESS FOR A PARTICULAR PURPOSE.  For details, type `warranty'.

Octave was configured for "x86_64-pc-linux-gnu".

Additional information about Octave is available at http://www.octave.org.

Please contribute if you find this software useful.
For more information, visit http://www.octave.org/help-wanted.html

Report bugs to <bug@octave.org> (but first, please read
http://www.octave.org/bugs.html to learn how to write a helpful report).

For information about changes from previous versions, type `news'.

The value of 'k' is 1
The value of 'k' is 2
The value of 'k' is 3
The value of 'k' is 4
The value of 'k' is 5

jspaaks@login2:~$
```

2.5   Jobscripts and the scheduler

So far, we've executed all our commands on just one machine, 'login2'. As long as the task at hand is a small one, this isn't a problem, but if the task takes a long time to run, it can be advantageous to divide the task into smaller parts, and let each part be computed by a separate machine. The way this works on LISA is as follows: you write a small text file, referred to as a *jobscript*. The jobscript lays out the requirements of the task, such

as the number of nodes that are needed, the program that you want to run, and where the necessary data can be found. The jobscript is then sent to a program known as the *scheduler*. The scheduler runs on LISA and manages the requests from all users, such that the computation resources are used in an optimal way, while taking into account things like different priority levels, the number and type of nodes that are needed, and so on.

Listing 2.2 is an example of a simple jobscript.

Listing 2.2: Example of a jobscript.

```
 1  #PBS -lwalltime=00:05:00
 2  #PBS -lnodes=1:cores8:ppn=1
 3  #PBS -S /bin/bash
 4
 5  echo `date`: job starts
 6
 7  # let octave execute the disp and pause commands:
 8  octave --silent --no-window-system --eval "disp('hello world');pause(90)"
 9
10  echo `date`: job ends
11
12  exit
```

This jobscript asks the scheduler for a time slot of 5 minutes (`lwalltime=00:05:00`), and will be using one machine (`lnodes=1`) with 8 cores in its CPU (`cores8`). Only one of these cores will actually be doing something though, because the number of processes per node is just 1 (`ppn=1`). The next line tells the scheduler that the rest of the jobscript is written in a scripting language called 'bash', which is a very common scripting language on Linux. Incidentally, you already know it, since the shell program you have been using is in fact bash. The script then echoes the current date and time plus the message ': job starts' to the standard output (more about standard output later). Line 8 is the core of the script, in that it specifies what program needs to be run. In our case, it says that it wants to start an instance of the Octave software (`octave`) and that this instance needs to be started with the `--silent` and `--no-window-system` options, such that it will not display the usual welcome message and that it will not use any of the graphical output methods (i.e. Octave's `figure` command will not yield the usual output). The string following the `--eval` option specifies the Octave command that will be run by the Octave software. Here, it is simply the `disp('hello world')` command, but it could be any string that qualifies as valid Octave code, including function names and script names. (In a minute, it will become apparent why I added the `pause(90)`). The `disp` command always writes to the standard output, which normally equates to saying that it outputs to your screen, but on the LISA system it actually is a file which we will check later. The script then echoes the current date and time plus the message ': job ends' to the standard output, before exiting the script.

OK, so now that we have a jobscript file (which I saved as '˜/tutorial/simple-batch/jobscript.pbs'—LISA uses the OpenPBS/Torque scheduler[1], so I usually save my jobscripts as *.pbs), let's send it to the scheduler with the `qsub` command (`qsub` is an abbreviation for 'submit to the queue', the queue in question being the scheduler's):

```
jspaaks@login2:~/tutorial/simple-batch$ qsub jobscript.pbs
6388734.batch1.irc.surfsara.nl
```

---

[1]http://www.adaptivecomputing.com/products/open-source/torque/

```
jspaaks@login2:~/tutorial/simple-batch$
```

As you can see above, `qsub` prints a number `6388734` to the shell. This number is referred to as the *job id*. You can check the status of the job by typing the `qstat` command, followed by the job id, like so:

```
jspaaks@login2:~/tutorial/simple-batch$ qstat 6388734
Job id                    Name             User            Time Use S Queue
------------------------- ---------------- --------------- -------- - -----
6388734.batch1            jobscript.pbs    jspaaks                0 Q express
jspaaks@login2:~/tutorial/simple-batch$
```

or, you can ask for the status of all jobs that are owned by a specific user, using `qstat`'s `-u` option, like so:

```
jspaaks@login2:~/tutorial/simple-batch$ qstat -u jspaaks
Job ID            Username Queue    Jobname       SessID NDS TSK Memory Time  S Time
----------------- -------- ------- -------------- ------ --- --- ------ ----- - -----
6388734.batch1.i jspaaks  express jobscript.pbs    --    1   1    --   00:05 Q   --
```

This is where the `pause(90)` comes in: it is to make sure that the job runs sufficiently long for you to check the job's statistics, because the LISA system can't show any statistics for jobs that are finished already. Once you've seen how the `qstat` command works, you can remove the `pause(90)` if you like.

The `S` column lists the status of the job. In this case, the job is queued, hence its status is listed in the table as `Q`. Besides queued, it can be `R`unning, `C`ompleted, or `H`eld. (There are a few more statuses which are more obscure, see `man qstat`). `qstat`'s `-n` option shows the nodes that are allocated for your job (here: 'gb-r2n14'):

```
jspaaks@login2:~/tutorial/simple-batch$ qstat -u jspaaks -n

batch1.irc.surfsara.nl:
                                                        Req'd  Req'd   Elap
Job ID            Username Queue    Jobname       SessID NDS TSK Memory Time  S Time
----------------- -------- ------- ------------------- ------ --- --- ------ ----- - -----
6388734.batch1.i  jspaaks  express jobscript.pbs 15291    1   1    --   00:05 R 00:00
   gb-r2n14/0
jspaaks@login2:~/tutorial/simple-batch$
```

You can look up statistics for a given node at https://ganglia.surfsara.nl/?r=hour&cs=&ce=&s=by+name&c=LISA%2520Cluster&tab=m&vn=, for example if you want to check its performance (see also Fig. 2.5).

Because `6388734` is such a tiny job in terms of walltime and number of nodes, the scheduler adds the job to the 'express queue'. Depending on the requirements layed out in the jobscript, your job may end up in one of 3 different queues:

1. the express queue

2. the serial queue

3. the parallel queue

Your job ends up in the express queue if it asks for less than 5 minutes walltime and doesn't use more than one node. If the system is not too busy, jobs in the express queue are usually executed without delay. The express queue is primarily meant for development work. If your job asks for more than 5 minutes on one node, you end up in the serial queue. Despite its name, you can still run parallel jobs, but they will be limited to the cores of the one node that was allocated to you (in LISA's current configuration, that means a maximum of 16
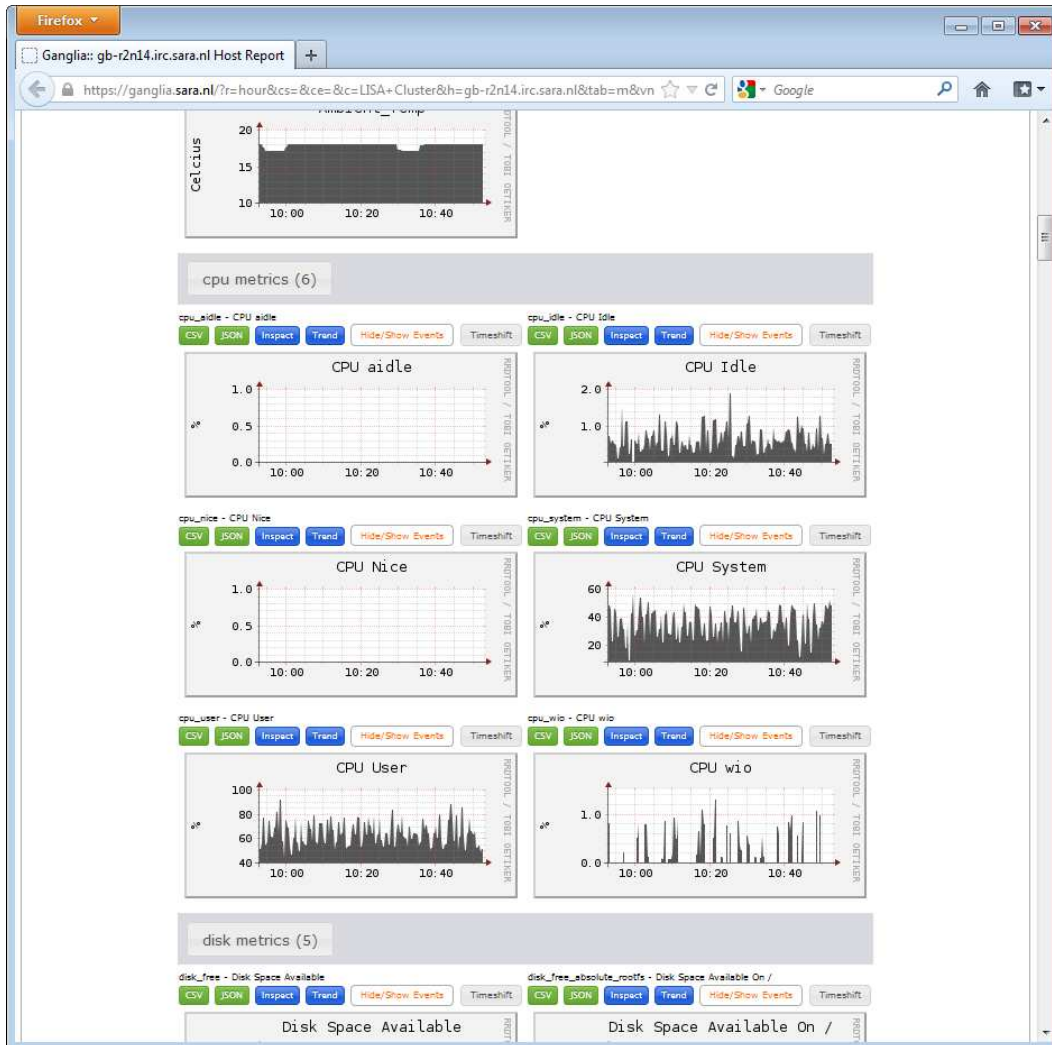
Figure 2.5: Ganglia visualizes a wide array of performance indices for the LISA system. The plots can be viewed in a web browser such as Firefox.

parallel processes). Your job ends up in the parallel queue if you ask for more than one node. Jobs that are in the serial or parallel queues can take a long time to start, but when they finally do, you can unleash the full computing power of the cluster, without performance loss due to other users.

If you need to develop software that requires testing on multiple machines, you can start an interactive session using the `-I` option as follows:

```
jspaaks@login2:~/tutorial$ qsub -I -lnodes=2:cores8 -lwalltime=00:59:00
qsub: waiting for job 6388157.batch1.irc.surfsara.nl to start
```

The above command asks for a 59-minute session with 2 nodes of the core8 type. Note that the information that is normally passed to `qsub` through the first few lines in a jobscript (i.e. the lines that start with `#PBS`) must now be entered as options. After a delay, you will get a prompt on a different machine, in this case 'gb-r7n32':

```
qsub: job 6388157.batch1.irc.surfsara.nl ready

jspaaks@gb-r7n32:~$
```

At this prompt, you can manually enter your commands, just like you were doing earlier, except you're no longer on 'login2' anymore, but on one of the computing nodes within the cluster. Either one of the login nodes may have many users on them at any given time, whereas the nodes that you get through the `qsub` command are exclusively yours (at least for a limited time). This means that you can take full advantage of the computing power and available memory.

When your time is up, the following message will appear:

```
jspaaks@gb-r7n32:~$ echo $PBS_O=>> PBS: job killed: walltime 3575 exceeded limit 3540
```

and you will return to 'login2' (or 'login1' if that's where you were before).

The `showq` command lets you view (your part of) the queue, for example:

```
jspaaks@login2:~/tutorial/simple-batch$ showq -u jspaaks
ACTIVE JOBS--------------------
JOBNAME             USERNAME        STATE   PROC   REMAINING              STARTTIME

6388079             jspaaks     Running     8     00:01:00   Thu Aug 23 15:41:24

    1 Active Job     6444 of 6684 Processors Active (96.41%)
                      617 of  647 Nodes Active      (95.36%)

IDLE JOBS----------------------
JOBNAME             USERNAME        STATE   PROC     WCLIMIT             QUEUETIME


0 Idle Jobs

BLOCKED JOBS----------------
JOBNAME             USERNAME        STATE   PROC     WCLIMIT             QUEUETIME


Total Jobs: 1   Active Jobs: 1   Idle Jobs: 0   Blocked Jobs: 0
jspaaks@login2:~/tutorial/simple-batch$
```

Also, `showq` shows whether the cluster is very busy or not (Friday afternoons are usually the busiest; Sundays, Mondays and Tuesdays are quiet in comparison). The statistics displayed by `showq` are updated every 30 seconds or so.

Some other commands that come in handy from time to time are:

```
jspaaks@login2:~/tutorial/simple-batch$ qdel 6388079
```

This deletes job `6388079` from the queue. Very useful if you accidentally requested too many

nodes, or when you realize you made a mistake in your program but the job was submitted already. It's not possible to delete a job that was not submitted by you, so you don't have to worry about accidentally deleting other people's jobs if you type the job id wrong.

checkjob gives a more detailed overview of the job:

```
jspaaks@login2:~/tutorial/simple-batch$ checkjob 6388672


checking job 6388672

State: Running
Creds:  user:jspaaks  group:lisa_uva  class:express  qos:DEFAULT
WallTime: 00:00:00 of 00:01:00
SubmitTime: Thu Aug 23 17:17:24
  (Time Queued  Total: 00:00:01  Eligible: 00:00:01)

StartTime: Thu Aug 23 17:17:25
Total Tasks: 1

Req[0]  TaskCount: 1  Partition: DEFAULT
Network: [NONE]  Memory >= 0  Disk >= 0  Swap >= 0
Opsys: [NONE]  Arch: x86_64  Features: [q_express][cores8]
Allocated Nodes:
[gb-r7n32:1]


IWD: [NONE]  Executable:  [NONE]
Bypass: 0  StartCount: 1
PartitionMask: [ALL]
Flags:       BACKFILL RESTARTABLE

Reservation '6388672' (00:00:00 -> 00:01:00  Duration: 00:01:00)
PE:  1.00  StartPriority:  -8641

jspaaks@login2:~/tutorial/simple-batch$
```

Finding out when your job is scheduled to start can be accomplished with the showstart command like this (although the estimate is quite inaccurate in my experience):

```
showstart 6388079
```

If you want to check how much computing time your **acc**ount has **use**d, you can use the accuse command, or the **acc**ount **info**rmation (accinfo) command.

This concludes the Linux tutorial part of this manual. The next chapters cover the general concept of parallel optimization (Chapter 3) and the MMSODA software (Chapter 4).

Chapter 3

Parallel optimization

Optimization algorithms such as SCEM-UA (Vrugt et al., 2003b), SODA (Vrugt et al., 2005a), Differential Evolution (Storn and Price, 1997), or DREAM (Vrugt et al., 2009) repeatedly sample the parameter space. In this chapter, we look at how such a sampling algorithm may be parallelized, and we introduce a law that describes the speedup that can be expected from parallelizing a particular piece of software.

Most parameter optimization algorithms sample the parameter space in generations of independent samples. When the optimization is implemented as a *serial* or *sequential* algorithm, the members of a generation are evaluated one after the other. For example, if the tasks that need to be evaluated each consist of one parameter set and there are 10 such tasks, the walltime that is needed to evaluate these tasks is equivalent to the sum of the CPU time that individual tasks need (Figure 3.1). In contrast, if the optimization algorithm employs a parallel strategy for evaluating the tasks, and the tasks are started simultaneously on 10 CPUs, then the walltime is determined by the CPU time of the slowest task (including the overhead introduced by the parallelization). The maximum speed-up S that be gained from executing a task in parallel is expressed by *Amdahl's Law*:

$$S = \frac{1}{\alpha} \tag{3.1}$$

in which α is the fraction of the program that cannot be parallelized.

For the example in Figure 3.1, each task is about 10% of the total walltime when executed sequentially, so α is about 0.1 (not counting the overhead due to parallelization), therefore the theoretical maximum speedup is about 10x. When executed in parallel, a relatively large part of the time is spent in communication ('parallelization overhead'). When this is the case, the application is said to be *fine-grained*. In contrast, if a parallel implementation of a program spends most of its time on calculation (as opposed to on communication), it is said to be *coarse-grained*. Most Monte-Carlo based optimization problems are coarse-grained, since the model CPU time is usually at least a few seconds, or sometimes even hours—in any case, much less than the time needed to send a parameter set over the network. Problems for which the communication time is negligible compared to the calculation time are said to be *embarassingly parallel*.
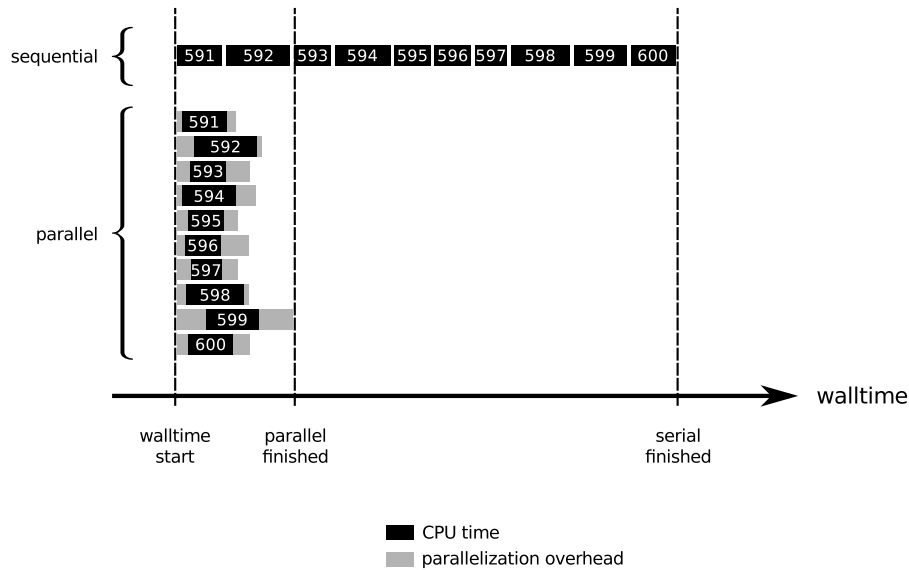
Figure 3.1: Walltime needed to complete 10 tasks 591–600 when evaluated sequentially or in parallel. The actual speedup that is achieved in parallelizing this problem is less than the theoretical maximum speedup due to parallelization overhead.

3.1 The Master-Worker paradigm

For Monte-Carlo type optimization, the Master-Worker paradigm (see Fig. 3.2; sometimes also referred to as Master-Slave paradigm) is the most common. In the Master-Worker paradigm, one of the available nodes is assigned the role of Master, while all the other nodes assume Worker roles.

3.1.1 Master side

The Master node is responsible for keeping track of the status of all Worker nodes with regard to what program a given Worker should run next, as well as to the logistics of the optimization, i.e. whether all nodes are connected, which nodes are busy calculating, which have finished, which are waiting for a new task, etc. Furthermore, the Master node is the brains of the optimization algorithm: the Master decides which tasks should be evaluated next. At the very beginning of the optimization, the Master typically checks whether all the nodes are online. After that, the Master will send each node all data that the Worker needs to complete its tasks. This typically includes things like the observations against which the model result will be compared, as well as the model's initial and boundary conditions—basically everything that is constant for all tasks. The Master also sends the model structure itself. Once all Workers have received the data and the model structure, the Master node determines what parameter combinations need to be sampled first. This is

entirely dependent on which algorithm is used for the optimization. In any case, the Master compiles a list of all parameter combinations that need to be evaluated (i.e. for which the model structure needs to be run). It then distributes these parameter combinations over the available Workers, and waits for the Workers to start returning results. A result is usually in the form of an objective score or likelihood function value, but can in principle be any variable, or even a collection of variables.

3.1.2 Worker side

On the Worker side, things are pretty simple: when the Worker starts, it loads all the data that it received from the Master, after which it goes into a never-ending loop. The never-ending loop consists of just a few components: first, it waits for a new task, i.e., a new parameter combination. After it receives a parameter combination, it runs the model structure with it. After the model finishes, the Worker will typically run some sort of objective function to calculate the likelihood function value, for instance by comparing it to observations (which the Master sent to the Worker at the very beginning). The objective function's result is then sent back to the Master node, and the Worker returns to the beginning of the never-ending loop where it either continues with the next task, or waits until it receives a new one.
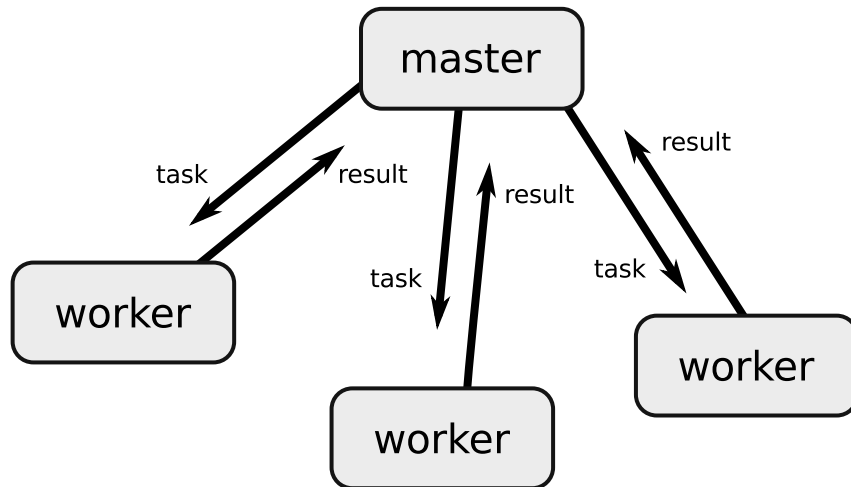

Figure 3.2: Message passing between a master node and its workers.

Chapter 4

The MMSODA Toolbox for MATLAB

There are various softwares that implement the Master-Worker paradigm. The most commonly used Master-Worker software is probably MPI, which stands for *Message Passing Interface*. Most cluster computers have some form of MPI installed. We will use the GNU version of OpenMPI, since this is the default MPI package at the LISA cluster computer.

We have developed a parallel MATLAB version of SODA (e.g. Vrugt et al., 2005a) that makes use of MPI. The software package is called 'The MMSODA Toolbox for MATLAB', or MMSODA for short (MMSODA stands for MATLAB-MPI-SODA). In this chapter, we will look at how to set it up.

MMSODA offers the functionality of a number of previously separate softwares, namely SCEM-UA (Vrugt et al., 2003b), SODA (Vrugt et al., 2005a,b; Clark and Vrugt, 2006), MOSCEM-UA (Vrugt et al., 2003a), multi-objective SODA (Vrugt et al., 2008), the MPITB-parallel version of SCEM-UA implemented in Octave (Vrugt et al., 2006b), and the MPITB-parallel version of SODA implemented in Octave (Vrugt et al., 2006a). Additionally, MMSODA offers a parallel version of multi-objective SCEM-UA, and a parallel version of multi-objective SODA, both of which did not exist previously. Moreover, MMSODA does not use Octave when running in parallel, because Octave does not evaluate code as quickly as does MATLAB. MMSODA circumvents (in a legal fashion) the license requirements that are often an impediment to parallel computation by compiling the MATLAB code into a binary which can be run without any license. Compiling the binary, however, does require a license, both for the MATLAB program itself, as well as for the MATLAB Compiler Runtime Toolbox. Fortunately, the required licenses are available on most cluster environments targeting a scientific and engineering audience.

In short, the acronyms mentioned above mean that: MMSODA can do parameter tuning with or without intermediate state updating by an ensemble Kalman Filter; that MMSODA supports both single-objective and multi-objective optimization; and that the optimization can be run either sequentially on a local machine, or in parallel on a cluster computer.

The serial/parallel capability is particularly attractive, since it allows the users to set up

their optimizations locally on their own machines, thus ensuring a familiar development environment without the need to make the code compatible with Octave syntax. When the user finishes setting up the optimization, running it on a cluster computer is simply a matter of copying the relevant directory to the cluster storage using standard tools (e.g. WinSCP) and compiling the software by executing a script that comes with the software. Furthermore, MMSODA is fully documented with HTML documentation which can be accessed in the same way as MATLAB's built-in commands, namely through the `doc` command.

The remainder of this chapter explains how to set up increasingly sophisticated optimizations within the MMSODA framework. Let's start off with a single-objective SCEM-UA optimization of a benchmark function `calcLikelihood()`, and let's not do anything in parallel just yet.

4.1   MMSODA in 'bypass' mode; sequential execution

▶ 4. In your file explorer program, navigate to the directory where you unzipped the file from https://github.com/NLeSC/esibayes.

As you can see, the 'esibayes-master' directory contains a number of subdirectories. Among these, the 'src/mmsoda-toolbox' and 'examples' subdirectories are probably the most important: the former contains the MATLAB toolbox that this chapter is about, while the latter contains a couple of examples of how to use the MMSODA toolbox for MATLAB with different models and different configurations. There are a few other directories, such as 'manual', 'testing' and 'code-quality-metrics'. The 'manual' directory contains all the files pertaining to the document you have before you. The 'testing' and 'code-quality-metrics' directories are part of the software quality control process: whenever we change something in MMSODA's code, a number of tests from the 'testing' directory are run automatically. The test results are subsequently posted in 'code-quality-metrics'. With this so-called unit-testing, we can verify that updates to one part of the algorithm do not accidentally break other parts.

▶ 5. Let's get started by making a new directory that will hold all of our MMSODA projects. Let's call this directory 'mmsoda-projects' (you can put this directory anywhere you have write access on your system). Change directory into 'mmsoda-projects', create a subdirectory 'example1', with three subdirectories in it called 'data', 'model', and 'results'. (We won't always use all three directories, but MMSODA expects all three to be present regardless of whether they are used). So now you have a directory somewhere on your local storage device that has at least the following subdirectories:

- mmsoda-projects/example1
- mmsoda-projects/example1/data
- mmsoda-projects/example1/model
- mmsoda-projects/example1/results

▶ 6. Open MATLAB and set your working directory to 'example1'.

▶ 7. Before we can use the functionality provided by the MMSODA Toolbox for MATLAB, we need to tell MATLAB about its existence by adding the main directory to the MATLAB

search path. You must do this using the `addpath` command as follows:
`>> addpath('s')`, in which `s` indicates the location of the MMSODA directory. For example, it could be:
`>> addpath('C:\Users\jspaaks\esibayes-master\src\mmsoda-toolbox')`
on a Windows machine or
`>> addpath('/home/jspaaks/esibayes-master/src/mmsoda-toolbox')`
on Linux.

▶ 8. At the MATLAB prompt, type:
`>> mmsoda --docinstall`
to complete the MMSODA setup. In principle, you only have to run this command once per MATLAB session, as long as you do not change the location of the 'mmsoda-toolbox' directory on your storage.

▶ 9. Test whether everything works as it should by typing:
`>> doc mmsoda`
at the MATLAB command prompt. This should bring up MATLAB's help browser. Click on the link 'View HTML documentation for this function in the help browser'. You should now see an overview of the functions comprising the MMSODA Toolbox for MATLAB.

▶ 10. Spend at least 12 minutes to browse through the documentation. In any case, make sure to read the documentation on 'mmsoda.m'.

The function that we want to maximize implements the double-normal probability distribution:

$$p = \frac{1}{2} \cdot \frac{1}{\sqrt{2\pi\sigma_1^2}} e^{-\frac{1}{2}\left(\frac{x-\mu_1}{\sigma_1}\right)^2} + \ldots$$
$$\frac{1}{2} \cdot \frac{1}{\sqrt{2\pi\sigma_2^2}} e^{-\frac{1}{2}\left(\frac{x-\mu_2}{\sigma_2}\right)^2} \tag{4.1}$$

with $\mu_1 = -10$, $\sigma_1 = 3$, $\mu_2 = 5$, $\sigma_2 = 1$, respectively. The parameter that is optimized (or, equivalently, whose probability distribution we will estimate by means of the MMSODA Toolbox for MATLAB) is x. For example, for $x = 4.5$, $p = 0.1760$.

Because MMSODA expects the objective function to return a log-likelihood l, we must actually take the natural logarithm of p as the objective score:

$$l = \ln(p) \tag{4.2}$$

4.1.1 Creating the 'constants.mat' and 'conf.mat' files

Before we actually start writing any code for this objective function however, let's first create the 'conf.mat' and 'constants.mat' files that are always needed for running `mmsoda()`.

▶ 11. Start a new text file in the MATLAB editor and save it as 'makeconf.m' in the current working directory ('mmsoda-projects/example1').

▶ 12. At the first line in 'makeconf.m', add the following:
`function makeconf()`

Now we need to edit the contents of 'makeconf.m' as follows.

▶ 13. At the MATLAB prompt, type
```
doc mmsoda
```
and bring up the HTML documentation for the `mmsoda()` function.

Near the bottom of the documentation, there is an overview of the configuration variables that must be specified for a given type of optimization. For our double-normal example, we will use MMSODA in 'bypass' mode. This mode is used when the log-likelihood can be estimated directly from the parameter vector, without the need to run a (dynamic) model structure.

▶ 14. If you look in the table with the configuration variables, you'll see that only 5 variables are required for running MMSODA in 'bypass' mode. These are `modeStr`, `objCallStr`, `parNames`, `parSpaceHiBound`, and `parSpaceLoBound`. Make sure you understand the description for each of these.

▶ 15. Return to 'makeconf.m' and add the following:
```
modeStr = 'bypass';
objCallStr = 'calcLikelihood';
parNames = {'x'};
parSpaceHiBound = [10];
parSpaceLoBound = [-30];
```


With the above settings we specify that we want MMSODA to do a bypass run, in which the function 'calcLikelihood.m' (which we will create shortly) is optimized. `calcLikelihood` has one tunable parameter, `x`. The bounds that we set on the search for the optimal value of `x` are `[-30,10]`.

▶ 16. At the last line in 'makeconf.m', add the following:
```
save('./results/conf.mat')
```


▶ 17. Save and close 'makeconf.m'.

Next, we need to create 'constants.mat' by a similar procedure.

▶ 18. Create a new m-file in the current working directory called 'makeconstants.m'.

▶ 19. At the first line in 'makeconstants.m', type:
```
function makeconstants()
```

Now we need to assign the constants, i.e. the variables that `calcLikelihood` needs in order to calculate the log-likelihood according to equations 4.1–4.2.

▶ 20. In 'makeconstants.m', add:
```
parMu1 = -10;
parSigma1 = 3;
parMu2 = 5;
```

```
parSigma2 = 1;
```
i.e. the two means and two standard deviations for the double normal distribution.

► 21. At the last line in 'makeconstants.m', add
```
save('./data/constants.mat')
```

► 22. Save and close 'makeconstants.m'.

Finally, we need to create the objective function m-file that implements equations 4.1 and 4.2.

4.1.2   Creating the objective function m-file

► 23. Create a new m-file, called 'calcLikelihood.m' and save it in the subdirectory './model'.

► 24. Open './model/calcLikelihood.m'. MMSODA uses a standardized way of passing the input and output arguments to and from the objective function, so the first line is always exactly the same (with the exception of the name of the function `calcLikelihood`, which may vary), like so:
```
function objScore = calcLikelihood(conf,constants,modelOutput,parVec)
```

► 25. As a second line, type:
```
mmsodaUnpack()
```
`mmsodaUnpack` uses the information from the input arguments to construct the variable `x` and to assign it a value based on the value of `parVec`. Similarly, it uses information from the `constants` variable to construct the model constants and to assign them the correct values.

Now that we have `parMu1`, `parSigma1`, `parMu2`, `parSigma2`, and `x` we can calculate the probability density `dens` as follows:

```
dens = (1/(sqrt(2*pi*parSigma1^2))*exp(-(1/2)*((x-parMu1)/parSigma1)^2) + ...
        1/(sqrt(2*pi*parSigma2^2))*exp(-(1/2)*((x-parMu2)/parSigma2)^2))/2;
```

► 26. Add this calculation to your `calcLikelihood` function.

► 27. Don't forget that MMSODA expects a log-likelihood however, so as a final line in `calcLikelihood`, add:
```
objScore = log(dens);
```

► 28. Save and close 'calcLikelihood.m'.

4.1.3   Running the optimization locally

► 29. Make sure that the current working directory is the 'example1' directory. At the MATLAB command prompt, type:
```
>> makeconf()
```
and check that a new file 'conf.mat' is created in subdirectory './results'.

▶ 30. At the MATLAB command prompt, type:
```
>> makeconstants()
```
and check that a new file 'constants.mat' is created in subdirectory './data'.

▶ 31. At the command prompt, type `clear` to clear the workspace if there are any variables in it.

▶ 32. Now, we are ready to run the optimization. At the MATLAB command prompt, type:
```
>> [evalResults,critGelRub,sequences,metropolisRejects,conf] = mmsoda();
```
and wait for the optimization to finish. Input arguments to `mmsoda` are not required, since `mmsoda` knows to look in './results/conf.mat' for the configuration, in './data/constants.mat' for the model constants, and in './model' for the model functions and objective functions.

4.1.4   Interpreting the results

Once the optimization finishes, you should have 5 variables in your workspace: `evalResults`, `critGelRub`, `sequences`, `metropolisRejects`, and `conf`. Refer to the `mmsoda()` documentation for a description of what these variables are and how they are laid out.

Let's explore the results by making a histogram of the occurence of certain parameter values. You could simply use MATLAB's built-in `hist()` function to do this, but it is often more convient to use a specialized function that comes pre-packaged with MMSODA like so:
```
>> mmsodaSubplotScreen(2,2,1);
>> mmsodaMargHist(conf,evalResults);
```

▶ 33. Refer to the documentation of these two functions to see how they work and use the optional `'nHistory'` argument to show the marginal histogram based on the last quarter of the `evalResults` record. Your result should look like Fig. 4.1.
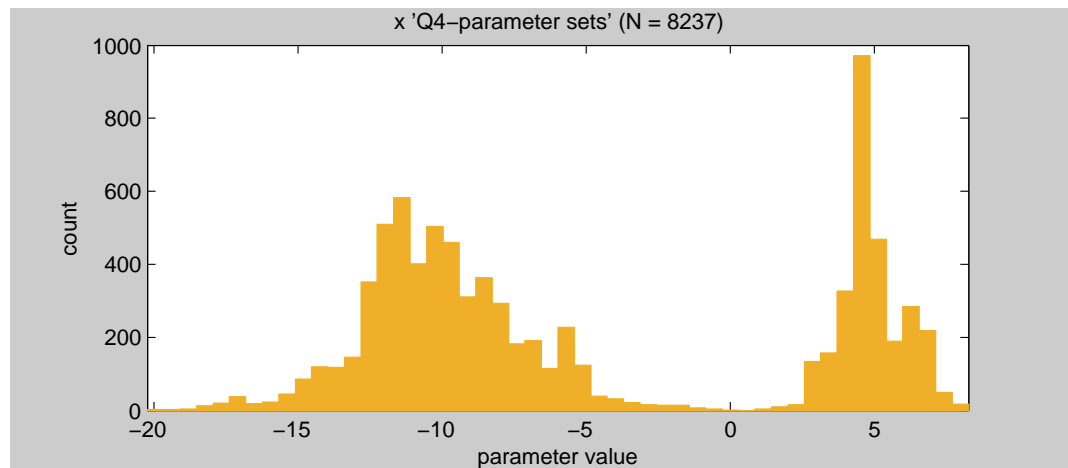

Figure 4.1: Histogram for the Q4 parameter sets for the double-normal model.

▶ 34. Refer to the documentation on how to use `mmsodaPlotSeq`. Create another figure on the right

side of your screen, in which you visualize the record of sequences. Use the `'showRejects'` option to hide the samples that were rejected as part of the Metropolis scheme. Your result should look like Fig. 4.2.
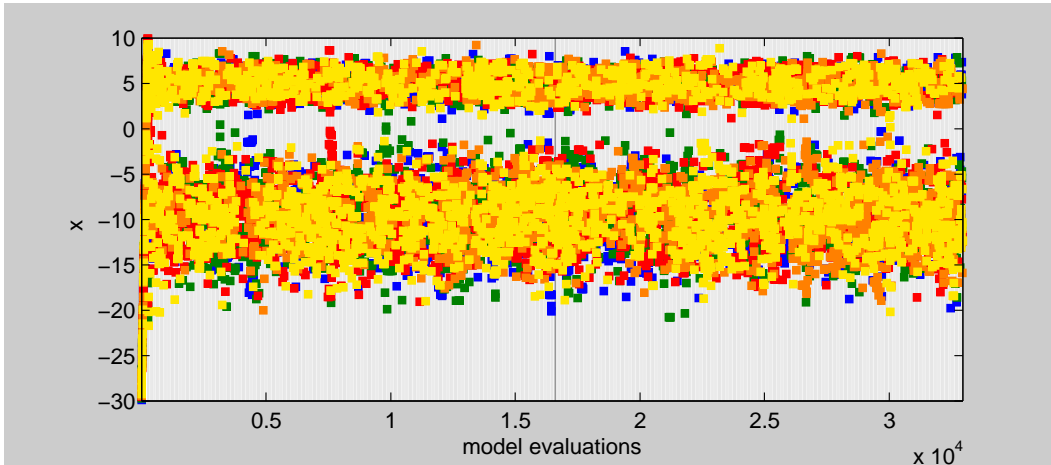

Figure 4.2: History of samples taken from the 1-D parameter space by SCEM-UA during optimization of the double-normal model.

▶ 35. Refer back to the documentation on the `mmsoda` function; specifically, browse through some of the configuration options for running MMSODA in 'bypass' mode. Alter your 'makeconf.m' with the options that you find useful, and re-run the optimization.

▶ 36. When you are satisfied with the way you set up MMSODA locally, you can make preparations for running it in parallel on the LISA cluster computer. Running on LISA requires a so-called 'Makefile' as well as a jobscript, both of which are tricky to write yourself. Therefore, the MMSODA Toolbox for MATLAB comes with a function that helps you generate the correct files by asking a series of questions. At the MATLAB prompt, type:
`>> mmsodaPrepParallelFiles('s')`
but substitute `s` with the location of the MMSODA Toolbox for MATLAB as used on the LISA cluster. So for me, it would be:
`>> mmsodaPrepParallelFiles('/home/jspaaks/esibayes-master/src/mmsoda-toolbox')`
Now use the following information to answer `mmsodaPrepParallelFiles`'s questions:

1. the optimization will run on one of the login nodes;

2. we want not much verbal feedback from the program;

3. we don't want to use all the cores on the login node;

4. we want to start 4 processes;

5. we don't want to save the timing information.

(Note that `mmsodaPrepParallelFiles()` indicates the default answer with brackets, and that you can accept the default by simply pressing Enter.)

When `mmsodaPrepParallelFiles()` finishes, it prints a message in the command window that tells you what file it has just created. This file should be located in the current working

directory. We will use it shortly to start the optimization on the cluster. You can take a look a its contents in Notepad or a similar program, but make sure not to change anything. Besides the jobscript, there should also be a new file called 'Makefile'. Just like the jobscript, this is also a plain text file, so you can view its contents in Notepad as well. Again, make sure not to accidentally change anything.

4.2 MMSODA in 'bypass' mode; parallel execution

▶ 37. Use WinSCP or the alternative program of your choice to copy the 'example1' and 'mmsoda' directories, including all of their contents, to your storage on the cluster, i.e. anywhere under the '/home/<username>/' directory.

When you are satisfied with the way you set up MMSODA locally, you can run it on the LISA cluster computer. In order to do so, we must first compile the software into a so-called 'binary' or 'executable'. You do not need to worry about how this works in detail, it is just a matter of running the Linux `make` command. `make` looks for a file called 'Makefile' that was just created by `mmsodaPrepParallelFiles()`. Based on the contents of 'Makefile', `make` collects all the relevant software (your model files, your objective functions, the MMSODA code, as well as the code that enables communication between the Master and the Workers) and creates two files that are necessary to run your code within MMSODA using multiple cores.

4.2.1 Compiling MMSODA and your model code into a binary

▶ 38. Use PuTTY to start an SSH connection to the LISA cluster.

▶ 39. In the PuTTY terminal, load the MATLAB program and MPI programs by typing:
`module load matlab/2013a`
This command will not give any feedback on the success or otherwise of the command, but you could check by typing the following command:
`module list`
which should now include MATLAB. Next, type
`module load openmpi/gnu/1.6.5`
to load the MPI software.

▶ 40. Use the `cd` command to set 'example1' as your current directory if you hadn't already done so.

▶ 41. Now we are ready to compile. At the terminal, type:
`make`
You should see some text scrolling over your screen—it takes about 60 seconds or so to complete. The `make` command looks for a file called 'Makefile' in the current directory, and uses the information in it to correctly build the binary 'matlabprog' and the library that it needs, called 'libmmpi.so'.

▶ 42. After `make` finishes, list the directory contents with `ls -l` and verify that you now have two extra files 'matlabprog' and 'libmmpi.so'.

Starting the optimization requires that we adjust the 'permission bits' for the 'run-mmsoda.sh' file that was just created by `mmsodaPrepParallelFiles()`. Permission bits indicate what a specific user is allowed to do with a particular file. (You may know the same concept from Windows, where you can sometimes have 'Read-only' versions of a file). The permission bits are listed as the first 10 columns in the output from `ls -l`:

```
jspaaks@login1:~/esibayes-master/example1$ ls -l
total 204
drwxr-xr-x 2 jspaaks jspaaks     26 Jan 16 16:09 data
-rwxrwxr-x 1 jspaaks jspaaks 172792 Jan 18 11:57 libmmpi.so
-rw-r--r-- 1 jspaaks jspaaks    176 Jan 16 16:02 makeconf.m
-rw-r--r-- 1 jspaaks jspaaks    120 Jan 16 15:06 makeconstants.m
-rw-rw-r-- 1 jspaaks jspaaks   1357 Jan 16 16:10 Makefile
-rwxrwxr-x 1 jspaaks jspaaks  11969 Jan 18 11:57 matlabprog
drwxr-xr-x 2 jspaaks jspaaks     29 Jan 16 16:09 model
drwxr-xr-x 2 jspaaks jspaaks   4096 Jan 16 17:36 results
-rw-r--r-- 1 jspaaks jspaaks    580 Jan 18 13:26 run-mmsoda.sh
jspaaks@login1:~/esibayes-master/example1$
```

For 'run-mmsoda.sh', the permissions are set to `-rw-r--r--`. The first character `-` indicates that 'run-mmsoda.sh' is a file (as opposed to a `d` which would indicate a directory). Characters 2, 3 and 4 (`rw-`) indicate what you, the currently logged-in user, is allowed to do with 'run-mmsoda.sh'. Currently, you are allowed to read from (`r`) and write to (`w`) 'run-mmsoda.sh'. The `-` character from the fourth column of `ls -l` indicates that you are currently not allowed to execute 'run-mmsoda.sh' as a script.

▶ 43. Change the permission bit for 'run-mmsoda.sh' by typing at the prompt:
`chmod u+x run-mmsoda.sh`
In normal English, this command translates to "`Ch`ange the `mod`e of file 'run-mmsoda.sh' by adding (`+`) the executable permission (`x`) for the current user (`u`)". Check that the permissions have changed to `-rwxr--r--`.

▶ 44. Now we are ready to start the optimization in parallel on the login node. At the beginning of the optimization, you will see a lot of text scrolling over your terminal screen which at this stage probably does not make much sense. Don't worry if you don't understand it— we will look at it in greater detail later. Eventually, you'll get messages along the lines of 'Evaluating parameter sets 1-100', 'Evaluating parameter sets 101-120', etc. Start the optimization by typing at the terminal:
`./run-mmsoda.sh`
(Don't omit the `./` at the beginning, otherwise it won't work.)

▶ 45. After the optimization finishes, the results need to be transferred to your local system. Copy the contents of 'example1/results/' from the remote system to 'example1/results/' on your local machine (you can overwrite the old files in 'example1/results/' on your local machine if you want).

▶ 46. On your local machine, clear the workspace, and load MMSODA's output variables using:
`>> load('./results/bypass-so-results.mat')`
You can now use any of the MMSODA visualizations (or MATLAB visualizations for that matter), in just the same way as if the results had been calculated locally.

▶ 47. Now that you know what information goes where for MMSODA in 'bypass' mode, it may be useful to review some of the 'bypass' examples in the 'esibayes-master/examples' directory. Try running MMSODA for those configurations, but make sure MATLAB is set to the correct working directory when `mmsoda` is started.

4.3 MMSODA in 'scemua' mode; sequential execution

Now that we have a working example of MMSODA in 'bypass' mode, let's try our hand at something a little more difficult: optimizing the parameters of a dynamic model. This works in more or less the same way as the bypass mode, except that the likelihood is determined by comparing a model prediction to observations, while taking into account the uncertainty of the latter. Let's first make a small digression and look at the general structure of dynamic models. Such models simulate the behavior of a number of states over time. As an example, Fig. 4.3 shows a system in which there are two states. The first state is the water level in a tank which has a small hole in the bottom. The second state is the water level in a tank that has no leaks. The first tank discharges into the second. The rate of discharge Q is dependent on the volume of water in the tank V_{tank_1} and on a resistance parameter R (if there is a big leak in the first tank, the resistance is low, but if the leak is only small, the resistance is high). The model simulates discharge as follows:

$$Q = \frac{V_{tank_1}}{-R} \tag{4.3}$$

Given the state of the upper tank at a given point in time $V_{tank_1}(t)$, Eq. 4.3 may be used to calculate the corresponding flow at time t. Furthermore, the current state $V_{tank_1}(t)$ and flow $Q(t)$ may be used to simulate the state at a later time, $t + \Delta t_{sim}$, provided that Δt_{sim} is sufficiently small:

$$V_{tank_1}(t + \Delta t_{sim}) = V_{tank_1}(t) + Q(t) * \Delta t_{sim} \tag{4.4}$$

$$V_{tank_2}(t + \Delta t_{sim}) = V_{tank_2}(t) - Q(t) * \Delta t_{sim} \tag{4.5}$$

If the initial state of the system $V_{tank_1}(t_0)$ and $V_{tank_2}(t_0)$ is known, and if the resistance parameter R has been assigned, repeated application of Eqs. 4.3–4.5 thus enables constructing a time series of simulated values for V_{tank_1} and V_{tank_2}.

It is quite common that not all the parameter values are known beforehand, so in order to make predictions with the model, it becomes necessary to estimate the model parameter values by comparing simulation results to observations of the system's states. The model must therefore be set up such that it returns the system's state at the times for which an observation is available, otherwise the comparison isn't much use. Since the time interval between observations Δt_{obs} can be (much) larger than the model integration interval Δt_{sim}, multiple model integration steps are often needed in between observation times. Listing 4.1 shows a simple MATLAB script that implements the system depicted in Figure 4.3. A copy of the script has been included as 'esibayes-master/manual/other/lintank_script.m'.

Over the next few exercises, we will:

1. prepare a 'constants.mat',

2. prepare a 'conf.mat',

3. prepare the main model m-file by adapting 'lintank_script.m' such that it can be used within the MMSODA framework,

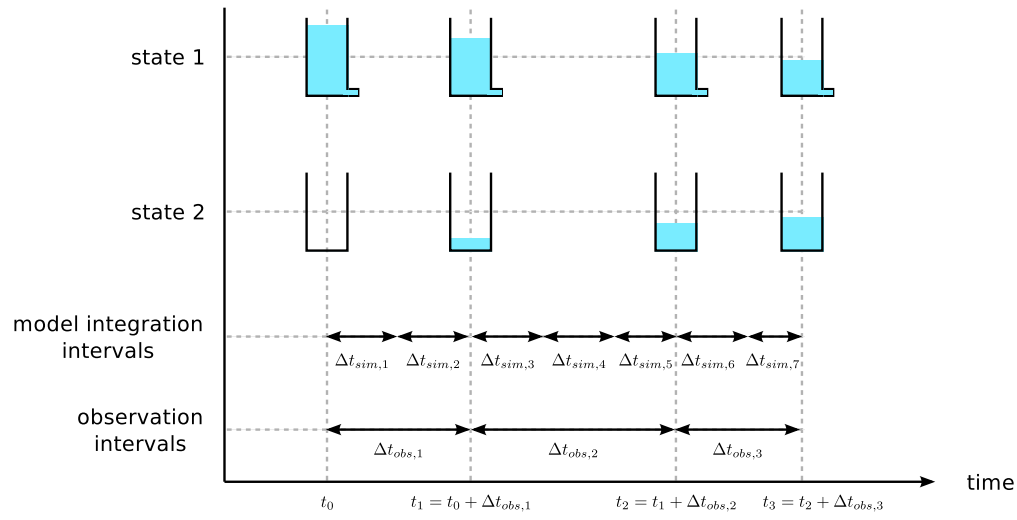4. construct a likelihood function.

Figure 4.3: The general structure of dynamic models.

▶ 48. Before we start, make sure you understand how the 'lintank_script.m' works by studying Listing 4.1 and running through it line-by-line using MATLAB's debugging capabilities.

Listing 4.1: Simple MATLAB script that implements the system depicted in Figure 4.3. A copy of this script has been included as 'esibayes-master/manual/other/lintank_script.m'.

```matlab
1  clear          % clear old variables
2  close all      % close any open figures
3  clc            % clean the command window
4
5  % assign the resistance parameter a value of 100
6  R = 100;
7
8  % initial value of the upper tank
9  state1Init = 30.0;
10 % initial value of the lower tank
11 state2Init = 0;
12
13 % initialize 'priorTimes', the array that contains the time of the initial state (0) as well
14 % as all times at which the model should return a prediction of state1 and state2.
15 priorTimes = [0,61,147,200];
16 % initialize the current simulated time as the first entry in 'priorTimes'
17 tNow = priorTimes(1);
18 % initialize the last simulated time as the last entry in 'priorTimes'
19 tEnd = priorTimes(end);
20
21 % set the default model integration step
22 dtSimDefault = 30.5;
23
24 % assign the upper tank state variable its initial value
25 state1 = state1Init;
26 % assign the lower tank state variable its initial value
27 state2 = state2Init;
28
29 % initialize an array for recording 'tNow', 'state1', and 'state2'
30 rec = [tNow,state1,state2];
31
32 while tNow < tEnd
33
34     % retrieve the index in 'priorTimes' of the next observation time:
35     iPriorNext = find(tNow<priorTimes,1,'first');
36
37     % In principle, the model proceeds by time steps of 'dtSimDefault'. However, if that
38     % results in values of 'tNow' beyond the next time of observation
39     % 'priorTimes(iPriorNext)', then we use a shorter model integration time step
40     % 'dtSim = priorTimes(iPriorNext) - tNow' instead.
41     dtSim = min([dtSimDefault,priorTimes(iPriorNext) - tNow]);
42
43     % calculate the instantaneous discharge from 'state1' and the resistance parameter 'R':
44     Q = state1/-R;
45
46     % integrate the discharge from the first tank over the interval dtSim
47     dState = Q * dtSim;
48
49     % decrease the volume in the first tank by dState (which is negative, hence the + sign)
50     state1 = state1 + dState;
51
52     % increase the volume in the first tank by dState (which is negative, hence the - sign)
53     state2 = state2 - dState;
54
55     % increment the current time by the model integration time step
56     tNow = tNow + dtSim;
57
58     % record the current time, state1 and state2
59     rec = [rec;tNow,state1,state2];
60
61 end
62
63 figure(1)
64 plot(rec(:,1),rec(:,2),'-b.',rec(:,1),rec(:,3),'-m.')
65 set(gca,'xtick',rec(:,1))
66 xlabel('Time')
67 ylabel('State')
68 legend('state 1','state 2')
```
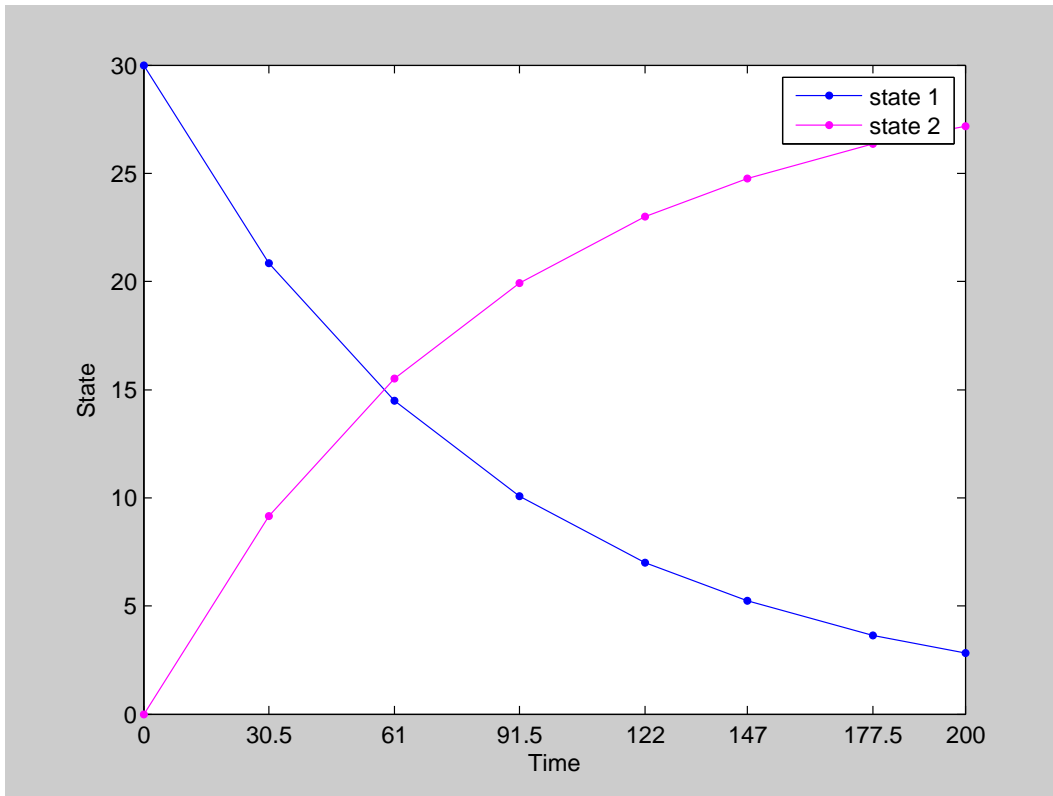
Figure 4.4: Result of running the code from Listing 4.1.

▶ 49. Create a new directory 'example2' in 'mmsoda-projects'. Make sure that the 'example2' directory has the required subdirectories just like you did before.

▶ 50. Read the MMSODA documentation on 'the dynamic model' (see Figure 4.5).

In the initialization part of Listing 4.1, 10 variables (R, state1Init, state2Init, priorTimes, tNow, tEnd, dtSimDefault, rec, state1, and state2) are created, but only some of these need to be included in 'constants.mat'. For example, R does not need to be in 'constants.mat' because its value will be determined by MMSODA: the variable R is assigned by mmsodaUnpack (which uses the input argument parVec to do so). Similarly, priorTimes and its derivatives tNow and tEnd do not need to be in 'constants.mat' because priorTimes is an input argument, too. state1, state2, and rec are all derived from other variables, so they do not need to be part of 'constants.mat' either. Essentially, all we need is state1Init, state2Init, and dtSimDefault.

▶ 51. Write 'makeconstants.m'.

▶ 52. Create a new m-file called 'makeconf.m' just like you did before, but this time make sure that the m-file lists the necessary configuration variables for a 'scemua' optimization. Refer to the configuration variables table in the MATLAB documentation of mmsoda, and use the information below to set up the optimization:
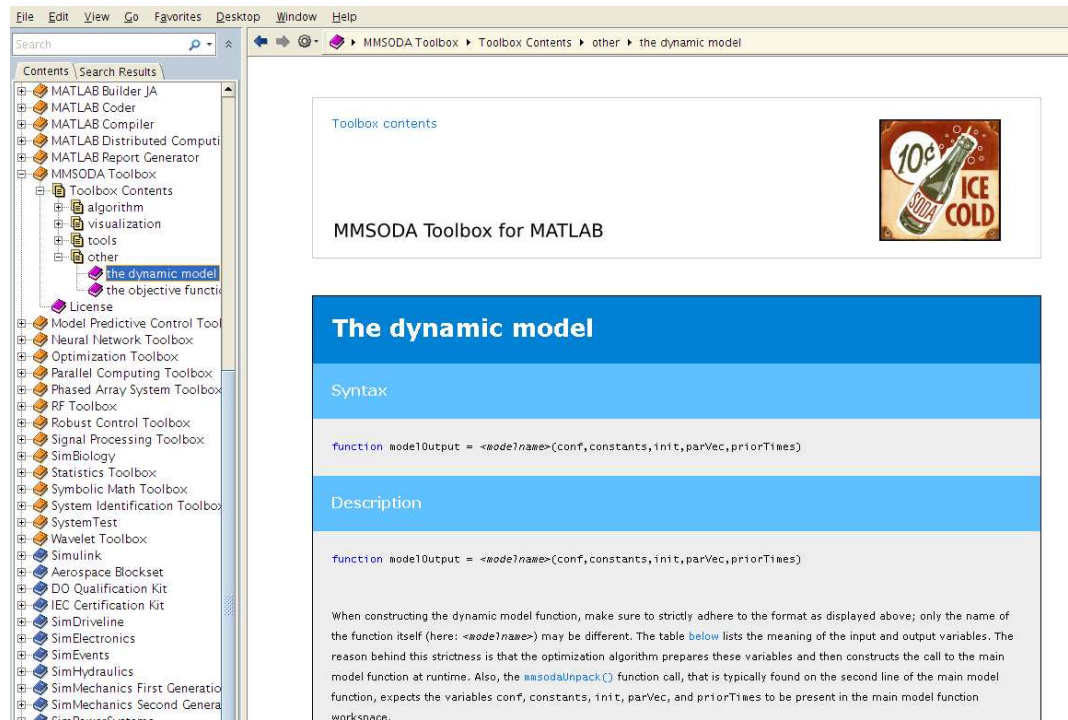
Figure 4.5: MATLAB documentation on how to set up the dynamic model.

1. Set `modeStr` to `'scemua'`;

2. Set `modelName` to `'lintank'`. (We will create 'lintank.m' later);

3. Set `objCallStr` to `'calcLikelihoodState'`. (We will create 'calcLikelihoodState.m' later);

4. Set `parNames` to a cell array of strings with the name of the resistance parameter exactly as used in the dynamic part of the model: `{'R'}`. `R` is the only parameter that will be optimized;

5. For the upper boundary of the parameter space, use 1000.0;

6. For the lower boundary of the parameter space, use 80.0;

7. Fill in the `priorTimes` values by copying from 'lintank_script.m';

8. Set `nOutputs` to 2.

▶ 53. Copy 'lintank_script.m' to your 'model' subdirectory. Rename it to 'lintank.m'.

▶ 54. Adapt 'lintank.m' to be a function. Refer to the MMSODA documentation on the dynamic model for the proper way of constructing the function's input and output arguments. Remove all lines from the initialization part that are obsolete given that we want to run it within the MMSODA framework. Afterwards, your code should look like that of Listing 4.2.

Listing 4.2: First 19 lines of 'lintank.m'. You can find a copy of this
script at 'other/lintank.m'.

```
1   function modelOutput = lintank(conf,constants,init,parVec,priorTimes)
2
3   % unpack the information from the input arguments and assign it to the correct variables
4   mmsodaUnpack()
5
6   % initialize the current simulated time as the first entry in 'priorTimes'
7   tNow = priorTimes(1);
8
9   % initialize the last simulated time as the last entry in 'priorTimes'
10  tEnd = priorTimes(end);
11
12  % assign the upper tank state variable its initial value
13  state1 = state1Init;
14
15  % assign the lower tank state variable its initial value
16  state2 = state2Init;
17
18  % initialize an array for recording 'tNow', 'state1', and 'state2'
19  rec = [tNow,state1,state2];
```

Next, we need to make sure that the function returns the correct values—we want it to return
an array of size nOutputs x nPrior. The nth column in the output argument modelOutput
must contain the values pertaining to the nth time in priorTimes. Listing 4.3 shows a
simple way of accomplishing this.

Listing 4.3: Last 10 lines of 'lintank.m'. You can find a copy of this
script at 'other/lintank.m'.

```
61  % transpose 'rec' because the output argument 'modelOutput' must have 'nOutputs' rows
62  % and nPrior columns
63  rec = rec';
64  % find the columns in the transposed 'rec' array that contain the values of 'state1' and
65  % 'state2' at the times listed in 'priorTimes':
66  c = ismember(rec(1,:),priorTimes);
67  % extract those columns from 'rec' and assign to the output argument 'modelOutput'
68  modelOutput = rec(2:3,c);
69  % overwrite with NaN to comply with what MMSODA expects
70  modelOutput(1:conf.nStatesKF,1) = NaN;
```

▶ 55. Now it's time to test if everything works so far. Make sure MATLAB is in the correct
working directory (i.e. one level higher than your 'data', 'model', and 'results' directories).
Run makeconstants and makeconf in order to create the necessary configuration files. Then
type:
>> [evalResults,critGelRub,sequences,metropolisRejects,conf] = mmsoda()
and press Enter. If all goes well, MMSODA will start printing various messages to your
screen. You should see the message 'Evaluating parameter sets 1–250', and if you
haven't commented out the visualization part in 'lintank.m', you should see 250 plots being
made before MMSODA crashes with the following error:

```
Error using eval
Undefined function 'calcLikelihoodState' for input arguments of type 'struct'.
>>
```

The error is because MMSODA refers to the configuration variable objCallStr, which
you set to 'calcLikelihoodState' earlier on. When MMSODA attempts to run
calcLikelihoodState, this results in an error because we still have to create 'calcLike-
lihoodState.m'.

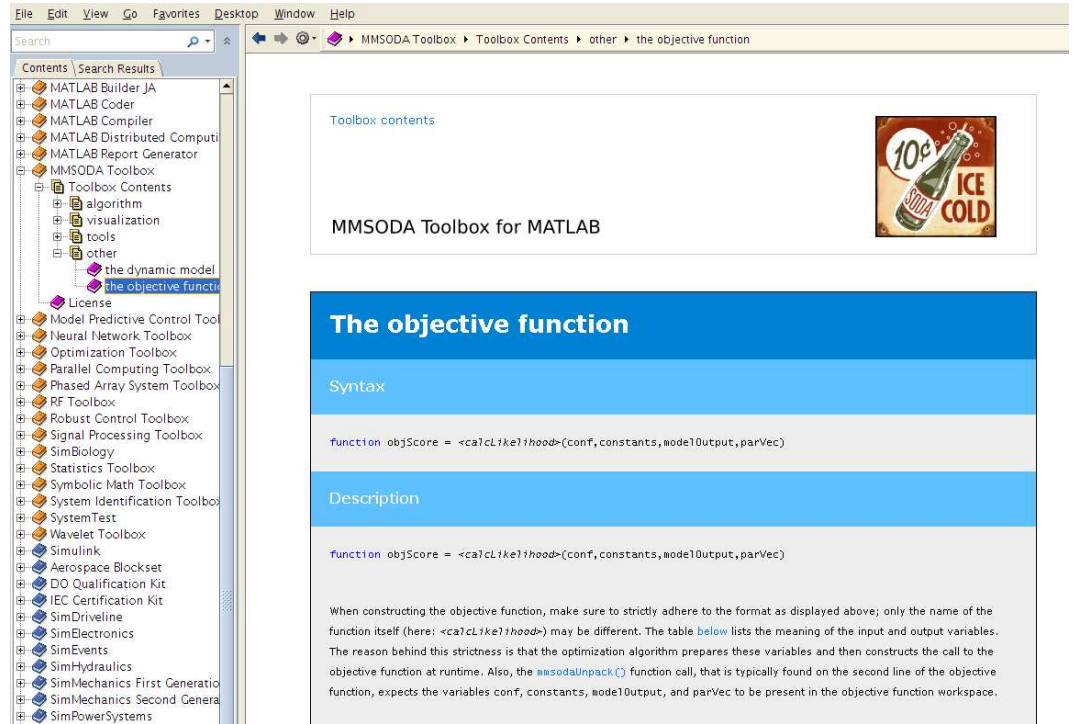▶ 56. Read the documentation about the objective function (see Figure 4.6).

Figure 4.6: MATLAB documentation on how to set up the objective function.

▶ 57. Create a new m-file in the './model' subdirectory, and call this file 'calcLikelihoodState.m'. Refer to the documentation and make sure the first line of the objective function is correct.

The objective function we will use is related to the sum of squared residuals or SSR:

$$\text{SSR} = \sum_{t=1}^{n_o} (\hat{x}_t - \tilde{x}_t)^2 \tag{4.6}$$

with $\hat{x}_t$ the tth predicted value of x, $\tilde{x}_t$ the tth observed value of x, and n_o the total number of observations. Note that the number of observations n_o is one less than the number of elements in `conf.nPrior`, since the first column in `modelOutput` is not calculated by the model, but instead contains the initial values of the model output variables.

However, we can't use the SSR directly as an objective score, because the SSR is not a log-likelihood (or a probability, for that matter). This problem is easily resolved though, by

using the following objective function[1]:

$$\ell = -\frac{1}{2} \cdot n_o \cdot \ln(\text{SSR}) \tag{4.7}$$

In order to calculate the SSR, we need some observations. These have been prepared already and are located in the 'other' directory.

▶ 58. Copy 'other/lintank-obs.mat' to your './data' directory.

▶ 59. In 'calcLikelihoodState.m', add
   `load('./data/lintank-obs.mat','obs','obsTimes')`

Now that we have the observations in the workspace, we still need to select the corresponding simulations from the `modelOutput` variable. Refer to the documentation on the objective function for a description. We want to select all values pertaining to the first state (since this is the state that we have observations for). We can do so by:

```
% row of interest in 'modelOutput' is #1
r = 1;
nPriors = size(modelOutput,2);
nObs = nPriors-1;

% extract the relevant row from 'modelOutput'
sim = modelOutput(r,1:nPriors);

% Calculate the SSR, but ignore the first entry in 'obs' and 'sim' because those are always
% exactly the same anyway
ssr = sum((obs(1,2:nPriors)-sim(1,2:nPriors)).^2);

% use the SSR to calculate the likelihood
objScore = -(1/2) * nObs * log(ssr);
```

▶ 60. Add the command lines above to your `calcLikelihoodState` in order to let it calculate the SSR and the objective score according to Eq. 4.7.

▶ 61. Make sure you are still in the right working directory. At the MATLAB prompt, type:
   `>> [evalResults,critGelRub,sequences,metropolisRejects,conf] = mmsoda()`

Currently, `calcLikelihoodState` loads the observations from file every time it needs to calculate the `objScore`. Since file operations are much slower than memory operations, it is more efficient to load the observations just once (during creation of the constants), and then keep them in the computer's memory.

▶ 62. Cut the `load` statement from `calcLikelihoodState` and paste it into 'makeconstants.m'. Make sure to re-run `makeconstants()`, otherwise './data/constants.mat' will remain unchanged.

▶ 63. Re-read the documentation on MMSODA's `mmsodaUnpack()` function. Go back to 'calcLikelihoodState.m' and use `mmsodaUnpack()` to make the observations available in the objective

---

[1]Skip forward to Appendix B to see how this was derived.

function's workspace. Restart the optimization to check if everything works. The marginal parameter distribution should show a high density in a narrow band around `R = 333`.

4.4   MMSODA in 'scemua' mode; parallel execution

▶ 64. Generate a 'Makefile' and a jobscript using `mmsodaPrepParallelFiles()`. Use the same answers as those given on page 28.

▶ 65. Copy the working directory to LISA using WinSCP or an alternative program. Make sure the directory is at the same level as the 'mmsoda-toolbox' directory that should still be present on the remote system.

▶ 66. Use PuTTY to start an SSH connection to the LISA cluster.

▶ 67. Load the necessary software modules and compile your m-files together with the MMSODA m-files.

▶ 68. Add the executable permission to 'run-mmsoda.sh'.

▶ 69. Start the optimization on the login node.

So far, we've run our optimizations on one of the login nodes. These nodes are intended for testing small problems and for development work. However, if you want to do some real calculations, then it becomes necessary to submit your job to the PBS queue (as discussed in Chapter 2).

▶ 70. Submitting your optimization to the PBS scheduler requires a slightly different jobscript. On your local system, run `mmsodaPrepParallelFiles`, but this time indicate that you want to run your optimization as a PBS jobscript, without much verbal feedback, and that you want 00:15:00 walltime on 1 node. We are not interested in saving the timings for the moment. When `mmsodaPrepParallelFiles` finishes, it prints the name of the file it just created ('jobscript-mmsoda.pbs') to the command window. Copy this file to the working directory on the remote system.

▶ 71. Make sure that PuTTY is in the right directory and type:
`qsub jobscript-mmsoda.pbs`
to add the optimization to the scheduler's queue. Note that it is not necessary to change the permission bits for 'jobscript-mmsoda.pbs' when it is simply an input argument to `qsub`, rather than a program in its own right. Furthermore, it is also not necessary to re-compile your program, since we did not change anything in the code—we're just submitting to a different queue.

▶ 72. Use the tools discussed in Chapter 2 (e.g. `qstat`, `showq`, `showstart`, `checkjob`) to check on the status of your job.

4.4.1   Standard output and standard error

This is probably as good a time as any to look in more detail at some of the outputs that MMSODA generates. On the remote machine, there should now be a file './results/jobscript-

mmsoda.pbs.**o**XXXXXXX' (those X's represent the job id number). This file contains the standard **o**utput of our parallel optimization program. Whenever any of the parallel processes would normally print some message to the command window, on LISA that text will instead end up in the standard output file. The standard output file (and its sister, the standard **e**rror file './results/jobscript-mmsoda.pbs.**e**XXXXXXX') is interesting because it is the first place to look if something is not going like it should.

It is not necessary for you to fully understand what all lines in the standard output mean, but having just a general idea can save you a lot of time and frustration when you run into trouble. Most often, tracking an error is just a matter of spotting the difference between the output that you see when everything is working and when it's not. If nothing else, you can send the standard output file to one of the LISA administrators, such that (s)he may assist you better in solving your problem.

The standard output files that are generated during MMSODA optimizations typically consist of three parts: first, there is the output that was written when everything was being set up for the MMSODA run; second, there is a middle part that contains output that would be displayed in MATLAB's command window if you were running MMSODA on your local machine. Finally, the third part contains some text that the LISA system adds to every job's standard output. Listings 4.4 and 4.5 show the most interesting parts of the standard output for a single-objective MMSODA optimization in 'scemua' mode. Much of the lines in the first part are generated by bash commands[1] from the jobscript. For example, it includes the directory in which the job was started (PBS_WORK_DIR; lines 4–5), an `ls -l` overview of the files in that directory (lines 6–17), a message stating which modules will be loaded (lines 20 and 22). the identifier for the node on which the job ran (line 24), an overview of the nodes that participated in the execution of the job (lines 27–38); the name of each node occurs as many times as there are CPUs in it, so in this case there are 12 'r36n27' entries). Next, lines 40–43 add the PBS_WORK_DIR directory to the environment variable LD_LIBRARY_PATH to make sure that 'libmmpi.so' can be located by the compiled MATLAB program. Lines 45–331 provide the outputs from running the `nm` and `ldd` Linux commands on the binary 'matlabprog' and the library it uses, 'libmmpi.so'. After every => sign in the `ldd` result, there should be an entry; if it says 'not found', something is wrong. For example, if we would not have added the current directory to the LD_LIBRARY_PATH, line 50 would say '`libmmpi.so => not found`'. The `nm` results are included to enable checking whether 'matlabprog' and 'libmmpi.so' are not missing any functions. Lines 333–336 show the modules that are currently loaded. These should include at least the MATLAB Compiler Runtime (`mcr/v81`) and OpenMPI/GNU (`openmpi/gnu/1.6.5`). Lines 343–426 show the environment variables that currently exist. There are only a couple that are relevant to what we are doing, e.g. PBS_WORK_DIR, PBS_JOBID, and maybe a few others.

The middle part of the standard output (lines 433–1054) is what you normally see in the command window; it starts with a disclaimer message that is generated by the MMSODA code (lines 433–434). Line 438 states what kind of run this is: 'scemua', 'reset', or 'soda'; and whether it is a single-objective run ('so') or a multi-objective run ('mo'). Most of

---

[1]See page 14 in Chapter 2.

the remainder of the middle part consists of 'Evaluating parameter sets X-Y' messages (lines 439–1051), indicating the progress of the MMSODA algorithm.

The last part of the standard output file (lines 1055–1069) is always added by the LISA system. It provides an overview of the resources that were used in executing the job.

Listing 4.4: First part of the standard output file. Lines that were too long to fit on the page were wrapped; this is indicated with the line break ✓ and line continuation → symbols.

```
 1  Current dir ($PWD) is:
 2  /home/jspaaks
 3  Changing into $PBS_O_WORKDIR
 4  Current dir is ($PWD):
 5  /home/jspaaks/tmp/mmsoda-projects/example2
 6  Result of 'ls -l' is:
 7  total 220
 8  drwxr-xr-x 2 jspaaks jspaaks      48 Nov  5 11:33 data
 9  -rw-r--r-- 1 jspaaks jspaaks    1941 Nov  5 11:38 jobscript-mmsoda.pbs
10  -rwxrwxr-x 1 jspaaks jspaaks 189309 Nov  5 11:35 libmmpi.so
11  -rw-r--r-- 1 jspaaks jspaaks     276 Nov  5 11:29 makeconf.m
12  -rw-r--r-- 1 jspaaks jspaaks     271 Nov  4 19:19 makeconstants.m
13  -rw-r--r-- 1 jspaaks jspaaks    1770 Nov  5 11:32 Makefile
14  -rwxrwxr-x 1 jspaaks jspaaks   11832 Nov  5 11:35 matlabprog
15  drwxr-xr-x 2 jspaaks jspaaks      50 Nov  5 11:33 model
16  drwxr-xr-x 2 jspaaks jspaaks      51 Nov  5 11:40 results
17  -rwxr--r-- 1 jspaaks jspaaks    1363 Nov  5 11:32 run-mmsoda.sh
18  Unloading module matlab
19
20  Loading module openmpi/gnu/1.6.5
21
22  Loading module mcr/v81
23
24  Starting MPI job on node r36n27.lisa.surfsara.nl
25  node r36n27 has 12 CPUs.
26  Starting interactive MPI job on 1 batch nodes with a total of 12 CPUs.
27  r36n27
28  r36n27
29  r36n27
30  r36n27
31  r36n27
32  r36n27
33  r36n27
34  r36n27
35  r36n27
36  r36n27
37  r36n27
38  r36n27
39
40  Adding the current workdir to the library path environment variable
41
42  The current LD_LIBRARY_PATH is:
43  /sara/sw/mcr/64/v81/runtime/glnxa64:/sara/sw/mcr/64/v81/bin/glnxa64:/sara/sw/mcr/64/ ✓
    → v81/sys/os/glnxa64:/sara/sw/mcr/64/v81/sys/java/jre/glnxa64/jre/lib/amd64/ ✓
    → native_threads:/sara/sw/mcr/64/v81/sys/java/jre/glnxa64/jre/lib/amd64/server:/sara ✓
    → /sw/mcr/64/v81/sys/java/jre/glnxa64/jre/lib/amd64:/sara/sw/openmpi-gnu-1.6.5/lib:/ ✓
    → sara/sw/ofed/1.5.2/64/lib64:/sara/sw/libgfortran/32/1/lib:/home/jspaaks/tmp/mmsoda ✓
    → -projects/example2
44
45  Result of 'ldd matlabprog' is:
46      linux-vdso.so.1 =>  (0x00007fffe4af5000)
47      libmwmclmcrrt.so.8.1 => /sara/sw/mcr/64/v81/runtime/glnxa64/libmwmclmcrrt.so.8.1 ✓
    → (0x00002b00f760e000)
48      libm.so.6 => /lib/x86_64-linux-gnu/libm.so.6 (0x00002b00f787c000)
49      libmpi.so.1 => /sara/sw/openmpi-gnu-1.6.5/lib/libmpi.so.1 (0x00002b00f7afe000)
50      libmmpi.so => /home/jspaaks/tmp/mmsoda-projects/example2/libmmpi.so (0 ✓
    → x00002b00f80a9000)
51      libpthread.so.0 => /lib/x86_64-linux-gnu/libpthread.so.0 (0x00002b00f82b1000)
52      libc.so.6 => /lib/x86_64-linux-gnu/libc.so.6 (0x00002b00f84cd000)
```

```
53      libmwcpp11compat.so => /sara/sw/mcr/64/v81/runtime/glnxa64/../../bin/glnxa64/  ✓
   ↪   libmwcpp11compat.so (0x00002b00f8858000)
54      libdl.so.2 => /lib/x86_64-linux-gnu/libdl.so.2 (0x00002b00f8a61000)
55      libstdc++.so.6 => /sara/sw/mcr/64/v81/runtime/glnxa64/../../sys/os/glnxa64/  ✓
   ↪   libstdc++.so.6 (0x00002b00f8c65000)
56      libgcc_s.so.1 => /sara/sw/mcr/64/v81/runtime/glnxa64/../../sys/os/glnxa64/  ✓
   ↪   libgcc_s.so.1 (0x00002b00f8f75000)
57      libibverbs.so.1 => /sara/sw/ofed/1.5.2/64/lib64/libibverbs.so.1 (0  ✓
   ↪   x00002b00f918b000)
58      libtorque.so.2 => /usr/lib/libtorque.so.2 (0x00002b00f9398000)
59      libnuma.so.1 => /usr/lib/libnuma.so.1 (0x00002b00f96a4000)
60      librt.so.1 => /lib/x86_64-linux-gnu/librt.so.1 (0x00002b00f98af000)
61      libnsl.so.1 => /lib/x86_64-linux-gnu/libnsl.so.1 (0x00002b00f9ab7000)
62      libutil.so.1 => /lib/x86_64-linux-gnu/libutil.so.1 (0x00002b00f9cd0000)
63      /lib64/ld-linux-x86-64.so.2 (0x00002b00f73ec000)
64
65 Result of 'nm matlabprog' is:
66                  U MPI_Comm_rank
67                  U MPI_Comm_size
68                  U MPI_Finalize
69                  U MPI_Init_thread
70 0000000000601540 d _DYNAMIC
71 0000000000601788 d _GLOBAL_OFFSET_TABLE_
72 0000000000401258 R _IO_stdin_used
73                  w _ITM_deregisterTMCloneTable
74                  w _ITM_registerTMCloneTable
75                  w _Jv_RegisterClasses
76 0000000000401520 r __FRAME_END__
77 0000000000601538 d __JCR_END__
78 0000000000601538 d __JCR_LIST__
79 0000000000601858 D __TMC_END__
80 0000000000601858 A __bss_start
81 0000000000601848 D __data_start
82 0000000000400e80 t __do_global_dtors_aux
83 0000000000601530 t __do_global_dtors_aux_fini_array_entry
84 0000000000601850 D __dso_handle
85 0000000000601528 t __frame_dummy_init_array_entry
86                  w __gmon_start__
87 0000000000601530 t __init_array_end
88 0000000000601528 t __init_array_start
89 00000000004011b0 T __libc_csu_fini
90 00000000004011c0 T __libc_csu_init
91                  U __libc_start_main@@GLIBC_2.2.5
92 0000000000601858 A _edata
93 0000000000601c88 A _end
94 000000000040124c T _fini
95 0000000000400c50 T _init
96 0000000000400dc0 T _start
97 0000000000400dec t call_gmon_start
98 0000000000601c70 b completed.6092
99 0000000000601848 W data_start
100 0000000000400e10 t deregister_tm_clones
101 0000000000400ea0 t frame_dummy
102                  U fwrite@@GLIBC_2.2.5
103                  U getopt@@GLIBC_2.2.5
104                  U libmmpiInitialize
105                  U libmmpiTerminate
106 0000000000401010 T main
107                  U mclInitializeApplication_proxy
108                  U mclRunMain_proxy
109                  U mclTerminateApplication_proxy
110                  U mclmcrInitialize_proxy
111                  U mlfMatlabmain
112                  U mlfSetmpistuff
113 0000000000601c7c B mpi_rank
114 0000000000601c80 B mpi_size
115                  U mxCreateDoubleMatrix_730_proxy
116                  U mxDestroyArray_proxy
117                  U mxGetPr_proxy
118 0000000000601860 B ompi_mpi_comm_world
119 0000000000601c60 B optarg@@GLIBC_2.2.5
120                  U printf@@GLIBC_2.2.5
121                  U puts@@GLIBC_2.2.5
```

```
122  0000000000400e40 t register_tm_clones
123  0000000000400ed0 T run_main
124  0000000000601c74 B savetimings
125  0000000000601c68 B stderr@@GLIBC_2.2.5
126                   U strtol@@GLIBC_2.2.5
127  0000000000601c78 B verbosity
128
129  Result of 'ldd libmmpi.so' is:
130      linux-vdso.so.1 =>  (0x00007fff59d54000)
131      libmwmclmcrrt.so.8.1 => /sara/sw/mcr/64/v81/runtime/glnxa64/libmwmclmcrrt.so.8.1   ✓
  → (0x00002ba2f37b3000)
132      libm.so.6 => /lib/x86_64-linux-gnu/libm.so.6 (0x00002ba2f3a21000)
133      libpthread.so.0 => /lib/x86_64-linux-gnu/libpthread.so.0 (0x00002ba2f3ca3000)
134      libc.so.6 => /lib/x86_64-linux-gnu/libc.so.6 (0x00002ba2f3ebf000)
135      libmwcpp11compat.so => /sara/sw/mcr/64/v81/runtime/glnxa64/../../bin/glnxa64/   ✓
  → libmwcpp11compat.so (0x00002ba2f424a000)
136      libdl.so.2 => /lib/x86_64-linux-gnu/libdl.so.2 (0x00002ba2f4453000)
137      libstdc++.so.6 => /sara/sw/mcr/64/v81/runtime/glnxa64/../../sys/os/glnxa64/   ✓
  → libstdc++.so.6 (0x00002ba2f4658000)
138      libgcc_s.so.1 => /sara/sw/mcr/64/v81/runtime/glnxa64/../../sys/os/glnxa64/   ✓
  → libgcc_s.so.1 (0x00002ba2f4967000)
139      /lib64/ld-linux-x86-64.so.2 (0x00002ba2f3388000)
140
141  Result of 'nm libmmpi.so' is:
142  0000000000206658 a _DYNAMIC
143  0000000000206898 a _GLOBAL_OFFSET_TABLE_
144                   w _ITM_deregisterTMCloneTable
145                   w _ITM_registerTMCloneTable
146                   w _Jv_RegisterClasses
147  0000000000006638 r __FRAME_END__
148  0000000000206650 d __JCR_END__
149  0000000000206650 d __JCR_LIST__
150  0000000000206918 d __TMC_END__
151  0000000000206918 A __bss_start
152                   w __cxa_finalize@@GLIBC_2.2.5
153  0000000000002f20 t __do_global_dtors_aux
154  0000000000206648 t __do_global_dtors_aux_fini_array_entry
155  0000000000206910 d __dso_handle
156  0000000000206640 t __frame_dummy_init_array_entry
157                   w __gmon_start__
158  0000000000206918 A _edata
159  0000000000206928 A _end
160  0000000000004d70 T _fini
161  0000000000002da8 T _init
162  0000000000206920 b _mcr_inst
163  0000000000002e90 t call_gmon_start
164  0000000000206918 b completed.6092
165  0000000000002eb0 t deregister_tm_clones
166  0000000000002f60 t frame_dummy
167  00000000000030d0 T libmmpiInitialize
168  0000000000003034 T libmmpiInitializeWithHandlers
169  000000000000310c T libmmpiPrintStackTrace
170  00000000000030ec T libmmpiTerminate
171  0000000000002fbb t mclDefaultErrorHandler
172  0000000000002f90 t mclDefaultPrintHandler
173                   U mclDestroyStream_proxy
174                   U mclFeval_proxy
175                   U mclFreeStackTrace_proxy
176                   U mclGetEmbeddedCtfStream_proxy
177                   U mclGetStackTrace_proxy
178                   U mclInitializeComponentInstanceEmbedded_proxy
179                   U mclMlfFeval_proxy
180                   U mclTerminateInstance_proxy
181                   U mclWrite_proxy
182                   U mclmcrInitialize_proxy
183  0000000000003e81 T mlfBcastvar
184  0000000000003f68 T mlfCalcLikelihoodState
185  0000000000003ce2 T mlfGetverbosity
186  0000000000003f1a T mlfLintank
187  0000000000003d7c T mlfMatlabmain
188  00000000000041ca T mlfMmsoda
189  0000000000003fac T mlfMmsodaAbortOptim
190  0000000000003fe6 T mlfMmsodaAllComb
```

```
191   00000000000047ab  T  mlfMmsodaAnalyzeTimings
192   00000000000047df  T  mlfMmsodaAnalyzeTimings_old
193   000000000000401b  T  mlfMmsodaCalcCbWb
194   0000000000004b06  T  mlfMmsodaCalcEnsembleCov
195   0000000000004b40  T  mlfMmsodaCalcInnovations
196   0000000000004b98  T  mlfMmsodaCalcKalmanGain
197   0000000000004bdc  T  mlfMmsodaCalcMeasErrCov
198   0000000000004055  T  mlfMmsodaCalcObjScore
199   0000000000004cdd  T  mlfMmsodaCalcPareto
200   000000000000434f  T  mlfMmsodaCheckForOldResults
201   000000000000408f  T  mlfMmsodaContinue
202   0000000000004383  T  mlfMmsodaCreateMakefile
203   00000000000043b7  T  mlfMmsodaDiffStruct
204   0000000000004c16  T  mlfMmsodaEnKF
205   00000000000040c9  T  mlfMmsodaEvolveComplex
206   0000000000004117  T  mlfMmsodaGelmanRubin
207   0000000000004151  T  mlfMmsodaGenerateOffspring
208   00000000000043f6  T  mlfMmsodaHostnameReturnsLisa
209   0000000000004195  T  mlfMmsodaInitialize
210   0000000000004427  T  mlfMmsodaIsColumn
211   000000000000445c  T  mlfMmsodaLoadSettings
212   0000000000004813  T  mlfMmsodaMakeColors
213   0000000000004848  T  mlfMmsodaMargHist
214   0000000000004887  T  mlfMmsodaMatrixOfScatter
215   0000000000004496  T  mlfMmsodaOpenBrowser
216   00000000000044ca  T  mlfMmsodaOpenPdf
217   00000000000044fe  T  mlfMmsodaPack
218   000000000000452f  T  mlfMmsodaParetoPrinciple
219   0000000000004560  T  mlfMmsodaParsePairs
220   00000000000041fd  T  mlfMmsodaPartComplexes
221   00000000000048d5  T  mlfMmsodaPlotEnsemble
222   0000000000004914  T  mlfMmsodaPlotGelmanRubin
223   0000000000004951  T  mlfMmsodaPlotPaCo
224   0000000000004990  T  mlfMmsodaPlotSeq
225   0000000000004591  T  mlfMmsodaPrepParallelFiles
226   0000000000004237  T  mlfMmsodaPrepRejArray
227   0000000000004271  T  mlfMmsodaPrepSeqArray
228   0000000000004c50  T  mlfMmsodaProcessBundle
229   0000000000004d17  T  mlfMmsodaRecalcPareto
230   00000000000045f6  T  mlfMmsodaSaveConf
231   00000000000042ab  T  mlfMmsodaStratDraw
232   00000000000042e0  T  mlfMmsodaStratRandDraw
233   0000000000004627  T  mlfMmsodaSubplotScreen
234   0000000000004315  T  mlfMmsodaUnifRandDraw
235   000000000000466b  T  mlfMmsodaUnpack
236   0000000000004c8f  T  mlfMmsodaUpdateStates
237   000000000000469c  T  mlfMmsodaVerifyFieldNames
238   00000000000049d4  T  mlfMmsodaVisSequences
239   0000000000004a11  T  mlfMmsodaVisualization1
240   0000000000004a42  T  mlfMmsodaVisualization2
241   0000000000004a73  T  mlfMmsodaVisualization3
242   0000000000004aa4  T  mlfMmsodaVisualization4
243   0000000000004ad5  T  mlfMmsodaVisualization5
244   00000000000046d6  T  mlfMmsodaWriteJobscript
245   00000000000045c5  T  mlfMmsodaroot
246   0000000000003eb4  T  mlfReceivevar
247   0000000000003db4  T  mlfRunmpirank0
248   0000000000003de5  T  mlfRunmpirank1
249   0000000000003e50  T  mlfRunmpirankOther
250   0000000000003e16  T  mlfRunmpirankOtherFun
251   0000000000003ee7  T  mlfSendvar
252   0000000000003d13  T  mlfSetmpistuff
253   0000000000004707  T  mlfSubaxes
254   0000000000004749  T  mlfUimatlab
255   000000000000477a  T  mlfUioctave
256   0000000000003d4b  T  mlfWhoami
257   00000000000032d4  T  mlxBcastvar
258   0000000000003370  T  mlxCalcLikelihoodState
259   000000000000319c  T  mlxGetverbosity
260   0000000000003349  T  mlxLintank
261   0000000000003211  T  mlxMatlabmain
262   00000000000034f6  T  mlxMmsoda
263   0000000000003397  T  mlxMmsodaAbortOptim
```

```
264  00000000000033be T mlxMmsodaAllComb
265  000000000000393a T mlxMmsodaAnalyzeTimings
266  0000000000003961 T mlxMmsodaAnalyzeTimings_old
267  00000000000033e5 T mlxMmsodaCalcCbWb
268  0000000000003b83 T mlxMmsodaCalcEnsembleCov
269  0000000000003baa T mlxMmsodaCalcInnovations
270  0000000000003bd1 T mlxMmsodaCalcKalmanGain
271  0000000000003bf8 T mlxMmsodaCalcMeasErrCov
272  000000000000340c T mlxMmsodaCalcObjScore
273  0000000000003c94 T mlxMmsodaCalcPareto
274  0000000000003607 T mlxMmsodaCheckForOldResults
275  0000000000003433 T mlxMmsodaContinue
276  000000000000362e T mlxMmsodaCreateMakefile
277  0000000000003655 T mlxMmsodaDiffStruct
278  0000000000003c1f T mlxMmsodaEnKF
279  000000000000345a T mlxMmsodaEvolveComplex
280  0000000000003481 T mlxMmsodaGelmanRubin
281  00000000000034a8 T mlxMmsodaGenerateOffspring
282  000000000000367c T mlxMmsodaHostnameReturnsLisa
283  00000000000034cf T mlxMmsodaInitialize
284  00000000000036a3 T mlxMmsodaIsColumn
285  00000000000036ca T mlxMmsodaLoadSettings
286  0000000000003988 T mlxMmsodaMakeColors
287  00000000000039af T mlxMmsodaMargHist
288  00000000000039d6 T mlxMmsodaMatrixOfScatter
289  00000000000036f1 T mlxMmsodaOpenBrowser
290  0000000000003718 T mlxMmsodaOpenPdf
291  000000000000373f T mlxMmsodaPack
292  0000000000003766 T mlxMmsodaParetoPrinciple
293  000000000000378d T mlxMmsodaParsePairs
294  000000000000351d T mlxMmsodaPartComplexes
295  00000000000039fd T mlxMmsodaPlotEnsemble
296  0000000000003a24 T mlxMmsodaPlotGelmanRubin
297  0000000000003a4b T mlxMmsodaPlotPaCo
298  0000000000003a72 T mlxMmsodaPlotSeq
299  00000000000037b4 T mlxMmsodaPrepParallelFiles
300  0000000000003544 T mlxMmsodaPrepRejArray
301  000000000000356b T mlxMmsodaPrepSeqArray
302  0000000000003c46 T mlxMmsodaProcessBundle
303  0000000000003cbb T mlxMmsodaRecalcPareto
304  0000000000003802 T mlxMmsodaSaveConf
305  0000000000003592 T mlxMmsodaStratDraw
306  00000000000035b9 T mlxMmsodaStratRandDraw
307  0000000000003829 T mlxMmsodaSubplotScreen
308  00000000000035e0 T mlxMmsodaUnifRandDraw
309  0000000000003850 T mlxMmsodaUnpack
310  0000000000003c6d T mlxMmsodaUpdateStates
311  0000000000003877 T mlxMmsodaVerifyFieldNames
312  0000000000003a99 T mlxMmsodaVisSequences
313  0000000000003ac0 T mlxMmsodaVisualization1
314  0000000000003ae7 T mlxMmsodaVisualization2
315  0000000000003b0e T mlxMmsodaVisualization3
316  0000000000003b35 T mlxMmsodaVisualization4
317  0000000000003b5c T mlxMmsodaVisualization5
318  000000000000389e T mlxMmsodaWriteJobscript
319  00000000000037db T mlxMmsodaroot
320  00000000000032fb T mlxReceivevar
321  0000000000003238 T mlxRunmpirank0
322  000000000000325f T mlxRunmpirank1
323  00000000000032ad T mlxRunmpirankOther
324  0000000000003286 T mlxRunmpirankOtherFun
325  0000000000003322 T mlxSendvar
326  00000000000031c3 T mlxSetmpistuff
327  00000000000038c5 T mlxSubaxes
328  00000000000038ec T mlxUimatlab
329  0000000000003913 T mlxUioctave
330  00000000000031ea T mlxWhoami
331  0000000000002ee0 t register_tm_clones
332
333  Currently Loaded Modulefiles:
334   1) libgfortran/32/1   4) licenses/default   7) openmpi/gnu/1.6.5
335   2) stdenv/1.1         5) sara/1              8) mcr/v81
336   3) compilerwrappers   6) ofed/64/1.5.2
```

```
337  Setting MCR_CACHE_ROOT to: /scratch/mmsoda-hTmsClGn
338
339  The current MCR_CACHE_ROOT is:
340  /scratch/mmsoda-hTmsClGn
341
342
343  --------------------------------------------------
344  The environment variables are (env|sort)
345  }
346  ENVIRONMENT=BATCH
347  GIT_EDITOR=nano
348  HOME=/home/jspaaks
349  IBV_FORK_SAFE=1
350  INTEL_LICENSE_FILE_modshare=/opt/intel/licenses:1
351  INTEL_LICENSE_FILE=/opt/intel/licenses
352  LANG=en_US.UTF-8
353  LC_ALL=en_US.UTF-8
354  LC_TIME=en_DK.UTF-8
355  LD_LIBRARY_PATH_modshare=/sara/sw/mcr/64/v81/sys/java/jre/glnxa64/jre/lib/amd64/  ↙
   →   server:1:/sara/sw/openmpi-gnu-1.6.5/lib:1:/sara/sw/ofed/1.5.2/64/lib64:1:/sara/sw/  ↙
   →   mcr/64/v81/runtime/glnxa64:1:/sara/sw/mcr/64/v81/sys/os/glnxa64:1:/sara/sw/mcr/64/  ↙
   →   v81/bin/glnxa64:1:/sara/sw/mcr/64/v81/sys/java/jre/glnxa64/jre/lib/amd64/  ↙
   →   native_threads:1:/sara/sw/mcr/64/v81/sys/java/jre/glnxa64/jre/lib/amd64:1:/sara/sw  ↙
   →   /libgfortran/32/1/lib:1
356  LD_LIBRARY_PATH=/sara/sw/mcr/64/v81/runtime/glnxa64:/sara/sw/mcr/64/v81/bin/glnxa64:/  ↙
   →   sara/sw/mcr/64/v81/sys/os/glnxa64:/sara/sw/mcr/64/v81/sys/java/jre/glnxa64/jre/lib  ↙
   →   /amd64/native_threads:/sara/sw/mcr/64/v81/sys/java/jre/glnxa64/jre/lib/amd64/  ↙
   →   server:/sara/sw/mcr/64/v81/sys/java/jre/glnxa64/jre/lib/amd64:/sara/sw/openmpi-gnu  ↙
   →   -1.6.5/lib:/sara/sw/ofed/1.5.2/64/lib64:/sara/sw/libgfortran/32/1/lib:/home/  ↙
   →   jspaaks/tmp/mmsoda-projects/example2
357  LD_RUN_PATH_modshare=/sara/sw/openmpi-gnu-1.6.5/lib:1:/sara/sw/ofed/1.5.2/64/lib64:1
358  LD_RUN_PATH=/sara/sw/openmpi-gnu-1.6.5/lib:/sara/sw/ofed/1.5.2/64/lib64
359  _LMFILES__modshare=/sara/sw/modules-ng-64/modulefiles/tools/ofed/64/1.5.2:2:/sara/sw/  ↙
   →   modules-ng-64/modulefiles/environment/licenses/default:2:/sara/sw/modules-ng-64/  ↙
   →   modulefiles/environment/libgfortran/32/1:2:/sara/sw/modules-ng-64/modulefiles/  ↙
   →   environment/compilerwrappers:1:/sara/sw/modules-ng-64/modulefiles/tools/mcr/v81:1
360  _LMFILES_=/sara/sw/modules-ng-64/modulefiles/environment/libgfortran/32/1:/sara/sw/  ↙
   →   modules-ng-64/modulefiles/environment/compilerwrappers:/sara/sw/modules-ng-64/  ↙
   →   modulefiles/environment/licenses/default:/sara/sw/modules-ng-64/modulefiles/tools/  ↙
   →   ofed/64/1.5.2:/sara/sw/modules-ng-64/modulefiles/tools/mcr/v81
361  LOADEDMODULES=libgfortran/32/1:stdenv/1.1:compilerwrappers:licenses/default:sara/1:  ↙
   →   ofed/64/1.5.2:openmpi/gnu/1.6.5:mcr/v81
362  LOADEDMODULES_modshare=mcr/v81:1:openmpi/gnu/1.6.5:1:ofed/64/1.5.2:1:licenses/default  ↙
   →   :1:libgfortran/32/1:1:sara/1:1:compilerwrappers:1:stdenv/1.1:1
363  LOGNAME=jspaaks
364  LS_COLORS=
365  MANPATH_modshare=:1:/usr/man:1:/sara/sw/ofed/1.5.2/64/share/man:1:/usr/share/man:1:/  ↙
   →   usr/local/man:1:/sara/sw/openmpi-gnu-1.6.5/share/man:1
366  MANPATH=/sara/sw/openmpi-gnu-1.6.5/share/man::/sara/sw/ofed/1.5.2/64/share/man:/usr/  ↙
   →   share/man:/usr/man:/usr/local/man
367  MCR_CACHE_ROOT=/scratch/mmsoda-hTmsClGn
368  MODULE_BIN=/sara/sw/modules-ng-64/module/bin
369  module=() {  eval $($MODULE_BIN/modulecmd bash $*)
370  MODULEFILES=/sara/sw/modules-ng-64/modulefiles
371  MODULE_INCLUDE=/sara/sw/modules-ng-64/module/../include
372  MODULEPATH=/sara/sw/modules-ng-64/modulefiles/applications:/sara/sw/modules-ng-64/  ↙
   →   modulefiles/compilers:/sara/sw/modules-ng-64/modulefiles/environment:/sara/sw/  ↙
   →   modules-ng-64/modulefiles/libraries:/sara/sw/modules-ng-64/modulefiles/tools:/sara  ↙
   →   /sw/modules-ng-64/modulefiles/deprecated:/sara/sw/modules-ng-64/modulefiles/  ↙
   →   unsupported
373  MODULES_BASE=/sara/sw/modules-ng-64
374  MODULESHOME=/sara/sw/modules-ng-64/module
375  MODULES_PREFIX=SARA
376  MODULE_VERSION=4.0.0
377  MODULE_VERSION_STACK=4.0.0
378  OLDPWD=/home/jspaaks
379  OMPI_MCA_btl_base_warn_component_unused=0
380  PATH_modshare=/sara/sw/ofed/1.5.2/64/bin:1:/bin:1:/sara/sw/modules-ng-64/wrappers/  ↙
   →   sara:1:/usr/bin:1:/sara/sw/openmpi-gnu-1.6.5/bin:1:/usr/bin/X11:1:/sara/sw/ofed  ↙
   →   /1.5.2/64/sbin:1:/usr/local/bin:1
381  PATH=/sara/sw/modules-ng-64/wrappers/sara:/sara/sw/openmpi-gnu-1.6.5/bin:/sara/sw/  ↙
   →   ofed/1.5.2/64/sbin:/sara/sw/ofed/1.5.2/64/bin:/bin:/usr/bin:/usr/bin/X11:/usr/  ↙
   →   local/bin
```

```
382  PBS_ENVIRONMENT=PBS_BATCH
383  PBS_GPUFILE=/var/spool/torque/aux//7228630.batch1.lisa.surfsara.nlgpu
384  PBS_JOBCOOKIE=F5EBE03BCE49A38B57E22065BDC39E48
385  PBS_JOBID=7228630.batch1.lisa.surfsara.nl
386  PBS_JOBNAME=jobscript-mmsoda.pbs
387  PBS_MOMPORT=15003
388  PBS_NODEFILE=/var/spool/torque/aux//7228630.batch1.lisa.surfsara.nl
389  PBS_NODENUM=0
390  PBS_NP=1
391  PBS_NUM_NODES=1
392  PBS_NUM_PPN=1
393  PBS_O_HOME=/home/jspaaks
394  PBS_O_HOST=login2.lisa.surfsara.nl
395  PBS_O_LANG=en_US
396  PBS_O_LOGNAME=jspaaks
397  PBS_O_MAIL=/var/mail/jspaaks
398  PBS_O_PATH=/sara/sw/modules-ng-64/wrappers/sara:/sara/sw/openmpi-gnu-1.6.5/bin:/sara/ ↙
     → sw/ofed/1.5.2/64/sbin:/sara/sw/ofed/1.5.2/64/bin:/sara/sw/matlab/64/2013a/bin:/bin ↙
     → :/usr/bin:/usr/bin/X11:/usr/local/bin
399  PBS_O_QUEUE=batch
400  PBS_O_SHELL=/bin/bash
401  PBS_O_WORKDIR=/home/jspaaks/tmp/mmsoda-projects/example2
402  PBS_QUEUE=serial
403  PBS_SERVER=batch
404  PBS_TASKNUM=1
405  PBS_VERSION=TORQUE-2.5.13
406  PBS_VNODENUM=0
407  PBS_WALLTIME=900
408  PWD=/home/jspaaks/tmp/mmsoda-projects/example2
409  SARA_INCLUDE_PATH_modshare=/sara/sw/openmpi-gnu-1.6.5/include:1:/sara/sw/ofed ↙
     → /1.5.2/64/include:1
410  SARA_INCLUDE_PATH=/sara/sw/openmpi-gnu-1.6.5/include:/sara/sw/ofed/1.5.2/64/include
411  SARA_LIBRARY_PATH_modshare=/sara/sw/openmpi-gnu-1.6.5/lib:1:/sara/sw/ofed/1.5.2/64/ ↙
     → lib64:1
412  SARA_LIBRARY_PATH=/sara/sw/openmpi-gnu-1.6.5/lib:/sara/sw/ofed/1.5.2/64/lib64
413  SARA_OFED_INCLUDE=/sara/sw/ofed/1.5.2/64/include
414  SARA_OFED_LIB=/sara/sw/ofed/1.5.2/64/lib64
415  SARA_OFED_ROOT=/sara/sw/ofed/1.5.2/64
416  SARA_OPENMPI_INCLUDE=/sara/sw/openmpi-gnu-1.6.5/include
417  SARA_OPENMPI_LIB=/sara/sw/openmpi-gnu-1.6.5/lib
418  SARA_OPENMPI_ROOT=/sara/sw/openmpi-gnu-1.6.5
419  SHELL=/bin/bash
420  SHLVL=2
421  TMPDIR=/scratch/7228630.batch1.lisa.surfsara.nl
422  USER=jspaaks
423  _=/usr/bin/env
424  XAPPLRESDIR_modshare=/sara/sw/mcr/64/v81/X11/app-defaults:1
425  XAPPLRESDIR=/sara/sw/mcr/64/v81/X11/app-defaults
426  ------------------------------------------------
427
428
429  Starting MPI run
430  Setting verbosity to level 0.
431  Warning: application is running on a locale different from the original platform ↙
     → locale.
432
433  % This is a pre-alpha release of the MMSODA simultaneous
434  % parameter optimization and data assimilation software.
435
436  Setting value of 'conf.nMembers' to 1.
437
438  SCEMUA-SO run started on: November 05, 2013 11:40:49
439  +00s: Evaluating parameter sets 1-250
440  +01s: Evaluating parameter sets 251-300
441  +01s: Evaluating parameter sets 301-350
442  +01s: Evaluating parameter sets 351-400
443  +01s: Evaluating parameter sets 401-450
444  +01s: Evaluating parameter sets 451-500
```

Listing 4.5: Last part of the standard output file. Lines that were too long to fit on the page were wrapped; this is indicated with the line break ✓ and line continuation → symbols.

```
1048  +01m 15s: Evaluating parameter sets 30651-30700
1049  +01m 15s: Evaluating parameter sets 30701-30750
1050  +01m 15s: Evaluating parameter sets 30751-30800
1051  +01m 15s: Evaluating parameter sets 30801-30850
1052  Convergence achieved.
1053  SCEMUA-SO run completed on: November 05, 2013 11:42:05
1054  The run took 0d 0h 1m 15s.
1055  Q: "...sara_stats": -------------------Begin of SARA epilogue  ✓
      →  ---------------------------------
1056  Q: "...sara_stats": This output was generated by the SARA epilogue script
1057  Q: "...sara_stats": Your job [jobscript-mmsoda.pbs] has been executed in queue [  ✓
      →  serial] with
1058  Q: "...sara_stats": the following PBS arguments:
1059  Q: "...sara_stats":    ncpus=1,neednodes=1,nodes=1,walltime=00:15:00
1060  Q: "...sara_stats":    .
1061  Q: "...sara_stats": Resources used in job [7228630.batch1.lisa.surfsara.nl] with name  ✓
      →  [jobscript-mmsoda.pbs]:
1062  Q: "...sara_stats":    cput=00:15:40,mem=1117536kb,vmem=7739088kb,walltime=00:01:26
1063  Q: "...sara_stats":    r36n27
1064  Q: "...sara_stats":    .
1065  Q: "...sara_stats": Job start and end time:
1066  Q: "...sara_stats":   Job start time: Tue Nov  5 11:40:41 CET 2013
1067  Q: "...sara_stats":   Job end time  : Tue Nov  5 11:42:08 CET 2013
1068  Q: "...sara_stats": --------------------End of SARA epilogue  ✓
      →  ---------------------------------
1069  I: Last 14 quoted lines were generated by promiser "/var/spool/torque/mom_priv/  ✓
      →  epilogue.d/sara_stats"
```

4.4.2   Analyzing the parallelization overhead

When dealing with parallel programs, it is often useful to monitor how much time is lost in parallelization overhead in relation to the CPU time (recall Fig. 3.1). The MMSODA Toolbox for MATLAB enables you to record and visualize the timings of all relevant events (sending and receiving data, serializing[1] and deserializing, waiting for input, etc.) on all nodes that have been assigned to the job. Recording the timings does slow the optimization down slightly, so the default behavior is not to record any events. However, enabling the time-keeping functionality is simply a matter of re-running the `mmsodaPrepParallelFiles()` function, and answering 'a : yes' to the last question 'Would you like to save the timings?'.

▶ 73. Re-run `mmsodaPrepParallelFiles()` and enable time-keeping. Copy the newly created jobscript to the cluster. Submit the new jobscript using `qsub`.

▶ 74. After the job finishes, copy the contents of the './results' directory from the remote system to your local system.

▶ 75. Read the documentation on `mmsodaAnalyzeTimings` and visualize the timings for the linear tank example. Would you say that parallel optimization of the linear tank model is a coarse-grained or a fine-grained problem?

---

[1]Serialization is the process of collecting all the arrays that need to be sent over to a different machine, such that the arrays occupy a consecutive part of the computer's memory. This part of the memory can then be sent to another machine.

At this point, you are familiar with MMSODA in 'bypass' mode and in 'scemua' mode, and you know how to run MMSODA optimizations locally as well as on the LISA cluster. In the next few sections, we will cover the 'reset' mode and 'soda' modes, but the important point is that the workflow as you know it from the previous projects (as summarized in Fig. 4.7) is the same for all MMSODA projects.
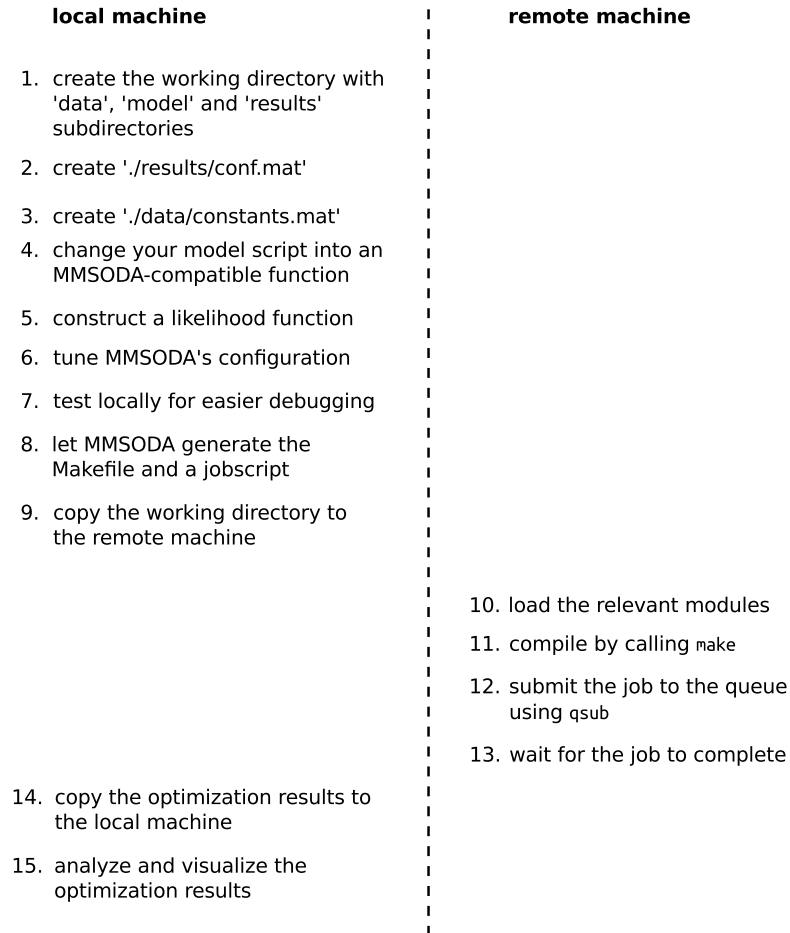
local machine | **remote machine**

1. create the working directory with 'data', 'model' and 'results' subdirectories

2. create './results/conf.mat'

3. create './data/constants.mat'

4. change your model script into an MMSODA-compatible function

5. construct a likelihood function

6. tune MMSODA's configuration

7. test locally for easier debugging

8. let MMSODA generate the Makefile and a jobscript

9. copy the working directory to the remote machine

      10. load the relevant modules

      11. compile by calling `make`

      12. submit the job to the queue using `qsub`

      13. wait for the job to complete

14. copy the optimization results to the local machine

15. analyze and visualize the optimization results

Figure 4.7: Typical workflow for setting up MMSODA optimizations. Note that the items under 'remote machine' are executed in a terminal program such as PuTTY.

▶ 76. Now that you know what information goes where for MMSODA in 'scemua' mode, it may be useful to review some of the other examples in the 'esibayes-master/examples' directory. On your local machine, explore the configurations for a few of the other 'scemua' mode directories. Run MMSODA for those configurations, but make sure MATLAB is set to the correct working directory when `mmsoda` is started.

4.5   MMSODA in 'reset' mode; sequential execution

► 77. On your local system, make a copy of the 'example2' directory, and rename the copy to 'example3'. Clean up the 'example3' directory by removing 'matlabprog', 'libmmpi.so', 'Makefile', 'jobscript-mmsoda.pbs' as well as any results pertaining to the 'example2' case. Set your MATLAB working directory to the newly created 'example3' directory.

► 78. Remove the 'constants.mat' and 'lintank-obs.mat' files from the 'example3/data' directory. Copy 'lintank-obs-unobserved-input.mat' from the 'esibayes-master/manual/other' directory to 'example3/data'.

► 79. On the MATLAB command line, load the `obsTimes` and `obs` variables from the './data/lintank-obs-unobserved-input.mat' file by typing:
```
>> load('./data/lintank-obs-unobserved-input.mat','obsTimes','obs')
```

► 80. Visualize the data that were just loaded by:
```
>> plot(obsTimes,obs(1,:),'-b.')
```
Your figure should be similar to Fig. 4.8.
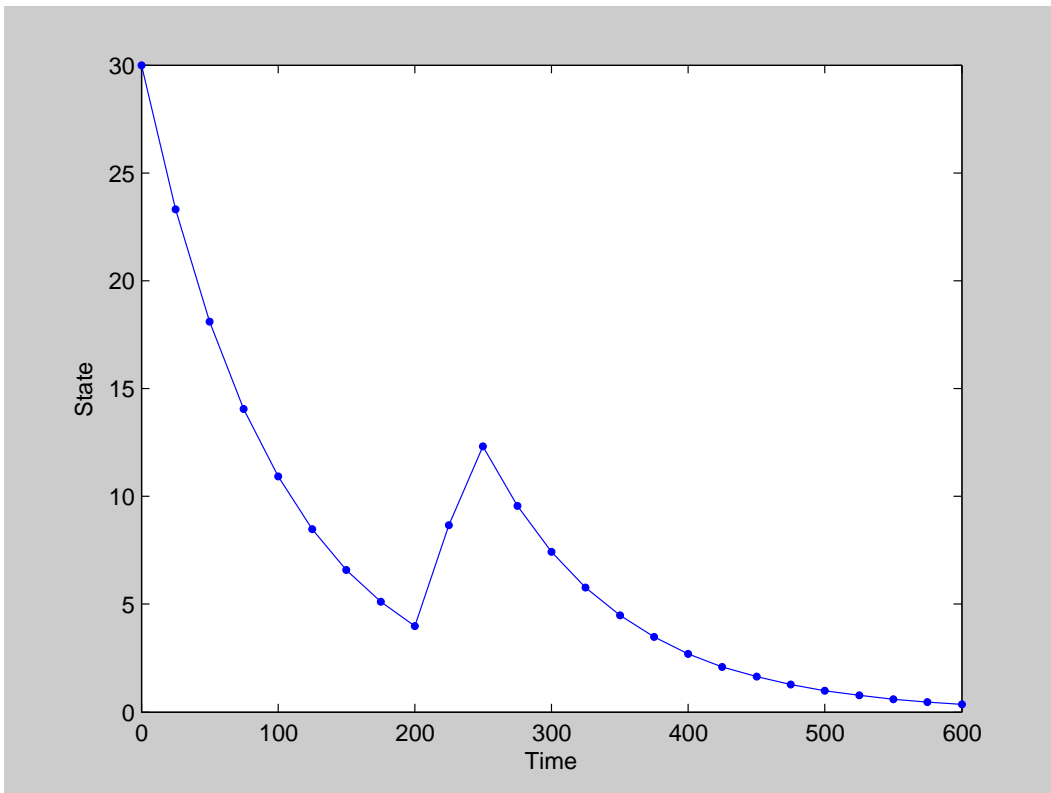
Figure 4.8: Simple `plot` of the data in './data/lintank-obs-unobserved-input.mat'. The true value of the resistance parameter in this figure is 100.

From Fig. 4.8, it is clear that something happened around Time=200–250. It seems that water was added to the upper tank—that is to say, the upper tank has been subjected to an

unobserved input. This kind of error is very common in hydrology; for example if the linear tank simulates the streamflow from a particular catchment, it can sometimes happen that streamflow in the river increases (as in Fig. 4.8), without any rain being recorded during the preceding days. Most often, these kinds of apparent impossibilities are explained by a rainstorm which did indeed pass over (some of) the catchment, but which missed the location of the rain gauge. Observational error like that can play havoc with the effectiveness of the calibration, as we shall see shortly.

In this section, we will look at what happens if we take a naive approach to calibrating the lin-tank model to the data of Fig. 4.8. For this, we need to make a few changes in the MMSODA configuration. For example, we need the model to generate predictions at `priorTimes = [0:25:600]`, and we want to use the data from './data/lintank-obs-unobserved-input.mat' in the objective function.

▶ 81. Make the necessary changes to 'makeconf.m' and 'makeconstants.m' to implement these changes. Also change the value of the `dtSimDefault` model constant to 2.0 and set the lower and upper boundaries of the parameter space to 10 and 500, respectively. Furthermore, set the `doPlot` configuration variable to `true`, such that MMSODA will produce some standardized visualizations as the optimization progresses. Finally, set `nModelEvalsMax` to `7000`.

▶ 82. Run the updated versions of 'makeconf.m' and 'makeconstants.m' and verify that the necessary files are created. Then, start the SCEM-UA optimization in the regular way from the MATLAB command window.

Listing 4.6 on page 52 demonstrates how parameter uncertainty intervals can be constructed using the information in `evalResults`. A copy of the listing has been included as 'calcUncertaintyIntervals.m' in the 'esibayes-master/manual/other' directory.

▶ 83. Study the script and use it to visualize the model prediction for the best parameter set, along with the parameter uncertainty intervals for the case of Fig. 4.8.

```matlab
1  % load the MMSODA configuration and the 'evalResults' array
2  load('./results/scemua-so-results.mat','conf','evalResults')
3
4  % load the model constants from the data subdirectory
5  constants = load('./data/constants.mat');
6
7  % set the initial state to empty for scemua run (nStatesKF = 0);
8  init = [];
9
10 % define the number of model outputs to include in the construction of the
11 % parameter uncertainty intervals:
12 nModelOutputs = 250;
13
14 % count the number of rows in 'evalResults'
15 nRows = size(evalResults,1);
16
17 % pre-allocate the array that will hold the model outputs
18 allModelOutputs = repmat(NaN,[nModelOutputs,conf.nPrior]);
19
20 % iterate over the last 'nModelOutputs' rows in 'evalResults', retrieve the
21 % parameter set, re-run the model structure, and store the model output
22 for k = nRows+(-nModelOutputs+1:1:0)
23
24     % retrieve the k-th parameter set
25     parVec = evalResults(k,conf.parCols);
26
27     % % re-run the model with the k-th parameter set
28     modelOutput = lintank(conf,constants,init,parVec,conf.priorTimes);
29
30     % store the first row of the model output
31     allModelOutputs(k+nModelOutputs-nRows,1:conf.nPrior) = modelOutput(1,:);
32
33 end
34 % calculate the 2.5, 50, and 97.5 percent parameter uncertainty percentiles
35 % using MMSODA's 'mmsodaPrctile' function:
36 percentiles = mmsodaPrctile(allModelOutputs,[2.5,50,97.5]);
37
38 % retrieve a list of unique parameter combinations that have the best
39 % objective scores using MMSODA's 'mmsodaBestParsets' function
40 bestsets = mmsodaBestParsets(conf,evalResults,'unique');
41
42 % pre-allocate the array that holds the model outputs associated with the
43 % best objective scores
44 bestModelOutputs = repmat(NaN,[size(bestsets,1),conf.nPrior]);
45
46 % use the same principle as before to iterate over the rows in the list of
47 % best parameter sets, re-run the model, and store the output
48 for k = 1:size(bestsets,1)
49
50     parVec = bestsets(k,1:conf.nOptPars);
51     modelOutput = lintank(conf,constants,init,parVec,conf.priorTimes);
52     bestModelOutputs(k,1:conf.nPrior) = modelOutput(1,:);
53
54 end
55
56 % plot the observations along with the 2.5% parameter uncertainty
57 % percentile, the median, the 97.5% parameter uncertainty percentile, and
58 % the best model output associated with the best parameter combination
59 figure
60 h = plot(constants.obsTimes,constants.obs,'om-',...
61     conf.priorTimes,percentiles(1,1:conf.nPrior),'--k',...
62     conf.priorTimes,percentiles(2,1:conf.nPrior),'-k',...
63     conf.priorTimes,percentiles(3,1:conf.nPrior),'--k',...
64     conf.priorTimes,bestModelOutputs,'-b.');
65 xlabel('Time')
66 ylabel('State')
67 legend([h([1,2,3,5])],'obs','95% parameter uncetainty interval','median','best sim')
```

As you can see from the resulting figure, optimizing the model without allowing for the unobserved input to the upper tank can lead to biased parameter estimates—even though the best parameter set minimizes the residuals, the corresponding model output is plainly wrong. In the rest of this section, we will look at data assimilation. Data assimilation provides a way of dealing with uncertain model states (for example as a result of uncertain model forcings, initial state or model structure error). MMSODA supports two types of data assimilation: in the first, full confidence is placed on the observation, i.e. whenever the simulated time reaches a time at which an observation is available, the model state pertaining to that time (known as *prior* state or *forecast* state) is abandoned, and the value of the model state is reset to the value of the observation. In MMSODA parlance, this mode is known as the 'reset' mode. The second type of data assimilation that MMSODA supports is the 'soda' mode, which we will study in greater detail in section 4.6.

According to `mmsoda`'s documentation, the following configuration variables are required for running MMSODA in 'reset' mode when using one objective (we do not use `initMethodNOKF`, `initValuesNOKF` and `namesNOKF` since we are only interested in the model state for the moment and do not bother with any additional variables):

1. `initMethodKF`
2. `initValuesKF`
3. `modeStr`
4. `modelName`
5. `objCallStr`
6. `obsState`
7. `parNames`
8. `parSpaceHiBound`
9. `parSpaceLoBound`
10. `priorTimes`
11. `stateNamesKF`
12. `stateSpaceHiBound`
13. `stateSpaceLoBound`

As you can see, you are already familiar with most of these, but there are a few new ones as well. `initMethodKF` and `initValuesKF` always go together. Their purpose is to initialize the correct initial values to those state variables which are subject to state updating. For our case, that means that `initMethodKF` must be set to `'reference'` (this is currently the only supported method), and that `initValuesKF` must be set to `30.0` (the initial value of the `state1` variable). This implies that `state1Init` no longer needs to be part of the model constants, and that `state1` no longer needs to be initialized by assigning `state1Init` to `state1` in 'lintank.m'.

Configuration variable `obsState` is used to tell MMSODA what the observed values of the state are for every time in `priorTimes`. For our case, that means that `obsState` must be assigned the values from variable `obs` from './data/lintank-unobserved-input.mat'.

You also have to indicate which model variables you want to be part of the Ensemble Kalman Filter scheme (Note that we are using the simplest scheme here, i.e. the 'reset' scheme). This is done through the `stateNamesKF` variable, which is simply a list of variable names as they are used in the model. We only have one variable, so you need to set `stateNamesKF` to `{'state1'}`.

Finally, you need to specify the limits on the state space, i.e. for each state, you define what the maximum and minimum values are, using `stateSpaceHiBound` and `stateSpaceLoBound`, respectively. For this data set, reasonable values are 40.0 and 0.0, respectively.

▶ 84. Make the necessary changes to 'makeconf.m', 'makeconstants.m', and 'lintank.m'. Start the 'reset' mode optimization from the command line like you did before. MMSODA will most likely not run just yet; a couple of things need to be resolved first. Interpret the error messages and make the required changes until MMSODA will start without any errors. TIP: One particularly tricky thing is that when running in 'scemua' mode, you can have the model return as many outputs as you like, but in 'reset' and 'soda' modes, you need to adhere to a strictly enforced format. See the documentation of 'the dynamic model' mentioned earlier.

▶ 85. Once the optimization completes after 7000 model evaluations, use 'calcUncertaintyIntervals.m' to visualize the parameter uncertainty (but change the name of the *.mat file from 'scemua-so-results.mat' to 'reset-so-results.mat' and change the value of `init = []` to `init = 30`, the initial value of the first state). If the result is not quite what you hoped it would be; don't worry, this is just because 'calcUncertaintyIntervals.m' does not reset the values of the prior states when constructing the uncertainty intervals. Luckily, there is an easy way around this problem.

▶ 86. Read the description of the `saveEnKFResults` and `startFromUniform` configuration variables in `mmsoda`'s documentation.

▶ 87. Change 'makeconf.m' such that it will evaluate an additional 500 parameter combinations. Make sure to set `startFromUniform` to `false` (we want to resume the previous run) and set `saveEnKFResults` to `true`, to be able to plot uncertainty intervals for the prior state values later on. Re-run 'makeconf.m' and start the optimization as usual.

▶ 88. When the additional 500 parameter sets have been evaluated, verify that you have a bunch of new files in the './results' directory, whose names are formatted like 'reset-so-results-enkf-evals-Z-Z.mat', with Z representing an integer number.

▶ 89. Read the documentation on `mmsodaPlotEnsemble`. Make a new figure using `mmsodaSubplotScreen(2,2,1)` and visualize the prior state values associated with the last parameter combination.

▶ 90. Once that works, try to visualize the last 20 parameter sets using `mmsodaPlotEnsemble`'s optional parameters.

As you can see, there are quite a few parameter combinations that do not result in a very good fit. It would seem then that the uncertainty intervals associated with these model outputs are quite large. This is not the case, though; it is simply because the default behavior for `mmsodaPlotEnsemble` is to include all model outputs in the figure, regardless of whether they were accepted or rejected by the Metropolis part of MMSODA. If you want to view only the model outputs that were accepted by the Metropolis part of MMSODA, you should use `mmsodaPlotEnsemble`'s `'replaceRejected'` optional parameter.

▶ 91. Make a new figure using `mmsodaSubplotScreen(2,2,2)`. Visualize the same selection of parameter combinations as you did previously, but this time, let `mmsodaPlotEnsemble` replace the rejected outputs with model outputs that were accepted. Note that the model evaluation number in the figure's title is no longer simply `[7481:7500]` but instead shows

the model evaluation numbers that replaced the Metropolis-rejected ones.

▶ 92. Make a new figure using `mmsodaSubplotScreen(2,1,2)`. Use `mmsodaMatrixOfScatter` to plot the evaluation number on the x-axis against the parameter value on the y-axis for the last part of the record (see optional parameter `'nHistory'`). Use the resulting figure to verify that `mmsodaPlotEnsemble` replaced the correct model outputs.

Now that we have some idea about what sort of model outputs are probable, let's calculate the 95% parameter uncertainty intervals. MMSODA comes prepackaged with a function that retrieves the correct model outputs from the relevant files in './results' and that calculates time series of arbitrary percentiles, while taking into account the intermediate state updating that has been performed by MMSODA.

▶ 93. Read the MMSODA documentation on `mmsodaCalcUncertInts` and use it to calculate the 2.5%, 50% and 97.5% percentiles. The code snippet in Listing 4.7 may serve as an example of how `mmsodaCalcUncertInts`'s result may be used, while Fig. 4.9 shows what the result looks like.

Listing 4.7: MATLAB code snippet for visualizing parameter uncertainty intervals for the lintank model. A copy of this script has been included as 'esibayes-master/manual/other/patch_uncertainty_snippet.m'.

```
1  % load variables 'conf','evalResults', 'sequences', and 'metropolisRejects'
2  % from the reset-mode optimization results:
3  load('./results/reset-so-results.mat','conf','evalResults',...
4      'sequences','metropolisRejects')
5
6  % load the observations from file:
7  constants = load('./data/constants');
8
9  % define the percentiles:
10 prc = [2.5,50,97.5];
11
12 % define the number of model outputs to include in the construction of the
13 % parameter uncertainty intervals:
14 nIntervals = 250;
15
16 % count the number of rows in 'evalResults':
17 nRows = size(evalResults,1);
18
19 % calculate the evaluation numbers of the parameter combinations whose
20 % associated output are used in constructing the uncertainty intervals:
21 evalNumbers = nRows + (-nIntervals+1:1:0);
22
23 % use the 'mmsodaCalcUncertInts' function to retrieve the correct
24 % data and to calculate precentiles:
25 [x,y] = mmsodaCalcUncertInts(conf,evalResults,metropolisRejects,prc,evalNumbers);
26
27 % compose the x and y data for the patch object:
28 xp = [x(1,2:2*conf.nPrior),fliplr(x(1,2:2*conf.nPrior)),x(1,2)];
29 yp = [y(1,2:2*conf.nPrior),fliplr(y(3,2:2*conf.nPrior)),y(1,2)];
30
31 % make the figure:
32 mmsodaSubplotScreen(2,2,2)
33 clf
34 h1 = patch(xp,yp,'k');
35 hold on
36 h2 = plot(x,y(2,:),'-k');
37 h3 = plot(constants.obsTimes,constants.obs,'sm');
38 set(h1,'facecolor',0.5*[1,1,1],'edgecolor',0.5*[1,1,1])
39 set(h3,'markerfacecolor','none','markersize',8)
40 xlabel('Time')
```

```
41    ylabel('State')
42    box on
43    legend([h1,h2,h3],'95% parameter uncertainty interval','median','obs')
```
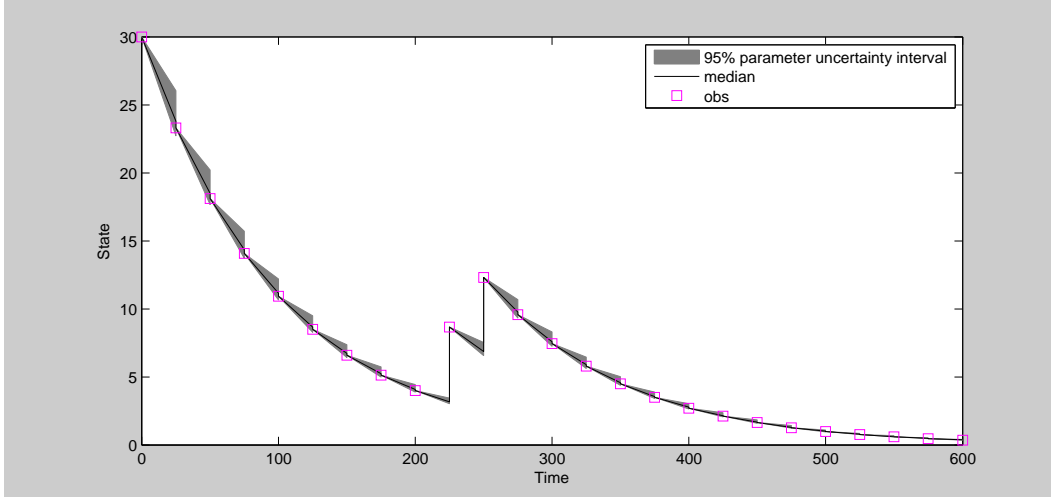

Figure 4.9: Result of running the code from Listing 4.7.

4.6   MMSODA in 'soda' mode; sequential execution

▶ 94. On your local machine, copy the 'example3' directory to a new directory, 'example4'. Clean up the './results' subdirectory, and remove any old files pertaining to 'example3'.

The 'soda' mode is the most complex and most compute-intensive mode. It is similar to the 'reset' mode in that it updates the model states during the simulation. The way the updating is performed, however, is different. The difference between 'scemua', 'reset', and 'soda' modes essentially comes down to how much confidence is placed on the observed values of the state in comparison to how much confidence is placed on the simulated values of the state. For example, in 'scemua' mode, all of the confidence is placed on the simulated values—the model can be run from the time of the initial state (`conf.priorTimes(1)`) to the time at which the last prediction is required (`conf.priorTimes(end)`), without the need for temporarily halting the model at `conf.priorTimes(2:end-1)` to do any state updating. In contrast to this, the 'reset' mode places full condidence on the observations: at the times when an observation is available, the model is temporarily halted, and its states are reset to the value of the observed state. The 'soda' mode then, provides sort of a middle ground between MMSODA's 'scemua' and 'reset' modes: instead of placing all of the confidence on one or the other, a little confidence is placed on both the simulated and the observed value of the states. A weighted average of the two is then calculated, and the simulated state (i.e. the prior state) is adjusted in the direction of the observed state. The magnitude of the adjustment is sometimes referred to as the 'state *innovation*' or simply 'state *update*'. Adding the state update to the prior state results in a new state value, which is known as the '*posterior* state' or the '*analysis* state'.

In terms of setup, the 'soda' mode is not so different from the 'reset' mode that you are familiar with. In fact, a quick look at the table of configuration variables in `mmsoda`'s documentation reveals that only 3 additional configuration variables are needed: `covObsPert`, `covModelPert`, and `nMembers`.

▶ 95. Read the description in `mmsoda`'s documentation for these three options.

▶ 96. Include `covObsPert`, `covModelPert`, and `nMembers` in your 'makeconf.m', and assign them values of `0.02`, `0.10` and `10`, respectively. Don't forget to change `modeStr` to `'soda'`, otherwise MMSODA will overwrite the values of `covObsPert` and `covModelPert` with `0`. Set `nModelEvalsMax` to 150 for now, re-run 'makeconf.m', and verify that './results/conf.mat' was indeed written.

▶ 97. Re-read the documentation on the objective function (see Figure 4.6), in particular the description of the input argument `modelOutput`, which is 3-D if `modeStr` is `'soda'`.

▶ 98. Adapt the objective function such that the SSR is calculated based on the ensemble-member mean of the prior state. Note: calculating the mean over the 3$^{\rm rd}$ dimension of an N-dimensional array `X` in MATLAB is easily achieved by `mu = mean(X,3)`.

▶ 99. Test your configuration locally until it works. Then set `nModelEvals` to 7000 and re-run 'makeconf.m'.

▶ 100. Call `mmsodaPrepParallelFiles` to write the jobscript and the Makefile.

▶ 101. Copy your 'example4' working directory to the cluster.

4.7 MMSODA in 'soda' mode; parallel execution

▶ 102. Use PuTTY to set up an SSH connection to the LISA cluster. Make sure the necessary modules are loaded before compiling the binary. Submit your jobscript to the queue and wait for the optimization to finish.

▶ 103. Once the job finishes, edit 'makeconf.m' on your local machine by setting `saveEnKFResults` to `true` and `startFromUniform` to `false`. Increase the maximum number of model evaluations by `500`. Run `makeconf` and copy the new MMSODA configuration to the remote system. Submit the jobscript to the queue once more, and wait for the results.

▶ 104. Copy the optimization results back to your local machine.

▶ 105. Copy the code snippet from Listing 4.7 to your working directory. Adapt the filename from which the optimization results are read, and run the snippet on the results of the 'soda' mode optimization. The result should look like Fig. 4.10.
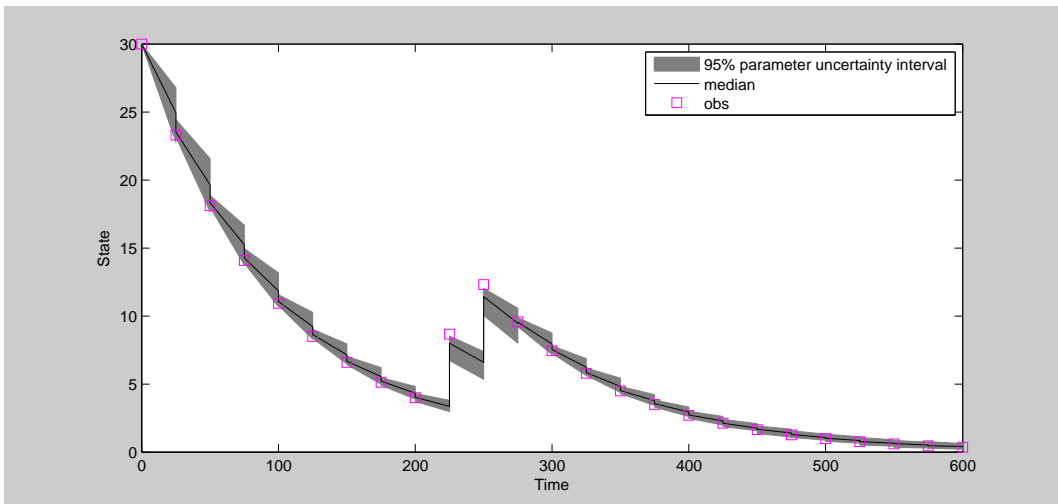
Figure 4.10: Parameter uncertainty intervals for the 'soda' mode optimization of the lintank model.

Appendices

Appendix A

Remote graphical applications

Up to this point, we've issued commands through the terminal. The terminal is a powerful tool, but sometimes it's also useful to run graphical programs (as opposed to text-based terminal programs) remotely, for example when you want to use the graphical debugging capabilities that the MATLAB GUI offers to debug some of your code on LISA, or if you want to view remotely generated MATLAB figures. Amazingly, this is possible through a process called *X forwarding over SSH*. Here, 'X' refers to the program that takes care of visualization on Linux. The Linux operating system is telling X what to visualize, and then X figures out which pixels on what screen should be what color, and whether a particular pixel is part of, say, a button, drop-down list, or some other user interface element. It is possible to re-route messages to the X system through your SSH connection, such that they end up on your local machine. If your local system is Linux, the X messages that your system receives can be interpreted by your local copy of the X program, and the user interface of a graphical application that is running on the remote machine will be displayed locally. However, you are probably running Windows, so you need to install a Windows version of X first.

Download Xming from http://sourceforge.net/projects/xming/files/Xming/6.9.0. 31/Xming-6-9-0-31-setup.exe/download and install it. Now go to the Windows start menu and click XLaunch (Fig. A.1). This will bring up a wizard (Fig. A.2). Follow the steps outlined in Figs. A.3–A.5.
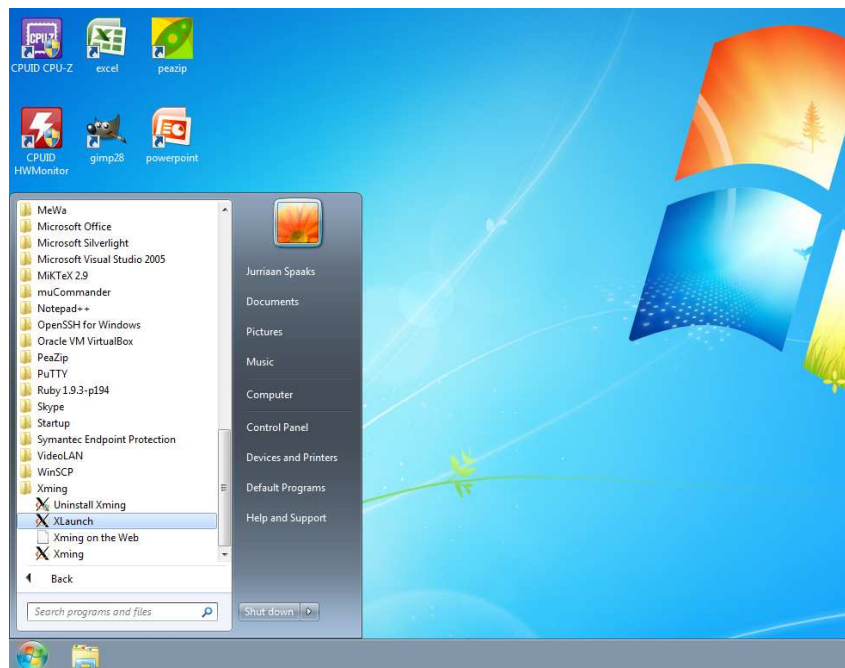
Figure A.1: Starting XLaunch from the Windows 7 start menu.
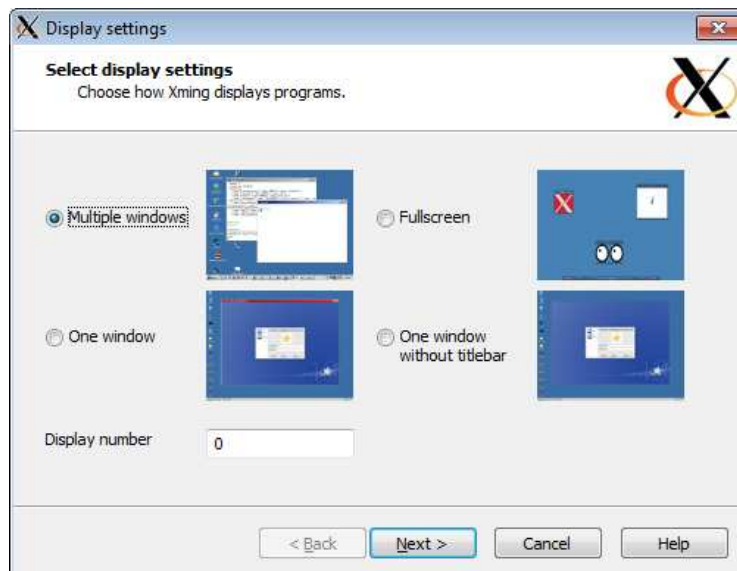
Figure A.2: The XLaunch configuration wizard page 1.
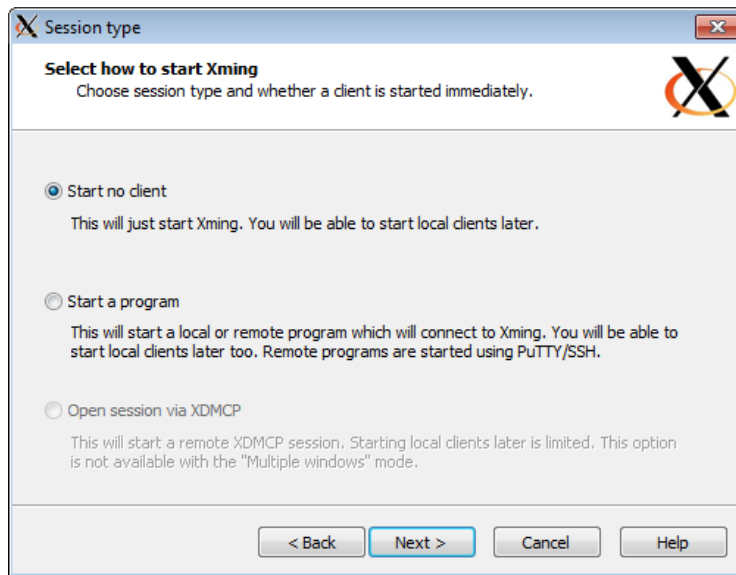
Figure A.3: The XLaunch configuration wizard page 2.
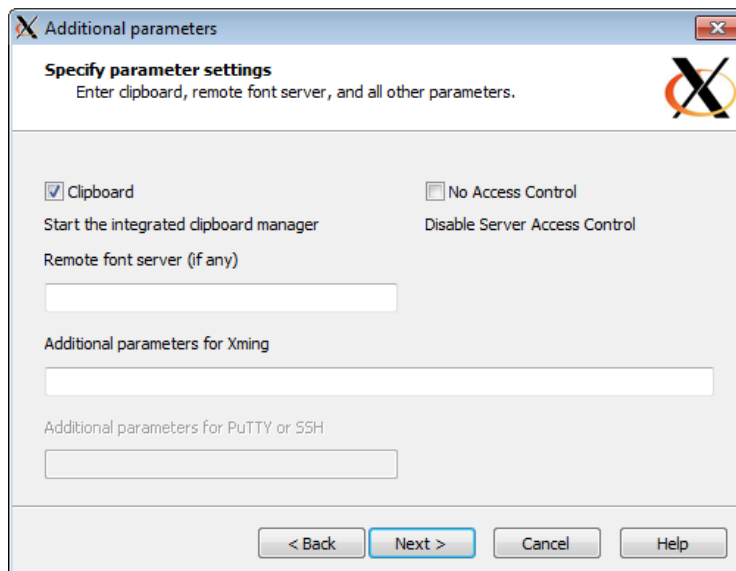
Figure A.4: The XLaunch configuration wizard page 3.
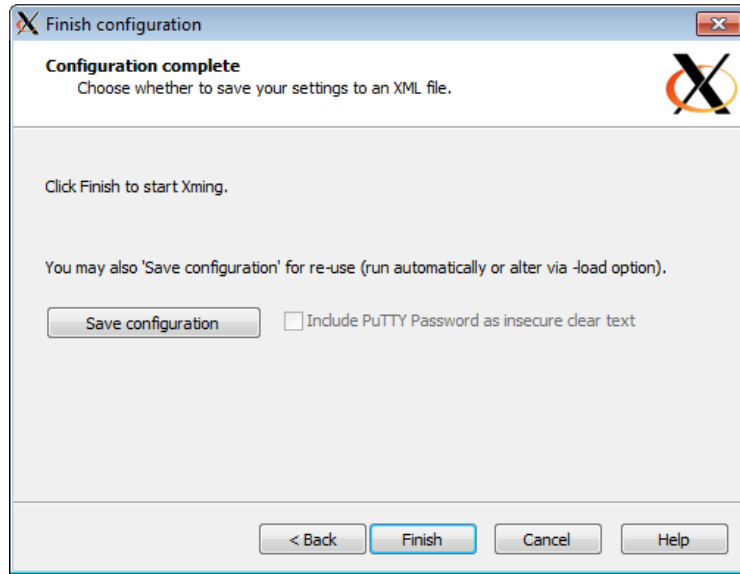
Figure A.5: The XLaunch configuration wizard page 4.

After you go through the XLaunch wizard, there should be an X icon in your icon tray.

Now that we have an X server for Windows running locally, we still need to tell the remote system that we want it to route its X messages through the SSH connection to our local system. For this, you need to start a new SSH connection. Start PuTTY, and type in the 'lisa.surfsara.nl' host name, exactly as before (recall Fig. 2.4). However, before clicking the 'Open' button, expand the plus sign symbol for 'SSH' in the bottom part of the left pane (see Fig. A.6). Find the item labeled 'X11' (X is sometimes referred to as 'X11'), and in the right pane, enable the checkbox that says 'Enable X11 forwarding' before clicking the 'Open' button.

At the prompt, you can quickly test whether the remote system is connected to your local X server by typing:

```
jspaaks@login2:~$ echo $DISPLAY
```

which should result in a message like this (the numbers could be different):

```
localhost:10.0
```

If the connection was unsuccessful, the shell returns an empty message.

Start Octave in silent mode by:

```
jspaaks@login2:~$ octave --silent
octave:1>
```

and then run the `peaks(30)` function.

```
octave:1> peaks(30)
octave:2>
```

After a few moments (depending on the bandwidth of your connection to LISA), it will show you Fig. A.7.
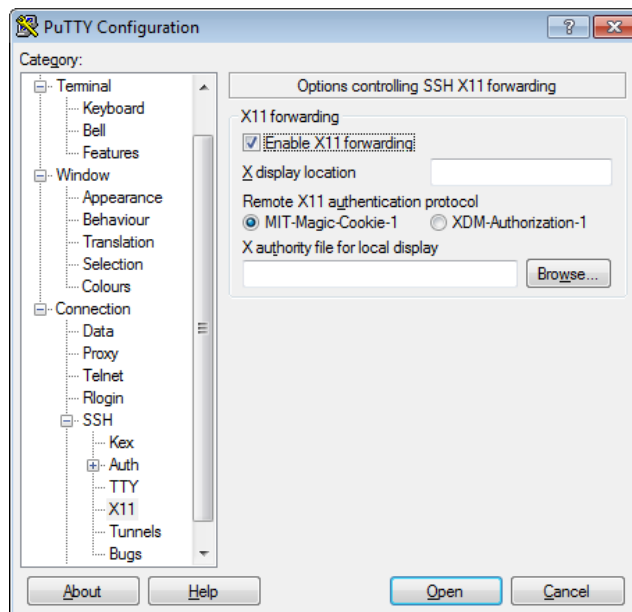
Figure A.6: Configure PuTTY for X forwarding over SSH.
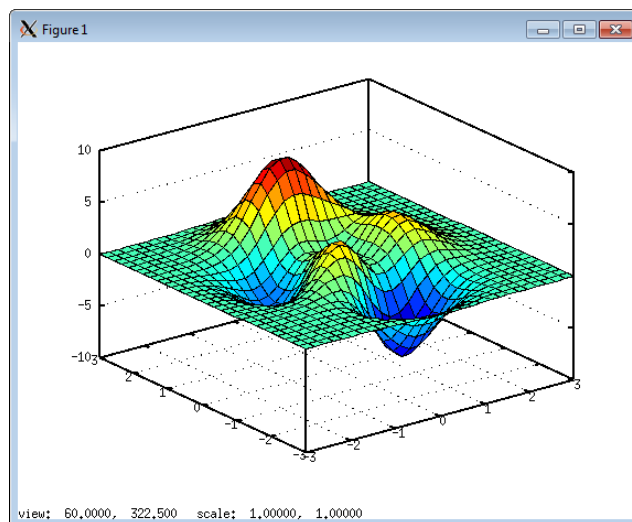
Figure A.7: After Octave generated this `peaks(30)` figure remotely, the remote system sent it to the local machine over SSH where it was displayed with Xming.

Let's see if we can do the same thing in MATLAB:

```
octave:2> exit

jspaaks@login2:~$ matlab
-bash: matlab: command not found
```

The reason this does not work is that MATLAB is only used by some users, therefore it is

not available by default[1]. However, it's easy enough to make MATLAB available, like so:

```
jspaaks@login2:~$ module load matlab
jspaaks@login2:~$ matlab
```

It is considered good practice to `unload` MATLAB once you are done with it:

```
jspaaks@login2:~$ module unload matlab
```

This frees up one of the MATLAB licenses, such that other users may use it. There are currently enough MATLAB licenses to run 32 instances of MATLAB simultaneously; however, some of the toolboxes require a separate license. For some toolboxes there are only 3 licenses available, so if your program happens to use one of those, you can only use 3 MATLAB instances simultaneously.

If you are just using the MATLAB licenses to run your programs on LISA, as opposed to doing development work, you can (legally) circumvent licensing problems by compiling your m-code, and running the compiled code with the *MATLAB Compiler Runtime* or *MCR*. The MCR can be loaded in a similar fashion as the full MATLAB suite:

```
jspaaks@login2:~$ module load mcr
```
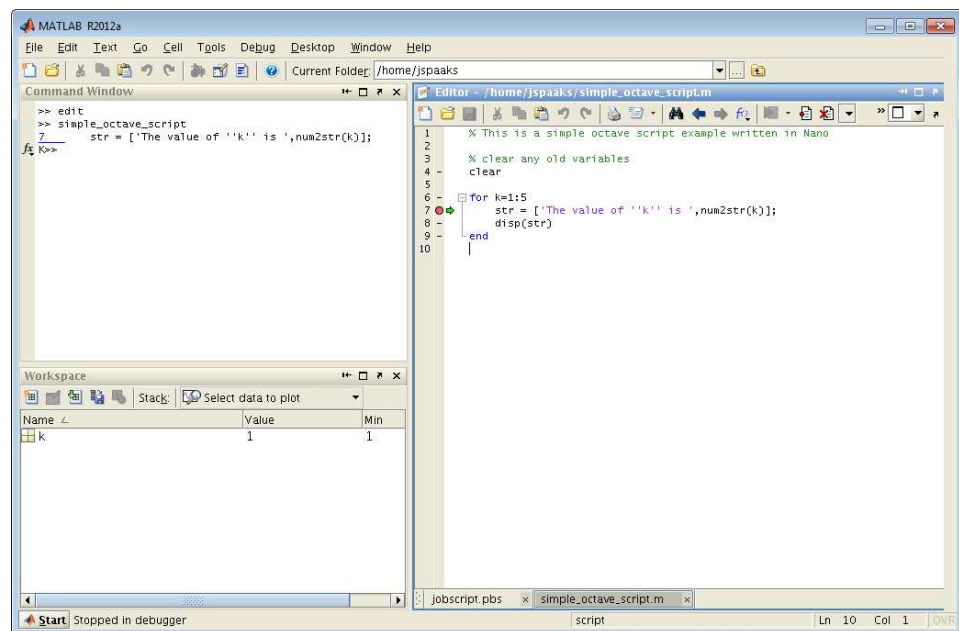

Figure A.8: Even MATLAB's debugging capabilities can be used remotely!

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[1]In fact, you must be a member of the 'MATLAB users group' that exist on LISA. Any of LISA's administrators can add you to this group, but it usually involves some administration.

Appendix B

Likelihoods in optimization

B.1 Definition of the system

The discrete-time state-space formulation of a nonlinear dynamic system is[1]:

$$x_{t+1} = f(x_t, u_t, \boldsymbol{\theta}) \tag{B.1}$$

$$y_{t+1} = h(x_{t+1}, \boldsymbol{\phi}) \tag{B.2}$$

To keep notation as simple as possible, we consider a system in which the state, the forcing and the output at any given time can be represented as scalars. Further note that the 'state' of the system at a given time can include history. Since it is generally impossible to observe the true state, the true forcing, and the true output of a system, we have to make do with the observed state, observed forcing, and the observed output instead:

$$\tilde{x}_{t+1} = x_{t+1} + \omega_{t+1} \tag{B.3}$$

$$\tilde{u}_{t+1} = u_{t+1} + \psi_{t+1} \tag{B.4}$$

$$\tilde{y}_{t+1} = y_{t+1} + \nu_{t+1} \tag{B.5}$$

Note that Eqs. B.3–B.5 assume that the dimensionality of x_{t+1}, u_{t+1} and y_{t+1} is the same as their observed counterparts, and that they do indeed represent the same entities (in other words, there is no *incommensurability*). Furthermore, we do not know the mechanism by which x_t leads to x_{t+1} in Eq. B.1, so instead we propose a mechanism $\hat{f}(\cdot)$; similarly we do not know how x_{t+1} leads to y_{t+1} in Eq. B.2, so we propose $\hat{h}(\cdot)$. Typically, $\hat{f}(\cdot)$ and $\hat{h}(\cdot)$ are part of the same computer model structure. Because of philosophical reasons (e.g. Popper, 2009), it is impossible to prove that $\hat{f}(\cdot)$ and $\hat{h}(\cdot)$ are in fact the correct functions $f(\cdot)$ and

---

[1]Refer to Appendix C for the meaning of the symbols used in this Chapter.

$h(\cdot)$—instead, we can only subject $\hat{f}(\cdot)$ and $\hat{h}(\cdot)$ to increasingly difficult tests, and if $\hat{f}(\cdot)$ and $\hat{h}(\cdot)$ are not falsified by these tests, then the confidence in the correctness of $\hat{f}(\cdot)$ and $\hat{h}(\cdot)$ increases.

B.2 Constructing a likelihood for a simple error model

The probability of sampling a value x from a normal distribution is calculated with:

$$p(x \mid \mu, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2} \tag{B.6}$$

Within the context of calibration, this is equivalent to:

$$p(\hat{x} \mid \tilde{x}, \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{1}{2}\left(\frac{\hat{x}-\tilde{x}}{\sigma}\right)^2} \tag{B.7}$$

Note that this assumes that the true mean of the distribution can be observed, i.e. $\tilde{x} = \mu$.

For the case where we have not just 1 observation, but instead have a time series of n_o observations, the probability $p(\hat{\mathbf{x}} \mid \tilde{\mathbf{x}}, \boldsymbol{\sigma})$ is calculated as the product of all individual probabilities[1]:

$$p(\hat{\mathbf{x}} \mid \tilde{\mathbf{x}}, \sigma) = \prod_{t=1}^{n_o} \frac{1}{\sqrt{2\pi\sigma^2}}\, e^{-\frac{1}{2}\left(\frac{\hat{x}_t-\tilde{x}_t}{\sigma}\right)^2} \tag{B.8}$$

Note that the multiplication of individual probabilities in Eq. B.7 reflects the implicit assumption that the errors are independent—an assumption that is often violated.

Since $\frac{1}{\sqrt{2\pi\sigma^2}}$ is constant for homoscedastic problems, Eq. B.7 can be rearranged as follows:

$$p(\hat{\mathbf{x}} \mid \tilde{\mathbf{x}}, \sigma) = \left[\frac{1}{\sqrt{2\pi\sigma^2}}\right]^{n_o} \cdot \prod_{t=1}^{n_o} e^{-\frac{1}{2}\left(\frac{\hat{x}_t-\tilde{x}_t}{\sigma}\right)^2} \tag{B.9}$$

and since:

$$\left[\frac{1}{\sqrt{2\pi\sigma^2}}\right]^{n_o} = \left[\sqrt{2\pi\sigma^2}\right]^{-n_o}$$

---

[1]Note that this can be extended to deal with non-constant variance (*heteroscedasticity*) by making σ into a vector $\boldsymbol{\sigma}$:

$$p(\hat{\mathbf{x}} \mid \tilde{\mathbf{x}}, \boldsymbol{\sigma}) = \prod_{t=1}^{n_o} \frac{1}{\sqrt{2\pi\sigma_t^2}}\, e^{-\frac{1}{2}\left(\frac{\hat{x}_t-\tilde{x}_t}{\sigma_t}\right)^2}$$

Eq. B.9 can be rewritten as:

$$p\left(\hat{\mathbf{x}}\,|\,\tilde{\mathbf{x}},\sigma\right) = \left[\sqrt{2\pi\sigma^2}\right]^{-n_o} \cdot \prod_{t=1}^{n_o} e^{-\frac{1}{2}\left(\frac{\hat{x}_t - \tilde{x}_t}{\sigma}\right)^2} \tag{B.10}$$

Furthermore,

$$e^a \cdot e^b = e^{a+b} \tag{B.11}$$

so Eq. B.10 may be written as:

$$p\left(\hat{\mathbf{x}}\,|\,\tilde{\mathbf{x}},\sigma\right) = \left[\sqrt{2\pi\sigma^2}\right]^{-n_o} \cdot e^{-\frac{1}{2}\sum_{t=1}^{n_o}\left(\frac{\hat{x}_t - \tilde{x}_t}{\sigma}\right)^2} \tag{B.12}$$

The probability density in Eq. B.12 is related to the *log-likelihood* according to[1]:

$$\ell\left(\hat{\mathbf{x}}\,|\,\tilde{\mathbf{x}},\sigma\right) = \ln\left(p\left(\hat{\mathbf{x}}\,|\,\tilde{\mathbf{x}},\sigma\right)\right) \tag{B.13}$$

$$= \ln\left(\left[\sqrt{2\pi\sigma^2}\right]^{-n_o} \cdot e^{-\frac{1}{2}\sum_{t=1}^{n_o}\left(\frac{\hat{x}_t - \tilde{x}_t}{\sigma}\right)^2}\right) \tag{B.14}$$

and since:

$$\ln\left(a \cdot b\right) = \ln\left(a\right) + \ln\left(b\right), \tag{B.15}$$

$$\ln\left(a^b\right) = b \cdot \ln\left(a\right), \tag{B.16}$$

$$\ln\left(e^a\right) = a, \tag{B.17}$$

Eq. B.13 can be rewritten as:

$$\ell\left(\hat{\mathbf{x}}\,|\,\tilde{\mathbf{x}},\sigma\right) = -n_o \cdot \ln\left[\sqrt{2\pi\sigma^2}\right] + \left[-\frac{1}{2}\sum_{t=1}^{n_o}\left(\frac{\hat{x}_t - \tilde{x}_t}{\sigma}\right)^2\right] \tag{B.18}$$

Subsequently applying Eqs. B.16 and B.15, Eq. B.18 can be rewritten as:

$$\ell\left(\hat{\mathbf{x}}\,|\,\tilde{\mathbf{x}},\sigma\right) = -\frac{1}{2}n_o \cdot \ln\left(2\pi\right) - \frac{1}{2}n_o \cdot \ln\left(\sigma^2\right) - \frac{1}{2}\sum_{t=1}^{n_o}\left(\frac{\hat{x}_t - \tilde{x}_t}{\sigma}\right)^2 \tag{B.19}$$

to yield the Gaussian log-likelihood function with unknown standard deviation σ of the residuals $\hat{x}_t - \tilde{x}_y$. It is convenient to rewrite Eq. B.19 as follows:

$$\ell\left(\hat{\mathbf{x}}\,|\,\tilde{\mathbf{x}},\sigma\right) = -\frac{1}{2}n_o \cdot \ln\left(2\pi\right) - \frac{1}{2}n_o \cdot \ln\left(\sigma^2\right) - \frac{1}{2}\sum_{t=1}^{n_o}\frac{\left(\hat{x}_t - \tilde{x}_t\right)^2}{\sigma^2} \tag{B.20}$$

For many measuring devices, σ^2 is either known or can be determined by simple experiments.

---

[1] Note that $\hat{\mathbf{x}}$ in Eq. B.13 is only dependent on the parameter vector $\boldsymbol{\theta}$, while the observations $\tilde{\mathbf{x}}$ and σ are given. When a probability is a function of the parameter value, 'likelihood' is preferred over 'probability'.

If necessary, σ^2 can also be estimated from the observations according to[2]:

$$s^2 = \frac{1}{n_o - 1} \sum_{t=1}^{n_o} (\hat{x}_t - \tilde{x}_t)^2 \tag{B.21}$$

Replacing σ^2 with s^2 in Eq. B.22 yields:

$$\ell(\hat{\mathbf{x}} \,|\, \tilde{\mathbf{x}}) = -\frac{1}{2} n_o \cdot \ln(2\pi) - \frac{1}{2} n_o \cdot \ln(s^2) - \frac{1}{2} \sum_{t=1}^{n_o} \frac{(\hat{x}_t - \tilde{x}_t)^2}{s^2} \tag{B.22}$$

which is equal to:

$$\ell(\hat{\mathbf{x}} \,|\, \tilde{\mathbf{x}}) = -\frac{1}{2} n_o \cdot \ln(2\pi) - \frac{1}{2} n_o \cdot \ln\left(\frac{1}{n_o - 1} \sum_{t=1}^{n_o} (\hat{x}_t - \tilde{x}_t)^2 \right) - \frac{1}{2} \frac{\sum_{t=1}^{n_o} (\hat{x}_t - \tilde{x}_t)^2}{\frac{1}{n_o - 1} \sum_{t=1}^{n_o} (\hat{x}_t - \tilde{x}_t)^2} \tag{B.23}$$

Simplification of the last term in Eq. B.23 yields:

$$\ell(\hat{\mathbf{x}} \,|\, \tilde{\mathbf{x}}) = -\frac{1}{2} n_o \cdot \ln(2\pi) - \frac{1}{2} n_o \cdot \ln\left(\frac{1}{n_o - 1} \sum_{t=1}^{n_o} (\hat{x}_t - \tilde{x}_t)^2 \right) - \frac{1}{2} (n_o - 1) \tag{B.24}$$

Application of Eq. B.15 to the second term in Eq. B.24 yields:

$$-\frac{1}{2} n_o \cdot \ln\left(\frac{1}{n_o - 1} \sum_{t=1}^{n_o} (\hat{x}_t - \tilde{x}_t)^2 \right) = -\frac{1}{2} n_o \cdot \ln\left(\frac{1}{n_o - 1} \right) - \frac{1}{2} n_o \cdot \ln\left(\sum_{t=1}^{n_o} (\hat{x}_t - \tilde{x}_t)^2 \right) \tag{B.25}$$

and since

$$\ln\left(\frac{a}{b} \right) = \ln(a) - \ln(b) \tag{B.26}$$

and

$$\ln(1) = 0, \tag{B.27}$$

Eq. B.25 thus becomes:

$$-\frac{1}{2} n_o \cdot \ln\left(\frac{1}{n_o - 1} \sum_{t=1}^{n_o} (\hat{x}_t - \tilde{x}_t)^2 \right) = +\frac{1}{2} n_o \cdot \ln(n_o - 1) - \frac{1}{2} n_o \cdot \ln\left(\sum_{t=1}^{n_o} (\hat{x}_t - \tilde{x}_t)^2 \right) \tag{B.28}$$

Filling Eq. B.28 back into Eq. B.24 yields:

$$\ell(\hat{\mathbf{x}} \,|\, \tilde{\mathbf{x}}) = -\frac{1}{2} n_o \cdot \ln(2\pi) + \frac{1}{2} n_o \cdot \ln(n_o - 1) - \frac{1}{2} n_o \cdot \ln\left(\sum_{t=1}^{n_o} (\hat{x}_t - \tilde{x}_t)^2 \right) - \frac{1}{2} (n_o - 1) \tag{B.29}$$

---

[2]This implicitly assumes that parameter uncertainty is the only source of uncertainty.

For a given number of observations n_o, terms 1, 2, and 4 from Eq. B.29 may be collected into a constant C as follows:

$$\ell \left(\hat{\mathbf{x}} \,|\, \tilde{\mathbf{x}} \right) = -\frac{1}{2} n_o \cdot \ln \left(\sum_{t=1}^{n_o} (\hat{x}_t - \tilde{x}_t)^2 \right) + C \tag{B.30}$$

with

$$C = -\frac{1}{2} n_o \cdot \ln (2\pi) + \frac{1}{2} n_o \cdot \ln (n_o - 1) - \frac{1}{2} (n_o - 1) \tag{B.31}$$

When constructing log likelihood functions for MMSODA, we may safely leave out the C term. This is because MMSODA uses the Metropolis algorithm to determine whether a new sample of the parameter space should be accepted or rejected. Whether a new sample is accepted depends on how its likelihood ℓ_{new} compares to the likelihood associated with a previous sample ℓ_{prev}. A sample is accepted if

$$\ell_{new} - \ell_{prev} \;>\; \ln(z) \tag{B.32}$$

with z a draw from a uniform distribution between 0 and 1:

$$z \;\sim\; U(0,1) \tag{B.33}$$

In other words, if ℓ_{new} is an improvement relative to ℓ_{prev}, the new point is always accepted; if ℓ_{new} is slightly worse than ℓ_{prev}, it is still quite likely that the new point will be accepted; if ℓ_{new} is much worse than ℓ_{prev} it is unlikely, but not impossible, that the new point will be accepted.

Since raising both ℓ_{new} and ℓ_{prev} by the constant C has no effect on the distance $\ell_{new} - \ell_{prev}$, C may be left out of the objective function entirely.

Appendix C

Definition of terms

Table C.1: Definition of terms.

e^x	Euler's e raised to the power x, or in MATLAB syntax `exp(x)`
$\ln(x)$	natural logarithm of a variable x, or in MATLAB syntax `log(x)`
$f(\cdot)$	true state operator (nonlinear function)
$\hat{f}(\cdot)$	supposed state operator (nonlinear function)
$h(\cdot)$	true measurement operator (nonlinear function)
$\hat{h}(\cdot)$	supposed measurement operator (nonlinear function)
$\boldsymbol{\theta}$	true parameter values pertaining to the state operator
$\hat{\boldsymbol{\theta}}$	estimate of the parameter values pertaining to the state operator
$\boldsymbol{\phi}$	true parameter values pertaining to the measurement operator
σ	standard deviation of the normal distribution
μ	mean of the normal distribution
ν_{t+1}	random perturbation of the true output at time t
ψ_{t+1}	random perturbation of the true forcing at time t
ω_{t+1}	random perturbation of the true state at time t
u_t	true forcing at time t
$\tilde{u}_t$	observed forcing at time t
x_t	true state at time t
$\tilde{x}_t$	observed state at time t

Table C.1: Definition of terms (continued).

$\hat{x}_t$ predicted state at time t

y_t true output at time t

$\tilde{y}_t$ observed output at time t

$\hat{y}_t$ predicted output at time t

ε observation-prediction residual vector

$\mathcal{N}(\mu, \sigma^2)$ normal probability distribution with mean μ and variance σ^2

$\ell(\cdot)$ log likelihood

s^2 estimator of variance σ^2

n_o number of observations in the vector $\tilde{\mathbf{x}}$

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