TH LFNS toolbox, as well as examples and this very tutorial can be found on github, it can be downloaded using

git clone https://github.com/Mijan/LFNS.git

This allows in particular to use

git pull

to get all latest versions and updates.

1 Installation

The first exercise is to get the LFNS toolbox ready to be used. This can be done in one of the following three ways:

1.1 Install the toolbox on a Unix-based system

The most straight forward way to use the toolbox is to install it using cmake. On Linux systems (and for the most part Mac systems) this can be done fairly easily by first cloning the git repository (by typing git clone https://github.com/Mijan/LFNS.git) and following the instructions on https://mijan.github.io/LFNS/.

1.2 Use LFNS in a Docker container (all system)

You can download and install Docker for any operating system and running the LFNS Docker image. For this follow the following steps:

- Download Docker from https://www.docker.com/get-started and install it using the instruction.
- Download the docker image file lfns.tar from https://polybox.ethz.ch/index.php/s/XOwXhgB10BRbY and the run script from https://polybox.ethz.ch/index.php/s/EPOkSU0Z7EhL0sJ.
- Put the lfns.tar file and the run_lfns.sh into the same folder, which we will refer to /lfns.
- Make sure the script run_lfns.sh is executable. This can be done in most OS by right clicking it and clicking a button.
- Load the docker image lfns.tar by typing docker load < lfns.tar.
- Run the docker image by running the provided script by typing sh run_lfns.sh.
 This will run the docker image in interactive mode and will mount the current folder on docker. Now you should be able to just type the lfns commands in the console. To test this you can type simulate --help. If this produces a help message, everything went well!

1.3 Install LFNS on Euler

It might be the easiest to install the LFNS toolbox on Euler and use it there.

- Log into Euler (from a console you can type ssh your-user-name@euler.ethz.ch)
- Clone the git repository by typing

```
git clone https://github.com/Mijan/LFNS.git
```

• The git repository comes with a script file to install all the required libraries and toolbox on euler. To run the script change the directory to \$HOME/LFNS/scripts and call the script euler_install_script.sh

```
cd LFNS/scripts
source euler_installation_script.sh
```

• To make sure that Euler saves the location of the installation path, open the .bashrc file in the home folder and add the following lines

```
module load open_mpi boost/1.59.0
export LD_LIBRARY_PATH=$HOME/local/lib:$HOME/local/lib64:$LD_LIBRARY_PATH
export LIBRARY_PATH=$HOME/local/lib:$HOME/local/lib64:$LIBRARY_PATH
export CPATH=$HOME/local/include:$CPATH
export PATH=$HOME/local/bin:$PATH
export CPPFLAGS="${CPPFLAGS} -I${BOOST_INCLUDEDIR}"
export LDFLAGS="-L${BOOST_LIBRARYDIR} ${LDFLAGS}"
```

• You can test if everything has worked by typing simulate --help, which should produce a help message.

2 The antithetic controller

In this exercise you will write the model files for the antithetic controller and simulate it. For information about the files see the document doc.pdf (either online or in the folder LFNS/Documentation).

2.1 Write the model files

The model reaction for the antithetic controller has 3 species z1, z2 and x1, The reactions follow mass action kinetics and the reaction are

Use the templates in the antithetic/folder and edit the files antithetic_model.txt, antithetic_initial.txt and antithetic_measurement.txt to represent the above model. As initial conditions, set all the species to 0, and for a measurement take the species x1 and add a Gaussion noise with mean 0 and standard deviation 0.1.

2.2 Write the config file

- Modify the <model> and the <Simulation> block of the file antithetic_config_file.xml to contain the relative paths of your model files and specify the parameter to be simulated to all be set to 1. Specify the model type to be deterministic <type>DET</type>
- Simulate the antithetic model by typing simulate antithetic_config_file.xml. This command should simulate the system and produce a number of output files in the same folder as the simulate antithetic_config_file.xml file.
- Take a look at the results_model_summary.txt file to make sure the simulated system is the correct one.
- You can use the script LFNS/scripts/plotSystem.m to plot the system using matlab. For this type plotSystem(results_model_summary.txt).
- Change the model type in the antithetic_config_file.xml under <type> to STOCH to simulate the system using SSA. Call the simulate command with the option -n 100 to simulate 100 SSA trajectories. Use again the plotSystem command to plot the simulation outcome.
- You can simulate the system again and play around with the option (you can see a list of them by typing simulate --help.

2.3 Add a perturbation to the antithetic model

Now modify the model files to contain a system perturbation.

• Modify the antithetic_model.txt file by adding another parameter pert that is added to the propensity of the production propensity of x1.

- Add an <inputs> block to the antithetic_config_file.xml that defines a new experiment and sets the parameter value of pert to 1 in the times between 10 and 50 minutes.
- Add an <experiments> entry to the <Simulation> block in the antithetic_config_file.xml and make sure the experiment name is the same as in the <experiments> entry in the <input> block.
- Simulate the new experiment and plot the system states.