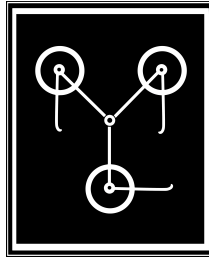


Flux Capacitor Toolkit for Systems Biology



User Manual

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CHAPTER 1

INTRODUCTION

Flux Capacitor is an open source software toolkit for systems biology and flux balance analysis. Flux Capacitor is focused on the application of FBA to study metabolism.

1.1 Toolkit Features

The toolkit includes the following features:

- FBA implementation for metabolic models in SBML format.
- Implementation of tissue specific FBA (Shlomi et al. [2008](#)).
- Flux Variability Analysis (FVA) implementation.
- Techniques to accelerate FVA calculations including parallel execution.
- Automated techniques to generate metabolic network representations.
- Metabolic network reduction methods.

1.2 Distribution Details

Flux Capacitor has been coded using C, C++, Python, R and shell scripting. Flux Capacitor is known to compile on Unix-like and Windows (using Cygwin) systems. As future work we plan to port the code to other platforms. See Section [1.4](#) section of this file if you experience problems during compilation.

It is released under the GNU Lesser General Public License (LGPL)^a.

^a<http://www.gnu.org/copyleft/lgpl.html>

1.3 Current Status

The Flux Capacitor toolkit is under development. Basic usage instructions are being added. In addition to this, there are some toolkit extensions currently in preparation:

- Incorporate interactive Python mode (currently the toolkit offers a command-line interface).
- Enable use of alternative mathematical solvers for FBA and FVA (current version only supports CPLEX).

1.4 Documentation and Support

Project documentation is being developed. Such documentation include:

- Flux Capacitor website^b.
- The Flux Capacitor manual (`flux_capacitor_manual.pdf` under the `doc` directory).
- Daniel Ortiz' MSc thesis in bioinformatics^c: the thesis explains the theoretical foundations of the functionality implemented in the toolkit and uses it to report results.
- MSc thesis slides^d: provide a summary of the above mentioned MSc thesis.

If you need additional help, you can:

- use the github issue tracker^e.
- send an e-mail to the author^f.

^b<http://daormar.github.io/flux-capacitor/>

^chttps://daormar.github.io/flux-capacitor/docsupport/dortiz_bio_msc_thesis.pdf

^dhttps://daormar.github.io/flux-capacitor/docsupport/dortiz_bio_msc_thesis_slides.pdf

^e<https://github.com/daormar/flux-capacitor/issues>

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CHAPTER 2

INSTALLATION

2.1 Basic Installation Procedure

The code of the Flux Capacitor toolkit is hosted on [github](https://github.com/daormar/flux-capacitor)^a. To install Flux Capacitor, first you need to install the autotools (autoconf, autoconf-archive, automake and libtool packages in Ubuntu). If you are planning to use Flux Capacitor on a Windows platform, you also need to install the Cygwin environment^b. Alternatively, Flux Capacitor can also be installed on Mac OS X systems using MacPorts^c.

On the other hand, Flux Capacitor can be combined with third party software so as to enable extended functionality, see more information in Section [2.2](#).

Once the autotools are available (as well as other required software such as Cygwin, MacPorts), the user can proceed with the installation of Flux Capacitor by following the next sequence of steps:

1. Obtain the package using git:

```
$ git clone https://github.com/daormar/flux-capacitor.git
```

Additionally, Flux Capacitor can be downloaded in a zip file^d.

2. `cd` to the directory containing the package's source code and type `./reconf`.
3. Type `./configure` to configure the package.
4. Type `make` to compile the package.

^a<https://github.com/daormar/flux-capacitor/>

^b<https://www.cygwin.com/>

^c<https://www.macports.org/>

^d<https://github.com/daormar/flux-capacitor/archive/master.zip>

5. Type `make install` to install the programs and any data files and documentation.
6. You can remove the program binaries and object files from the source code directory by typing `make clean`.

By default the files are installed under the `/usr/local` directory (or similar, depending of the OS you use); however, since Step 5 requires root privileges, another directory can be specified during Step 3 by typing:

```
$ configure --prefix=<absolute-installation-path>
```

For example, if `user1` wants to install the Flux Capacitor package in the directory `/home/user1/flux-capacitor`, the sequence of commands to execute should be the following:

```
$ make clean # This is recommended if the package has already been built
$ ./reconf
$ configure --prefix=/home/user1/flux-capacitor
$ make
$ make install
```

The installation process also creates three directories with additional information:

- **`${PREFIX}/share/flux-capacitor/cfg_templates`**: contains configuration files to be used with different Flux Capacitor utilities (see Chapter 3 for more details).
- **`${PREFIX}/share/flux-capacitor/doc`**: contains the documentation of Flux Capacitor, which currently consists in the Flux Capacitor manual (`flux-capacitor.manual.pdf`).

IMPORTANT NOTE: if Flux Capacitor is being installed in a PBS cluster (a cluster providing `qsub` and other related tools), it is important that the `configure` script is executed in the main cluster node, so as to properly detect the cluster configuration (do not execute it in an interactive session).

2.2 Third Party Software

Flux Capacitor internally uses CPLEX^e as a mathematical solver to obtain the solutions required by FBA and FVA procedures. Therefore, users also need to install this package to be able to access most of the functionality of the toolkit.

^e<https://www-01.ibm.com/software/commerce/optimization/cplex-optimizer/>

2.3 Add Flux Capacitor to the System PATH

To end the installation process, it might be useful to add Flux Capacitor to the system PATH. This will allow us to easily execute commands provided in the package without the necessity of providing the whole Flux Capacitor installation path.

For this purpose, we can execute the following commands:

```
$ FCAP_HOME_DIR=<absolute-installation-path>
$ export PATH=$PATH:${FCAP_HOME_DIR}
```

These variable definitions can be added to the `.bashrc` user profile file, so as to define them automatically whenever a new interactive shell session is started.

CHAPTER 3

USER GUIDE

BIBLIOGRAPHY

Shlomi, T., M. N. Cabili, M. J. Herrgård, B. Ø. Palsson, and Eytan Ruppin (2008). “Network-based prediction of human tissue-specific metabolism”. In: *Nat. Biotechnol.* 26(9), pp. 1003–10.