Installation Guide for ByoDyn version 4.8

Adrián López García de Lomana, Alex Gómez-Garrido, Miguel Hernández, Pau Rué Queralt and Jordi Villà-Freixa

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This document specifies the requirements and different steps to install ByoDyn on a Linux box (Fedora Core 2, 4 and 6).

Computational Biochemistry and Biophysics Laboratory
Research Unit on Biomedical Informatics
Universitat Pompeu Fabra - Institut Municipal d'Investigació Mèdica
c/ Dr. Aiguader 88, 08003, Barcelona, Spain
http://cbbl.imim.es

Contents

1 ByoDyn Requirements

1.1 Mandatory

- **Python**: version 2.5 or newer is required http://www.python.org/download.
- **SciPy**: version 0.6.0 or newer available at http://www.scipy.org/. To install SciPy you also need `numpy` available at http://numeric.scipy.org/. Please install `numpy` version 1.1.0 or newer. For an smooth use of SciPy, make sure you have built BLAS and LAPACK libraries as explained at http://www.scipy.org/Installing_SciPy/BuildingGeneral.
- **libSBML**: version 3.2.0 or newer available at http://www.sbml.org/libsbml.html. Make sure you use at least the Python binder adding the flag `--with-python` while configuring.
- **PORT Library**: from Netlib. Please follow the requiered specified steps for the correct functioning of the local search routines of `ByoDyn`:
  - Use the following command to download the code:
    `rsync -avz netlib.org::netlib/port .`
  - Modify the `Makefile`:
    * If your Fortran compiler is not `f77` add the following line at the top the file:

      `FC=gfortran`

      `gfortran` is the default Fortran compiler in the latest Fedora distribution. If you have another compiler, change `gfortran` by the one you have.
    * Change the line

      `LIB=portP`

      by

      `LIB=port`

      we are simply changing the name of the library.
    * Remove the line

      `n5err.o\`

      the file `n5err.f` was not found in the server and is not required in this case
    * Change the line

      `update lib$(LIB).a $?`

      by

      `ar rcs lib$(LIB).a $?`
    * Change the line

      `FFLAGS=-O`

      by

FFLAGS=-O -fPIC

if your architecture is 64 bits.

- Execute `make`.

Once you compile the source code, the file called `libport.a` has to be copied to the `byodyn/lib/local_search/PORT` directory.

- **Gnuplot**: Gnuplot 3.7 or newer needed to create the output graphs. Available at http://www.gnuplot.i
- **matplotlib**: Version 0.91.1 or newer is required. You can download it from http://matplotlib.sourcef It is required for the plots output by `ByoDyn`.

1.2 Optional

In addition to this, other pieces of software add extra functionality to the `ByoDyn` platform:

- **Doxygen:** required to build the API of `ByoDyn` in HTML and PDF formats. It has been tested under Doxygen version 1.5.2.
- **Octave**: is an optional tool to substitute SciPy functions for the integration of systems of ordinary differential equations (ODEs). On the contrary Octave is required for the solution of differential-algebraic equations (DAEs). Moreover Octave is compulsory required for clustering. Octave version 3.0.1 or newer is required. Octave is available at http://www.octave.org/.
- **OpenModelica**: version 1.4.3 or newer is required for the resolution of ODEs, DAEs and DAEs with events. Information for the installation can be found at http://www.ida.liu.se/~pelab/mod Some environmental variables are required:
  - `OPENMODELICAHOME`: pointing to the the `openmodelica` directory.
  - `PATH`: `omc` and `./` should be on the `PATH` for a correct execution of the software.
- **XPP/XPPAUT**: version 5.91 or newer is required for solving SBML models with delays. Information for the installation can be found at http://www.math.pitt.edu/~bard/xpp/xpp.html.
- **Open MPI**: the command `mpirun` is required to run `ByoDyn` in parallel. Version 1.2.3 or higher should be available.
- **ScientificPython**: the module `Scientific.MPI` is required for launching parallel calculations. Version 2.6 or newer is required. Please check http://dirac.cnrs-orleans.fr/plone/software/ for further information. Be sure you also create and call the executable `mpipython`. To build it please follow the instructions described in the `README.MPI` file of Scientific. If you will run `ByoDyn` on a single processor machine, the installation of this software is not required.

2 Installation of ByoDyn

Once all those software pieces have been installed into the machine and are accessible by ByoDyn you should set up a few things before you run it.

- First, add the ByoDyn executable to your path. For bash this would be done by:
  - edit your $HOME/.bashrc.
  - define the ByoDyn path: export BYODYN_PATH=$HOME/where_ByoDyn_is
    For example if you have ByoDyn at $HOME/a_directory/another_directory you should add the line
    export BYODYN_PATH=$HOME/a_directory/another_directory/byodyn
    at the .bashrc file.
  - Add ByoDyn executable file to the path: export PATH="$BYODYN_PATH/bin:$PATH"
- Make sure that the file libport.a is at the correct directory as specified at the Section 1.1.
- Finally, execute the command byodyn. The following lines should prompt:

```
ByoDyn version 4.6 is running ...
Run byodyn -h for help.
...  exiting from ByoDyn.
```

At the case of a newly installed ByoDyn, we suggest to run the ByoDyn tests in order check the correct functioning of the program. For that, type byodyn --testing on your terminal.