

▼ BPL_CHO_Fedbatch script with PyFMI ver 2.7.4

The key library PyFMI v2.7.4 is installed and downgrading is done Numpy v1.19.1. To simplify this we first install conda.

After the installation a small application BPL_CHO_Fedbatch is loaded and run. You can continue with this example if you like.

```
!lsb_release -a # Actual VM Ubuntu version used by Google
```

```
No LSB modules are available.
Distributor ID: Ubuntu
Description:   Ubuntu 18.04.6 LTS
Release:      18.04
Codename:     bionic
```

```
%env PYTHONPATH=
```

```
env: PYTHONPATH=
```

```
!wget https://repo.anaconda.com/miniconda/Miniconda3-py37_4.12.0-Linux-x86_64.sh
!chmod +x Miniconda3-py37_4.12.0-Linux-x86_64.sh
!bash ./Miniconda3-py37_4.12.0-Linux-x86_64.sh -b -f -p /usr/local
import sys
sys.path.append('/usr/local/lib/python3.7/site-packages/')
```

```
🔗 --2022-08-29 12:20:17-- https://repo.anaconda.com/miniconda/Miniconda3-py37_4
Resolving repo.anaconda.com (repo.anaconda.com)... 104.16.131.3, 104.16.130.3,
Connecting to repo.anaconda.com (repo.anaconda.com)|104.16.131.3|:443... conn
HTTP request sent, awaiting response... 200 OK
Length: 104996770 (100M) [application/x-sh]
Saving to: 'Miniconda3-py37_4.12.0-Linux-x86_64.sh'
```

```
Miniconda3-py37_4.1 100%[=====>] 100.13M 251MB/s in 0.4s
```

```
2022-08-29 12:20:17 (251 MB/s) - 'Miniconda3-py37_4.12.0-Linux-x86_64.sh' save
```

```
PREFIX=/usr/local
Unpacking payload ...
Collecting package metadata (current_repodata.json): done
Solving environment: done
```

```
## Package Plan ##
```

```
environment location: /usr/local
```

```
added / updated specs:
```

```
- _libgcc_mutex==0.1=main
- _openmp_mutex==4.5=1_gnu
- brotli==0.7.0=py37h27cfd23_1003
- ca-certificates==2022.3.29=h06a4308_1
- certifi==2021.10.8=py37h06a4308_2
```

```

- cffi==1.15.0=py37hd667e15_1
- charset-normalizer==2.0.4=pyhd3eb1b0_0
- colorama==0.4.4=pyhd3eb1b0_0
- conda-content-trust==0.1.1=pyhd3eb1b0_0
- conda-package-handling==1.8.1=py37h7f8727e_0
- conda==4.12.0=py37h06a4308_0
- cryptography==36.0.0=py37h9cele76_0
- idna==3.3=pyhd3eb1b0_0
- ld_impl_linux-64==2.35.1=h7274673_9
- libffi==3.3=he6710b0_2
- libgcc-ng==9.3.0=h5101ec6_17
- libgomp==9.3.0=h5101ec6_17
- libstdcxx-ng==9.3.0=hd4cf53a_17
- ncurses==6.3=h7f8727e_2
- openssl==1.1.1n=h7f8727e_0
- pip==21.2.2=py37h06a4308_0
- pycosat==0.6.3=py37h27cfd23_0
- pycparser==2.21=pyhd3eb1b0_0
- pyopenssl==22.0.0=pyhd3eb1b0_0
- pysocks==1.7.1=py37_1
- python==3.7.13=h12debd9_0
- readline==8.1.2=h7f8727e_1
- requests==2.27.1=pyhd3eb1b0_0
- ruamel_yaml==0.15.100=py37h27cfd23_0
- setuptools==61.2.0=py37h06a4308_0
- six==1.16.0=pyhd3eb1b0_1
- sqlite==3.38.2=hc218d9a_0
- tk==8.6.11=h1ccaba5_0
- tqdm==4.63.0=pyhd3eb1b0_0
- urllib3==1.26.8=pyhd3eb1b0_0
- wheel==0.37.1=pyhd3eb1b0_0

```

```
!conda update -n base -c defaults conda --yes
```

```
Collecting package metadata (current_repodata.json): done
```

```
Solving environment: done
```

```
## Package Plan ##
```

```
environment location: /usr/local
```

```
added / updated specs:
```

```
- conda
```

```
The following packages will be downloaded:
```

package	build	
-----	-----	
_openmp_mutex-5.1	1_gnu	21 KB
ca-certificates-2022.07.19	h06a4308_0	124 KB
certifi-2022.6.15	py37h06a4308_0	153 KB
cffi-1.15.1	py37h74dc2b5_0	227 KB
conda-4.14.0	py37h06a4308_0	909 KB
cryptography-37.0.1	py37h9cele76_0	1.3 MB
cytoolz-0.11.0	py37h7b6447c_0	328 KB
ld_impl_linux-64-2.38	h1181459_1	654 KB
libgcc-ng-11.2.0	h1234567_1	5.3 MB
libgomp-11.2.0	h1234567_1	474 KB

libstdcxx-ng-11.2.0	h1234567_1	4.7 MB
ncurses-6.3	h5eee18b_3	781 KB
openssl-1.1.1q	h7f8727e_0	2.5 MB
pip-22.1.2	py37h06a4308_0	2.4 MB
requests-2.28.1	py37h06a4308_0	92 KB
setuptools-63.4.1	py37h06a4308_0	1.1 MB
sqlite-3.39.2	h5082296_0	1.1 MB
tk-8.6.12	h1ccaba5_0	3.0 MB
toolz-0.11.2	pyhd3eb1b0_0	49 KB
tqdm-4.64.0	py37h06a4308_0	126 KB
urllib3-1.26.11	py37h06a4308_0	181 KB
xz-5.2.5	h7f8727e_1	339 KB
zlib-1.2.12	h7f8727e_2	106 KB

Total:		25.9 MB

The following NEW packages will be INSTALLED:

cytoolz	pkgs/main/linux-64::cytoolz-0.11.0-py37h7b6447c_0
toolz	pkgs/main/noarch::toolz-0.11.2-pyhd3eb1b0_0

The following packages will be REMOVED:

colorama-0.4.4-pyhd3eb1b0_0
conda-content-trust-0.1.1-pyhd3eb1b0_0
six-1.16.0-pyhd3eb1b0_1

The following packages will be UPDATED:

_openmp_mutex	4.5-1_gnu --> 5.1-1_gnu
ca-certificates	2022.3.29-h06a4308_1 --> 2022.07.19-h06
certifi	2021.10.8-py37h06a4308_2 --> 2022.6.15-py37
conda	4.15.0-py37h06a4308_1 --> 4.15.1-py37h7b

```
!conda --version
!python --version
```

```
conda 4.14.0
Python 3.7.13
```

```
!conda install -c conda-forge pyfmi==2.7.4 --yes # Install the key package
```

liblapack	conda-forge/linux-64::liblapack-3.9.0-15_linux64_openblas
libopenblas	conda-forge/linux-64::libopenblas-0.3.20-pthreads_h78a641
libxml2	conda-forge/linux-64::libxml2-2.9.12-h72842e0_0
libxslt	conda-forge/linux-64::libxslt-1.1.33-h15afd5d_2
lxml	conda-forge/linux-64::lxml-4.8.0-py37h540881e_2
metis	conda-forge/linux-64::metis-5.1.0-h58526e2_1006
mpfr	conda-forge/linux-64::mpfr-4.1.0-h9202a9a_1
numpy	conda-forge/linux-64::numpy-1.21.6-py37h976b520_0
pyfmi	conda-forge/linux-64::pyfmi-2.7.4-py37h161383b_0
python_abi	conda-forge/linux-64::python_abi-3.7-2_cp37m
scipy	conda-forge/linux-64::scipy-1.7.3-py37hf2a6cf1_0
suitesparse	conda-forge/linux-64::suitesparse-5.10.1-h9e50725_1
sundials	conda-forge/linux-64::sundials-5.8.0-h558c624_0
tbb	conda-forge/linux-64::tbb-2021.5.0-h924138e_1

The following packages will be UPDATED:

certifi	pkgs/main/linux-64::certifi-2022.6.15~ --> conda-forge/nc
---------	---

The following packages will be SUPERSEDED by a higher-priority channel:

```
ca-certificates      pkgs/main::ca-certificates-2022.07.19~ --> conda-forge::c
conda                pkgs/main::conda-4.14.0-py37h06a4308_0 --> conda-forge::c
openssl              pkgs/main::openssl-1.1.1q-h7f8727e_0 --> conda-forge::c
```

Downloading and Extracting Packages

```
metis-5.1.0          | 4.1 MB      | : 100% 1.0/1 [00:00<00:00, 1.01it/s]
libgfortran5-12.1.0  | 1.8 MB      | : 100% 1.0/1 [00:00<00:00, 2.53it/s]
libcblas-3.9.0       | 12 KB       | : 100% 1.0/1 [00:00<00:00, 20.78it/s]
libblas-3.9.0        | 12 KB       | : 100% 1.0/1 [00:00<00:00, 23.40it/s]
tbb-2021.5.0         | 1.9 MB      | : 100% 1.0/1 [00:00<00:00, 2.02it/s]
numpy-1.21.6         | 6.1 MB      | : 100% 1.0/1 [00:01<00:00, 1.73s/it]
ca-certificates-2022 | 149 KB      | : 100% 1.0/1 [00:00<00:00, 15.92it/s]
liblapack-3.9.0      | 12 KB       | : 100% 1.0/1 [00:00<00:00, 20.64it/s]
assimulo-3.2.9       | 2.6 MB      | : 100% 1.0/1 [00:00<00:00, 1.63it/s]
gmp-6.2.1            | 806 KB      | : 100% 1.0/1 [00:00<00:00, 5.31it/s]
libiconv-1.16        | 1.4 MB      | : 100% 1.0/1 [00:00<00:00, 4.28it/s]
libopenblas-0.3.20   | 10.1 MB     | : 100% 1.0/1 [00:02<00:00, 2.78s/it]
fmlib-2.2.3          | 532 KB      | : 100% 1.0/1 [00:00<00:00, 4.36it/s]
scipy-1.7.3          | 21.8 MB     | : 100% 1.0/1 [00:04<00:00, 4.92s/it]
lxml-4.8.0           | 1.4 MB      | : 100% 1.0/1 [00:00<00:00, 2.42it/s]
libxml2-2.9.12       | 772 KB      | : 100% 1.0/1 [00:00<00:00, 5.18it/s]
icu-68.2             | 13.1 MB     | : 100% 1.0/1 [00:02<00:00, 2.45s/it]
python_abi-3.7       | 4 KB        | : 100% 1.0/1 [00:00<00:00, 21.27it/s]
libxslt-1.1.33       | 522 KB      | : 100% 1.0/1 [00:00<00:00, 3.69it/s]
libgfortran-ng-12.1. | 23 KB       | : 100% 1.0/1 [00:00<00:00, 19.28it/s]
certifi-2022.6.15    | 154 KB      | : 100% 1.0/1 [00:00<00:00, 16.21it/s]
sundials-5.8.0       | 1.0 MB      | : 100% 1.0/1 [00:00<00:00, 2.22it/s]
conda-4.14.0         | 1010 KB     | : 100% 1.0/1 [00:00<00:00, 2.38it/s]
suitesparse-5.10.1   | 2.4 MB      | : 100% 1.0/1 [00:00<00:00, 1.35it/s]
mpfr-4.1.0           | 2.6 MB      | : 100% 1.0/1 [00:00<00:00, 1.97it/s]
pyfmi-2.7.4          | 12.4 MB     | : 100% 1.0/1 [00:02<00:00, 2.37s/it]
openssl-1.1.1o       | 2.1 MB      | : 100% 1.0/1 [00:00<00:00, 2.07it/s]
```

Preparing transaction: done

Verifying transaction: done

Executing transaction: done

Retrieving notices: ...working... done

```
!conda install numpy=1.19.1 --yes # Need to downgrade numpy
```

Collecting package metadata (current_repodata.json): done

Solving environment: failed with initial frozen solve. Retrying with flexible

Collecting package metadata (repodata.json): done

Solving environment: done

Package Plan

environment location: /usr/local

added / updated specs:

- numpy=1.19.1

The following packages will be downloaded:

package

build

```

-----|-----
blas-1.0                |                openblas                46 KB
numpy-1.19.1            |                py37h30dfecb_0           21 KB
numpy-base-1.19.1      |                py37h75fe3a5_0          4.1 MB
-----|-----
Total:                  |                4.2 MB

```

The following NEW packages will be INSTALLED:

```

blas                pkgs/main/linux-64::blas-1.0-openblas
numpy-base         pkgs/main/linux-64::numpy-base-1.19.1-py37h75fe3a5_0

```

The following packages will be UPDATED:

```

ca-certificates    conda-forge::ca-certificates-2022.6.1~ --> pkgs/main::ca-
openssl            conda-forge::openssl-1.1.1o-h166bdaf_0 --> pkgs/main::ope

```

The following packages will be SUPERSEDED by a higher-priority channel:

```

certifi            conda-forge/noarch::certifi-2022.6.15~ --> pkgs/main/linux-64::certifi
conda              conda-forge::conda-4.14.0-py37h89c186~ --> pkgs/main::conda
numpy              conda-forge::numpy-1.21.6-py37h976b52~ --> pkgs/main::numpy

```

Downloading and Extracting Packages

```

numpy-base-1.19.1    | 4.1 MB | : 100% 1.0/1 [00:00<00:00, 2.88it/s]
numpy-1.19.1         | 21 KB  | : 100% 1.0/1 [00:00<00:00, 16.55it/s]
blas-1.0             | 46 KB  | : 100% 1.0/1 [00:00<00:00, 12.34it/s]
Preparing transaction: done
Verifying transaction: done
Executing transaction: done
Retrieving notices: ...working... done

```

▼ BPL_CHO_Fedbatch demo

Now specific installation and the run simulations. Start with connecting to Github. Then upload the two files:

- FMU - BPL_CHO_Fedbatch_linux_jm_cs.fmu
- Setup-file - BPL_CHO_Fedbatch_explore

```

# Filter out DeprecationWarnings for 'np.float as alias' is needed - wish I could m
import warnings
warnings.filterwarnings("ignore")

```

```

%%bash
git clone https://github.com/janpeter19/BPL_CHO_Fedbatch

```

```

Cloning into 'BPL_CHO_Fedbatch'...

```

```

%cd BPL_CHO_Fedbatch

```

```
/content/BPL_CHO_Fedbatch/BPL_CHO_Fedbatch
```

```
run -i BPL_CHO_Fedbatch_explore.py
```

```
Linux - run FMU pre-comiled JModelica 2.4
```

```
Model for bioreactor has been setup. Key commands:
```

- par() - change of parameters and initial values
- init() - change initial values only
- simu() - simulate and plot
- newplot() - make a new plot
- show() - show plot from previous simulation
- disp() - display parameters and initial values from the last simulation
- describe() - describe culture, broth, parameters, variables with values /

```
Note that both disp() and describe() takes values from the last simulation
```

```
Brief information about a command by help(), eg help(simu)
```

```
Key system information is listed with the command system_info()
```

```
%matplotlib inline
```

```
plt.rcParams['figure.figsize'] = [25/2.54, 20/2.54]
```

```
describe('culture'); print(); describe('liquidphase')
```

```
Reactor culture CHO-MAB - cell line HB-58 American Culture Collection ATCC
```

```
Reactor broth substances included in the model
```

```
Cells viable index = 1 molecular weight = 24.6 Da
Cells dead    index = 2 molecular weight = 24.6 Da
Glucose       index = 3 molecular weight = 180.0 Da
Glutamine    index = 4 molecular weight = 146.1 Da
Lactate       index = 5 molecular weight = 90.1 Da
Ammonia       index = 6 molecular weight = 17.0 Da
Protein       index = 7 molecular weight = 150000.0 Da
```

```
# Slide 3
```

```
newplot('CHO fedbatch cultivation - protein expression', plotType='Textbook_3')
```

```
# Data from Table 1 and 2 for experiment 3
```

```
V_0=0.35
```

```
init(V_0=V_0, VXv_0=V_0*0.29, VXd_0=V_0*0.010)
```

```
init(VG_0=V_0*17.17, VGn_0=V_0*3.02, VL_0=V_0*1.12, VN_0=V_0*0.29)
```

```
# Feeding
```

```
Feed=0.1/24
```

```
par(G_in=15, Gn_in=9.3)
```

```
par(t0=0, F0=0, t1=35, F1=Feed, t2=100, F2=Feed, t3=300, F3=Feed)
```

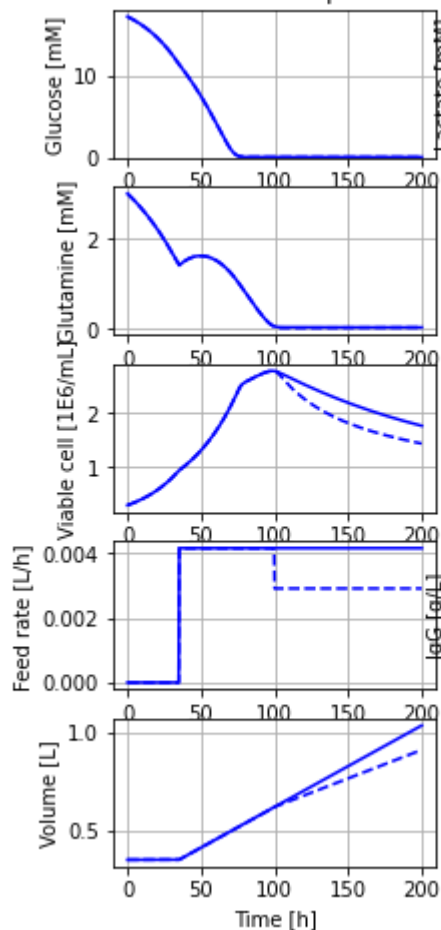
```
# Culture parameters
```

```
par(alpha=-1.0, beta=0.01)
```

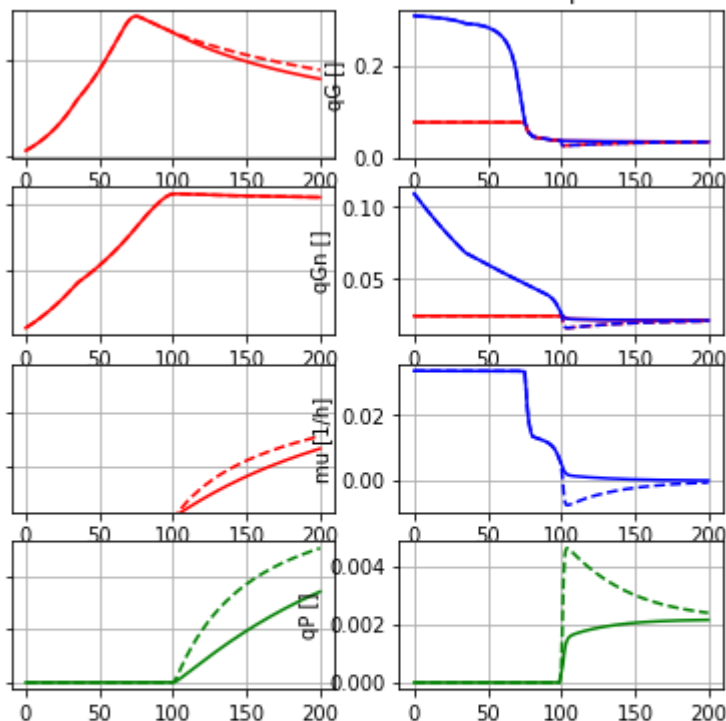
```
# Simulation
simu(200)
par(t2=100, F2=0.7*Feed, t3=300, F3=0.7*Feed); simu(200)
par(F2=Feed, F3=Feed)
```

```
Simulation interval      : 0.0 - 200.00000000000003 seconds.
Elapsed simulation time: 0.023053809999510122 seconds.
Simulation interval      : 0.0 - 200.00000000000003 seconds.
Elapsed simulation time: 0.01600876800057449 seconds.
```

CHO fedbatch cultivation - protein expression



- microscopic world



```
disp('culture', decimals=4)
```

```
qG_max1 : 0.2971
qG_max2 : 0.0384
qGn_max1 : 0.1238
qGn_max2 : 0.0218
mu_d_max : 0.1302
alpha : -1.0
beta : 0.01
```

```
system_info()
```

```
System information
-OS: Linux
-Python: 3.7.13
-PyFMI: 2.7.4
-FMU by: JModelica.org
-FMI: 2.0
```

```
-Type: FMUModelCS2
-Name: BPL_CHO.Fedbatch
-Generated: 2022-08-29T12:13:26
-MSL: 3.2.2 build 3
-Description: Bioprocess Library version 2.1.0 beta
-Interaction: FMU-explore ver 0.9.2
```

Double-click (or enter) to edit

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✓ 0s completed at 14:24

