

✓ BPL_TEST2_Batch script with FMPy

The key library FMPy is installed.

After the installation a small application BPL_YEAST_COB_Batch 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 22.04.3 LTS
Release:        22.04
Codename:       jammy

%env PYTHONPATH=

env: PYTHONPATH=

!wget https://repo.anaconda.com/miniconda/Miniconda3-py310_23.1.0-1-Linux-x86_64.sh
!chmod +x Miniconda3-py310_23.1.0-1-Linux-x86_64.sh
!bash ./Miniconda3-py310_23.1.0-1-Linux-x86_64.sh -b -f -p /usr/local
import sys
sys.path.append('/usr/local/lib/python3.10/site-packages/')

--2024-03-07 16:47:24-- https://repo.anaconda.com/miniconda/Miniconda3-py310_23.1.0-1-Linux-x86_64.sh
Resolving repo.anaconda.com (repo.anaconda.com)... 104.16.130.3, 104.16.131.3, 2606:4700::6810:8203, ...
Connecting to repo.anaconda.com (repo.anaconda.com)|104.16.130.3|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 74403966 (71M) [application/x-sh]
Saving to: 'Miniconda3-py310_23.1.0-1-Linux-x86_64.sh'

Miniconda3-py310_23 100%[=====] 70.96M 145MB/s in 0.5s

2024-03-07 16:47:25 (145 MB/s) - 'Miniconda3-py310_23.1.0-1-Linux-x86_64.sh' saved [74403966/74403966]

PREFIX=/usr/local
Unpacking payload ...

Installing base environment...

Downloading and Extracting Packages

Downloading and Extracting Packages

Preparing transaction: done
Executing transaction: done
installation finished.

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

```
Preparing transaction: done  
Verifying transaction: done  
Executing transaction: done
```

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

```
conda 24.1.2  
Python 3.10.13
```

```
!conda install -c conda-forge fmpy --yes # Install the key package
```

```
Preparing transaction: done
Verifying transaction: done
Executing transaction: done

!conda install matplotlib --yes

Channels:
- defaults
- conda-forge
Platform: linux-64
Collecting package metadata (repodata.json): done
Solving environment: done

## Package Plan ##

environment location: /usr/local

added / updated specs:
- matplotlib

The following packages will be downloaded:

package | build | size
-----|-----|-----
matplotlib-3.8.0 | py310h06a4308_0 | 8 KB
matplotlib-base-3.8.0 | py310h1128e8f_0 | 6.8 MB
pyparsing-3.0.9 | py310h06a4308_0 | 153 KB
Total: 7.0 MB

The following NEW packages will be INSTALLED:

matplotlib pkgs/main/linux-64::matplotlib-3.8.0-py310h06a4308_0

The following packages will be UPDATED:

matplotlib-base conda-forge::matplotlib-base-3.5.2-py~ --> pkgs/main::matplotlib-base-3.8.0-py310h1128e8f_0

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

certifi conda-forge/noarch::certifi-2024.2.2~ --> pkgs/main/linux-64::certifi-2024.2.2-py310h06a4308_0
conda conda-forge::conda-24.1.2-py310hff520~ --> pkgs/main::conda-24.1.2-py310h06a4308_0
pyparsing conda-forge/noarch::pyparsing-3.1.2-p~ --> pkgs/main/linux-64::pyparsing-3.0.9-py310h06a4308_0

Downloading and Extracting Packages:
matplotlib-base-3.8.0 | 6.8 MB | : 0% 0/1 [00:00<?, ?it/s]
pyparsing-3.0.9 | 153 KB | : 0% 0/1 [00:00<?, ?it/s]

matplotlib-3.8.0 | 8 KB | : 0% 0/1 [00:00<?, ?it/s]

matplotlib-base-3.8.0 | 6.8 MB | : 6% 0.05732043213112497/1 [00:00<00:01, 1.76s/it]
pyparsing-3.0.9 | 153 KB | : 100% 1.0/1 [00:00<00:00, 7.78it/s]

Preparing transaction: done
Verifying transaction: done
Executing transaction: done

#!conda install scipy --yes

#!conda install xlrd --yes

#!conda install openpyxl --yes

# For some reason conda installation does not work for optlang
!pip install optlang

Collecting optlang
  Downloading optlang-1.8.1-py2.py3-none-any.whl (142 kB)
    142.0/142.0 kB 10.2 MB/s eta 0:00:00
Requirement already satisfied: six>=1.9 in /usr/local/lib/python3.10/site-packages (from optlang) (1.16.0)
Collecting swiglpk>=5.0.8
  Downloading swiglpk-5.0.10-cp310-cp310-manylinux_2_17_x86_64.manylinux2014_x86_64.whl (2.3 MB)
    2.3/2.3 MB 49.5 MB/s eta 0:00:00
Collecting sympy>=1.12.0
  Downloading sympy-1.12-py3-none-any.whl (5.7 MB)
    5.7/5.7 MB 42.1 MB/s eta 0:00:00
Collecting mpmath>=0.19
```

Downloading mpmath-1.3.0-py3-none-any.whl (536 kB)

536.2/536.2 kB 47.0 MB/s eta 0:00:00

Installing collected packages: swiglpk, mpmath, sympy, optlang

Successfully installed mpmath-1.3.0 optlang-1.8.1 swiglpk-5.0.10 sympy-1.12

WARNING: Running pip as the 'root' user can result in broken permissions and conflicting behaviour with the system packa

✓ BPL_YEAST_COB_Batch setup

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

- FMU - BPL_YEAST_COB_Batch_linux_om_me.fmu
- Setup-file - BPL_YEAST_COB_Batch_fmipy_explore.py

```
%%bash
```

```
git clone https://github.com/janpeter19/BPL_YEAST_COB_Batch
```

```
Cloning into 'BPL_YEAST_COB_Batch'...
```

```
%cd BPL_YEAST_COB_Batch
```

```
/content/BPL_YEAST_COB_Batch
```

```
run -i BPL_YEAST_COB_Batch_fmipy_explore.py
```

```
Linux - run FMU pre-comiled OpenModelica 1.21.0
```

```
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/units

```
Note that both disp() and describe() takes values from the last simulation
and the command process_diagram() brings up the main configuration
```

```
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]
```

```
import warnings
```

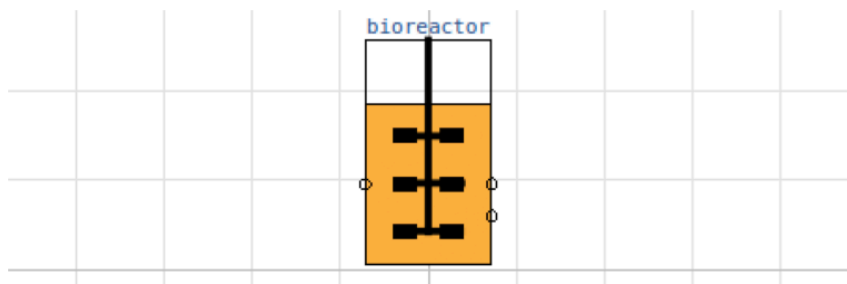
```
warnings.filterwarnings("ignore")
```

✓ BPL_YEAST_COB_Batch - demo

```
from optlang import Model, Variable, Constraint, Objective
```

```
process_diagram()
```

```
No processDiagram.png file in the FMU, but try the file on disk.
```



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

```
# Pump schedule parameter
```

```
Saccharomyces cerevisiae - default parameters for strain H1022
```

```

# Define culture constraint-based model
def culture(G, E):

    # LP calculation of the optimal qGr, qEr based on G and E values

    # - parameters
    q02max = 6.9e-3; kog = 2.3; koe = 1.6; YGr = 3.5; YEr = 1.32;
    alpha = 0.01; beta = 1.0

    # - transfer data from dynamic reactor model to static LP model
    qGr_opt = Variable('qGr_opt', lb=0)
    qEr_opt = Variable('qEr_opt', lb=0)

    # - LP model constraint and objective
    mu_max = Objective(YGr*qGr_opt + YEr*qEr_opt, direction='max')
    q02lim = Constraint(kog*qGr_opt + koe*qEr_opt, ub=q02max)
    qGlim = Constraint(qGr_opt, ub=alpha*max(0,G))
    qElim = Constraint(qEr_opt, ub=beta*max(0,E))

    # - put together the LP model
    yeast_model = Model(name='Yeast bottleneck model')
    yeast_model.objective = mu_max
    yeast_model.add(q02lim)
    yeast_model.add(qGlim)
    yeast_model.add(qElim)

    # - do LP optimization
    yeast_model.optimize()

    return (yeast_model.objective.value, yeast_model.variables.qGr_opt.primal, yeast_model.variables.qEr_opt.primal, q02lim)

# Initialization
V_start=1.0
init(V_start=V_start, VX_start=V_start*2.0, VG_start=V_start*10, VE_start=V_start*3.0)

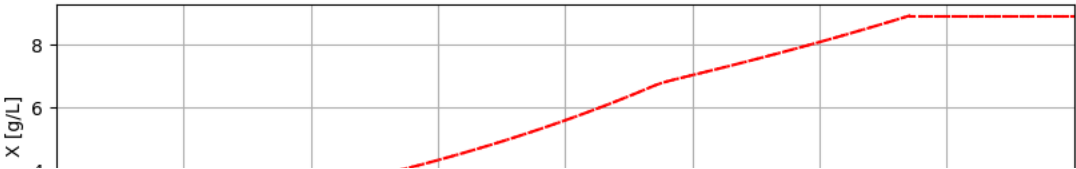
# Loop of simulations
t_final = 8.0
t_samp = 0.0333
n_samp = t_final/t_samp + 1

# Simulate n sample steps
newplot(title='Batch cultivation', plotType='TimeSeries2')
ax1.set_xlim([0, t_final]); ax2.set_xlim([0, t_final]); ax3.set_xlim([0, t_final])

simu(t_samp, options=opts_fast)
for i in range(int(n_samp)):
    (mum_opt, qGr_opt, qEr_opt, q02_opt) = culture(sim_res['bioreactor.c[2]'][-1], sim_res['bioreactor.c[3]'][-1])
    par(mum=mum_opt, qGr=qGr_opt, qEr=qEr_opt, q02=q02_opt)
    simu(t_samp, 'cont', options=opts_fast)

```

Batch cultivation



system_info()

```
System information
-OS: Linux
-Python: 3.10.12
-Scipy: not installed in the notebook
-FMPy: 0.3.19
-FMU by: OpenModelica Compiler OpenModelica 1.21.0
-FMI: 2.0
-Type: ME
-Name: BPL_YEAST_COB.Batch
-Generated: 2024-03-07T12:25:17Z
-MSL: 3.2.3
-Description: Bioprocess Library version 2.1.2 prel
-Interaction: FMU-explore for FMPy version 0.9.9
```

!conda list optlang

packages in environment at /usr/local:

#	Name	Version	Build	Channel
	optlang	1.8.1	pypi_0	pypi

Time [h]	Blue Line	Green Line
4.0	2	-
5.0	0	2
7.0	0	0
8.0	0	0