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-py312_24.3.0-0-Linux-x86_64.sh
!chmod +x Miniconda3-py312_24.3.0-0-Linux-x86_64.sh
!bash ./Miniconda3-py312_24.3.0-0-Linux-x86_64.sh -b -f -p /usr/local
import sys
sys.path.append('/usr/local/lib/python3.12/site-packages/')
```

```
--2024-08-13 11:22:49--  https://repo.anaconda.com/miniconda/Miniconda3-py312_24.3.0-0-Linux-x86_64.sh
Resolving repo.anaconda.com (repo.anaconda.com)... 104.16.32.241, 104.16.191.158, 2606:4700::6810:20f1, ...
Connecting to repo.anaconda.com (repo.anaconda.com)|104.16.32.241|:443... connected.
HTTP request sent, awaiting response... 200 OK
Length: 143351488 (137M) [application/octet-stream]
Saving to: ‘Miniconda3-py312_24.3.0-0-Linux-x86_64.sh’

Miniconda3-py312_24 100%[===================>] 136.71M   115MB/s    in 1.2s

2024-08-13 11:22:50 (115 MB/s) - ‘Miniconda3-py312_24.3.0-0-Linux-x86_64.sh’ saved [143351488/143351488]

PREFIX=/usr/local
Unpacking payload ...

Installing base environment...

Preparing transaction: ...working... done
Executing transaction: ...working... done
installation finished.
```

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

```
frozendict-2.4.2     | 36 KB     | : 100% 1.0/1 [00:00<00:00,  1.92it/s]
```

```
frozendict-2.4.2     | 36 KB     | : 100% 1.0/1 [00:00<00:00,  1.92it/s]
conda-24.7.1         | 1.2 MB    | : 100% 1.0/1 [00:01<00:00,  1.01s/it]
```

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

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

```
conda 24.7.1
Python 3.12.2
```

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

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

```
#!conda install matplotlib --yes
```

```
#!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-1.8.2-py2.py3-none-any.whl.metadata (8.1 kB)
Collecting swiglpk>=5.0.8 (from optlang)
  Downloading swiglpk-5.0.10-cp312-cp312-manylinux_2_17_x86_64.manylinux2014_x86_64.whl.metadata (5.5 kB)
Collecting sympy>=1.12.0 (from optlang)
  Downloading sympy-1.13.2-py3-none-any.whl.metadata (12 kB)
Collecting mpmath<1.4,>=1.1.0 (from sympy>=1.12.0->optlang)
  Using cached mpmath-1.3.0-py3-none-any.whl.metadata (8.6 kB)
Downloading optlang-1.8.2-py2.py3-none-any.whl (141 kB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 141.8/141.8 kB 1.5 MB/s eta 0:00:00
Downloading swiglpk-5.0.10-cp312-cp312-manylinux_2_17_x86_64.manylinux2014_x86_64.whl (2.3 MB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 2.3/2.3 MB 15.2 MB/s eta 0:00:00
Downloading sympy-1.13.2-py3-none-any.whl (6.2 MB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 6.2/6.2 MB 50.1 MB/s eta 0:00:00
Using cached mpmath-1.3.0-py3-none-any.whl (536 kB)
Installing collected packages: swiglpk, mpmath, sympy, optlang
Successfully installed mpmath-1.3.0 optlang-1.8.2 swiglpk-5.0.10 sympy-1.13.2
```

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_fmpy_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_fmpy_explore.py
```

```
Linux - run FMU pre-comiled OpenModelica 1.23.0-dev

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]
```

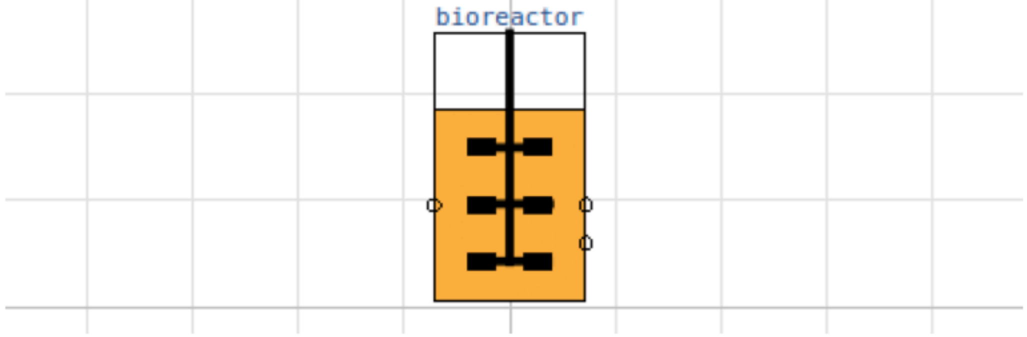
```
import warnings
warnings.filterwarnings("ignore")
```

BPL_YEAST_COB_Batch - demo

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

```
process_diagram()
```

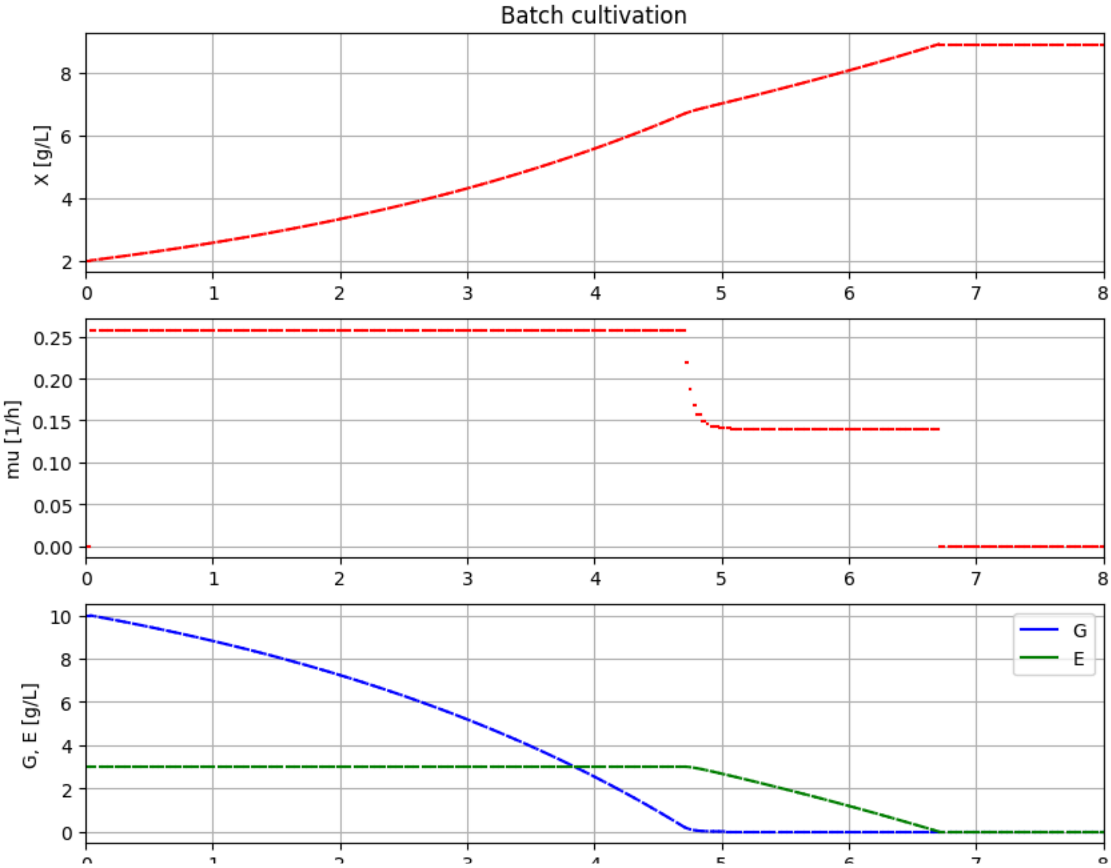
```
No processDiagram.png file in the FMU, but try the file on disk.
```



```
describe('culture'); print(); #describe('liquidphase')                                    # Pump schedule parameter
```

```
Saccharomyces cerevisae - 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
    qO2max = 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')
    qO2lim = Constraint(kog*qGr_opt + koe*qEr_opt, ub=qO2max)
    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(qO2lim)
    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, qO2lim.

# 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, qO2_opt) = culture(sim_res['bioreactor.c[2]'][-1], sim_res['bioreactor.c[3]'][-1])
    par(mum=mum_opt, qGr=qGr_opt, qEr=qEr_opt, qO2=qO2_opt)
    simu(t_samp, 'cont', options=opts_fast)
```



```
system_info()
```

```
System information
 -OS: Linux
 -Python: 3.10.12
 -Scipy: not installed in the notebook
 -FMPy: 0.3.20
 -FMU by: OpenModelica Compiler OpenModelica 1.23.0~dev.beta.1-1-g379f714
 -FMI: 2.0
 -Type: ME
 -Name: BPL_YEAST_COB.Batch
 -Generated: 2024-05-20T18:51:02Z
 -MSL: 3.2.3
 -Description: Bioprocess Library version 2.2.0
 -Interaction: FMU-explore for FMPy version 1.0.1
```

```
!conda list optlang
```

```
# packages in environment at /usr/local:
#
# Name                    Version                   Build  Channel
optlang                   1.8.2                    pypi_0    pypi
```