⌄ 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/')
```

> --2024-11-08 07:27:18-- 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:bf9e, ...
> 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   134MB/s   in 1.0s
>
> 2024-11-08 07:27:20 (134 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,  1.94it/s]

    certifi-2024.8.30     | 163 KB     | : 100% 1.0/1 [00:00<00:00,  1.94it/s]

    certifi-2024.8.30     | 163 KB     | : 100% 1.0/1 [00:00<00:00,  1.94it/s]
    conda-24.9.2          | 1.1 MB     | : 100% 1.0/1 [00:01<00:00,  1.09s/it]
```

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

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

⇥ conda 24.9.2
    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-1.13.3-py3-none-any.whl.metadata (12 kB)
Collecting mpmath<1.4,>=1.1.0 (from sympy>=1.12.0->optlang)
  Downloading 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 3.6 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 4.5 MB/s eta 0:00:00
Downloading sympy-1.13.3-py3-none-any.whl (6.2 MB)
  ──────────────────────────────────────── 6.2/6.2 MB 87.1 MB/s eta 0:00:00
Downloading mpmath-1.3.0-py3-none-any.whl (536 kB)
  ──────────────────────────────────────── 536.2/536.2 kB 30.1 MB/s eta 0:00:00
Installing collected packages: swiglpk, mpmath, sympy, optlang
Successfully installed mpmath-1.3.0 optlang-1.8.2 swiglpk-5.0.10 sympy-1.13.3
```

∨ 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

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")
```
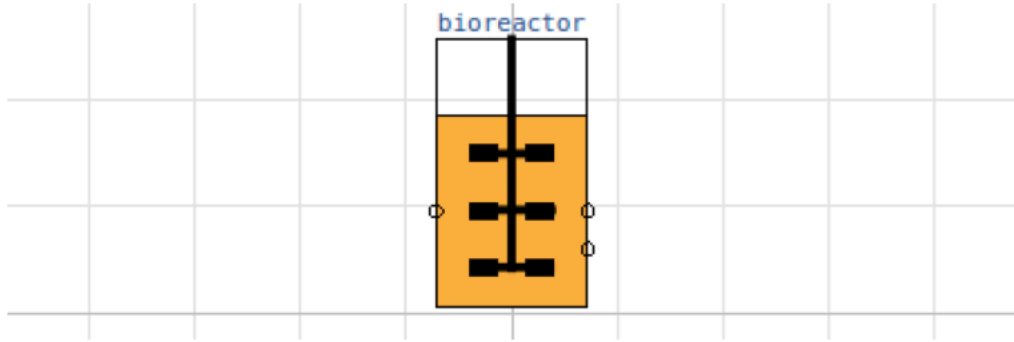
∨ BPL_YEAST_COB_Batch - demo

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

```python
process_diagram()
```

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


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

> Saccharomyces cerevisae – default parameters for strain H1022

```python
# 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)
```
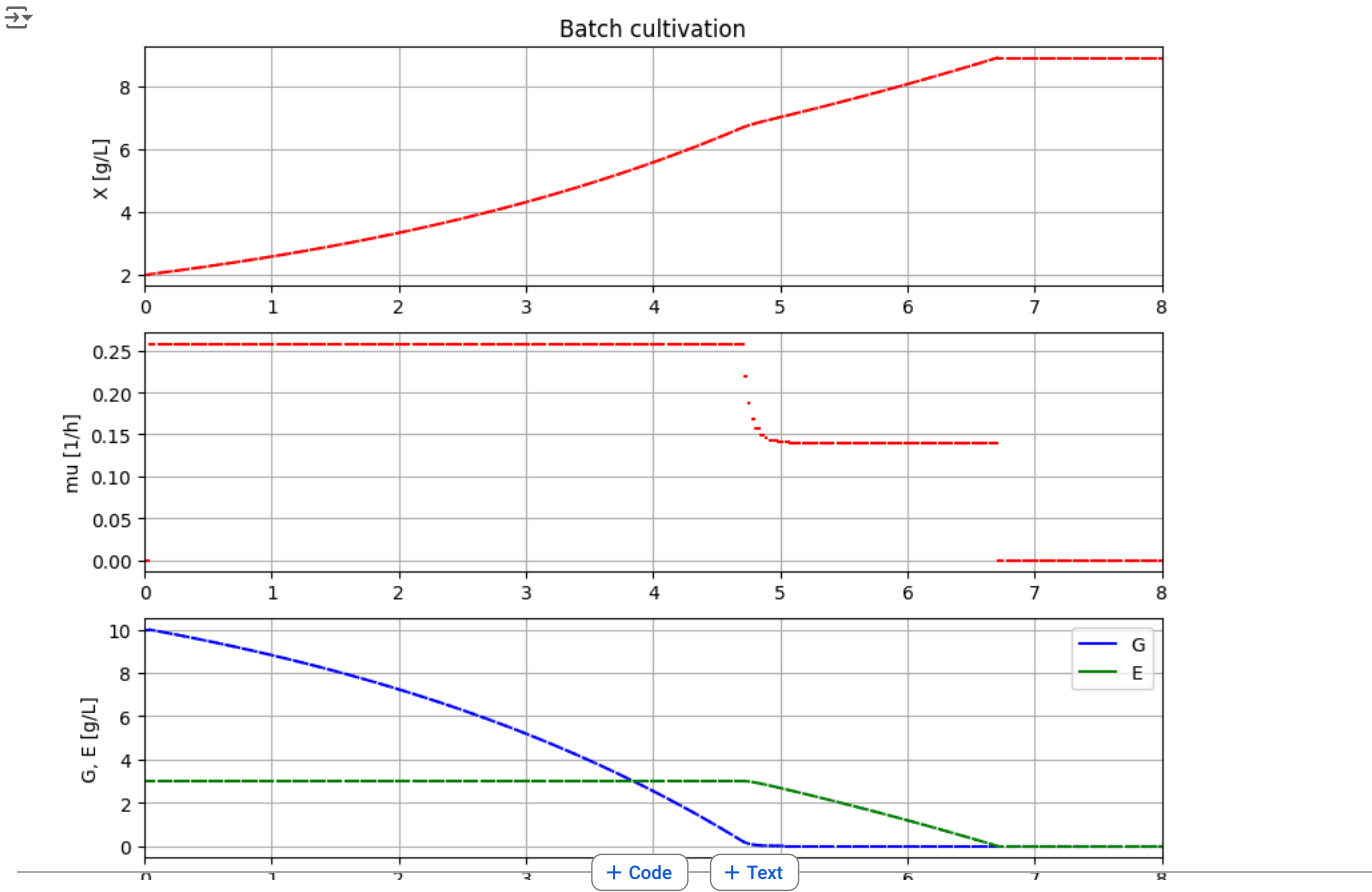
Batch cultivation

```
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 1.25.0~dev—133—ga5470be
 —FMI: 2.0
 —Type: ME
 —Name: BPL_YEAST_COB.Batch
 —Generated: 2024—11—08T08:21:20Z
 —MSL: 3.2.3
 —Description: Bioprocess Library version 2.3.0
 —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
```