## 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
                     Ubuntu 22.04.3 LTS
    Description:
    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/')
Show hidden output
!conda update -n base -c defaults conda --yes
Show hidden output
!conda --version
!python --version
    conda 23.11.0
    Pvthon 3.10.13
!conda install -c conda-forge fmpy --yes # Install the key package
Show hidden output
!conda install matplotlib --yes
Show hidden output
#!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 1.5 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 15.3 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 48.0 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 38.2 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\_fmpy\_explore.py

```
%bash
git clone https://github.com/janpeter19/CONF_2023_10_MODELICA15
    Cloning into 'CONF_2023_10_MODELICA15'...
%cd CONF_2023_10_MODELICA15
    /content/CONF_2023_10_MODELICA15
run -i BPL_YEAST_COB_Batch_fmpy_explore.py
    Linux - run FMU pre-comiled OpenModelica 1.21.0
    Model for bioreactor has been setup. Key commands:
                    - change of parameters and initial values
      - par()
     - init()
                   - change initial values only
     - simu()

    simulate and plot

     - newplot()
                  - make a new plot
     - show()
                   - show plot from previous simulation
                   - display parameters and initial values from the last simulation
     - disp()
     - 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
```

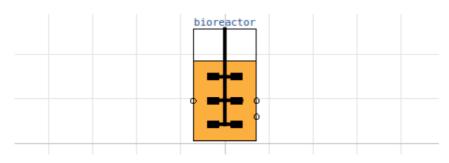
Brief information about a command by help(), eg help(simu) Key system information is listed with the command system\_info()

```
%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()

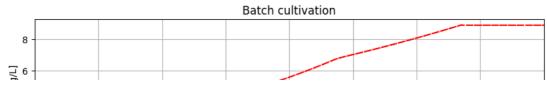


describe('culture'); print(); #describe('liquidphase')

# 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
   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, qO2lim.
# Initialization
V_0=1.0
init(V_0=V_0, VX_0=V_0*2.0, VG_0=V_0*10, VE_0=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)
```



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: 2023-05-31T09:43:28Z

-MSL: 3.2.3

-Description: Bioprocess Library version 2.1.1 -Interaction: FMU-explore for FMPy version 0.9.8

!conda list optlang

