

## ▾ BPL\_YEAST\_COB\_Batch script with PyFMI

The key library PyFMI 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.

```
lslsb_release -a # Actual VM Ubuntu version used by Google

No LSB modules are available.
Distributor ID: Ubuntu
Description:   Ubuntu 22.04.2 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/')

--2023-08-15 12:07:12--  https://repo.anaconda.com/miniconda/Miniconda3-py310\_23.1.0-1-Linux-x86\_64.sh
Resolving repo.anaconda.com (repo.anaconda.com)... 104.16.131.3, 104.16.130.3, 2606:4700::6810:8203, ...
Connecting to repo.anaconda.com (repo.anaconda.com)|104.16.131.3|: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 198MB/s in 0.4s

2023-08-15 12:07:13 (198 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
```

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

conda 23.7.2
Python 3.10.12

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

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

```
!pip install optlang
```

```
Collecting optlang
  Downloading optlang-1.7.0-py2.py3-none-any.whl (138 kB)
    ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 138.3/138.3 kB 5.2 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 57.7 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-5.0.8-cp310-cp310-manylinux_2_17_x86_64.manylinux2014_x86_64.whl (2.3 MB)
    ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 2.3/2.3 MB 24.4 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 42.8 MB/s eta 0:00:00
Installing collected packages: swiglpk, mpmath, sympy, optlang
Successfully installed mpmath-1.3.0 optlang-1.7.0 swiglpk-5.0.8 sympy-1.12
WARNING: Running pip as the 'root' user can result in broken permissions and conflicting behaviour with the system packag
```

## ▼ Notes YEAST\_COB\_Batch constraint-based approach

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

- FMU - BPL\_YEAST\_AIR\_Fedbatch\_linux\_jm\_cs.fmu
- Setup-file - BPL\_YEAST\_AIR\_Fedbatch\_explore

```
%%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_explore.py

Linux - run FMU pre-compiled 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

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

plt.rcParams['figure.figsize'] = [20/2.54, 16/2.54]
```

## ▼ Try using LP in each step

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

# 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.pr)

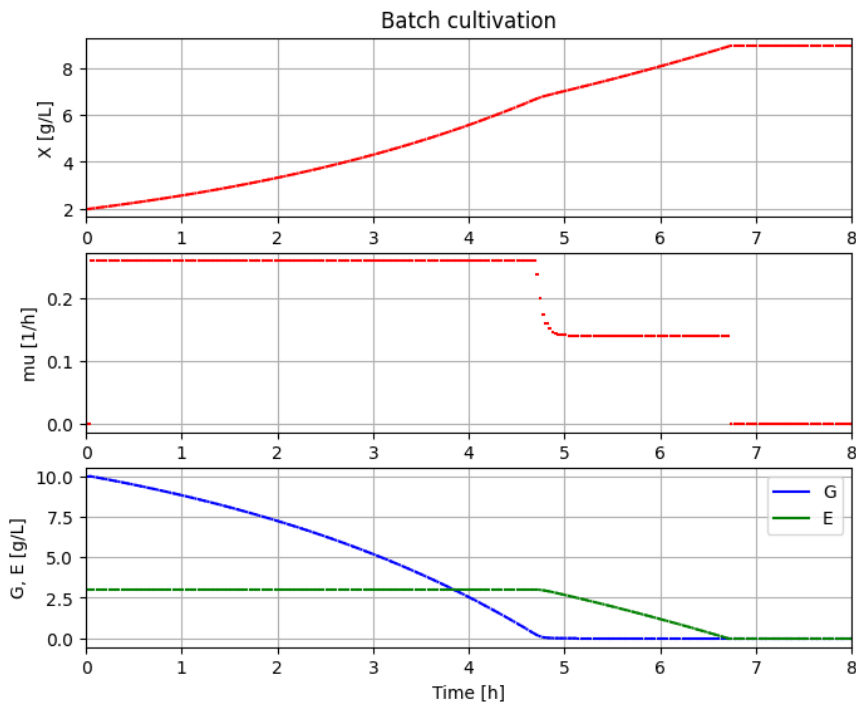
# Initialization
V_0=1.0
init(V_0=V_0, VX_0=V_0*2.0, VG_0=V_0*10, VE_0=3.0)

# 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, 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
-PyFMI: 2.11.0
-FMU by: OpenModelica Compiler OpenModelica 1.21.0
-FMI: 2.0

```

```
-Type: FMUModelME2
-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 version 0.9.7
```

```
!conda list optlang
```

```
# packages in environment at /usr/local:
#
# Name                      Version      Build    Channel
optlang                     1.7.0        pypi_0   pypi
```

✓ 1s completed at 14:10

● ×