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.

```
!lsb_release -a # Actual VM Ubuntu version used by Google
```

```
No LSB modules are available.
Distributor ID: Ubuntu
Description:    Ubuntu 22.04.4 LTS
Release:        22.04
Codename:       jammy
```

```
%env PYTHONPATH=
```

```
env: PYTHONPATH=
```

```
!python --version
```

```
Python 3.11.11
```

```
!wget https://repo.anaconda.com/miniconda/Miniconda3-py311_24.11.1-0-Linux-x86_64.sh
!chmod +x Miniconda3-py311_24.11.1-0-Linux-x86_64.sh
!bash ./Miniconda3-py311_24.11.1-0-Linux-x86_64.sh -b -f -p /usr/local
import sys
sys.path.append('/usr/local/lib/python3.11/site-packages/')
```

```
--2025-02-10 08:30:36--  https://repo.anaconda.com/miniconda/Miniconda3-py311_24.11.1-0-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: 145900576 (139M) [application/octet-stream]
Saving to: ‘Miniconda3-py311_24.11.1-0-Linux-x86_64.sh’

Miniconda3-py311_24 100%[===================>] 139.14M   123MB/s    in 1.1s

2025-02-10 08:30:38 (123 MB/s) - ‘Miniconda3-py311_24.11.1-0-Linux-x86_64.sh’ saved [145900576/145900576]

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
```

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

## Package Plan ##

  environment location: /usr/local

  added / updated specs:
    - conda


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    ca-certificates-2024.12.31 |       h06a4308_0         128 KB
    certifi-2025.1.31          |  py311h06a4308_0         163 KB
    ------------------------------------------------------------
```

```
  Total:         291 KB

  The following packages will be UPDATED:

    ca-certificates                    2024.11.26-h06a4308_0 --> 2024.12.31-h06a4308_0
    certifi                          2024.8.30-py311h06a4308_0 --> 2025.1.31-py311h06a4308_0



  Downloading and Extracting Packages:
  certifi-2025.1.31    | 163 KB    | :   0% 0/1 [00:00<?, ?it/s]
  certifi-2025.1.31    | 163 KB    | : 100% 1.0/1 [00:00<00:00, 18.92it/s]
  ca-certificates-2024 | 128 KB    | : 100% 1.0/1 [00:00<00:00, 18.52it/s]


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

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

```
conda 24.11.1
Python 3.11.11
```

```
!conda config --set channel_priority strict
```

```
!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-1.8.3-py2.py3-none-any.whl.metadata (8.2 kB)
Collecting swiglpk>=5.0.12 (from optlang)
  Downloading swiglpk-5.0.12-cp311-cp311-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-1.8.3-py2.py3-none-any.whl (141 kB)
Downloading swiglpk-5.0.12-cp311-cp311-manylinux_2_17_x86_64.manylinux2014_x86_64.whl (2.3 MB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 2.3/2.3 MB 54.9 MB/s eta 0:00:00
Downloading sympy-1.13.3-py3-none-any.whl (6.2 MB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 6.2/6.2 MB 94.9 MB/s eta 0:00:00
Downloading mpmath-1.3.0-py3-none-any.whl (536 kB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 536.2/536.2 kB 19.5 MB/s eta 0:00:00
Installing collected packages: swiglpk, mpmath, sympy, optlang
Successfully installed mpmath-1.3.0 optlang-1.8.3 swiglpk-5.0.12 sympy-1.13.3
```

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/CONF_2023_10_MODELICA15
```

```
Cloning into 'CONF_2023_10_MODELICA15'...
```

```
%cd CONF_2023_10_MODELICA15
```

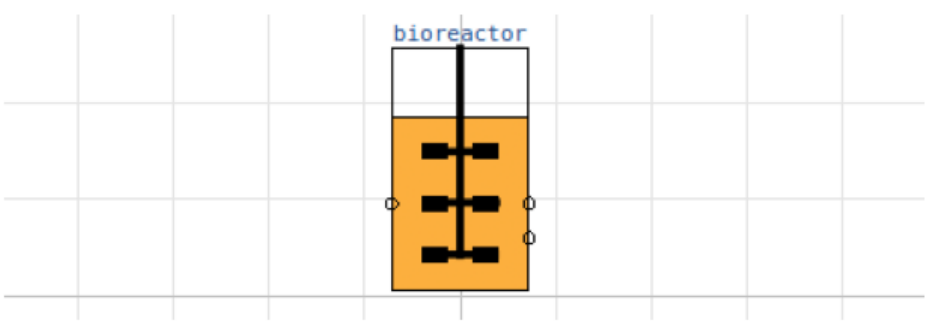
```
/content/CONF_2023_10_MODELICA15
```

```
run -i BPL_YEAST_COB_Batch_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()
```

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

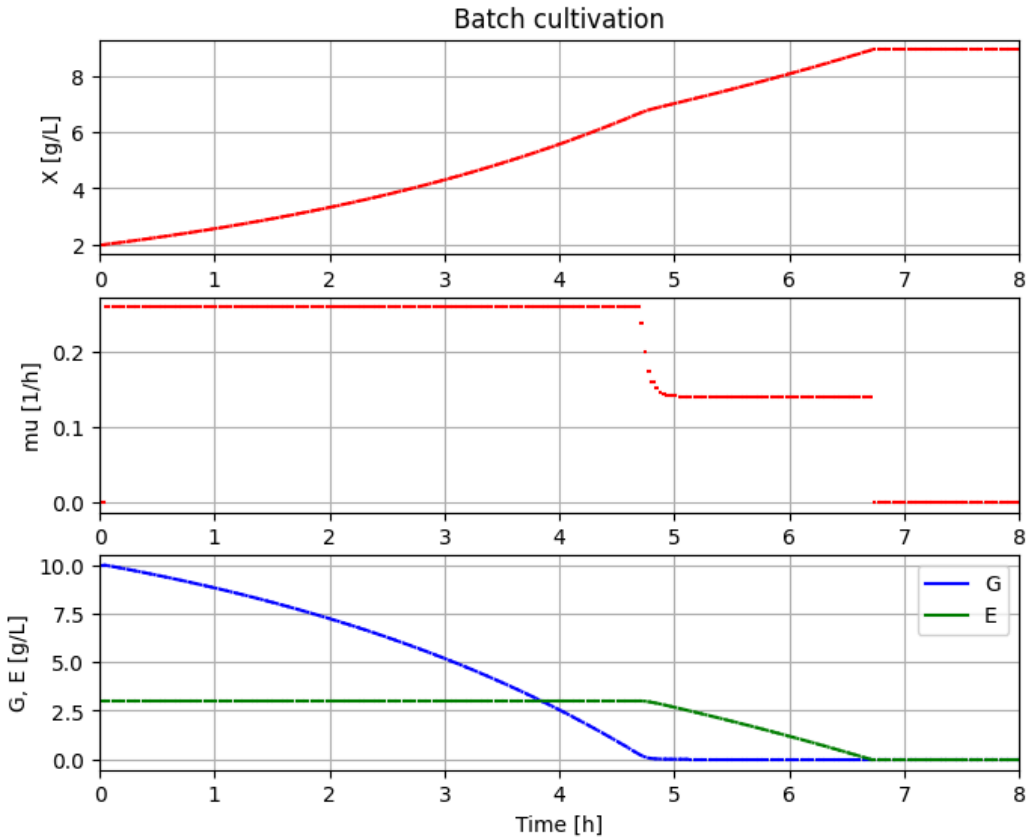
```
process_diagram()
```



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.


# 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]']
    par(mum=mum_opt, qGr=qGr_opt, qEr=qEr_opt, qO2=qO2_opt)
    simu(t_samp, 'cont', options=opts_fast)
```

```
Could not find cannot import name 'dopri5' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/as
Could not find cannot import name 'rodas' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/ass
Could not find cannot import name 'odassl' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/as
Could not find ODEPACK functions.
Could not find RADAR5
Could not find GLIMDA.
```




```
describe('MSL')
```

```
MSL: 3.2.3 - used components: none
```

```
system_info()
```

```
System information
 -OS: Linux
 -Python: 3.11.11
 -Scipy: not installed in the notebook
 -PyFMI: 2.16.3
 -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 0.9.8
```

```
!conda list optlang
```

```
# packages in environment at /usr/local:
#
# Name                    Version                   Build  Channel
optlang                   1.8.3                   pypi_0    pypi
```

Start coding or generate with AI.