BPL_YEAST_COB_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 22.04.4 LTS
    Description:
                      22.04
    Release:
    Codename:
                      iammv
%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 08:31:33-- <a href="https://repo.anaconda.com/miniconda/Miniconda3-py311_24.11.1-0-Linux-x86_64.sh">https://repo.anaconda.com/miniconda/Miniconda3-py311_24.11.1-0-Linux-x86_64.sh</a>
    Resolving repo.anaconda.com (repo.anaconda.com)... 104.16.191.158, 104.16.32.241, 2606:4700::6810:20f1, ...
     Connecting to repo.anaconda.com (repo.anaconda.com)|104.16.191.158|: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
                                                                 119MB/s
                                                                             in 1.2s
    2025-02-10 08:31:34 (119 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:
\rightarrow
     - 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:
                                                   build
        package
         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:

Downloading and Extracting Packages:

certifi-2025.1.31 | 163 KB | : 0% 0/1 [00:00<?, ?it/s] ca-certificates-2024 | 128 KB | : 0% 0/1 [00:00<?, ?it/s]

certifi-2025.1.31 | 163 KB | : 98% 0.9840122040576089/1 [00:00<00:00, 9.14it/s]

ca-certificates-2024 | 128 KB | : 100% 1.0/1 [00:00<00:00, 9.23it/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 fmpy --yes # Install the key package

 $\overline{2}$

```
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-1.8.3-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 40.1 MB/s eta 0:00:00
    Downloading sympy-1.13.3-py3-none-any.whl (6.2 MB)
                                                 6.2/6.2 MB 98.6 MB/s eta 0:00:00
     Downloading mpmath-1.3.0-py3-none-any.whl (536 kB)
                                                536.2/536.2 kB 16.9 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
```

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
The 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:
     - par()
                   - change of parameters and initial values
     - init()

    change initial values only

     - simu()
                   simulate and plot
     - newplot()

    make a new plot

                   - show plot from previous simulation
     - show()
                   - display parameters and initial values from the last simulation
     - disp()
                   - 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()

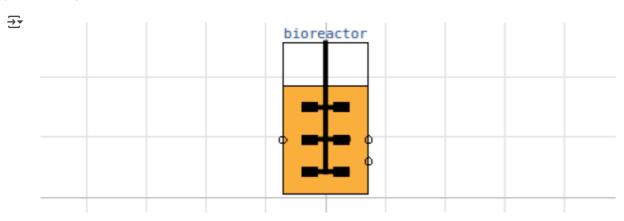
```
%matplotlib inline
plt.rcParams['figure.figsize'] = [25/2.54, 20/2.54]
```

```
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 param

→ Saccharomyces cerevisae - default parameters for strain H1022

```
# Define culture constraint-based model
def culture(G, E):
```

 $\mbox{\# LP}$ 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()
```

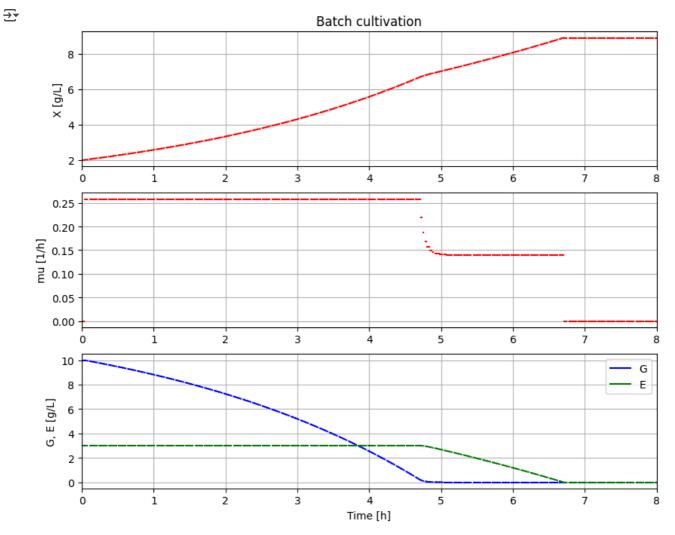
return (yeast_model.objective.value, yeast_model.variables.qGr_opt.primal, yeast_model.variables.qEr_opt.

```
# 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]']
    par(mum=mum_opt, qGr=qGr_opt, qEr=qEr_opt, q02=q02_opt)
    simu(t_samp, 'cont', options=opts_fast)
```



```
describe('MSL')

MSL: 3.2.3 - used components: RealInput, RealOutput

system_info()
```

System information
-OS: Linux
-Python: 3.11.11

-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

Error while loading conda entry point: conda-libmamba-solver (libarchive.so.20: cannot open shared object # packages in environment at /usr/local:

#

Name Version Build Channel optlang 1.8.3 pypi_0 pypi

Start coding or generate with AI.