

✓ 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/')
```

```
➦ --2025-02-07 07:20:06-- https://repo.anaconda.com/miniconda/Miniconda3-py311_24.11.1-0-Linux-x86_64.sh
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 71.1MB/s in 2.0s
```

```
2025-02-07 07:20:08 (71.1 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]
ca-certificates-2024	128 KB	: 0% 0/1 [00:00<?, ?it/s]
certifi-2025.1.31	163 KB	: 100% 1.0/1 [00:00<00:00, 9.54it/s]
ca-certificates-2024	128 KB	: 100% 1.0/1 [00:00<00:00, 8.22it/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 45.9 MB/s eta 0:00:00
Downloading sympy-1.13.3-py3-none-any.whl (6.2 MB)
6.2/6.2 MB 104.9 MB/s eta 0:00:00
Downloading mpmath-1.3.0-py3-none-any.whl (536 kB)
536.2/536.2 kB 17.5 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/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
```

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

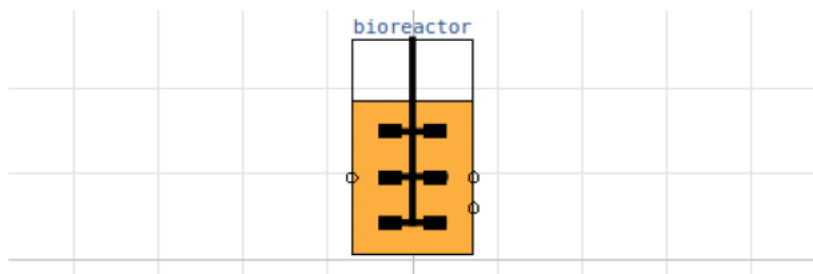
Note that both disp() and describe() takes values from the last simulation and the command process_diagram() brings up the main configuration

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()
```

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



✓ 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
```

```

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, q02lim)

# 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)

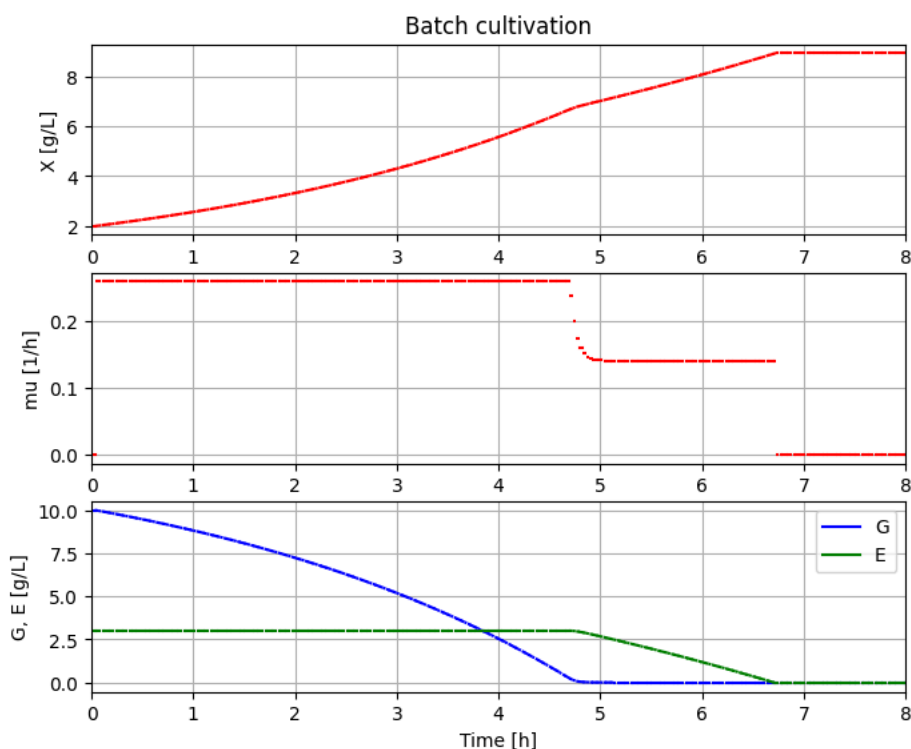
# Loop of simulations
t_final = 8.0
t_samp = 0.0333
n_samp = t_final/t_samp + 1

# 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, 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)

```

↗ Could not find cannot import name 'dopri5' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/assimulo/lib/__i
 Could not find cannot import name 'rodas' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/assimulo/lib/__i
 Could not find cannot import name 'odassl' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/assimulo/lib/__i
 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 1.25.0~dev-133-ga5470be
-FMI: 2.0
-Type: FMUModelME2
-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 version 1.0.0

```
!conda list optlang
```



packages in environment at /usr/local:

#	Name	Version	Build	Channel
#	optlang	1.8.3	pypi_0	pypi