

✓ 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/')
```

```
↳ --2025-03-25 13:13:07-- 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:bf9e, ...
   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 107MB/s in 1.3s
```

```
2025-03-25 13:13:08 (107 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-2025.2.25	h06a4308_0	129 KB
certifi-2025.1.31	py311h06a4308_0	163 KB
openssl-3.0.16	h5eee18b_0	5.2 MB
Total:		5.5 MB

The following packages will be UPDATED:

```

ca-certificates      2024.11.26-h06a4308_0 --> 2025.2.25-h06a4308_0
certifi              2024.8.30-py311h06a4308_0 --> 2025.1.31-py311h06a4308_0
openssl              3.0.15-h5eee18b_0 --> 3.0.16-h5eee18b_0

```

Downloading and Extracting Packages:

```

openssl-3.0.16      | 5.2 MB | : 0% 0/1 [00:00<?, ?it/s]
certifi-2025.1.31   | 163 KB | : 0% 0/1 [00:00<?, ?it/s]

openssl-3.0.16      | 5.2 MB | : 1% 0.011930375800648256/1 [00:00<00:09, 9.15s/it]
certifi-2025.1.31   | 163 KB | : 20% 0.1968024408115218/1 [00:00<00:00, 1.81it/s]

ca-certificates-2025 | 129 KB | : 99% 0.9905458612637259/1 [00:00<00:00, 8.94it/s]

ca-certificates-2025 | 129 KB | : 100% 1.0/1 [00:00<00:00, 8.94it/s]

ca-certificates-2025 | 129 KB | : 100% 1.0/1 [00:00<00:00, 8.94it/s]
certifi-2025.1.31    | 163 KB | : 100% 1.0/1 [00:00<00:00, 1.81it/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 41.5 MB/s eta 0:00:00
Downloading sympy-1.13.3-py3-none-any.whl (6.2 MB)
 6.2/6.2 MB 87.1 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
```

✓ 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-comiled OpenModelica
```

Model for the process 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

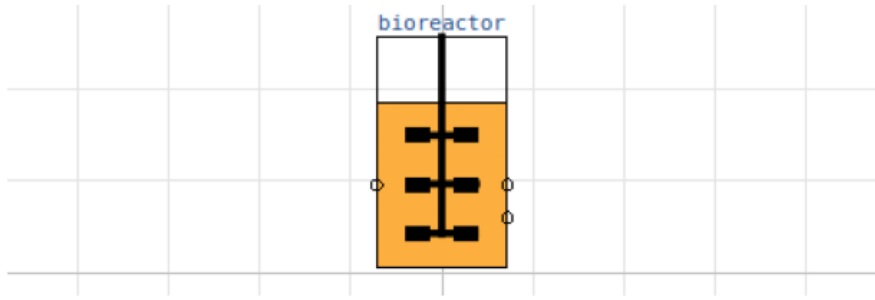
Note that both disp() and describe() takes values from the last simulation and the command process_diagram() brings up the main configuration

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)
```

```
# 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])
```

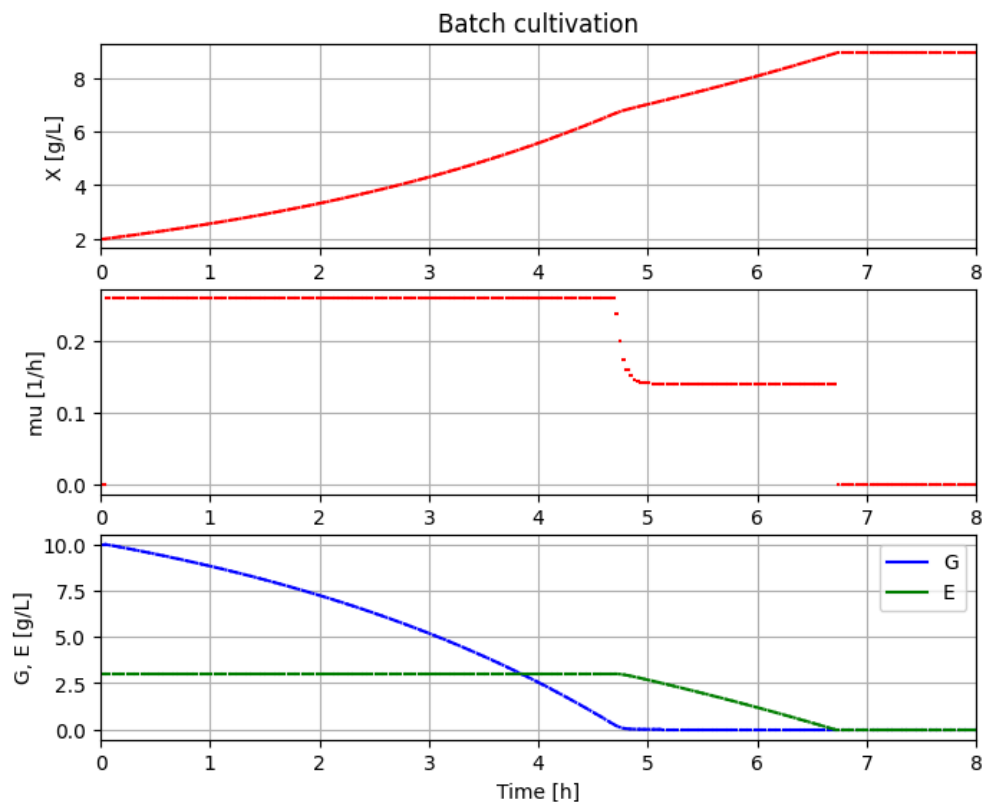
```
    par(mum=mum_opt, qGr=qGr_opt, qEr=qEr_opt, q02=q02_opt)
```

```
    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)
Could not find cannot import name 'rodas' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/assimulo)
Could not find cannot import name 'odassl' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/assimulo)
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

```

