

✓ 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 22.04.3 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.
!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/')
```

```
⇒ --2024-10-03 15:10:52-- https://repo.anaconda.com/miniconda/Miniconda3-py310
Resolving repo.anaconda.com (repo.anaconda.com)... 104.16.32.241, 104.16.191.1
Connecting to repo.anaconda.com (repo.anaconda.com)|104.16.32.241|:443... con
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 110MB/s in 0.6s
```

```
2024-10-03 15:10:53 (110 MB/s) - 'Miniconda3-py310_23.1.0-1-Linux-x86_64.sh' :
```

```
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
```



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

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

```
⇨ conda 23.1.0  
   Python 3.10.15
```

```
!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-1.8.2-py2.py3-none-any.whl (141 kB)
    _____ 141.8/141.8 kB 5.9 MB/s eta 0:00:00
Collecting sympy>=1.12.0
  Downloading sympy-1.13.3-py3-none-any.whl (6.2 MB)
    _____ 6.2/6.2 MB 57.3 MB/s eta 0:00:00
Collecting swiglpk>=5.0.8
  Downloading swiglpk-5.0.10-cp310-cp310-manylinux_2_17_x86_64.manylinux2014_
    _____ 2.3/2.3 MB 45.2 MB/s eta 0:00:00
Collecting mpmath<1.4,>=1.1.0
  Downloading mpmath-1.3.0-py3-none-any.whl (536 kB)
    _____ 536.2/536.2 kB 41.2 MB/s eta 0:
Installing collected packages: swiglpk, mpmath, sympy, optlang
Successfully installed mpmath-1.3.0 optlang-1.8.2 swiglpk-5.0.10 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 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

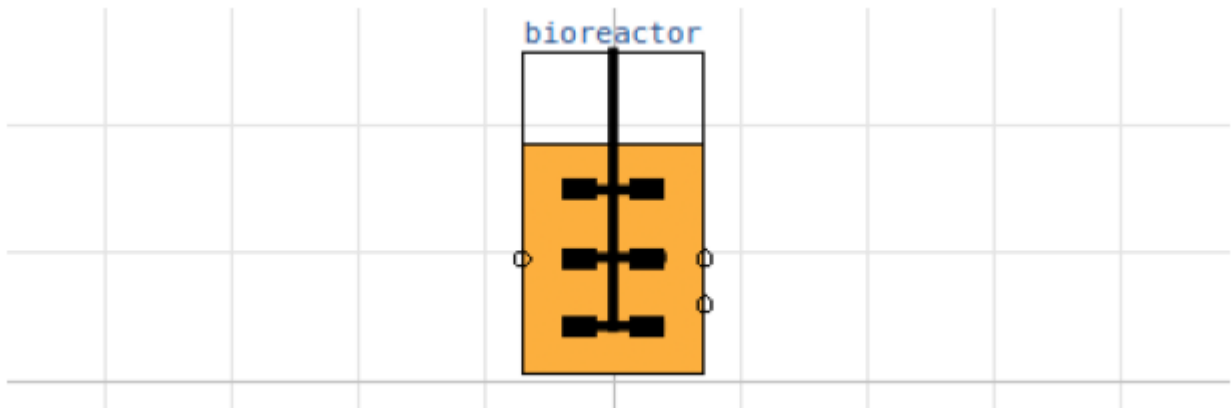
Note that both `disp()` and `describe()` takes values from the last simulation and the command `process_diagram()` brings up the main configuration

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(qO2lim)
yeast_model.add(qGlim)
yeast_model.add(qElim)

# - do LP optimization
yeast_model.optimize()

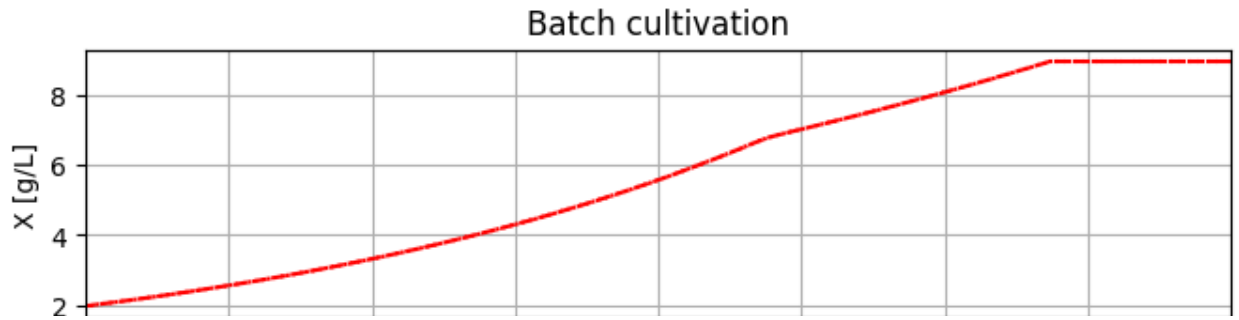
return (yeast_model.objective.value, yeast_model.variables.qGr_opt.primal, ye

# 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

# 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]
    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: 2.14.0
-FMU by: OpenModelica Compiler OpenModelica 1.25.0~dev-51-ge672d09
-FMI: 2.0
-Type: FMUModelME2
-Name: BPL_YEAST_COB.Batch
-Generated: 2024-10-03T17:06:18Z
-MSL: 3.2.3
-Description: Bioprocess Library version 2.2.1 - GUI
-Interaction: FMU-explore version 1.0.0
```

```
!conda list optlang
```



```
# packages in environment at /usr/local:
```

```
#
```

# Name	Version	Build	Channel
optlang	1.8.2	pypi_0	pypi