

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.

```
In [1]: !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
```

```
In [2]: !python --version
```

```
Python 3.11.11
```

```
In [3]: !pip install fmpy
```

```
Collecting fmpy
  Downloading FMPy-0.3.22-py3-none-any.whl.metadata (1.9 kB)
Requirement already satisfied: attrs in /usr/local/lib/python3.11/dist-packages (from fmpy) (25.3.0)
Requirement already satisfied: Jinja2 in /usr/local/lib/python3.11/dist-packages (from fmpy) (3.1.6)
Collecting lark (from fmpy)
  Downloading lark-1.2.2-py3-none-any.whl.metadata (1.8 kB)
Requirement already satisfied: lxml in /usr/local/lib/python3.11/dist-packages (from fmpy) (5.3.1)
Requirement already satisfied: msgpack in /usr/local/lib/python3.11/dist-packages (from fmpy) (1.1.0)
Requirement already satisfied: numpy in /usr/local/lib/python3.11/dist-packages (from fmpy) (2.0.2)
Requirement already satisfied: MarkupSafe>=2.0 in /usr/local/lib/python3.11/dist-packages (from Jinja2->fmpy) (3.0.2)
Downloading FMPy-0.3.22-py3-none-any.whl (4.9 MB)
----- 4.9/4.9 MB 30.6 MB/s eta 0:00:00
Downloading lark-1.2.2-py3-none-any.whl (111 kB)
----- 111.0/111.0 kB 3.6 MB/s eta 0:00:00
Installing collected packages: lark, fmpy
Successfully installed fmpy-0.3.22 lark-1.2.2
```

```
In [4]: # 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)
Requirement already satisfied: sympy>=1.12.0 in /usr/local/lib/python3.11/dist-packages (from optlang) (1.13.1)
Requirement already satisfied: mpmath<1.4,>=1.1.0 in /usr/local/lib/python3.11/dist-packages (from sympy>=1.12.0->optlang) (1.3.0)
Downloading optlang-1.8.3-py2.py3-none-any.whl (141 kB)
_____ 141.8/141.8 kB 2.8 MB/s eta 0:00:00
Downloading swiglpk-5.0.12-cp311-cp311-manylinux_2_17_x86_64.manylinux2014_x86_64.whl (2.3 MB)
_____ 2.3/2.3 MB 17.1 MB/s eta 0:00:00
Installing collected packages: swiglpk, optlang
Successfully installed optlang-1.8.3 swiglpk-5.0.12

```

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

```
In [5]: %%bash
git clone https://github.com/janpeter19/CONF_2023_10_MODELICA15
```

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

```
In [6]: %cd CONF_2023_10_MODELICA15
/content/CONF_2023_10_MODELICA15
```

```
In [7]: run -i BPL_YEAST_COB_Batch_fmpy_explore.py
```

Linux - run FMU pre-compiled 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()

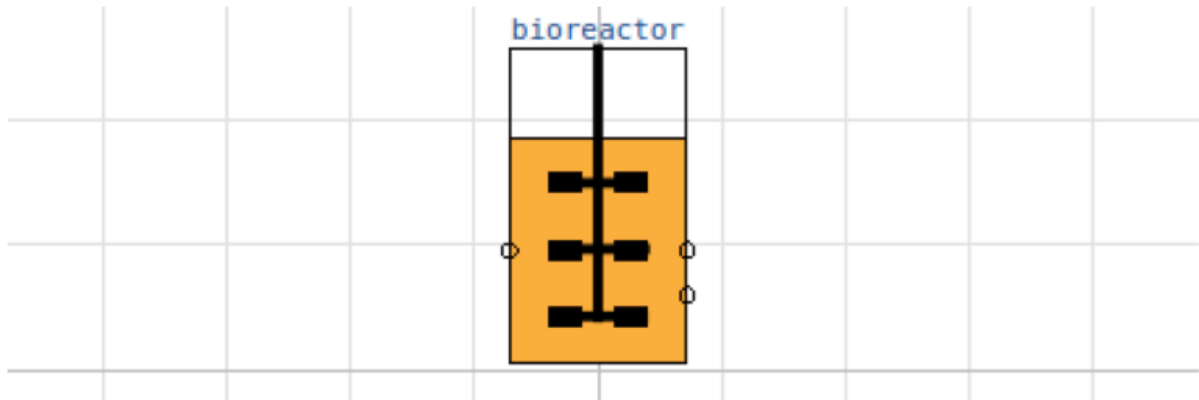
```
In [8]: %matplotlib inline
plt.rcParams['figure.figsize'] = [25/2.54, 20/2.54]
```

```
In [9]: import warnings
warnings.filterwarnings("ignore")
```

BPL_YEAST_COB_Batch - demo

```
In [10]: from optlang import Model, Variable, Constraint, Objective
```

```
In [11]: process_diagram()
```



```
In [12]: describe('culture'); print(); #describe('liquidphase')
```

Saccharomyces cerevisiae - default parameters for strain H1022

```
In [13]: # 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, yeas

```

```

In [14]: # 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)

```

```

In [15]: # Loop of simulations
t_final = 8.0
t_samp = 0.0333
n_samp = t_final/t_samp + 1

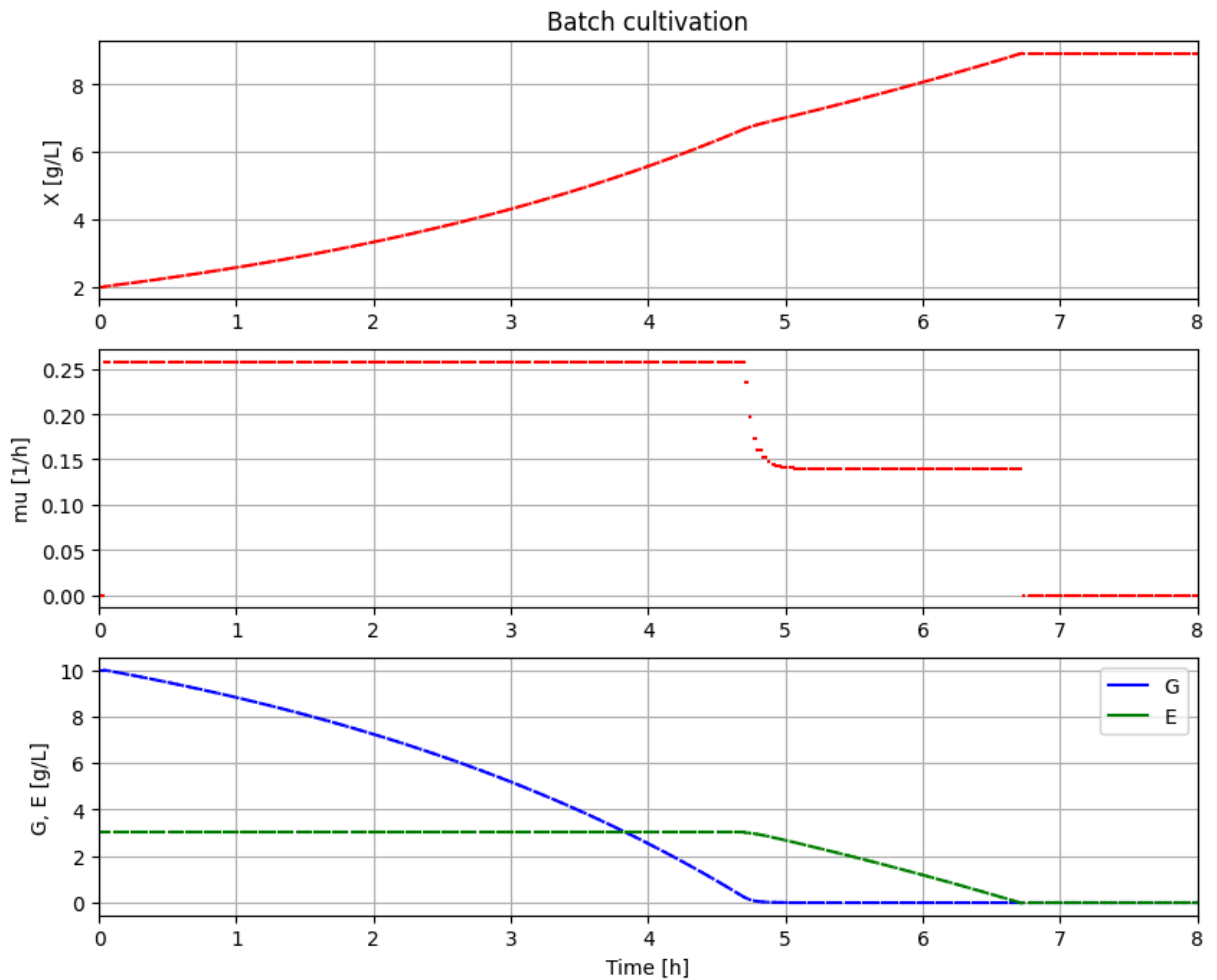
```

```

In [16]: # 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)

```



```
In [17]: describe('MSL')
```

MSL: 3.2.3 - used components: RealInput, RealOutput

```
In [18]: system_info()
```

System information

- OS: Linux
- Python: 3.11.11
- Scipy: not installed in the notebook
- FMPy: 0.3.22
- 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

```
In [19]: !pip show optlang|grep Version
```

Version: 1.8.3

```
In [19]:
```