

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.

```
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]: %env PYTHONPATH=
```

```
env: PYTHONPATH=
```

```
In [3]: !python --version
```

```
Python 3.11.11
```

```
In [4]: !wget https://repo.anaconda.com/miniconda/Miniconda3-py311_24.11.1-0-Linux-x86_64.s  
!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/')
```

```
--2025-03-27 08:38:47-- 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  139MB/s   in 1.0s

2025-03-27 08:38:48 (139 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.
```

```
In [5]: !conda update -n base -c defaults conda --yes
```

Channels:
- defaults
Platform: linux-64
Collecting package metadata (repodata.json): - 00\ 00| 00/ 00- 00\ 00| 00/ 00- 00\
00| 00/ 00- 00done
Solving environment: | 00/ 00done

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]
ca-certificates-2025	129 KB	: 0% 0/1 [00:00<?, ?it/s]
ca-certificates-2025	129 KB	: 100% 1.0/1 [00:00<00:00, 11.30it/s]
certifi-2025.1.31	163 KB	: 100% 1.0/1 [00:00<00:00, 9.87it/s]
certifi-2025.1.31	163 KB	: 100% 1.0/1 [00:00<00:00, 9.87it/s]
openssl-3.0.16	5.2 MB	: 6% 0.056669285053079214/1 [00:00<00:01, 1.89s/it]
ca-certificates-2025	129 KB	: 100% 1.0/1 [00:00<00:00, 9.58it/s]

Preparing transaction: - 00done
Verifying transaction: | 00/ 00- 00done
Executing transaction: | 00done

```
In [6]: !conda --version  
        !python --version
```

```
conda 24.11.1  
Python 3.11.11
```

```
In [7]: !conda config --set channel_priority strict
```

```
In [8]: !conda install -c conda-forge pyfmi --yes # Install the key package
```

```
Channels:
- conda-forge
- defaults
Platform: linux-64
Collecting package metadata (repodata.json): - 22\ 22| 22/ 22- 22\ 22| 22/ 22- 22\
22| 22/ 22- 22\ 22| 22/ 22- 22\ 22| 22/ 22- 22\ 22| 22/ 22- 22\ 22| 22/ 22- 22\ 22|
22/ 22- 22\ 22| 22/ 22- 22\ 22| 22/ 22- 22\ 22| 22/ 22- 22\ 22| 22/ 22- 22\ 22done
Solving environment: / 22- 22\ 22| 22/ 22done
```

Package Plan

environment location: /usr/local

added / updated specs:

- pyfmi

The following packages will be downloaded:

package	build		
-----	-----		
_x86_64-microarch-level-3	2_broadwell	8 KB	conda-forge
assimulo-3.6.0	py311h083bc19_0	1.1 MB	conda-forge
certifi-2025.1.31	pyhd8ed1ab_0	159 KB	conda-forge
conda-25.3.0	py311h38be061_0	1.1 MB	conda-forge
fmilib-2.4.1	hac33072_1	383 KB	conda-forge
gmp-6.3.0	hac33072_2	449 KB	conda-forge
libamd-3.3.3	haaf9dc3_7100102	49 KB	conda-forge
libblas-3.9.0	31_h59b9bed_openblas	16 KB	conda-forge
libbtf-2.3.2	h32481e8_7100102	27 KB	conda-forge
libcamd-3.3.3	h32481e8_7100102	46 KB	conda-forge
libcbblas-3.9.0	31_he106b2a_openblas	16 KB	conda-forge
libccolamd-3.3.4	h32481e8_7100102	42 KB	conda-forge
libcholmod-5.3.1	h59ddab4_7100102	1.1 MB	conda-forge
libcolamd-3.3.4	h32481e8_7100102	33 KB	conda-forge
libcxsparse-4.4.1	h32481e8_7100102	118 KB	conda-forge
libgcc-14.2.0	h767d61c_2	828 KB	conda-forge
libgcc-ng-14.2.0	h69a702a_2	52 KB	conda-forge
libgfortran-14.2.0	h69a702a_2	52 KB	conda-forge
libgfortran-ng-14.2.0	h69a702a_2	53 KB	conda-forge
libgfortran5-14.2.0	hf1ad2bd_2	1.4 MB	conda-forge
libgomp-14.2.0	h767d61c_2	449 KB	conda-forge
libklu-2.3.5	hf24d653_7100102	142 KB	conda-forge
liblapack-3.9.0	31_h7ac8fdf_openblas	16 KB	conda-forge
libldl-3.3.2	h32481e8_7100102	24 KB	conda-forge
libopenblas-0.3.29	pthreads_h94d23a6_0	5.6 MB	conda-forge
libparu-1.0.0	h17147ab_7100102	91 KB	conda-forge
librbio-4.3.4	h32481e8_7100102	47 KB	conda-forge
libspex-3.2.3	had10066_7100102	79 KB	conda-forge
libspqr-4.3.4	h852d39f_7100102	213 KB	conda-forge
libstdcxx-14.2.0	h8f9b012_2	3.7 MB	conda-forge
libstdcxx-ng-14.2.0	h4852527_2	53 KB	conda-forge
libsuitesparseconfig-7.10.1	h92d6892_7100102	42 KB	conda-forge
libumfpack-6.3.5	heb53515_7100102	424 KB	conda-forge
metis-5.1.0	hd0bcaf9_1007	3.7 MB	conda-forge
mpfr-4.2.1	h90cbb55_3	620 KB	conda-forge

numpy-2.2.4	py311h5d046bc_0	8.6 MB	conda-forge
openssl-3.4.1	h7b32b05_0	2.8 MB	conda-forge
pyfmi-2.16.3	py311h9f3472d_0	5.2 MB	conda-forge
python_abi-3.11	2_cp311	5 KB	conda-forge
scipy-1.15.2	py311h8f841c2_0	16.4 MB	conda-forge
suitesparse-7.10.1	ha0f6916_7100102	12 KB	conda-forge
sundials-7.1.1	ha52427a_0	907 KB	conda-forge

Total:		56.1 MB	

The following NEW packages will be INSTALLED:

_x86_64-microarch~	conda-forge/noarch::_x86_64-microarch-level-3-2_broadwell
assimulo	conda-forge/linux-64::assimulo-3.6.0-py311h083bc19_0
fmilib	conda-forge/linux-64::fmilib-2.4.1-hac33072_1
gmp	conda-forge/linux-64::gmp-6.3.0-hac33072_2
libamd	conda-forge/linux-64::libamd-3.3.3-haaf9dc3_7100102
libblas	conda-forge/linux-64::libblas-3.9.0-31_h59b9bed_openblas
libbtf	conda-forge/linux-64::libbtf-2.3.2-h32481e8_7100102
libcamd	conda-forge/linux-64::libcamd-3.3.3-h32481e8_7100102
libcbblas	conda-forge/linux-64::libcbblas-3.9.0-31_he106b2a_openblas
libccolamd	conda-forge/linux-64::libccolamd-3.3.4-h32481e8_7100102
libcholmod	conda-forge/linux-64::libcholmod-5.3.1-h59ddab4_7100102
libcolamd	conda-forge/linux-64::libcolamd-3.3.4-h32481e8_7100102
libcxsparse	conda-forge/linux-64::libcxsparse-4.4.1-h32481e8_7100102
libgcc	conda-forge/linux-64::libgcc-14.2.0-h767d61c_2
libgfortran	conda-forge/linux-64::libgfortran-14.2.0-h69a702a_2
libgfortran-ng	conda-forge/linux-64::libgfortran-ng-14.2.0-h69a702a_2
libgfortran5	conda-forge/linux-64::libgfortran5-14.2.0-hf1ad2bd_2
libklu	conda-forge/linux-64::libklu-2.3.5-hf24d653_7100102
liblapack	conda-forge/linux-64::liblapack-3.9.0-31_h7ac8fdf_openblas
libldl	conda-forge/linux-64::libldl-3.3.2-h32481e8_7100102
libopenblas	conda-forge/linux-64::libopenblas-0.3.29-pthreads_h94d23a6_0
libparu	conda-forge/linux-64::libparu-1.0.0-h17147ab_7100102
librbio	conda-forge/linux-64::librbio-4.3.4-h32481e8_7100102
libspex	conda-forge/linux-64::libspex-3.2.3-had10066_7100102
libspqr	conda-forge/linux-64::libspqr-4.3.4-h852d39f_7100102
libstdcxx	conda-forge/linux-64::libstdcxx-14.2.0-h8f9b012_2
libsuitesparsecon~	conda-forge/linux-64::libsuitesparseconfig-7.10.1-h92d6892_7100102
libumfpack	conda-forge/linux-64::libumfpack-6.3.5-heb53515_7100102
metis	conda-forge/linux-64::metis-5.1.0-hd0bc9f9_1007
mpfr	conda-forge/linux-64::mpfr-4.2.1-h90cbb55_3
numpy	conda-forge/linux-64::numpy-2.2.4-py311h5d046bc_0
pyfmi	conda-forge/linux-64::pyfmi-2.16.3-py311h9f3472d_0
python_abi	conda-forge/linux-64::python_abi-3.11-2_cp311
scipy	conda-forge/linux-64::scipy-1.15.2-py311h8f841c2_0
suitesparse	conda-forge/linux-64::suitesparse-7.10.1-ha0f6916_7100102
sundials	conda-forge/linux-64::sundials-7.1.1-ha52427a_0

The following packages will be UPDATED:

conda	pkgs/main::conda-24.11.1-py311h06a430~ --> conda-forge::conda-25.3.0-py311h38be061_0
libgcc-ng	pkgs/main::libgcc-ng-11.2.0-h1234567_1 --> conda-forge::libgcc-ng-14.2.0-h69a702a_2

```
libgomp                pkgs/main::libgomp-11.2.0-h1234567_1 --> conda-forge::libgomp
-14.2.0-h767d61c_2
libstdcxx-ng           pkgs/main::libstdcxx-ng-11.2.0-h12345~ --> conda-forge::libstdc
xx-ng-14.2.0-h4852527_2
openssl                pkgs/main::openssl-3.0.16-h5eee18b_0 --> conda-forge::openssl
-3.4.1-h7b32b05_0
```

The following packages will be SUPERSEDED by a higher-priority channel:

```
certifi                pkgs/main/linux-64::certifi-2025.1.31~ --> conda-forge/noarch::
certifi-2025.1.31-pyhd8ed1ab_0
```

Downloading and Extracting Packages:

```
scipy-1.15.2           | 16.4 MB | : 0% 0/1 [00:00<?, ?it/s]
numpy-2.2.4            | 8.6 MB  | : 0% 0/1 [00:00<?, ?it/s]
```

```
libopenblas-0.3.29    | 5.6 MB  | : 0% 0/1 [00:00<?, ?it/s]
```

```
pyfmi-2.16.3          | 5.2 MB  | : 0% 0/1 [00:00<?, ?it/s]
```

```
metis-5.1.0           | 3.7 MB  | : 0% 0/1 [00:00<?, ?it/s]
```

```
libstdcxx-14.2.0      | 3.7 MB  | : 0% 0/1 [00:00<?, ?it/s]
```

```
openssl-3.4.1         | 2.8 MB  | : 0% 0/1 [00:00<?, ?it/s]
```

```
libgfortran5-14.2.0   | 1.4 MB  | : 0% 0/1 [00:00<?, ?it/s]
```

```
conda-25.3.0          | 1.1 MB  | : 0% 0/1 [00:00<?, ?it/s]
```

assimulo-3.6.0 | 1.1 MB | : 0% 0/1 [00:00<?, ?it/s]

libcholmod-5.3.1 | 1.1 MB | : 0% 0/1 [00:00<?, ?it/s]

sundials-7.1.1 | 907 KB | : 0% 0/1 [00:00<?, ?it/s]

libgcc-14.2.0 | 828 KB | : 0% 0/1 [00:00<?, ?it/s]

mpfr-4.2.1 | 620 KB | : 0% 0/1 [00:00<?, ?it/s]

gmp-6.3.0 | 449 KB | : 0% 0/1 [00:00<?, ?it/s]

libgomp-14.2.0 | 449 KB | : 0% 0/1 [00:00<?, ?it/s]

libumfpack-6.3.5 | 424 KB | : 0% 0/1 [00:00<?, ?it/s]

fmilib-2.4.1	383 KB	:	0% 0/1 [00:00<?, ?it/s]
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libspqr-4.3.4	213 KB	:	0% 0/1 [00:00<?, ?it/s]
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... (more hidden) ...			
scipy-1.15.2	16.4 MB	:	0% 0.0038117559308295653/1 [00:00<00:28, 28.21s/it]
libopenblas-0.3.29	5.6 MB	:	1% 0.005535800927408837/1 [00:00<00:19, 19.42s/it]
pyfmi-2.16.3	5.2 MB	:	1% 0.005967906113297332/1 [00:00<00:17, 17.46s/it]
metis-5.1.0	3.7 MB	:	1% 0.008351599057998349/1 [00:00<00:12, 12.13s/it]
numpy-2.2.4	8.6 MB	:	22% 0.2201477554182317/1 [00:00<00:00, 1.28it/s]
scipy-1.15.2	16.4 MB	:	17% 0.17152901688733044/1 [00:00<00:00, 1.07

s/it]

pyfmi-2.16.3 t/s]	5.2 MB	: 41% 0.4058176157042186/1 [00:00<00:00, 2.30i
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metis-5.1.0 t/s]	3.7 MB	: 75% 0.7516439152198514/1 [00:00<00:00, 4.04i
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scipy-1.15.2 t/s]	16.4 MB	: 38% 0.38022265410024914/1 [00:00<00:00, 1.38i
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scipy-1.15.2 t/s]	16.4 MB	: 62% 0.6203632777425118/1 [00:00<00:00, 1.68i
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libstdcxx-14.2.0 58s/it]	3.7 MB	: 0% 0.0042177278432850495/1 [00:00<01:43, 103.
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libopenblas-0.3.29	5.6 MB	: 100% 1.0/1 [00:00<00:00, 2.15it/s]
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libopenblas-0.3.29	5.6 MB	: 100% 1.0/1 [00:00<00:00, 2.15it/s]
--------------------	--------	--------------------------------------

pyfmi-2.16.3	5.2 MB	: 100% 1.0/1 [00:00<00:00, 2.17it/s]
--------------	--------	--------------------------------------

pyfmi-2.16.3	5.2 MB	: 100% 1.0/1 [00:00<00:00, 2.17it/s]
--------------	--------	--------------------------------------

libgfortran5-14.2.0 s/it]	1.4 MB	: 1% 0.011206734985068174/1 [00:00<00:46, 47.21
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libstdcxx-14.2.0 t/s]	3.7 MB	: 46% 0.45551460707478536/1 [00:00<00:00, 1.12i
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scipy-1.15.2 t/s]	16.4 MB	: 79% 0.7871275997163052/1 [00:00<00:00, 1.48i
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libgfortran5-14.2.0 | 1.4 MB | : 100% 1.0/1 [00:00<00:00, 2.07it/s]

scipy-1.15.2 | 16.4 MB | : 98% 0.9777153962577835/1 [00:00<00:00, 1.60it/s]

conda-25.3.0 | 1.1 MB | : 1% 0.01395284272989957/1 [00:00<00:48, 49.14s/it]
numpy-2.2.4 | 8.6 MB | : 100% 1.0/1 [00:00<00:00, 1.20it/s]
numpy-2.2.4 | 8.6 MB | : 100% 1.0/1 [00:00<00:00, 1.20it/s]

openssl-3.4.1 | 2.8 MB | : 100% 1.0/1 [00:00<00:00, 1.60it/s]

openssl-3.4.1 | 2.8 MB | : 100% 1.0/1 [00:00<00:00, 1.60it/s]

libstdcxx-14.2.0 | 3.7 MB | : 100% 1.0/1 [00:00<00:00, 1.57it/s]

libstdcxx-14.2.0 | 3.7 MB | : 100% 1.0/1 [00:00<00:00, 1.57it/s]

conda-25.3.0 | 1.1 MB | : 100% 1.0/1 [00:00<00:00, 1.64it/s]

conda-25.3.0 | 1.1 MB | : 100% 1.0/1 [00:00<00:00, 1.64it/s]

assimulo-3.6.0 | 1.1 MB | : 1% 0.014703493605362324/1 [00:00<00:56, 57.55
s/it]

sundials-7.1.1 | 907 KB | : 2% 0.01763373830085844/1 [00:00<00:48, 48.89
s/it]

libcholmod-5.3.1 | 1.1 MB | : 1% 0.014870549794649543/1 [00:00<00:57, 58.15
s/it]

libgcc-14.2.0 | 828 KB | : 2% 0.01932337522187561/1 [00:00<00:44, 44.88
s/it]

libcholmod-5.3.1 | 1.1 MB | : 100% 1.0/1 [00:00<00:00, 58.15s/it]

assimulo-3.6.0 | 1.1 MB | : 100% 1.0/1 [00:00<00:00, 57.55s/it]

libgcc-14.2.0 | 828 KB | : 100% 1.0/1 [00:00<00:00, 44.88s/it]

sundials-7.1.1 | 907 KB | : 100% 1.0/1 [00:00<00:00, 48.89s/it]

gmp-6.3.0 | 449 KB | : 4% 0.03561313321233331/1 [00:00<00:26, 27.01
s/it]

mpfr-4.2.1 s/it]	620 KB	:	3% 0.025811696239942908/1 [00:00<00:37, 38.04
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libgomp-14.2.0 s/it]	449 KB	:	4% 0.03562807972826631/1 [00:00<00:26, 27.72
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libumfpack-6.3.5 s/it]	424 KB	:	4% 0.037731330084655984/1 [00:01<00:25, 26.42
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gmp-6.3.0 | 449 KB | : 100% 1.0/1 [00:01<00:00, 27.01s/it]

libgomp-14.2.0 | 449 KB | : 100% 1.0/1 [00:01<00:00, 27.72s/it]

libumfpack-6.3.5 | 424 KB | : 100% 1.0/1 [00:01<00:00, 26.42s/it]

mpfr-4.2.1 | 620 KB | : 100% 1.0/1 [00:01<00:00, 38.04s/it]

libspqr-4.3.4	213 KB	: 8% 0.07503068271326775/1 [00:01<00:13, 14.43s/it]
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libspqr-4.3.4	213 KB	: 100% 1.0/1 [00:01<00:00, 14.43s/it]
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... (more hidden) ...

fmilib-2.4.1	383 KB	: 4% 0.04180391656566945/1 [00:01<00:25, 26.16s/it]
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... (more hidden) ...

fmilib-2.4.1	383 KB	: 100% 1.0/1 [00:01<00:00, 26.16s/it]
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scipy-1.15.2	16.4 MB	: 100% 1.0/1 [00:01<00:00, 1.60it/s]
--------------	---------	--------------------------------------

pyfmi-2.16.3	5.2 MB	: 100% 1.0/1 [00:01<00:00, 2.17it/s]
--------------	--------	--------------------------------------

libopenblas-0.3.29	5.6 MB	: 100% 1.0/1 [00:01<00:00, 2.15it/s]
--------------------	--------	--------------------------------------

libgfortran5-14.2.0 | 1.4 MB | : 100% 1.0/1 [00:01<00:00, 2.07it/s]

openssl-3.4.1 | 2.8 MB | : 100% 1.0/1 [00:01<00:00, 1.60it/s]

libstdcxx-14.2.0 | 3.7 MB | : 100% 1.0/1 [00:02<00:00, 1.57it/s]

conda-25.3.0 | 1.1 MB | : 100% 1.0/1 [00:02<00:00, 1.64it/s]

libcholmod-5.3.1 | 1.1 MB | : 100% 1.0/1 [00:02<00:00, 2.19s/it]

libcholmod-5.3.1 | 1.1 MB | : 100% 1.0/1 [00:02<00:00, 2.19s/it]

assimulo-3.6.0 | 1.1 MB | : 100% 1.0/1 [00:02<00:00, 2.37s/it]

assimulo-3.6.0 | 1.1 MB | : 100% 1.0/1 [00:02<00:00, 2.37s/it]

libgcc-14.2.0 | 828 KB | : 100% 1.0/1 [00:02<00:00, 2.47s/it]

libgcc-14.2.0 | 828 KB | : 100% 1.0/1 [00:02<00:00, 2.47s/it]

sundials-7.1.1 | 907 KB | : 100% 1.0/1 [00:02<00:00, 2.65s/it]

sundials-7.1.1 | 907 KB | : 100% 1.0/1 [00:02<00:00, 2.65s/it]

gmp-6.3.0 | 449 KB | : 100% 1.0/1 [00:02<00:00, 2.67s/it]

gmp-6.3.0 | 449 KB | : 100% 1.0/1 [00:02<00:00, 2.67s/it]

libgomp-14.2.0 | 449 KB | : 100% 1.0/1 [00:03<00:00, 2.73s/it]

libgomp-14.2.0 | 449 KB | : 100% 1.0/1 [00:03<00:00, 2.73s/it]
numpy-2.2.4 | 8.6 MB | : 100% 1.0/1 [00:03<00:00, 1.20it/s]

libumfpack-6.3.5 | 424 KB | : 100% 1.0/1 [00:03<00:00, 2.76s/it]

libumfpack-6.3.5 | 424 KB | : 100% 1.0/1 [00:03<00:00, 2.76s/it]

libspqr-4.3.4 | 213 KB | : 100% 1.0/1 [00:03<00:00, 2.79s/it]

libspqr-4.3.4 | 213 KB | : 100% 1.0/1 [00:03<00:00, 2.79s/it]

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mpfr-4.2.1 | 620 KB | : 100% 1.0/1 [00:03<00:00, 2.82s/it]

mpfr-4.2.1 | 620 KB | : 100% 1.0/1 [00:03<00:00, 2.82s/it]

fmilib-2.4.1 | 383 KB | : 100% 1.0/1 [00:03<00:00, 2.85s/it]

scipy-1.15.2 | 16.4 MB | : 100% 1.0/1 [00:04<00:00, 1.60it/s]


```
Preparing transaction: - 00\ 00done
Verifying transaction: / 00- 00\ 00| 00/ 00done
Executing transaction: \ 00| 00/ 00- 00\ 00| 00/ 00- 00\ 00| 00/ 00- 00\ 00| 00/ 00-
00\ 00| 00done
```

In [9]: `!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.wh
l (2.3 MB)
_____ 2.3/2.3 MB 46.6 MB/s eta 0:00:00
Downloading sympy-1.13.3-py3-none-any.whl (6.2 MB)
_____ 6.2/6.2 MB 101.5 MB/s eta 0:00:00
Downloading mpmath-1.3.0-py3-none-any.whl (536 kB)
_____ 536.2/536.2 kB 20.5 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

```
In [10]: %%bash
git clone https://github.com/janpeter19/CONF_2023_10_MODELICA15
```

Cloning into 'CONF_2023_10_MODELICA15'...

```
In [11]: %cd CONF_2023_10_MODELICA15

/content/CONF_2023_10_MODELICA15
```

```
In [12]: run -i BPL_YEAST_COB_Batch_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

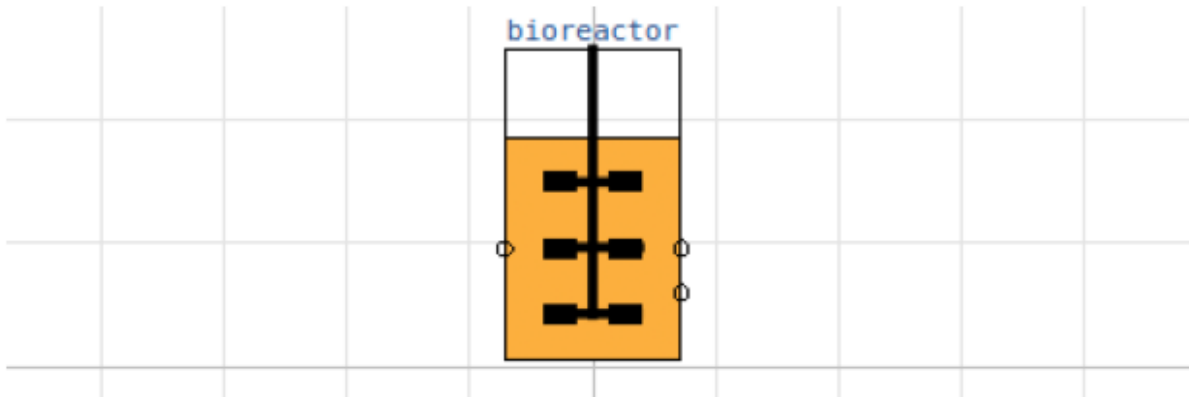
Note that both disp() and describe() takes values from the last simulation and the command process_diagram() brings up the main configuration

Brief information about a command by help(), eg help(simu)

Key system information is listed with the command system_info()

```
In [13]: plt.rcParams['figure.figsize'] = [20/2.54, 16/2.54]
```

```
In [14]: process_diagram()
```

Try using LP in each step

```
In [15]: from optlang import Model, Variable, Constraint, Objective
```

```
In [16]: # 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
```

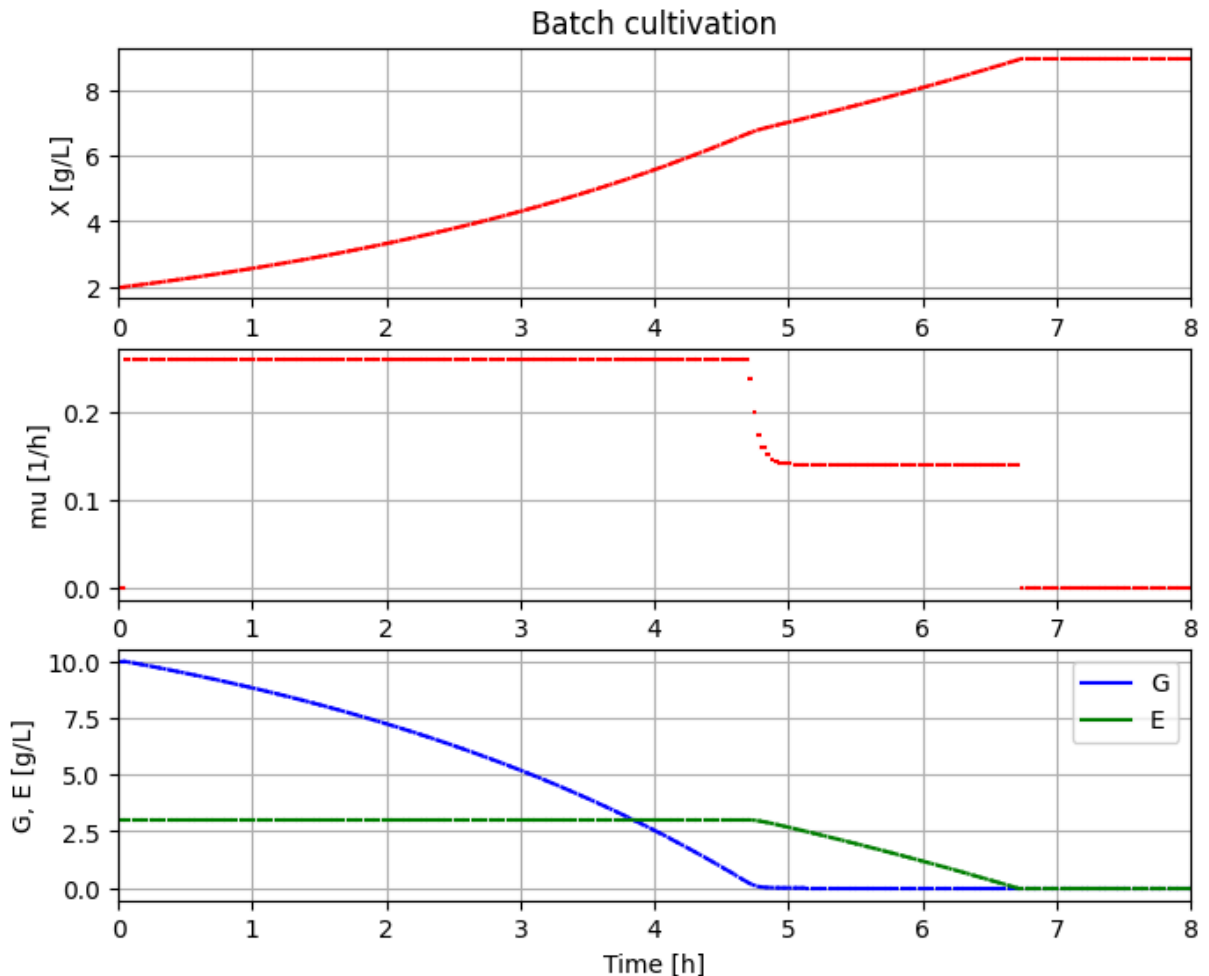
```
In [17]: # Initialization
V_0=1.0
init(V_0=V_0, VX_0=V_0*2.0, VG_0=V_0*10, VE_0=3.0)
```

```
In [18]: # Loop of simulations
t_final = 8.0
t_samp = 0.0333
n_samp = t_final/t_samp + 1
```

```
In [19]: # 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)
```

Could not find cannot import name 'dopri5' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/assimulo/lib/__init__.py)
 Could not find cannot import name 'rodas' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/assimulo/lib/__init__.py)
 Could not find cannot import name 'odassl' from 'assimulo.lib' (/usr/local/lib/python3.11/site-packages/assimulo/lib/__init__.py)
 Could not find ODEPACK functions.
 Could not find RADAR5
 Could not find GLIMDA.



```
In [20]: describe('MSL')
```

```
MSL: 3.2.3 - used components: none
```

```
In [21]: 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 1.21.0
```

```
-FMI: 2.0
```

```
-Type: FMUModelME2
```

```
-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 version 0.9.8
```

```
In [22]: !conda list optlang
```

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

```
#
```

# Name	Version	Build	Channel
optlang	1.8.3	pypi_0	pypi

```
In [22]:
```