Open in Colab

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/')
```

```
--2025-03-26 15:06:31--  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, 26
06:4700::6810:20f1, ...
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   137MB/s    in 1.0s

2025-03-26 15:06:32 (137 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): - \ | / - \ | / - \
| / - 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-py311h06a4
308_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, 18.44it/s]
certifi-2025.1.31    | 163 KB    | : 100% 1.0/1 [00:00<00:00, 13.09it/s]

ca-certificates-2025 | 129 KB    | : 100% 1.0/1 [00:00<00:00, 12.30it/s]
certifi-2025.1.31    | 163 KB    | : 100% 1.0/1 [00:00<00:00,  9.82it/s]



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

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): - ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\
▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒|
▒▒/ ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒- ▒▒\ ▒▒done
Solving environment: / ▒▒- ▒▒\ ▒▒| ▒▒/ ▒▒done

## 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-25.1.1               |  py311h38be061_1         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
    libcblas-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
  libcblas           conda-forge/linux-64::libcblas-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_7100
102
  libumfpack         conda-forge/linux-64::libumfpack-6.3.5-heb53515_7100102
  metis              conda-forge/linux-64::metis-5.1.0-hd0bcaf9_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-2
5.1.1-py311h38be061_1
  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-25.1.1          | 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]

libspqr-4.3.4         | 213 KB    | :   0% 0/1 [00:00<?, ?it/s]

scipy-1.15.2          | 16.4 MB   | :   8% 0.07623511861659131/1 [00:00<00:01,  1.31
s/it]
libopenblas-0.3.29    | 5.6 MB    | :  15% 0.14669872457633418/1 [00:00<00:00,  1.46i
t/s]

metis-5.1.0           | 3.7 MB    | :  25% 0.24637217221095128/1 [00:00<00:00,  2.45i
t/s]
numpy-2.2.4           | 8.6 MB    | :   0% 0.0018194029373407579/1 [00:00<01:01, 62.0
1s/it]

scipy-1.15.2          | 16.4 MB   | :  29% 0.28874051176033955/1 [00:00<00:00,  1.55i
t/s]
libopenblas-0.3.29    | 5.6 MB    | :  59% 0.5923306992327455/1 [00:00<00:00,  3.21i
t/s]
```

```
metis-5.1.0          | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  5.42it/s]
numpy-2.2.4          | 8.6 MB    | :  38% 0.3802552139042184/1 [00:00<00:00,  2.12i
t/s]


scipy-1.15.2         | 16.4 MB   | :  51% 0.5088694167657469/1 [00:00<00:00,  1.84i
t/s]



metis-5.1.0          | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  5.42it/s]
numpy-2.2.4          | 8.6 MB    | :  94% 0.9406313186051718/1 [00:00<00:00,  3.66i
t/s]




libstdcxx-14.2.0     | 3.7 MB    | :   0% 0.0042177278432850495/1 [00:00<01:21, 82.0
6s/it]

libopenblas-0.3.29   | 5.6 MB    | : 100% 1.0/1 [00:00<00:00,  2.59it/s]

scipy-1.15.2         | 16.4 MB   | :  72% 0.7156571760132509/1 [00:00<00:00,  1.93i
t/s]


pyfmi-2.16.3         | 5.2 MB    | : 100% 1.0/1 [00:00<00:00,  2.53it/s]


pyfmi-2.16.3         | 5.2 MB    | : 100% 1.0/1 [00:00<00:00,  2.53it/s]




openssl-3.4.1        | 2.8 MB    | :   1% 0.0055741049077571376/1 [00:00<01:16, 77.1
6s/it]



libstdcxx-14.2.0     | 3.7 MB    | :  73% 0.7296669168883136/1 [00:00<00:00,  2.13i
t/s]




scipy-1.15.2         | 16.4 MB   | :  92% 0.9195861183126326/1 [00:00<00:00,  1.91i
t/s]
```

```
libgfortran5-14.2.0  | 1.4 MB    | : 100% 1.0/1 [00:00<00:00, 41.60s/it]
numpy-2.2.4          | 8.6 MB    | : 100% 1.0/1 [00:00<00:00,  3.66it/s]

conda-25.1.1         | 1.1 MB    | :   1% 0.013622478419712683/1 [00:00<00:42, 42.85
s/it]

openssl-3.4.1        | 2.8 MB    | : 100% 1.0/1 [00:00<00:00,  2.17it/s]

openssl-3.4.1        | 2.8 MB    | : 100% 1.0/1 [00:00<00:00,  2.17it/s]

assimulo-3.6.0       | 1.1 MB    | :   1% 0.014703493605362324/1 [00:00<00:39, 39.93
s/it]

libstdcxx-14.2.0     | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  2.13it/s]

libcholmod-5.3.1     | 1.1 MB    | :   1% 0.014870549794649543/1 [00:00<00:41, 42.07
s/it]
```

```
conda-25.1.1          | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 42.85s/it]

sundials-7.1.1        | 907 KB    | :   2% 0.01763373830085844/1 [00:00<00:36, 37.32
s/it]

assimulo-3.6.0        | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 39.93s/it]

libgcc-14.2.0         | 828 KB    | :   2% 0.01932337522187561/1 [00:00<00:36, 37.13
s/it]

libcholmod-5.3.1      | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 42.07s/it]
```

```
sundials-7.1.1       | 907 KB    | : 100% 1.0/1 [00:00<00:00, 37.32s/it]

mpfr-4.2.1           | 620 KB    | :   3% 0.025811696239942908/1 [00:00<00:27, 28.49
s/it]

mpfr-4.2.1           | 620 KB    | : 100% 1.0/1 [00:00<00:00, 28.49s/it]

libgomp-14.2.0       | 449 KB    | :   4% 0.03562807972826631/1 [00:00<00:20, 21.41
s/it]
```

```
gmp-6.3.0            | 449 KB    | :   4% 0.03561313321233331/1 [00:00<00:20, 21.52
s/it]
```

```
gmp-6.3.0            | 449 KB    | : 100% 1.0/1 [00:00<00:00, 21.52s/it]
```

```
libgomp-14.2.0       | 449 KB    | : 100% 1.0/1 [00:00<00:00, 21.41s/it]
```

```
metis-5.1.0          | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  5.42it/s]
```

```
libgcc-14.2.0        | 828 KB    | : 100% 1.0/1 [00:00<00:00, 37.13s/it]
```

```
libumfpack-6.3.5     | 424 KB    | :   4% 0.037731330084655984/1 [00:00<00:21, 21.91
s/it]
```

```
libspqr-4.3.4        | 213 KB    | :   8% 0.07503068271326775/1 [00:00<00:10, 11.15
s/it]
```

```
libumfpack-6.3.5     | 424 KB    | : 100% 1.0/1 [00:00<00:00, 21.91s/it]
```

```
 ... (more hidden) ...
```

```
fmilib-2.4.1         | 383 KB    | :   4% 0.04180391656566945/1 [00:00<00:19, 20.22
s/it]
```

```
libspqr-4.3.4        | 213 KB    | : 100% 1.0/1 [00:00<00:00, 11.15s/it]
```

```
 ... (more hidden) ...


scipy-1.15.2         | 16.4 MB   | : 100% 1.0/1 [00:00<00:00,  1.91it/s]

pyfmi-2.16.3         | 5.2 MB    | : 100% 1.0/1 [00:01<00:00,  2.53it/s]
libopenblas-0.3.29   | 5.6 MB    | : 100% 1.0/1 [00:01<00:00,  2.59it/s]



libgfortran5-14.2.0  | 1.4 MB    | : 100% 1.0/1 [00:01<00:00,  1.23s/it]



libgfortran5-14.2.0  | 1.4 MB    | : 100% 1.0/1 [00:01<00:00,  1.23s/it]



openssl-3.4.1        | 2.8 MB    | : 100% 1.0/1 [00:01<00:00,  2.17it/s]



libstdcxx-14.2.0     | 3.7 MB    | : 100% 1.0/1 [00:01<00:00,  2.13it/s]
```

```
conda-25.1.1          | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.08s/it]
```


```
conda-25.1.1          | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.08s/it]
```


```
assimulo-3.6.0        | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.26s/it]
```


```
assimulo-3.6.0        | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.26s/it]
```


```
libcholmod-5.3.1      | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.30s/it]
```


```
libcholmod-5.3.1      | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.30s/it]
```

```
sundials-7.1.1       | 907 KB    | : 100% 1.0/1 [00:02<00:00,  2.49s/it]
```

```
sundials-7.1.1       | 907 KB    | : 100% 1.0/1 [00:02<00:00,  2.49s/it]
numpy-2.2.4          | 8.6 MB    | : 100% 1.0/1 [00:02<00:00,  3.66it/s]
```

```
gmp-6.3.0            | 449 KB    | : 100% 1.0/1 [00:02<00:00,  2.54s/it]
```


```
gmp-6.3.0            | 449 KB    | : 100% 1.0/1 [00:02<00:00,  2.54s/it]
```

```
mpfr-4.2.1           | 620 KB    | : 100% 1.0/1 [00:02<00:00,  2.55s/it]
```


```
mpfr-4.2.1           | 620 KB    | : 100% 1.0/1 [00:02<00:00,  2.55s/it]
```


```
libgomp-14.2.0       | 449 KB    | : 100% 1.0/1 [00:02<00:00,  2.66s/it]
```


```
libgomp-14.2.0       | 449 KB    | : 100% 1.0/1 [00:02<00:00,  2.66s/it]
```

```
libgcc-14.2.0        | 828 KB    | : 100% 1.0/1 [00:02<00:00,  2.69s/it]
```


```
libgcc-14.2.0        | 828 KB    | : 100% 1.0/1 [00:02<00:00,  2.69s/it]
```


```
libumfpack-6.3.5     | 424 KB    | : 100% 1.0/1 [00:02<00:00,  2.69s/it]
```


```
libumfpack-6.3.5     | 424 KB    | : 100% 1.0/1 [00:02<00:00,  2.69s/it]
```

```
libspqr-4.3.4        | 213 KB    | : 100% 1.0/1 [00:02<00:00,  2.73s/it]
```


```
libspqr-4.3.4        | 213 KB    | : 100% 1.0/1 [00:02<00:00,  2.73s/it]
```


```
 ... (more hidden) ...
```

```
 ... (more hidden) ...
```

```
fmilib-2.4.1         | 383 KB    | : 100% 1.0/1 [00:03<00:00,  2.79s/it]
```

```
scipy-1.15.2         | 16.4 MB   | : 100% 1.0/1 [00:04<00:00,  1.91it/s]
```

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

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 43.4 MB/s eta 0:00:00
Downloading sympy-1.13.3-py3-none-any.whl (6.2 MB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 6.2/6.2 MB 89.5 MB/s eta 0:00:00
Downloading mpmath-1.3.0-py3-none-any.whl (536 kB)
   ━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━━ 536.2/536.2 kB 20.6 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/BPL_YEAST_COB_Batch
```

```
Cloning into 'BPL_YEAST_COB_Batch'...
```

In [11]:
```
%cd BPL_YEAST_COB_Batch
```

```
/content/BPL_YEAST_COB_Batch
```

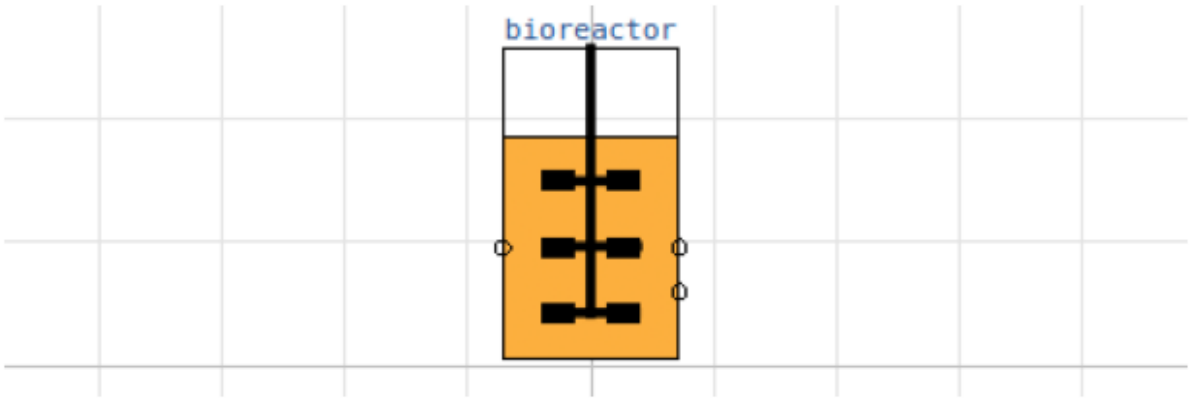
In [12]:
```
run -i BPL_YEAST_COB_Batch_explore.py
```

```
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()
```

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



Try using LP in each step

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

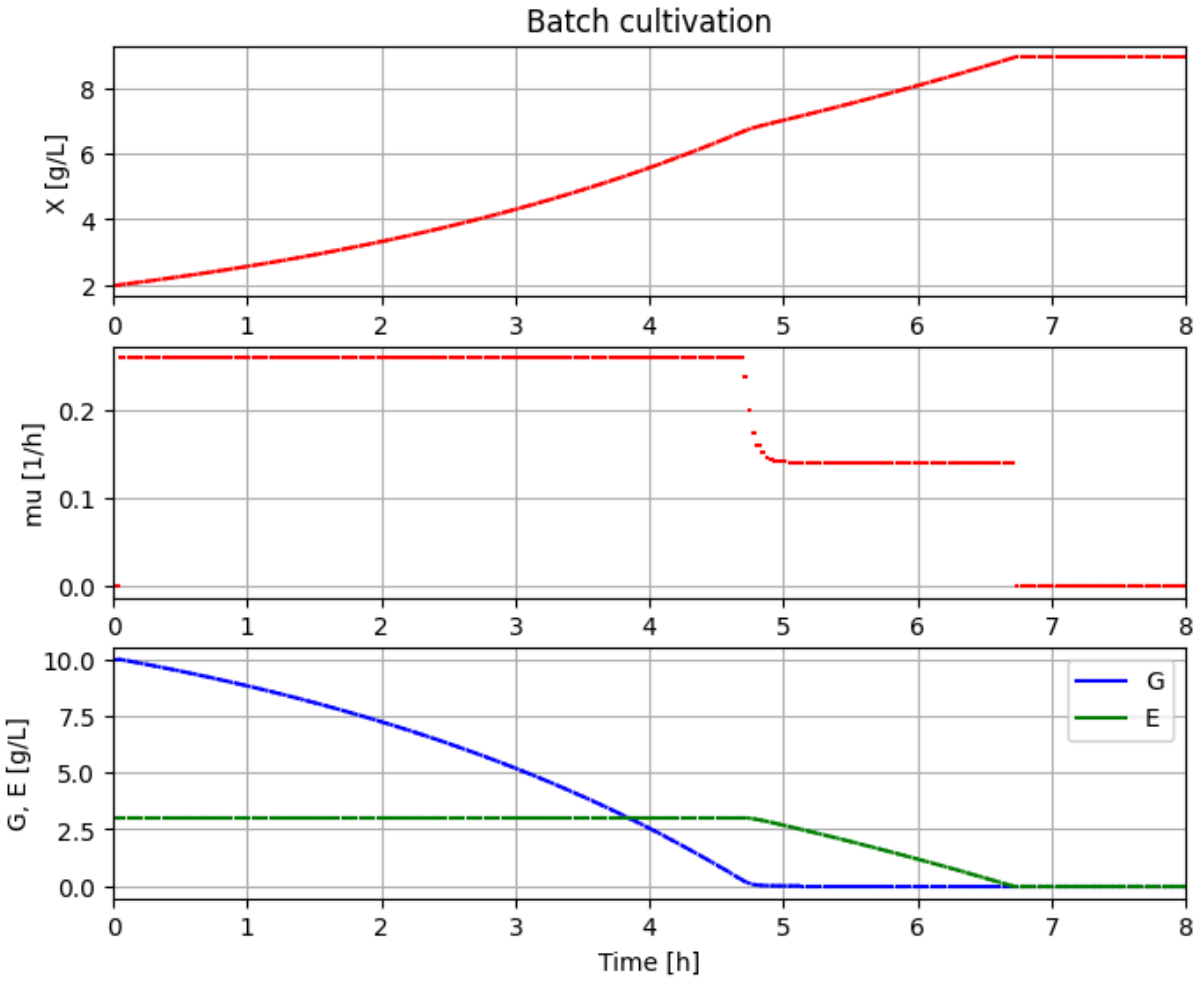
In [16]:
```
# Define culture constraint-based model
def culture(G, E):

    # 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_start=1.0
init(V_start=V_start, VX_start=V_start*2.0, VG_start=V_start*10, VE_start=V_start*3
```

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/pytho
n3.11/site-packages/assimulo/lib/__init__.py)
Could not find cannot import name 'rodas' from 'assimulo.lib' (/usr/local/lib/python
3.11/site-packages/assimulo/lib/__init__.py)
Could not find cannot import name 'odassl' from 'assimulo.lib' (/usr/local/lib/pytho
n3.11/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 1.25.0~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
```

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

```
# packages in environment at /usr/local:
#
# Name                    Version                   Build  Channel
optlang                   1.8.3                    pypi_0    pypi
```