Open in Colab

BPL_TEST2_Batch_calibration script with PyFMI

The key library PyFMI is installed.

After the installation a small application BPL_TEST2_Batch_calibration 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 10:26:56--  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   144MB/s    in 1.0s

2025-03-26 10:26:57 (144 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, 25.64it/s]
certifi-2025.1.31    | 163 KB    | : 100% 1.0/1 [00:00<00:00, 19.60it/s]

ca-certificates-2025 | 129 KB    | : 100% 1.0/1 [00:00<00:00, 12.44it/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]
```

```
 ... (more hidden) ...
scipy-1.15.2         | 16.4 MB   | :   8% 0.08099981353012826/1 [00:00<00:01,  1.24
s/it]

libopenblas-0.3.29   | 5.6 MB    | :  19% 0.1937530324593093/1 [00:00<00:00,  1.90i
t/s]


pyfmi-2.16.3         | 5.2 MB    | :  16% 0.16113346505902795/1 [00:00<00:00,  1.59i
t/s]



metis-5.1.0          | 3.7 MB    | :  38% 0.384173556667924/1 [00:00<00:00,  3.82it/
s]
scipy-1.15.2         | 16.4 MB   | :  30% 0.29826990158741346/1 [00:00<00:00,  1.60i
t/s]

libopenblas-0.3.29   | 5.6 MB    | :  82% 0.8192985372565079/1 [00:00<00:00,  4.44i
```

```
t/s]

pyfmi-2.16.3         | 5.2 MB    | :  90% 0.8951859169945998/1 [00:00<00:00,  4.92i
t/s]

metis-5.1.0          | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  4.07it/s]

metis-5.1.0          | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  4.07it/s]

scipy-1.15.2         | 16.4 MB   | :  58% 0.5765280845379718/1 [00:00<00:00,  2.13i
t/s]

pyfmi-2.16.3         | 5.2 MB    | : 100% 1.0/1 [00:00<00:00,  4.92it/s]

libopenblas-0.3.29   | 5.6 MB    | : 100% 1.0/1 [00:00<00:00,  4.44it/s]

openssl-3.4.1        | 2.8 MB    | :   1% 0.0055741049077571376/1 [00:00<01:03, 64.2
8s/it]

libgfortran5-14.2.0  | 1.4 MB    | :   1% 0.011206734985068174/1 [00:00<00:31, 32.27
s/it]

scipy-1.15.2         | 16.4 MB   | :  79% 0.78903347768172/1 [00:00<00:00,  1.98it/
s]

libgfortran5-14.2.0  | 1.4 MB    | : 100% 1.0/1 [00:00<00:00, 32.27s/it]
numpy-2.2.4          | 8.6 MB    | : 100% 1.0/1 [00:00<00:00,  4.38it/s]
```

```
conda-25.1.1         | 1.1 MB    | :   1% 0.013622478419712683/1 [00:00<00:34, 34.94
s/it]

libstdcxx-14.2.0     | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  3.33it/s]

assimulo-3.6.0       | 1.1 MB    | :   1% 0.014703493605362324/1 [00:00<00:33, 33.82
s/it]

openssl-3.4.1        | 2.8 MB    | : 100% 1.0/1 [00:00<00:00,  2.46it/s]

openssl-3.4.1        | 2.8 MB    | : 100% 1.0/1 [00:00<00:00,  2.46it/s]

scipy-1.15.2         | 16.4 MB   | :  99% 0.9891506640502722/1 [00:00<00:00,  1.79i
t/s]

libcholmod-5.3.1     | 1.1 MB    | :   1% 0.014870549794649543/1 [00:00<00:35, 36.27
s/it]
```

```
sundials-7.1.1       | 907 KB    | :   2% 0.017633738300858444/1 [00:00<00:30, 30.84
s/it]
```

```
assimulo-3.6.0       | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 33.82s/it]
```

```
libgcc-14.2.0        | 828 KB    | :   2% 0.01932337522187561/1 [00:00<00:28, 28.67
s/it]
```

```
sundials-7.1.1       | 907 KB    | : 100% 1.0/1 [00:00<00:00, 30.84s/it]
```

```
libcholmod-5.3.1     | 1.1 MB    | : 100% 1.0/1 [00:00<00:00, 36.27s/it]
```

```
mpfr-4.2.1           | 620 KB    | :   3% 0.025811696239942908/1 [00:00<00:22, 22.82
s/it]
```

```
libgcc-14.2.0        | 828 KB    | : 100% 1.0/1 [00:00<00:00, 28.67s/it]
```

```
mpfr-4.2.1           | 620 KB    | : 100% 1.0/1 [00:00<00:00, 22.82s/it]
```

```
libgomp-14.2.0       | 449 KB    | :   4% 0.03562807972826631/1 [00:00<00:16, 17.31
s/it]
```

```
gmp-6.3.0            | 449 KB    | :   4% 0.03561313321233331/1 [00:00<00:16, 17.40
s/it]
```

```
gmp-6.3.0            | 449 KB    | : 100% 1.0/1 [00:00<00:00, 17.40s/it]
```

```
fmilib-2.4.1         | 383 KB    | :   4% 0.04180391656566945/1 [00:00<00:14, 15.16
s/it]
```

```
libgomp-14.2.0       | 449 KB    | : 100% 1.0/1 [00:00<00:00, 17.31s/it]

libumfpack-6.3.5     | 424 KB    | :   4% 0.037731330084655984/1 [00:00<00:16, 17.18
s/it]

libumfpack-6.3.5     | 424 KB    | : 100% 1.0/1 [00:00<00:00, 17.18s/it]

fmilib-2.4.1         | 383 KB    | : 100% 1.0/1 [00:00<00:00, 15.16s/it]
```

```
libspqr-4.3.4        | 213 KB    | :   8% 0.07503068271326775/1 [00:00<00:08,  9.03
s/it]
```

... (more hidden) ...

... (more hidden) ...

```
libspqr-4.3.4        | 213 KB    | : 100% 1.0/1 [00:00<00:00,  9.03s/it]

metis-5.1.0          | 3.7 MB    | : 100% 1.0/1 [00:00<00:00,  4.07it/s]

scipy-1.15.2         | 16.4 MB   | : 100% 1.0/1 [00:00<00:00,  1.79it/s]

libgfortran5-14.2.0  | 1.4 MB    | : 100% 1.0/1 [00:01<00:00,  1.11it/s]

libgfortran5-14.2.0  | 1.4 MB    | : 100% 1.0/1 [00:01<00:00,  1.11it/s]
libopenblas-0.3.29   | 5.6 MB    | : 100% 1.0/1 [00:01<00:00,  4.44it/s]

libstdcxx-14.2.0     | 3.7 MB    | : 100% 1.0/1 [00:01<00:00,  3.33it/s]

openssl-3.4.1        | 2.8 MB    | : 100% 1.0/1 [00:01<00:00,  2.46it/s]

conda-25.1.1         | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.00s/it]
```

```
conda-25.1.1         | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.00s/it]
```

```
assimulo-3.6.0       | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.15s/it]
```

```
assimulo-3.6.0       | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.15s/it]
numpy-2.2.4          | 8.6 MB    | : 100% 1.0/1 [00:02<00:00,  4.38it/s]
```

```
libcholmod-5.3.1     | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.25s/it]
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libcholmod-5.3.1     | 1.1 MB    | : 100% 1.0/1 [00:02<00:00,  2.25s/it]
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sundials-7.1.1 | 907 KB | : 100% 1.0/1 [00:02<00:00, 2.33s/it]

sundials-7.1.1 | 907 KB | : 100% 1.0/1 [00:02<00:00, 2.33s/it]

libgcc-14.2.0 | 828 KB | : 100% 1.0/1 [00:02<00:00, 2.35s/it]

libgcc-14.2.0 | 828 KB | : 100% 1.0/1 [00:02<00:00, 2.35s/it]

gmp-6.3.0 | 449 KB | : 100% 1.0/1 [00:02<00:00, 2.40s/it]

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gmp-6.3.0            | 449 KB    | : 100% 1.0/1 [00:02<00:00,  2.40s/it]

mpfr-4.2.1           | 620 KB    | : 100% 1.0/1 [00:02<00:00,  2.42s/it]

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libumfpack-6.3.5     | 424 KB    | : 100% 1.0/1 [00:02<00:00,  2.44s/it]
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libumfpack-6.3.5     | 424 KB    | : 100% 1.0/1 [00:02<00:00,  2.44s/it]

libgomp-14.2.0       | 449 KB    | : 100% 1.0/1 [00:02<00:00,  2.48s/it]

libgomp-14.2.0       | 449 KB    | : 100% 1.0/1 [00:02<00:00,  2.48s/it]
```

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```

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

```
fmilib-2.4.1         | 383 KB    | : 100% 1.0/1 [00:02<00:00,  2.53s/it]
```

```
fmilib-2.4.1         | 383 KB    | : 100% 1.0/1 [00:02<00:00,  2.53s/it]
```

```
libspqr-4.3.4        | 213 KB    | : 100% 1.0/1 [00:02<00:00,  2.56s/it]
```

```
scipy-1.15.2         | 16.4 MB   | : 100% 1.0/1 [00:03<00:00,  1.79it/s]
```

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

Now specific installation and the run simulations. Start with connecting to Github. Then upload the four files:

- FMU - BPL_TEST2_Batch_linux_om_me.fmu
- Setup-file - BPL_TEST2_Batch_explore.py

In [9]:
```
%%bash
git clone https://github.com/janpeter19/BPL_TEST2_Batch_calibration
```

```
Cloning into 'BPL_TEST2_Batch_calibration'...
```

In [10]:
```
%cd BPL_TEST2_Batch_calibration
```

```
/content/BPL_TEST2_Batch_calibration
```

BPL_TEST2_Batch_calibration - demo

Author: Jan Peter Axelsson

This notebook shows the possibilities for calibration of the model BPL_TEST2_Batch using scipy.optimize.minimize() routine. There are several different methods to choose between. In this notebook we work with simulated data.

The text-book model of batch cultivation we simulate is the following where S is substrate, X is cell concentration, and V is volume of the broth

$$\frac{d(VS)}{dt} = -q_S(S) \cdot VX$$
$$\frac{d(VX)}{dt} = \mu(S) \cdot VX$$

and where specific cell growth rate μ and substrate uptake rate q_S are

$$\mu(S) = Y \cdot q_S(S)$$

$$q_S(S) = q_S^{max} \frac{S}{K_s + S}$$

where Y is the yield, q_S^{max} is the maximal specific substrate uptake rate and K_s is the corresponding saturation constant.

The parameter estimation is done with optimization methods that only require evaluation of the missmatch between simulation with given parameters and data. At start the allowed range for each parameter is given. The method used for optimization is Nelder-Mead but can easily be changed [1].

In the near future the FMU may provide first derivative gradient informaion, that will make it possible to choose corresponding method of minimize() for improved performance. This possibility is related to the upgrade to the FMI-standard ver 3.0 for the Modelica compiler.

The Python package PyFMI [2] that is the base for FMU-explore has a simplified built-in functionality for parameter estimation that also use scipy.optimize.minimize(). However, there is estimatation functionaly but the purpose seems to only address smaller examples. There is for instance no support to handle models that takes sub-models from libraries and necesssary changes of default parameters not to be estimated. Therefore we here define a Python function evaluate() that facilitate the formulation of the parameter estimation and also bring flexibility to choice of optimization method, default Nelder-Mead.

In [11]:
```
run -i BPL_TEST2_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()
```

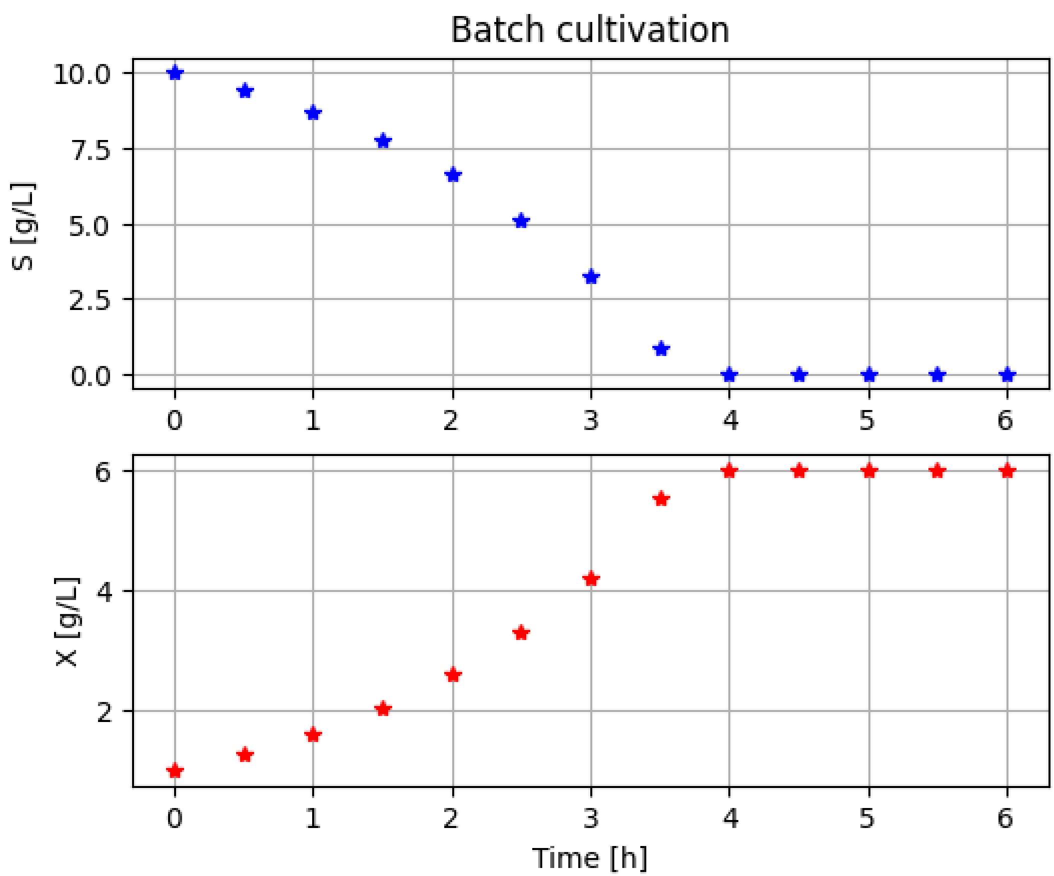
In [12]:
```
# Adjust the size of diagrams
plt.rcParams['figure.figsize'] = [15/2.54, 12/2.54]
```

1 Generate data later used for parameter estimation

In [13]:
```
import pandas as pd
```

In [14]:
```
# Data generated
simulationTime = 6.0
par(Y=0.50, qSmax=1.00, Ks=0.1)
init(V_start=1.0, VS_start=10, VX_start=1.0)
newplot(plotType='Demo_2')
simu(simulationTime, options=opts_data)
```

```
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 [15]:
```
# Store data in a DataFrame for later use
data = pd.DataFrame(data={'time':sim_res['time'], 'X':sim_res['bioreactor.c[1]'], '
data
```

Out[15]:

	time	X	S
0	0.0	1.000000	1.000000e+01
1	0.5	1.269848	9.438455e+00
2	1.0	1.615795	8.719839e+00
3	1.5	2.050445	7.800734e+00
4	2.0	2.601038	6.626389e+00
5	2.5	3.297304	5.128962e+00
6	3.0	4.195962	3.229259e+00
7	3.5	5.524388	8.813998e-01
8	4.0	6.000000	-2.037810e-08
9	4.5	6.000000	2.960320e-10
10	5.0	6.000000	1.200938e-10
11	5.5	6.000000	2.363337e-10
12	6.0	6.000000	-1.553435e-10

2 Simulation with initial guess of parameters compared with data

Here we define the parameters that should be estimated and specify allowed ranges. Nominal parameters are chosen as the mid-point of the allowed parameter range.

Simulation with these nominal parameter set and compare with data give an idea of who well the model fit data.

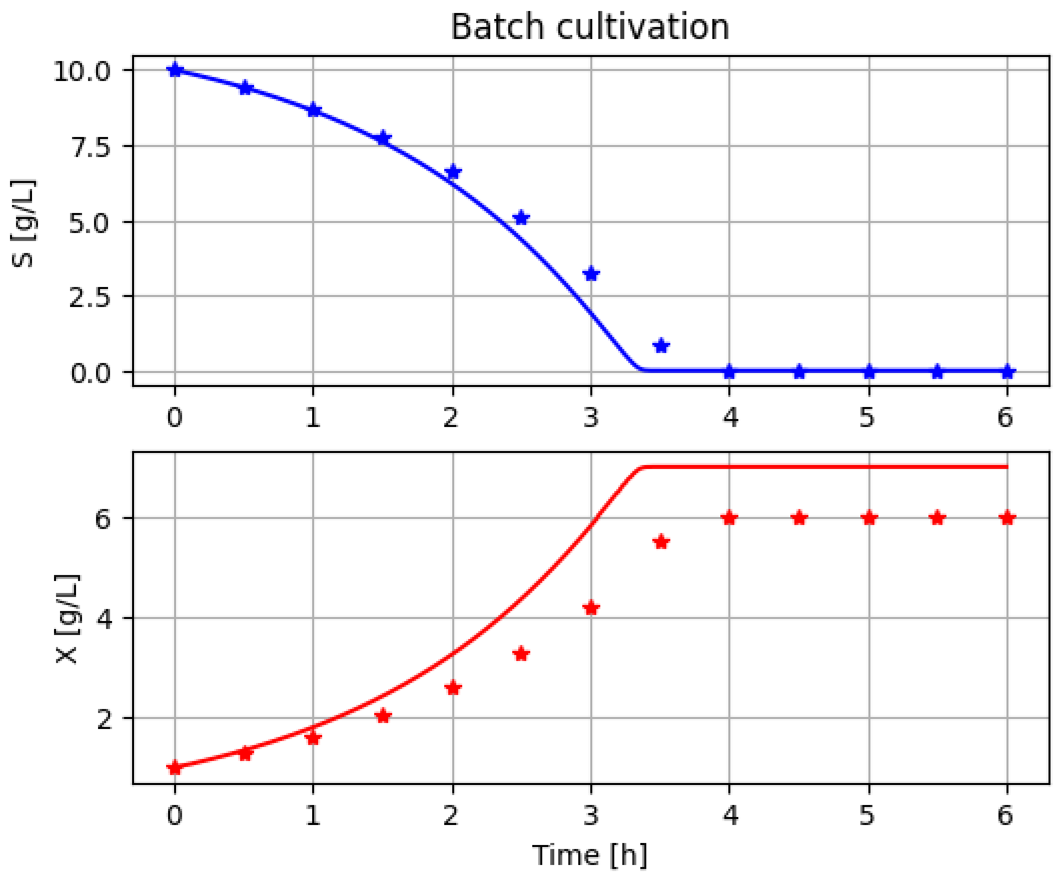
In [16]:

```
# Parameters to be estimated using parDict names and their bounds
parEstim = ['Y', 'qSmax', 'Ks']
parBounds = [(0.4, 0.8), (0.7, 1.3), (0.05, 0.20)]
parEstim_0 = [np.mean(parBounds[k]) for k in range(len(parBounds))]
```

In [17]:

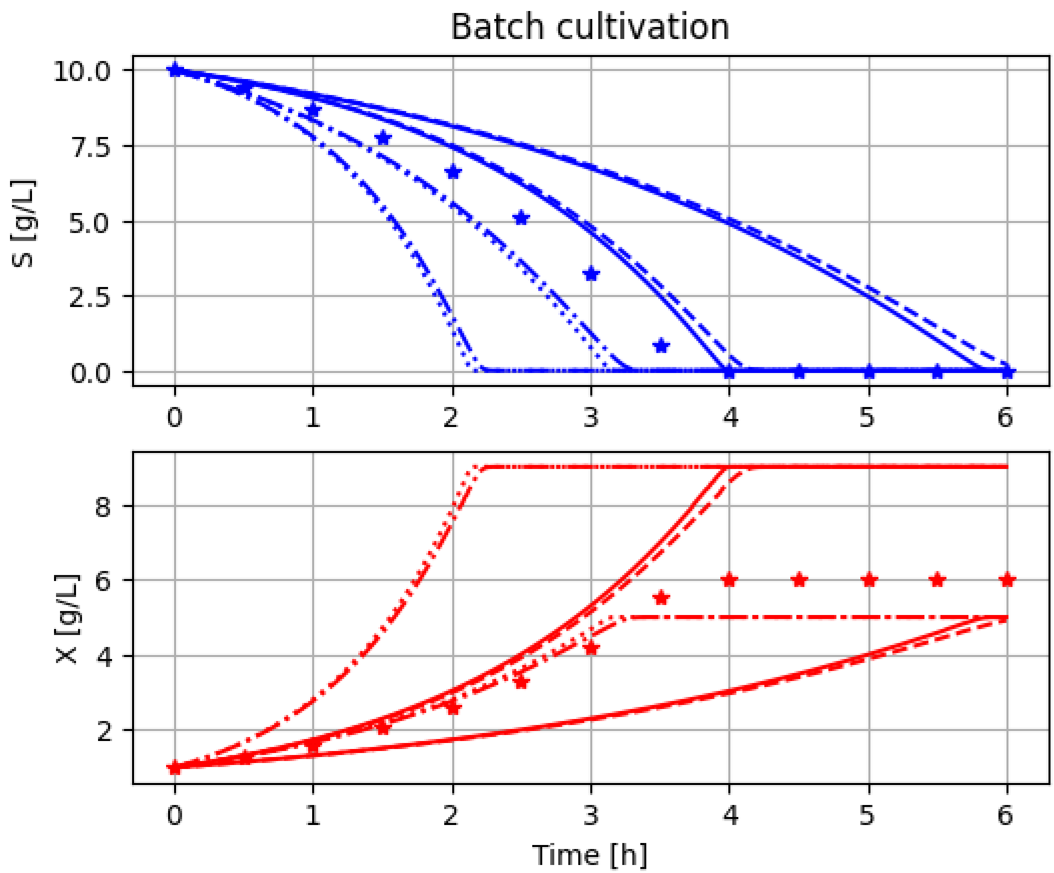
```
# Simulation with nominal parameters
newplot(plotType='Demo_1')
par(Y=parEstim_0[0], qSmax=parEstim_0[1], Ks=parEstim_0[2])
simu(simulationTime)

# Show data
ax1.plot(data['time'], data['S'],'b*')
ax2.plot(data['time'], data['X'],'r*')
plt.show()
```



In [18]:
```python
# Simulation over the parameter ranges given
newplot(plotType='Demo_1')
for Y_value in parBounds [0]:
    for qSmax_value in parBounds[1]:
        for Ks_value in parBounds[2]:
            par(Y=Y_value, qSmax=qSmax_value, Ks=Ks_value)
            simu(simulationTime)

# Show data
ax1.plot(data['time'], data['S'],'b*')
ax2.plot(data['time'], data['X'],'r*')
plt.show()
```



Simulation over the diferent parameter combinations of the parameter bounds shows that data is "covered" and we have good hope to find a parameter combination that fits data well.

3 Parameter estimation

Here we use the scipy.optimize.minimize() procedure which contain a family of different methods [1]. The default method is Nelder-Mead and is robust for fitting a model to data. Further we have chosen to work with bounds for the parameters to be estimated and the initial guess is chosen as the middle point in parameter space.

In [19]:
```
# Optimization routine import
import scipy.optimize
```

In [20]:
```
# Parameters to be estimated using parDict names and their bounds
extra_args = (parEstim, data, fmu_model, simulationTime)
```

In [21]:
```
# Modified evaluation function tailored for Python optimization algorithms
def objective(x, parEstim, data=data, fmu_model=fmu_model, simulationTime=simulatio
    """The parameter list is tailored for scipy optimization algorithms interface,
       where the first parameter x is an array with parameters that are tuned
       and evalauted and parEstim is a list of the names of these parameters.
       The code can be made 20-30% faster, but loner, using pyfmi-commands directly
```

```
    # Update parameters and simulate
    for i, p in enumerate(parEstim): par(**{p:x[i]})
    simu(simulationTime, options=opts_fast)

    # Calculate loss function V
    V={}
    V['X'] = np.linalg.norm(data['X'] - np.interp(data['time'], sim_res['time'], si
    V['S'] = np.linalg.norm(data['S'] - np.interp(data['time'], sim_res['time'], si

    return V['X'] + V['S']
```

In [22]:
```
import time
```

In [23]:
```
# Run minimize()
start_time = time.time()
result = scipy.optimize.minimize(objective, x0=parEstim_0, args=extra_args,
                                 method='Nelder-Mead', bounds=parBounds, options={"
print('CPU-time =', time.time()-start_time)
```

```
Optimization terminated successfully.
         Current function value: 0.148311
         Iterations: 66
         Function evaluations: 122
CPU-time = 0.5640532970428467
```

In [24]:
```
result.x
```

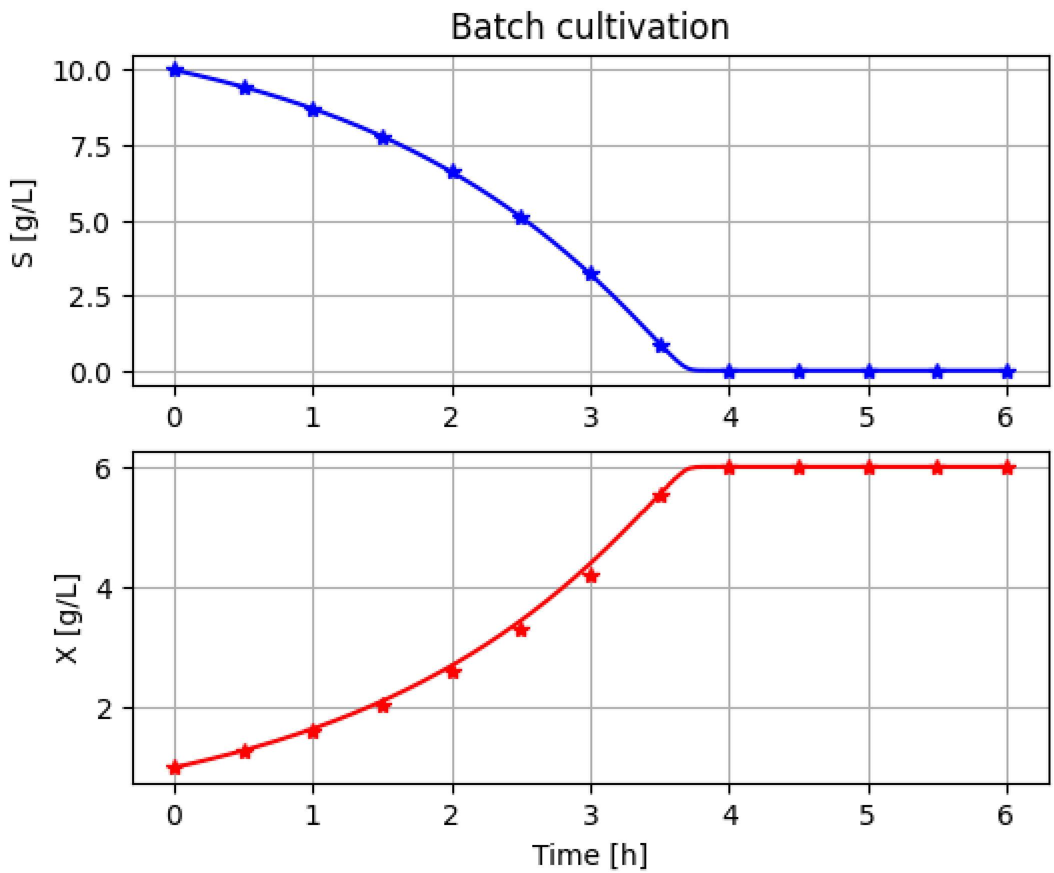
Out[24]:
```
array([0.49997276, 1.00731527, 0.14380564])
```

The estimated parameters result.x are very close to the original values and no surprise.

4 Simulation with estimated parameters compared with data

In [25]:
```
newplot(plotType='Demo_1')
par(Y=result.x[0], qSmax=result.x[1], Ks=result.x[2])
simu(simulationTime)

# Show data
ax1.plot(data['time'], data['S'],'b*')
ax2.plot(data['time'], data['X'],'r*')
plt.show()
```



In [26]:
```python
# The estimated parameters are
for i in range(len(parEstim)): print(parEstim[i],':', result.x[i])
```

```
Y : 0.4999727558733863
qSmax : 1.0073152667279195
Ks : 0.14380564144282715
```

5 Analysis of the loss function

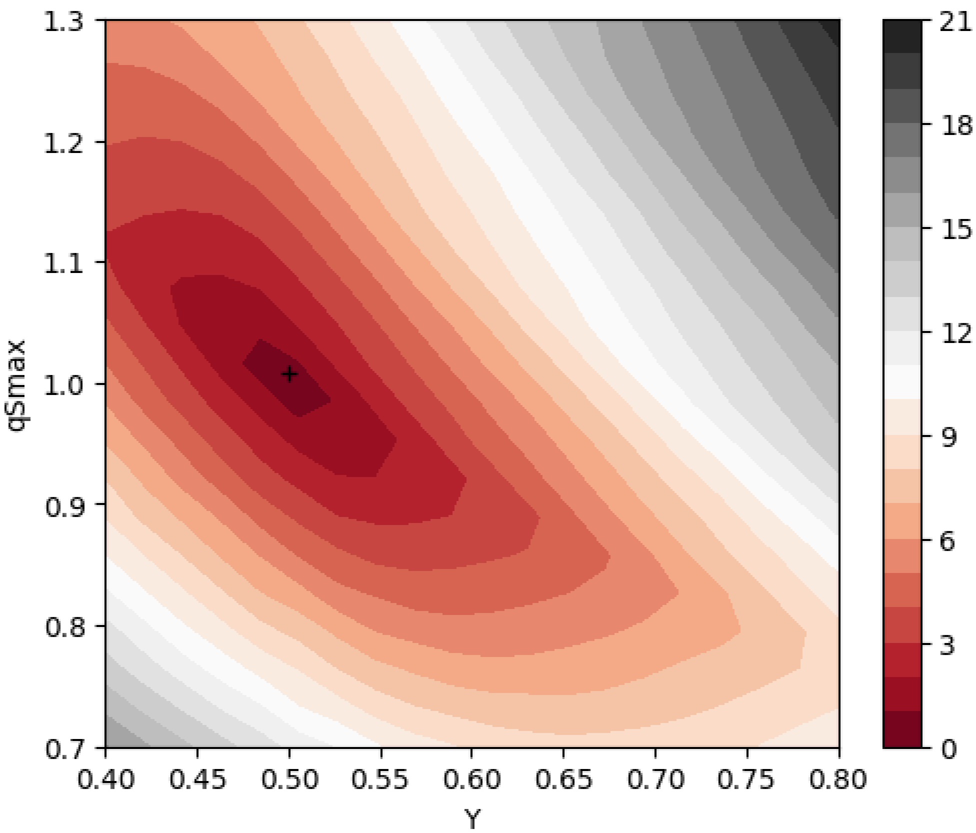
The problem is small and analysis of the loss function brings some insight. From the diagram above showing parameter sweep over combinations min- and max-parameters we see that the parameter K_s has little influence. Let use set that a fixed value and then plot the loss function in the parameters Y and $qSmax$. We do this by go through all the parametera combinations and evaluate each of them.

In [27]:
```python
# Sweep through Y and qSmax variation and store the value of the Loss-function for
nY = 20
nqSmax = 20
V = np.zeros((nY, nqSmax))

Y = np.linspace(parBounds[0][0],parBounds[0][1],nY)
qSmax = np.linspace(parBounds[1][0],parBounds[1][1],nqSmax)

for j in range(nY):
    for k in range(nqSmax):
        V[k,j] = objective([Y[j], qSmax[k], 0.1], parEstim)
```

```
# Contour plot
plt.figure()
plt.clf
plt.subplot(1,1,1)
plt.contourf(Y, qSmax, V, 20, cmap='RdGy')
plt.plot(result.x[0], result.x[1],'k+')
plt.colorbar()
plt.ylabel('qSmax')
plt.xlabel('Y')
plt.show()
```



We see the following in the contour diagram of the loss function simplified:

- The minima is unique in the range of parmaters we study. This is good news.
- The contour plot is ellipsoid and rather narrow. The more narrow the ellipsoid the more difficult and more time it takes to converge to the minima.
- The direction of the ellipsoid axis indicate the correlation you may get between the two parameters during the minimization process.

Note that the form of the contour plot change with the parameters (and initial values) of the actual proces. You can see the impact by changing the parameters in "cell # 4" where data is generated and then just choose to run that cell and the cells below. No need to restart the notebook.

6 Summary

A choice was made to work with allowed ranges of parameters to be estimated and a start value was defined as the center point in this parameter space. There are only three methods available in optimize.minimize() that can handle bounds on parameters.

An evaluate() function was created that define how the difference beween simulation and data is measured. The function is rather transparent and easy to modify and you may want to change weight on the loss in S and X, for instance. Here they have so far equal weight.

The FMU-explore workspace dictionaries partDict[] and parLocation[] are useful also here and simplify the code for the evaluation() function. But we also use the detailed PyFMI-functions to administrate and set parameters of the actual simulation.

The call optimize.minimize() has several parameters and can easily be modified, for instance change of method. For fitting a model to data Nelder-Mead is ao a robust and good choice, but can be somewhat slow.

The estimated parameters were close to perfect!

The contour plot of the simplified loss function shows that the minima is unique and should not be difficult too difficut to obtain. More narrow elliptical contour plots would indicate difficulties. Multiple local minima would also be a problem.

7 References

[1] Scipy Reference guide on optimize.minimize() here

[2] Andersson, C., Åkesson, J., Fuhrer C. : "PyFMI: A Python package for simulation of coupled dynamic models with the functional mock-up interface", Centre for Mathematical Sciences, Lund University, Report LUTFNA-5008-2016, 2016.

Appendix

In [28]:
```
describe('parts')
```

```
['bioreactor', 'bioreactor.culture']
```

In [29]:
```
describe('MSL')
```

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

In [30]:
```
system_info()
```

```
System information
 -OS: Linux
 -Python: 3.11.11
 -Scipy: 1.14.1
 -PyFMI: 2.16.3
 -FMU by: OpenModelica Compiler OpenModelica 1.25.0~dev-133-ga5470be
 -FMI: 2.0
 -Type: FMUModelME2
 -Name: BPL.Examples_TEST2.Batch
 -Generated: 2024-11-06T21:35:34Z
 -MSL: 3.2.3
 -Description: Bioprocess Library version 2.3.0
 -Interaction: FMU-explore version 1.0.0
```

In [30]:

```

```