Open in Colab

BPL_TEST2_Batch_calibration script with PyFMI ver 2.9.8

The key library PyFMI ver 2.9.8 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 [ ]:
```
!lsb_release -a # Actual VM Ubuntu version used by Google
```

```
No LSB modules are available.
Distributor ID: Ubuntu
Description:    Ubuntu 20.04.5 LTS
Release:        20.04
Codename:       focal
```

In [ ]:
```
%env PYTHONPATH=
```

```
env: PYTHONPATH=
```

In [ ]:
```
!wget https://repo.anaconda.com/miniconda/Miniconda3-py38_22.11.1-1-Linux
!chmod +x Miniconda3-py38_22.11.1-1-Linux-x86_64.sh
!bash ./Miniconda3-py38_22.11.1-1-Linux-x86_64.sh -b -f -p /usr/local
import sys
sys.path.append('/usr/local/lib/python3.8/site-packages/')
```

```
--2023-03-13 11:15:16--  https://repo.anaconda.com/miniconda/Miniconda3-
py38_22.11.1-1-Linux-x86_64.sh
Resolving repo.anaconda.com (repo.anaconda.com)... 104.16.130.3, 104.16.
131.3, 2606:4700::6810:8203, ...
Connecting to repo.anaconda.com (repo.anaconda.com)|104.16.130.3|:443...
connected.
HTTP request sent, awaiting response... 200 OK
Length: 64630241 (62M) [application/x-sh]
Saving to: ‘Miniconda3-py38_22.11.1-1-Linux-x86_64.sh’

Miniconda3-py38_22. 100%[===================>]  61.64M  34.7MB/s    in
1.8s

2023-03-13 11:15:18 (34.7 MB/s) - ‘Miniconda3-py38_22.11.1-1-Linux-x86_6
4.sh’ saved [64630241/64630241]

PREFIX=/usr/local
Unpacking payload ...

Installing base environment...


Downloading and Extracting Packages


Downloading and Extracting Packages

Preparing transaction: -   \   |   /   done
Executing transaction: \   |   /   -   \   |   /   -   \   |   /   -   \
  |   /   -   \   |   /   -   \   |   /   -   \   |   /   -   \   |   /
  -   \   |   /   -   \   |   done
installation finished.
```

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

```
Collecting package metadata (current_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-2023.01.10 |       h06a4308_0         120 KB
    conda-23.1.0               |   py38h06a4308_0         942 KB
    conda-package-handling-2.0.2|   py38h06a4308_0         267 KB
    conda-package-streaming-0.7.0|   py38h06a4308_0          26 KB
    cryptography-39.0.1        |   py38h9ce1e76_0         1.4 MB
    ncurses-6.4                |       h6a678d5_0         914 KB
    openssl-1.1.1t             |       h7f8727e_0         3.7 MB
    pyopenssl-23.0.0           |   py38h06a4308_0          96 KB
    sqlite-3.40.1              |       h5082296_0         1.2 MB
    urllib3-1.26.14            |   py38h06a4308_0         196 KB
    xz-5.2.10                  |       h5eee18b_1         429 KB
    zstandard-0.19.0           |   py38h5eee18b_0         474 KB
    ------------------------------------------------------------
                                           Total:         9.7 MB

The following NEW packages will be INSTALLED:

  conda-package-str~ pkgs/main/linux-64::conda-package-streaming-0.7.0-p
y38h06a4308_0
  zstandard          pkgs/main/linux-64::zstandard-0.19.0-py38h5eee18b_0

The following packages will be UPDATED:

  ca-certificates                     2022.10.11-h06a4308_0 --> 2023.01.
10-h06a4308_0
  conda                              22.11.1-py38h06a4308_4 --> 23.1.0-p
y38h06a4308_0
  conda-package-han~                   1.9.0-py38h5eee18b_1 --> 2.0.2-py
38h06a4308_0
  cryptography                        38.0.1-py38h9ce1e76_0 --> 39.0.1-p
y38h9ce1e76_0
  ncurses                                6.3-h5eee18b_3 --> 6.4-h6a6
78d5_0
  openssl                             1.1.1s-h7f8727e_0 --> 1.1.1t-h
7f8727e_0
  pyopenssl          pkgs/main/noarch::pyopenssl-22.0.0-py~ --> pkgs/mai
n/linux-64::pyopenssl-23.0.0-py38h06a4308_0
  sqlite                                 3.40.0-h5082296_0 --> 3.40.1-h
5082296_0
  urllib3                            1.26.13-py38h06a4308_0 --> 1.26.14-
py38h06a4308_0
  xz                                      5.2.8-h5eee18b_0 --> 5.2.10-h
5eee18b_1
```

```
Downloading and Extracting Packages
ca-certificates-2023 | 120 KB    | :   0% 0/1 [00:00<?, ?it/s]
pyopenssl-23.0.0     | 96 KB     | :   0% 0/1 [00:00<?, ?it/s]

openssl-1.1.1t       | 3.7 MB    | :   0% 0/1 [00:00<?, ?it/s]


conda-package-stream | 26 KB     | :   0% 0/1 [00:00<?, ?it/s]


xz-5.2.10            | 429 KB    | :   0% 0/1 [00:00<?, ?it/s]


urllib3-1.26.14      | 196 KB    | :   0% 0/1 [00:00<?, ?it/s]


ncurses-6.4          | 914 KB    | :   0% 0/1 [00:00<?, ?it/s]


conda-23.1.0         | 942 KB    | :   0% 0/1 [00:00<?, ?it/s]


cryptography-39.0.1  | 1.4 MB    | :   0% 0/1 [00:00<?, ?it/s]


conda-package-handli | 267 KB    | :   0% 0/1 [00:00<?, ?it/s]


zstandard-0.19.0     | 474 KB    | :   0% 0/1 [00:00<?, ?it/s]
```

```
sqlite-3.40.1        | 1.2 MB    | :   0% 0/1 [00:00<?, ?it/s]
pyopenssl-23.0.0     | 96 KB     | : 100% 0.997473440686737/1 [00:00<00:
00,  9.95it/s]

openssl-1.1.1t       | 3.7 MB    | :   2% 0.01671962984960089/1 [00:00<0
0:05,  6.05s/it]



xz-5.2.10            | 429 KB    | :  19% 0.18633724038004426/1 [00:00<0
0:00,  1.79it/s]




ncurses-6.4          | 914 KB    | :   2% 0.01750655534161504/1 [00:00<0
0:06,  6.16s/it]




conda-23.1.0         | 942 KB    | :   2% 0.01697734109389037 5/1 [00:00<
00:06,  6.89s/it]



urllib3-1.26.14      | 196 KB    | :   8% 0.0816656116198043/1 [00:00<0
0:01,  1.46s/it]

conda-package-stream | 26 KB     | : 100% 1.0/1 [00:00<00:00,  5.93it/s]

conda-package-stream | 26 KB     | : 100% 1.0/1 [00:00<00:00,  5.93it/s]




cryptography-39.0.1  | 1.4 MB    | :   1% 0.011057830211282578/1 [00:00<
00:15, 15.54s/it]
```

```
conda-package-handli | 267 KB    | :   6% 0.05994701947985423/1 [00:00<0
0:02,  3.09s/it]

openssl-1.1.1t       | 3.7 MB    | :  28% 0.27587389251841465/1 [00:00<0
0:00,  1.58it/s]
```

```
zstandard-0.19.0     | 474 KB    | :   3% 0.033766335474643305/1 [00:00<
00:06,  6.85s/it]
```

```
ca-certificates-2023 | 120 KB    | : 100% 1.0/1 [00:00<00:00,  3.91it/s]

openssl-1.1.1t       | 3.7 MB    | :  90% 0.8986801044160477/1 [00:00<0
0:00,  3.69it/s]
pyopenssl-23.0.0     | 96 KB     | : 100% 1.0/1 [00:00<00:00,  9.95it/s]
```

```
xz-5.2.10            | 429 KB    | : 100% 1.0/1 [00:00<00:00,  2.96it/s]
```

```
xz-5.2.10            | 429 KB    | : 100% 1.0/1 [00:00<00:00,  2.96it/s]
```

```
urllib3-1.26.14      | 196 KB    | : 100% 1.0/1 [00:00<00:00,  2.79it/s]
```

```
urllib3-1.26.14      | 196 KB    | : 100% 1.0/1 [00:00<00:00,  2.79it/s]
```

```
conda-23.1.0          | 942 KB    | : 100% 1.0/1 [00:00<00:00,  2.32it/s]
```


```
conda-23.1.0          | 942 KB    | : 100% 1.0/1 [00:00<00:00,  2.32it/s]
```


```
ncurses-6.4           | 914 KB    | : 100% 1.0/1 [00:00<00:00,  1.49it/s]
```


```
ncurses-6.4           | 914 KB    | : 100% 1.0/1 [00:00<00:00,  1.49it/s]
```


```
conda-package-handli | 267 KB    | : 100% 1.0/1 [00:00<00:00,  1.45it/s]
```


```
conda-package-handli | 267 KB    | : 100% 1.0/1 [00:00<00:00,  1.45it/s]
```


```
cryptography-39.0.1  | 1.4 MB    | : 100% 1.0/1 [00:00<00:00,  1.31it/s]
```


```
cryptography-39.0.1  | 1.4 MB    | : 100% 1.0/1 [00:00<00:00,  1.31it/s]
```

```
zstandard-0.19.0     | 474 KB    | : 100% 1.0/1 [00:00<00:00,  1.27it/s]
```


```
zstandard-0.19.0     | 474 KB    | : 100% 1.0/1 [00:00<00:00,  1.27it/s]
```


```
sqlite-3.40.1        | 1.2 MB    | : 100% 1.0/1 [00:00<00:00,  1.20it/s]
```


```
sqlite-3.40.1        | 1.2 MB    | : 100% 1.0/1 [00:00<00:00,  1.20it/s]
```

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

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

```
conda 23.1.0
Python 3.8.15
```

In [ ]:
```
!conda install -c conda-forge pyfmi=2.9.8 --yes # Install the key package
```

```
Collecting package metadata (current_repodata.json): -   \   |   /   -
  \   |   /   -   \   |   /   -   \   |   /   -   \   |   /   -   \   |
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  /   -   \   |   done
Solving environment: -   failed with initial frozen solve. Retrying with
flexible solve.
Collecting package metadata (repodata.json): |   /   -   \   |   /   -
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```

```
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Solving environment: |   /   -   \   |   /   -   \   |   /   -   \   |   /   -   \   |
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  / - \ | / - \ | done

## Package Plan ##

  environment location: /usr/local

  added / updated specs:
    - pyfmi=2.9.8


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
```

```
    _libgcc_mutex-0.1          |      conda_forge           3 KB  conda-
forge
    _openmp_mutex-4.5          |       2_kmp_llvm           6 KB  conda-
forge
    assimulo-3.4               |   py38ha96dddf_0         1.9 MB  conda-
forge
    ca-certificates-2022.12.7  |       ha878542_0         143 KB  conda-
forge
    certifi-2022.12.7          |     pyhd8ed1ab_0         147 KB  conda-
forge
    conda-23.1.0               |   py38h578d9bd_0         907 KB  conda-
forge
    fmilib-2.4.1               |       h27087fc_0         545 KB  conda-
forge
    gmp-6.2.1                  |       h58526e2_0         806 KB  conda-
forge
    icu-68.2                   |       h9c3ff4c_0        13.1 MB  conda-
forge
    libblas-3.9.0              |16_linux64_openblas          13 KB  cond
a-forge
    libcblas-3.9.0             |16_linux64_openblas          13 KB  cond
a-forge
    libgcc-ng-12.2.0           |      h65d4601_19         931 KB  conda-
forge
    libgfortran-ng-12.2.0      |      h69a702a_19          22 KB  conda-
forge
    libgfortran5-12.2.0        |      h337968e_19         1.8 MB  conda-
forge
    libiconv-1.17              |       h166bdaf_0         1.4 MB  conda-
forge
    liblapack-3.9.0            |16_linux64_openblas          13 KB  cond
a-forge
    libopenblas-0.3.21         |pthreads_h78a6416_3        10.1 MB  cond
a-forge
    libstdcxx-ng-12.2.0        |      h46fd767_19         4.3 MB  conda-
forge
    libxml2-2.9.12             |       h72842e0_0         772 KB  conda-
forge
    libxslt-1.1.33             |       h15afd5d_2         522 KB  conda-
forge
    llvm-openmp-12.0.1         |       h4bd325d_1         2.8 MB  conda-
forge
    lxml-4.8.0                 |   py38h0a891b7_2         1.4 MB  conda-
forge
    metis-5.1.0                |    h58526e2_1006         4.1 MB  conda-
forge
    mpfr-4.2.0                 |       hb012696_0         616 KB  conda-
forge
    numpy-1.24.2               |   py38h10c12cc_0         6.3 MB  conda-
forge
    openssl-1.1.1t             |       h0b41bf4_0         1.9 MB  conda-
forge
    packaging-23.0             |     pyhd8ed1ab_0          40 KB  conda-
forge
    platformdirs-3.1.1         |     pyhd8ed1ab_0          17 KB  conda-
forge
    pooch-1.7.0                |     pyhd8ed1ab_0          49 KB  conda-
forge
    pyfmi-2.9.8                |   py38h26c90d9_1        12.7 MB  conda-
forge
```

```
    python_abi-3.8             |           2_cp38           4 KB  conda-
forge
    scipy-1.10.1               |   py38h10c12cc_0        23.6 MB  conda-
forge
    suitesparse-5.10.1         |       h9e50725_1         2.4 MB  conda-
forge
    sundials-6.5.0             |       h6250759_0         823 KB  conda-
forge
    tbb-2021.7.0               |       h924138e_0         2.0 MB  conda-
forge
    typing-extensions-4.5.0    |       hd8ed1ab_0           9 KB  conda-
forge
    typing_extensions-4.5.0    |     pyha770c72_0          31 KB  conda-
forge
    ------------------------------------------------------------
                                           Total:        96.0 MB

The following NEW packages will be INSTALLED:

  assimulo           conda-forge/linux-64::assimulo-3.4-py38ha96dddf_0
  fmilib             conda-forge/linux-64::fmilib-2.4.1-h27087fc_0
  gmp                conda-forge/linux-64::gmp-6.2.1-h58526e2_0
  icu                conda-forge/linux-64::icu-68.2-h9c3ff4c_0
  libblas            conda-forge/linux-64::libblas-3.9.0-16_linux64_open
blas
  libcblas           conda-forge/linux-64::libcblas-3.9.0-16_linux64_ope
nblas
  libgfortran-ng     conda-forge/linux-64::libgfortran-ng-12.2.0-h69a702
a_19
  libgfortran5       conda-forge/linux-64::libgfortran5-12.2.0-h337968e_
19
  libiconv           conda-forge/linux-64::libiconv-1.17-h166bdaf_0
  liblapack          conda-forge/linux-64::liblapack-3.9.0-16_linux64_op
enblas
  libopenblas        conda-forge/linux-64::libopenblas-0.3.21-pthreads_h
78a6416_3
  libxml2            conda-forge/linux-64::libxml2-2.9.12-h72842e0_0
  libxslt            conda-forge/linux-64::libxslt-1.1.33-h15afd5d_2
  llvm-openmp        conda-forge/linux-64::llvm-openmp-12.0.1-h4bd325d_1
  lxml               conda-forge/linux-64::lxml-4.8.0-py38h0a891b7_2
  metis              conda-forge/linux-64::metis-5.1.0-h58526e2_1006
  mpfr               conda-forge/linux-64::mpfr-4.2.0-hb012696_0
  numpy              conda-forge/linux-64::numpy-1.24.2-py38h10c12cc_0
  packaging          conda-forge/noarch::packaging-23.0-pyhd8ed1ab_0
  platformdirs       conda-forge/noarch::platformdirs-3.1.1-pyhd8ed1ab_0
  pooch              conda-forge/noarch::pooch-1.7.0-pyhd8ed1ab_0
  pyfmi              conda-forge/linux-64::pyfmi-2.9.8-py38h26c90d9_1
  python_abi         conda-forge/linux-64::python_abi-3.8-2_cp38
  scipy              conda-forge/linux-64::scipy-1.10.1-py38h10c12cc_0
  suitesparse        conda-forge/linux-64::suitesparse-5.10.1-h9e50725_1
  sundials           conda-forge/linux-64::sundials-6.5.0-h6250759_0
  tbb                conda-forge/linux-64::tbb-2021.7.0-h924138e_0
  typing-extensions  conda-forge/noarch::typing-extensions-4.5.0-hd8ed1a
b_0
  typing_extensions  conda-forge/noarch::typing_extensions-4.5.0-pyha770
c72_0

The following packages will be REMOVED:

  libgomp-11.2.0-h1234567_1
```

```
The following packages will be UPDATED:

  libgcc-ng          pkgs/main::libgcc-ng-11.2.0-h1234567_1 --> conda-fo
rge::libgcc-ng-12.2.0-h65d4601_19
  libstdcxx-ng       pkgs/main::libstdcxx-ng-11.2.0-h12345~ --> conda-fo
rge::libstdcxx-ng-12.2.0-h46fd767_19

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

  _libgcc_mutex           pkgs/main::_libgcc_mutex-0.1-main --> conda-fo
rge::_libgcc_mutex-0.1-conda_forge
  _openmp_mutex          pkgs/main::_openmp_mutex-5.1-1_gnu --> conda-fo
rge::_openmp_mutex-4.5-2_kmp_llvm
  ca-certificates    pkgs/main::ca-certificates-2023.01.10~ --> conda-fo
rge::ca-certificates-2022.12.7-ha878542_0
  certifi            pkgs/main/linux-64::certifi-2022.12.7~ --> conda-fo
rge/noarch::certifi-2022.12.7-pyhd8ed1ab_0
  conda              pkgs/main::conda-23.1.0-py38h06a4308_0 --> conda-fo
rge::conda-23.1.0-py38h578d9bd_0
  openssl              pkgs/main::openssl-1.1.1t-h7f8727e_0 --> conda-fo
rge::openssl-1.1.1t-h0b41bf4_0



Downloading and Extracting Packages
openssl-1.1.1t       | 1.9 MB    | :   0% 0/1 [00:00<?, ?it/s]
tbb-2021.7.0         | 2.0 MB    | :   0% 0/1 [00:00<?, ?it/s]

_libgcc_mutex-0.1    | 3 KB      | :   0% 0/1 [00:00<?, ?it/s]


liblapack-3.9.0      | 13 KB     | :   0% 0/1 [00:00<?, ?it/s]



libgcc-ng-12.2.0     | 931 KB    | :   0% 0/1 [00:00<?, ?it/s]




icu-68.2             | 13.1 MB   | :   0% 0/1 [00:00<?, ?it/s]




libstdcxx-ng-12.2.0  | 4.3 MB    | :   0% 0/1 [00:00<?, ?it/s]




libopenblas-0.3.21   | 10.1 MB   | :   0% 0/1 [00:00<?, ?it/s]
```

```
mpfr-4.2.0           | 616 KB    | :   0% 0/1 [00:00<?, ?it/s]

certifi-2022.12.7    | 147 KB    | :   0% 0/1 [00:00<?, ?it/s]

ca-certificates-2022 | 143 KB    | :   0% 0/1 [00:00<?, ?it/s]

sundials-6.5.0       | 823 KB    | :   0% 0/1 [00:00<?, ?it/s]

_openmp_mutex-4.5    | 6 KB      | :   0% 0/1 [00:00<?, ?it/s]

typing_extensions-4. | 31 KB     | :   0% 0/1 [00:00<?, ?it/s]
```

```
libcblas-3.9.0       | 13 KB     | :   0% 0/1 [00:00<?, ?it/s]
```

```
suitesparse-5.10.1   | 2.4 MB    | :   0% 0/1 [00:00<?, ?it/s]
```

```
numpy-1.24.2         | 6.3 MB    | :   0% 0/1 [00:00<?, ?it/s]
```

```
libgfortran-ng-12.2. | 22 KB     | :   0% 0/1 [00:00<?, ?it/s]
```

```
gmp-6.2.1            | 806 KB    | :   0% 0/1 [00:00<?, ?it/s]
```

```
 ... (more hidden) ...
tbb-2021.7.0         | 2.0 MB    | :   1% 0.007970693689705332/1 [00:00<
00:14, 14.57s/it]

_libgcc_mutex-0.1    | 3 KB      | : 100% 1.0/1 [00:00<00:00,  8.66it/s]
```

```
openssl-1.1.1t       | 1.9 MB    | :   1% 0.00837250278759782/1 [00:00<0
0:15, 15.66s/it]
```

```
liblapack-3.9.0      | 13 KB     | : 100% 1.0/1 [00:00<00:00,  7.83it/s]
```

```
icu-68.2             | 13.1 MB   | :   0% 0.0011897319682882405/1 [00:00
<02:10, 130.57s/it]

_libgcc_mutex-0.1    | 3 KB      | : 100% 1.0/1 [00:00<00:00,  8.66it/s]
```

```
libstdcxx-ng-12.2.0  | 4.3 MB    | :   0% 0.003642462432659798/1 [00:00<
00:45, 45.20s/it]
openssl-1.1.1t       | 1.9 MB    | :  65% 0.6530552174326301/1 [00:00<0
0:00,  3.39it/s]
```

```
libopenblas-0.3.21   | 10.1 MB   | :   0% 0.0015489208557598652/1 [00:00
<02:37, 157.70s/it]
```

```
icu-68.2             | 13.1 MB   | :   8% 0.07614284597044739/1 [00:00<0
0:02,  2.82s/it]
```

```
liblapack-3.9.0      | 13 KB     | : 100% 1.0/1 [00:00<00:00,  7.83it/s]
```

```
libstdcxx-ng-12.2.0  | 4.3 MB    | :  25% 0.25132990785352605/1 [00:00<0
0:00,  1.15it/s]
```

```
mpfr-4.2.0           | 616 KB    | :   3% 0.02596525815495161/1 [00:00<0
0:10, 10.95s/it]
```

```
certifi-2022.12.7    | 147 KB    | :  11% 0.10862920603348251/1 [00:00<0
0:02,  2.91s/it]
```

```
libopenblas-0.3.21   | 10.1 MB   | :  16% 0.15798992728750624/1 [00:00<0
0:01,  1.73s/it]
```

```
ca-certificates-2022 | 143 KB    | :  11% 0.11222532741520083/1 [00:00<0
0:02,  3.16s/it]
```

```
sundials-6.5.0       | 823 KB    | :   2% 0.019441876691700773/1 [00:00<
00:18, 18.41s/it]
```

```
icu-68.2             | 13.1 MB   | :  17% 0.16656247556035367/1 [00:00<0
0:01,  1.75s/it]
```

```
libstdcxx-ng-12.2.0  | 4.3 MB    | :  55% 0.5500118273316295/1 [00:00<0
0:00,  1.86it/s]
```

```
_openmp_mutex-4.5    | 6 KB      | : 100% 1.0/1 [00:00<00:00,  2.54it/s]
```

```
libcblas-3.9.0       | 13 KB     | : 100% 1.0/1 [00:00<00:00,  2.36it/s]
```

```
typing_extensions-4. | 31 KB     | :  52% 0.5229993296517381/1 [00:00<0
0:00,  1.22it/s]
```

```
libopenblas-0.3.21   | 10.1 MB   | :  29% 0.286550358315575/1 [00:00<00:
00,  1.22s/it]
```

```
suitesparse-5.10.1   | 2.4 MB    | :   1% 0.006510694523092818/1 [00:00<
01:10, 70.48s/it]
```

```
icu-68.2             | 13.1 MB   | :  29% 0.2879151363257542/1 [00:00<0
0:00,  1.25s/it]
```

```
numpy-1.24.2         | 6.3 MB    | :   0% 0.00246386425166665/1 [00:00<0
3:08, 188.88s/it]
```

```
libstdcxx-ng-12.2.0  | 4.3 MB    | :  94% 0.9361128451935681/1 [00:00<0
0:00,  2.58it/s]
```

```
libgfortran-ng-12.2. | 22 KB     | :  72% 0.7159587484705471/1 [00:00<0
0:00,  1.35it/s]
```

```
libopenblas-0.3.21   | 10.1 MB   | :  40% 0.3965237390745255/1 [00:00<0
0:00,  1.10s/it]
```

```
suitesparse-5.10.1   | 2.4 MB    | :  57% 0.5664304235090752/1 [00:00<0
0:00,  1.34it/s]
```

```
icu-68.2             | 13.1 MB   | :  41% 0.40926779709115474/1 [00:00<0
0:00,  1.07s/it]
```

```
gmp-6.2.1            | 806 KB    | :   2% 0.019840539414665338/1 [00:00<
00:27, 28.26s/it]
```

```
numpy-1.24.2         | 6.3 MB    | :  30% 0.30305530295499794/1 [00:00<0
0:00,  1.41s/it]
```

```
libopenblas-0.3.21   | 10.1 MB   | :  56% 0.5576115080735514/1 [00:00<0
0:00,  1.13it/s]
```

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

```
icu-68.2             | 13.1 MB   | :  55% 0.5544150972223201/1 [00:00<0
0:00,  1.09it/s]
```

```
numpy-1.24.2         | 6.3 MB    | :  49% 0.49277285033332996/1 [00:00<0
0:00,  1.01s/it]
```

```
libopenblas-0.3.21   | 10.1 MB   | :  68% 0.6846230182458604/1 [00:00<0
0:00,  1.15it/s]
```

```
numpy-1.24.2         | 6.3 MB    | :  72% 0.7219122257383284/1 [00:00<0
0:00,  1.30it/s]
```

```
icu-68.2             | 13.1 MB   | :  67% 0.6674396342097029/1 [00:00<0
0:00,  1.03it/s]
```

```
libopenblas-0.3.21   | 10.1 MB   | :  86% 0.8565532332352054/1 [00:00<0
0:00,  1.32it/s]
```

```
icu-68.2              | 13.1 MB   | :  80% 0.7983101507214093/1 [00:00<0
0:00,  1.10it/s]
```

```
numpy-1.24.2          | 6.3 MB    | :  96% 0.9584431938983268/1 [00:00<0
0:00,  1.55it/s]
```

```
openssl-1.1.1t        | 1.9 MB    | : 100% 1.0/1 [00:01<00:00,  3.39it/s]
```

```
libgcc-ng-12.2.0      | 931 KB    | : 100% 1.0/1 [00:01<00:00,  1.14s/it]
```

```
libgcc-ng-12.2.0      | 931 KB    | : 100% 1.0/1 [00:01<00:00,  1.14s/it]
```

```
mpfr-4.2.0            | 616 KB    | : 100% 1.0/1 [00:01<00:00,  1.31s/it]
```

```
mpfr-4.2.0            | 616 KB    | : 100% 1.0/1 [00:01<00:00,  1.31s/it]
```

```
certifi-2022.12.7    | 147 KB    | : 100% 1.0/1 [00:01<00:00,  1.39s/it]
```


```
certifi-2022.12.7    | 147 KB    | : 100% 1.0/1 [00:01<00:00,  1.39s/it]
```


```
ca-certificates-2022 | 143 KB    | : 100% 1.0/1 [00:01<00:00,  1.51s/it]
```


```
ca-certificates-2022 | 143 KB    | : 100% 1.0/1 [00:01<00:00,  1.51s/it]
```


```
sundials-6.5.0       | 823 KB    | : 100% 1.0/1 [00:01<00:00,  1.74s/it]
```


```
sundials-6.5.0       | 823 KB    | : 100% 1.0/1 [00:01<00:00,  1.74s/it]
```

```
_openmp_mutex-4.5    | 6 KB      | : 100% 1.0/1 [00:01<00:00,  2.54it/s]

libcblas-3.9.0       | 13 KB     | : 100% 1.0/1 [00:01<00:00,  2.36it/s]

typing_extensions-4. | 31 KB     | : 100% 1.0/1 [00:01<00:00,  2.16s/it]

typing_extensions-4. | 31 KB     | : 100% 1.0/1 [00:01<00:00,  2.16s/it]
tbb-2021.7.0         | 2.0 MB    | : 100% 1.0/1 [00:02<00:00,  2.59s/it]
tbb-2021.7.0         | 2.0 MB    | : 100% 1.0/1 [00:02<00:00,  2.59s/it]
```

```
libgfortran-ng-12.2. | 22 KB     | : 100% 1.0/1 [00:02<00:00,  2.62s/it]
```


```
libgfortran-ng-12.2. | 22 KB     | : 100% 1.0/1 [00:02<00:00,  2.62s/it]
```


```
gmp-6.2.1            | 806 KB    | : 100% 1.0/1 [00:02<00:00,  2.38s/it]
```


```
gmp-6.2.1            | 806 KB    | : 100% 1.0/1 [00:02<00:00,  2.38s/it]
```

```
libstdcxx-ng-12.2.0  | 4.3 MB    | : 100% 1.0/1 [00:03<00:00,  2.58it/s]
```

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

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

```
suitesparse-5.10.1   | 2.4 MB    | : 100% 1.0/1 [00:03<00:00,  4.28s/it]
```

```
suitesparse-5.10.1   | 2.4 MB    | : 100% 1.0/1 [00:03<00:00,  4.28s/it]
```

```
numpy-1.24.2         | 6.3 MB    | : 100% 1.0/1 [00:06<00:00,  1.55it/s]
```

```
libopenblas-0.3.21   | 10.1 MB   | : 100% 1.0/1 [00:13<00:00, 28.16s/it]
```

```
libopenblas-0.3.21   | 10.1 MB   | : 100% 1.0/1 [00:13<00:00, 28.16s/it]
```

```
icu-68.2             | 13.1 MB   | : 100% 1.0/1 [00:15<00:00,  1.22it/s]
```

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

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

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

In [ ]:
```
%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 [1]:
```
run -i BPL_TEST2_Batch_explore.py
```

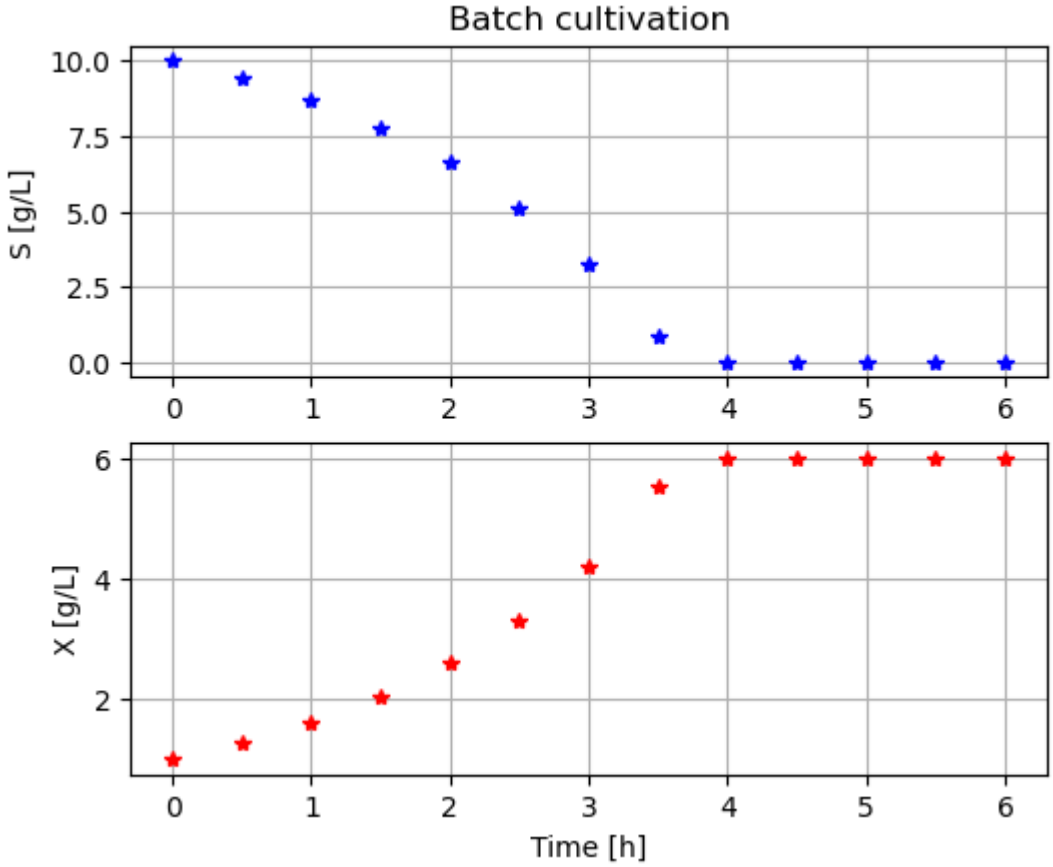
```
Linux - run FMU pre-comiled OpenModelica 1.21.0

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 sim
ulation
 - describe()  - describe culture, broth, parameters, variables with val
ues/units

Note that both disp() and describe() takes values from the last simulati
on

Brief information about a command by help(), eg help(simu)
Key system information is listed with the command system_info()
```

In [2]:
```
# Adjust the size of diagrams
plt.rcParams['figure.figsize'] = [15/2.54, 12/2.54]
```

1 Generate data later used for parameter estimation

In [3]:
```
import pandas as pd
```

In [4]:
```
# Data generated
simulationTime = 6.0
par(Y=0.50, qSmax=1.00, Ks=0.1)
init(V_0=1.0, VS_0=10, VX_0=1.0)
newplot(plotType='Demo_2')
simu(simulationTime, options=opts_data)
```



In [5]:
```
# Store data in a DataFrame for later use
data = pd.DataFrame(data={'time':sim_res['time'], 'X':sim_res['bioreactor
data
```

Out[5]:

	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

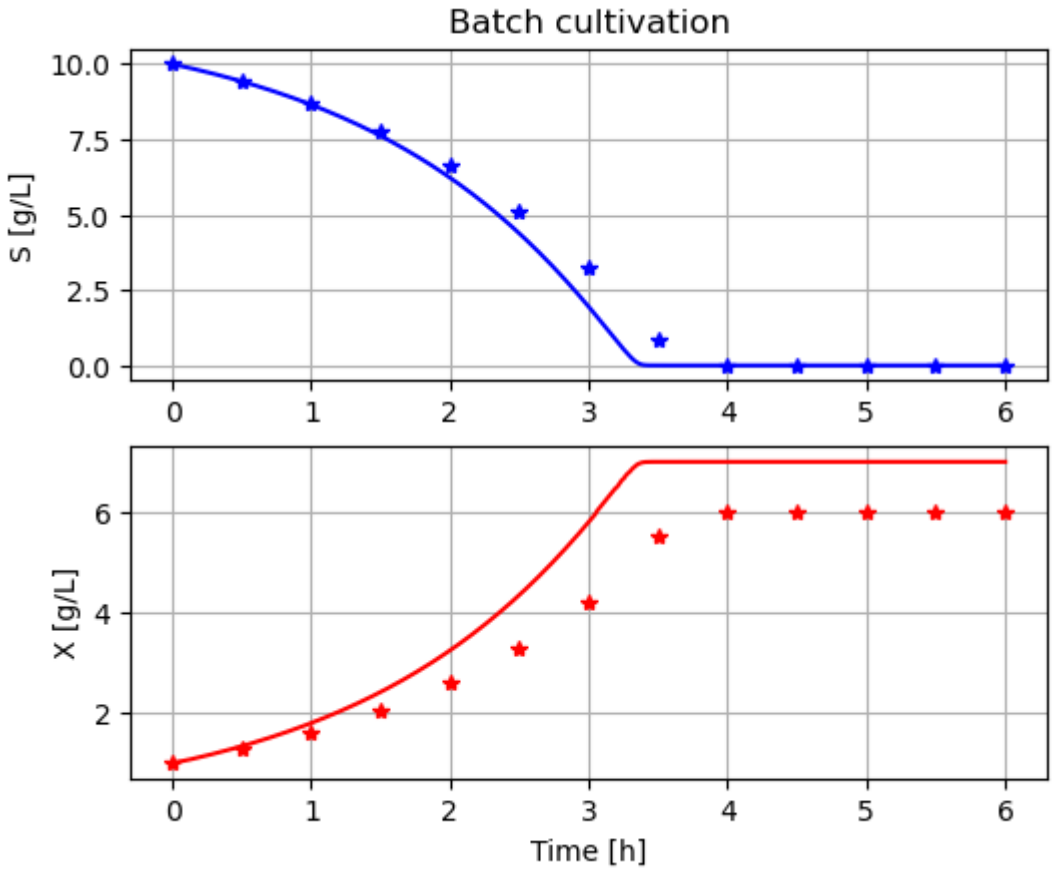
2 Simulation with initial guess of parameters compared with data

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.

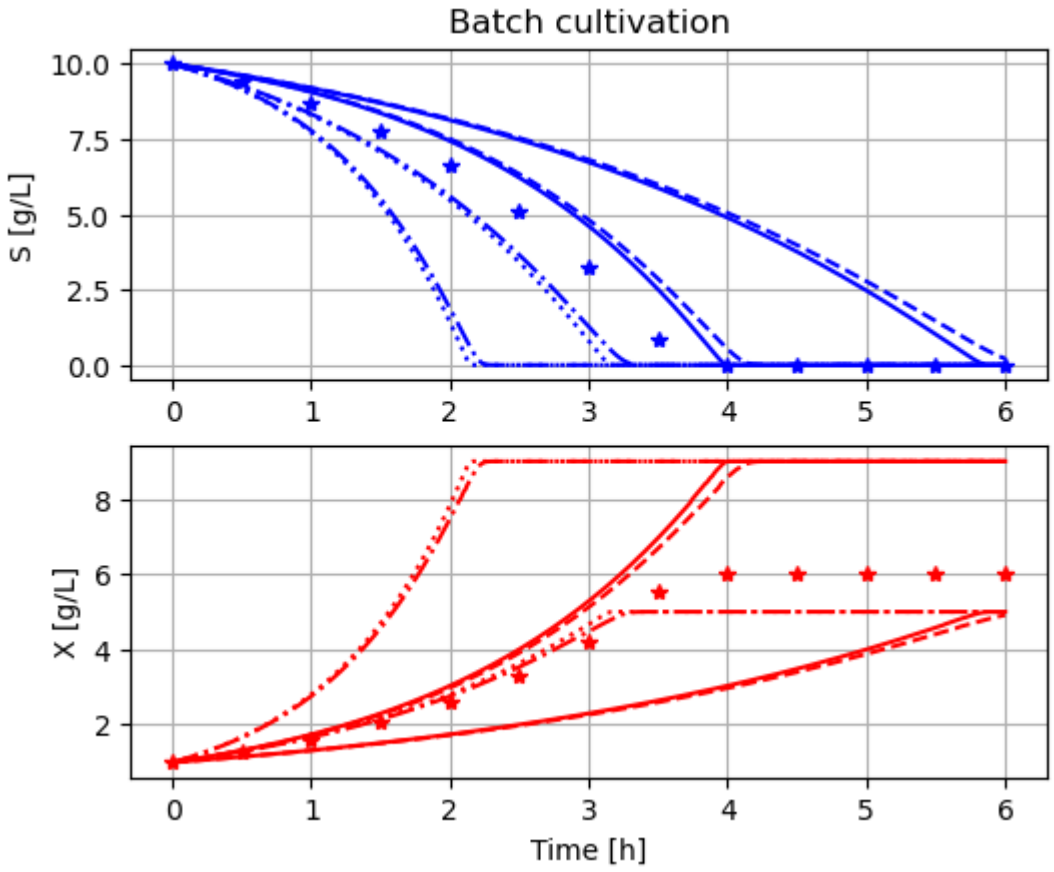
In [6]:
```
# Parameters to be estimated using parDict names and their bounds
parEstim = ['Y', 'qSmax', 'Ks']
parBounds = [(0.4, 0.8), (0.7, 1.3), (0.05, 0.20)]
parEstim_0 = [np.mean(parBounds[k]) for k in range(len(parBounds))]
```

In [7]:
```
# 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 [8]:
```
# 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 [9]:
```
# Optimization routine import
import scipy.optimize
```

In [10]:
```
# Parameters to be estimated using parDict names and their bounds
extra_args = (parEstim, data, fmu_model, simulationTime)
```

In [11]:
```
# Modified evaluation function tailored for Python optimization algorithm
def objective(x, parEstim, data=data, fmu_model=fmu_model, simulationTime
    """The parameter list is tailored for scipy optimization algorithms i
       where the first parameter x is an array with parameters that are t
       and evalauted and parEstim is a list of the names of these paramet
       The code can be made 20-30% faster, but loner, using pyfmi-command

    # 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['
    V['S'] = np.linalg.norm(data['S'] - np.interp(data['time'], sim_res['

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

In [12]:
```
import time
```

In [13]:
```
# Run minimize()
start_time = time.time()
result = scipy.optimize.minimize(objective, x0=parEstim_0, args=extra_arg
                                 method='Nelder-Mead', bounds=parBounds,
print('CPU-time =', time.time()-start_time)
```

```
Optimization terminated successfully.
         Current function value: 0.148311
         Iterations: 66
         Function evaluations: 122
CPU-time = 2.5193231105804443
```

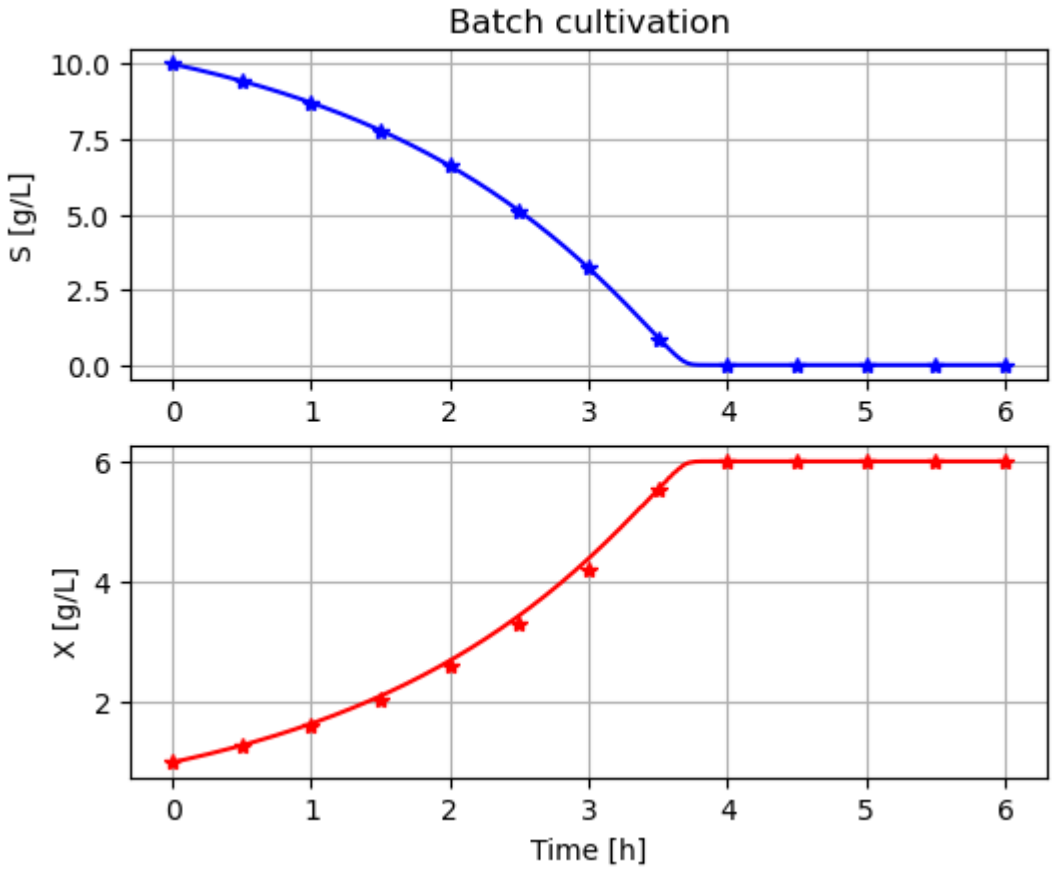
In [14]:
```
result.x
```

Out[14]:
```
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 [15]:
```
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 [16]:
```
# The estimated parameters are
for i in range(len(parEstim)): print(parEstim[i],':', result.x[i])
```

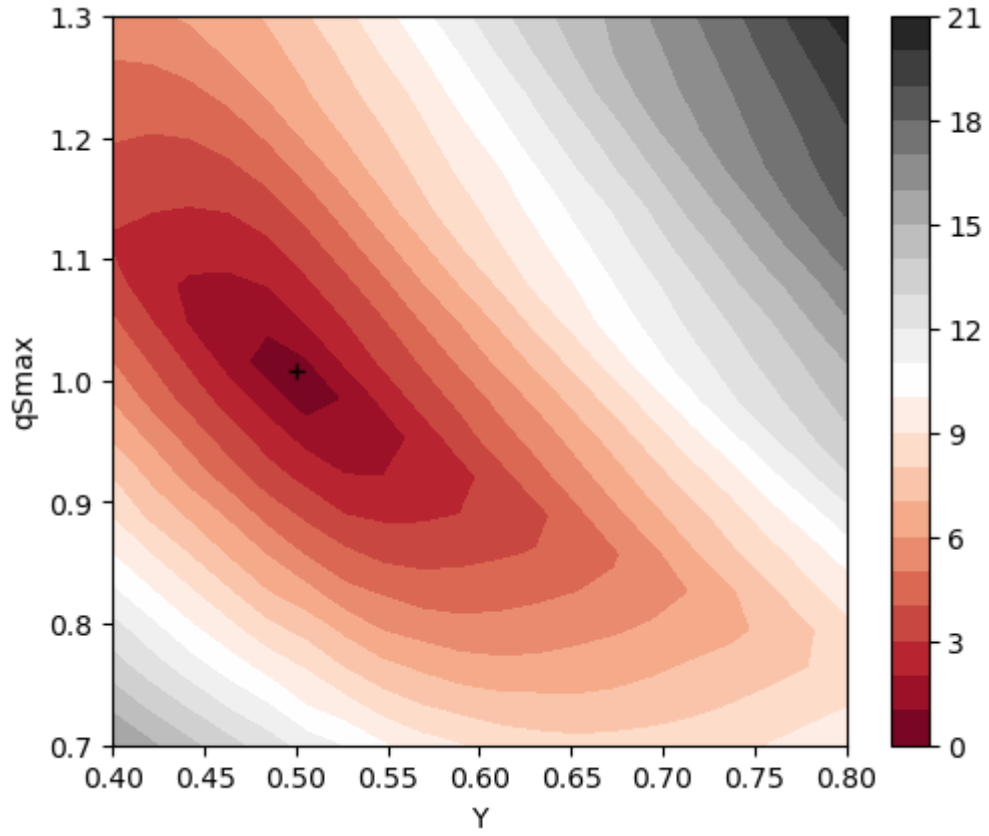
```
Y : 0.4999727558733863
qSmax : 1.0073152667279195
Ks : 0.14380564144282715
```

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 [17]:
```
# Sweep through Y and qSmax variation and store the value of the loss-fun
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 [18]:
```
describe('parts')
```

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

In [19]:
```
describe('MSL')
```

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

In [20]:
```
system_info()
```

```
System information
 -OS: Linux
 -Python: 3.8.16
 -Scipy: 1.10.0
 -PyFMI: 2.9.8
 -FMU by: OpenModelica Compiler OpenModelica 1.21.0~dev-185-g9d983b8
 -FMI: 2.0
 -Type: FMUModelME2
 -Name: BPL_TEST2.Batch
 -Generated: 2023-01-19T09:34:26Z
 -MSL: 3.2.3
 -Description: Bioprocess Library version 2.1.1-beta
 -Interaction: FMU-explore version 0.9.6
```

In [ ]: