janpeter19 / **BPL_TEST2_Batch_calibration** Public

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main

BPL_TEST2_Batch_calibration / BPL_TEST2_Batch_calibration_colab.ipynb

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1 contributor

1631 lines (1631 sloc) | 178 KB

BPL_TEST2_Batch_calibration script with PyFMI ver 2.7.4

The key library PyFMI v2.7.4 is installed and downgrading is done Numpy v1.19.1. To simplify this we first install conda.

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 18.04.6 LTS
Release:        18.04
Codename:       bionic
```

In [2]:
```
%env PYTHONPATH=
```

```
env: PYTHONPATH=
```

In [3]:
```
!wget https://repo.anaconda.com/miniconda/Miniconda3-py37_4.12.0-Linux
!chmod +x Miniconda3-py37_4.12.0-Linux-x86_64.sh
!bash ./Miniconda3-py37_4.12.0-Linux-x86_64.sh -b -f -p /usr/local
import sys
sys.path.append('/usr/local/lib/python3.7/site-packages/')
```

```
--2022-11-30 18:19:29--  https://repo.anaconda.com/miniconda/Miniconda
3-py37_4.12.0-Linux-x86_64.sh
Resolving repo.anaconda.com (repo.anaconda.com)... 104.16.130.3, 104.1
6.131.3, 2606:4700::6810:8203, ...
Connecting to repo.anaconda.com (repo.anaconda.com)|104.16.130.3|:44
3... connected.
HTTP request sent, awaiting response... 200 OK
Length: 104996770 (100M) [application/x-sh]
Saving to: ‘Miniconda3-py37_4.12.0-Linux-x86_64.sh’

Miniconda3-py37_4.1 100%[===================>] 100.13M   111MB/s    in
0.9s

2022-11-30 18:19:30 (111 MB/s) - ‘Miniconda3-py37_4.12.0-Linux-x86_64.
sh’ saved [104996770/104996770]

PREFIX=/usr/local
Unpacking payload ...
Collecting package metadata (current_repodata.json): - \ done
Solving environment: / - \ done

## Package Plan ##

  environment location: /usr/local

  added / updated specs:
```

```
    - _libgcc_mutex==0.1=main
    - _openmp_mutex==4.5=1_gnu
    - brotlipy==0.7.0=py37h27cfd23_1003
    - ca-certificates==2022.3.29=h06a4308_1
    - certifi==2021.10.8=py37h06a4308_2
    - cffi==1.15.0=py37hd667e15_1
    - charset-normalizer==2.0.4=pyhd3eb1b0_0
    - colorama==0.4.4=pyhd3eb1b0_0
    - conda-content-trust==0.1.1=pyhd3eb1b0_0
    - conda-package-handling==1.8.1=py37h7f8727e_0
    - conda==4.12.0=py37h06a4308_0
    - cryptography==36.0.0=py37h9ce1e76_0
    - idna==3.3=pyhd3eb1b0_0
    - ld_impl_linux-64==2.35.1=h7274673_9
    - libffi==3.3=he6710b0_2
    - libgcc-ng==9.3.0=h5101ec6_17
    - libgomp==9.3.0=h5101ec6_17
    - libstdcxx-ng==9.3.0=hd4cf53a_17
    - ncurses==6.3=h7f8727e_2
    - openssl==1.1.1n=h7f8727e_0
    - pip==21.2.2=py37h06a4308_0
    - pycosat==0.6.3=py37h27cfd23_0
    - pycparser==2.21=pyhd3eb1b0_0
    - pyopenssl==22.0.0=pyhd3eb1b0_0
    - pysocks==1.7.1=py37_1
    - python==3.7.13=h12debd9_0
    - readline==8.1.2=h7f8727e_1
    - requests==2.27.1=pyhd3eb1b0_0
    - ruamel_yaml==0.15.100=py37h27cfd23_0
    - setuptools==61.2.0=py37h06a4308_0
    - six==1.16.0=pyhd3eb1b0_1
    - sqlite==3.38.2=hc218d9a_0
    - tk==8.6.11=h1ccaba5_0
    - tqdm==4.63.0=pyhd3eb1b0_0
    - urllib3==1.26.8=pyhd3eb1b0_0
    - wheel==0.37.1=pyhd3eb1b0_0
    - xz==5.2.5=h7b6447c_0
    - yaml==0.2.5=h7b6447c_0
    - zlib==1.2.12=h7f8727e_1


The following NEW packages will be INSTALLED:

  _libgcc_mutex      pkgs/main/linux-64::_libgcc_mutex-0.1-main
  _openmp_mutex      pkgs/main/linux-64::_openmp_mutex-4.5-1_gnu
  brotlipy           pkgs/main/linux-64::brotlipy-0.7.0-py37h27cfd23_1
003
  ca-certificates    pkgs/main/linux-64::ca-certificates-2022.3.29-h06
a4308_1
  certifi            pkgs/main/linux-64::certifi-2021.10.8-py37h06a430
8_2
  cffi               pkgs/main/linux-64::cffi-1.15.0-py37hd667e15_1
  charset-normalizer pkgs/main/noarch::charset-normalizer-2.0.4-pyhd3e
b1b0_0
  colorama           pkgs/main/noarch::colorama-0.4.4-pyhd3eb1b0_0
  conda              pkgs/main/linux-64::conda-4.12.0-py37h06a4308_0
  conda-content-tru~ pkgs/main/noarch::conda-content-trust-0.1.1-pyhd3
eb1b0_0
  conda-package-han~ pkgs/main/linux-64::conda-package-handling-1.8.1-
py37h7f8727e_0
  cryptography       pkgs/main/linux-64::cryptography-36.0.0-py37h9ce1
e76_0
  idna               pkgs/main/noarch::idna-3.3-pyhd3eb1b0_0
  ld_impl_linux-64   pkgs/main/linux-64::ld_impl_linux-64-2.35.1-h7274
673_9
```

```
  _
  libffi             pkgs/main/linux-64::libffi-3.3-he6710b0_2
  libgcc-ng          pkgs/main/linux-64::libgcc-ng-9.3.0-h5101ec6_17
  libgomp            pkgs/main/linux-64::libgomp-9.3.0-h5101ec6_17
  libstdcxx-ng       pkgs/main/linux-64::libstdcxx-ng-9.3.0-hd4cf53a_1
7
  ncurses            pkgs/main/linux-64::ncurses-6.3-h7f8727e_2
  openssl            pkgs/main/linux-64::openssl-1.1.1n-h7f8727e_0
  pip                pkgs/main/linux-64::pip-21.2.2-py37h06a4308_0
  pycosat            pkgs/main/linux-64::pycosat-0.6.3-py37h27cfd23_0
  pycparser          pkgs/main/noarch::pycparser-2.21-pyhd3eb1b0_0
  pyopenssl          pkgs/main/noarch::pyopenssl-22.0.0-pyhd3eb1b0_0
  pysocks            pkgs/main/linux-64::pysocks-1.7.1-py37_1
  python             pkgs/main/linux-64::python-3.7.13-h12debd9_0
  readline           pkgs/main/linux-64::readline-8.1.2-h7f8727e_1
  requests           pkgs/main/noarch::requests-2.27.1-pyhd3eb1b0_0
  ruamel_yaml        pkgs/main/linux-64::ruamel_yaml-0.15.100-py37h27c
fd23_0
  setuptools         pkgs/main/linux-64::setuptools-61.2.0-py37h06a430
8_0
  six                pkgs/main/noarch::six-1.16.0-pyhd3eb1b0_1
  sqlite             pkgs/main/linux-64::sqlite-3.38.2-hc218d9a_0
  tk                 pkgs/main/linux-64::tk-8.6.11-h1ccaba5_0
  tqdm               pkgs/main/noarch::tqdm-4.63.0-pyhd3eb1b0_0
  urllib3            pkgs/main/noarch::urllib3-1.26.8-pyhd3eb1b0_0
  wheel              pkgs/main/noarch::wheel-0.37.1-pyhd3eb1b0_0
  xz                 pkgs/main/linux-64::xz-5.2.5-h7b6447c_0
  yaml               pkgs/main/linux-64::yaml-0.2.5-h7b6447c_0
  zlib               pkgs/main/linux-64::zlib-1.2.12-h7f8727e_1


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

In [4]:

```
!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
    ---------------------------|-----------------
    _openmp_mutex-5.1          |            1_gnu          21 KB
    ca-certificates-2022.10.11 |       h06a4308_0         124 KB
    certifi-2022.9.24          |   py37h06a4308_0         154 KB
    cffi-1.15.1                |   py37h74dc2b5_0         227 KB
    conda-22.9.0               |   py37h06a4308_0         878 KB
    conda-package-handling-1.9.0|   py37h5eee18b_1         945 KB
    cryptography-38.0.1        |   py37h9ce1e76_0         1.3 MB
    idna-3.4                   |   py37h06a4308_0          91 KB
    ld_impl_linux-64-2.38      |       h1181459_1         654 KB
    libgcc-ng-11.2.0           |       h1234567_1         5.3 MB
    libgomp-11.2.0             |       h1234567_1         474 KB
    libstdcxx-ng-11.2.0        |       h1234567_1         4.7 MB
```

```
    ncurses-6.3                |       h5eee18b_3         781 KB
    openssl-1.1.1s             |       h7f8727e_0         3.6 MB
    pip-22.2.2                 |   py37h06a4308_0         2.3 MB
    pycosat-0.6.4              |   py37h5eee18b_0          84 KB
    readline-8.2               |       h5eee18b_0         357 KB
    requests-2.28.1            |   py37h06a4308_0          92 KB
    setuptools-65.5.0          |   py37h06a4308_0         1.1 MB
    sqlite-3.40.0              |       h5082296_0         1.2 MB
    tk-8.6.12                  |       h1ccaba5_0         3.0 MB
    toolz-0.12.0               |   py37h06a4308_0         104 KB
    tqdm-4.64.1                |   py37h06a4308_0         126 KB
    urllib3-1.26.12            |   py37h06a4308_0         181 KB
    xz-5.2.6                   |       h5eee18b_0         394 KB
    zlib-1.2.13                |       h5eee18b_0         103 KB
    ------------------------------------------------------------
                                           Total:        28.2 MB

The following NEW packages will be INSTALLED:

  toolz              pkgs/main/linux-64::toolz-0.12.0-py37h06a4308_0

The following packages will be REMOVED:

  colorama-0.4.4-pyhd3eb1b0_0
  conda-content-trust-0.1.1-pyhd3eb1b0_0
  six-1.16.0-pyhd3eb1b0_1

The following packages will be UPDATED:

  _openmp_mutex                                 4.5-1_gnu --> 5.1-1_
gnu
  ca-certificates                       2022.3.29-h06a4308_1 --> 2022.1
0.11-h06a4308_0
  certifi                           2021.10.8-py37h06a4308_2 --> 2022.
9.24-py37h06a4308_0
  cffi                                 1.15.0-py37hd667e15_1 --> 1.15.1
-py37h74dc2b5_0
  conda                                4.12.0-py37h06a4308_0 --> 22.9.0
-py37h06a4308_0
  conda-package-han~                    1.8.1-py37h7f8727e_0 --> 1.9.0-
py37h5eee18b_1
  cryptography                         36.0.0-py37h9ce1e76_0 --> 38.0.1
-py37h9ce1e76_0
  idna               pkgs/main/noarch::idna-3.3-pyhd3eb1b0~ --> pkgs/m
ain/linux-64::idna-3.4-py37h06a4308_0
  ld_impl_linux-64                        2.35.1-h7274673_9 --> 2.38-h
1181459_1
  libgcc-ng                               9.3.0-h5101ec6_17 --> 11.2.0
-h1234567_1
  libgomp                                 9.3.0-h5101ec6_17 --> 11.2.0
-h1234567_1
  libstdcxx-ng                            9.3.0-hd4cf53a_17 --> 11.2.0
-h1234567_1
  ncurses                                    6.3-h7f8727e_2 --> 6.3-h5
eee18b_3
  openssl                                 1.1.1n-h7f8727e_0 --> 1.1.1s
-h7f8727e_0
  pip                                  21.2.2-py37h06a4308_0 --> 22.2.2
-py37h06a4308_0
  pycosat                               0.6.3-py37h27cfd23_0 --> 0.6.4-
py37h5eee18b_0
  readline                                 8.1.2-h7f8727e_1 --> 8.2-h5
eee18b_0
  requests           pkgs/main/noarch::requests-2.27.1-pyh~ --> pkgs/m
```

```
ain/linux-64::requests-2.28.1-py37h06a4308_0
  setuptools                         61.2.0-py37h06a4308_0 --> 65.5.0
-py37h06a4308_0
  sqlite                                3.38.2-hc218d9a_0 --> 3.40.0
-h5082296_0
  tk                                    8.6.11-h1ccaba5_0 --> 8.6.12
-h1ccaba5_0
  tqdm               pkgs/main/noarch::tqdm-4.63.0-pyhd3eb~ --> pkgs/m
ain/linux-64::tqdm-4.64.1-py37h06a4308_0
  urllib3            pkgs/main/noarch::urllib3-1.26.8-pyhd~ --> pkgs/m
ain/linux-64::urllib3-1.26.12-py37h06a4308_0
  xz                                     5.2.5-h7b6447c_0 --> 5.2.6-
h5eee18b_0
  zlib                                  1.2.12-h7f8727e_1 --> 1.2.13
-h5eee18b_0



Downloading and Extracting Packages
ca-certificates-2022 | 124 KB    | : 100% 1.0/1 [00:00<00:00,  7.57it/
s]
conda-package-handli | 945 KB    | : 100% 1.0/1 [00:00<00:00,  7.36it/
s]
openssl-1.1.1s       | 3.6 MB    | : 100% 1.0/1 [00:00<00:00,  2.91it/
s]
pycosat-0.6.4        | 84 KB     | : 100% 1.0/1 [00:00<00:00, 13.95it/
s]
toolz-0.12.0         | 104 KB    | : 100% 1.0/1 [00:00<00:00, 10.82it/
s]
libstdcxx-ng-11.2.0  | 4.7 MB    | : 100% 1.0/1 [00:00<00:00,  2.64it/
s]
ncurses-6.3          | 781 KB    | : 100% 1.0/1 [00:00<00:00,  3.12it/
s]
urllib3-1.26.12      | 181 KB    | : 100% 1.0/1 [00:00<00:00, 12.83it/
s]
requests-2.28.1      | 92 KB     | : 100% 1.0/1 [00:00<00:00, 12.32it/
s]
tk-8.6.12            | 3.0 MB    | : 100% 1.0/1 [00:00<00:00,  5.13it/
s]
idna-3.4             | 91 KB     | : 100% 1.0/1 [00:00<00:00, 15.84it/
s]
ld_impl_linux-64-2.3 | 654 KB    | : 100% 1.0/1 [00:00<00:00, 10.53it/
s]
_openmp_mutex-5.1    | 21 KB     | : 100% 1.0/1 [00:00<00:00, 13.40it/
s]
libgcc-ng-11.2.0     | 5.3 MB    | : 100% 1.0/1 [00:00<00:00,  4.63it/
s]
readline-8.2         | 357 KB    | : 100% 1.0/1 [00:00<00:00, 12.65it/
s]
pip-22.2.2           | 2.3 MB    | : 100% 1.0/1 [00:00<00:00,  3.12it/
s]
setuptools-65.5.0    | 1.1 MB    | : 100% 1.0/1 [00:00<00:00,  6.56it/
s]
tqdm-4.64.1          | 126 KB    | : 100% 1.0/1 [00:00<00:00, 11.13it/
s]
conda-22.9.0         | 878 KB    | : 100% 1.0/1 [00:00<00:00,  7.55it/
s]
xz-5.2.6             | 394 KB    | : 100% 1.0/1 [00:00<00:00, 11.07it/
s]
zlib-1.2.13          | 103 KB    | : 100% 1.0/1 [00:00<00:00, 12.10it/
s]
certifi-2022.9.24    | 154 KB    | : 100% 1.0/1 [00:00<00:00, 14.67it/
s]
libgomp-11.2.0       | 474 KB    | : 100% 1.0/1 [00:00<00:00,  6.50it/
s]
```

```
cryptography-38.0.1  | 1.3 MB    | : 100% 1.0/1 [00:00<00:00,  7.49it/
s]
sqlite-3.40.0        | 1.2 MB    | : 100% 1.0/1 [00:00<00:00,  9.66it/
s]
cffi-1.15.1          | 227 KB    | : 100% 1.0/1 [00:00<00:00, 14.12it/
s]
Preparing transaction: \ | / - done
Verifying transaction: | / - \ | / - \ | done
Executing transaction: - \ | / - \ | / - \ | / done
```

In [5]:

```
!conda --version
!python --version
```

```
conda 22.9.0
Python 3.7.13
```

In [6]:

```
!conda install -c conda-forge pyfmi==2.7.4 --yes # Install the key pac
```

```
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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- \ | / - \ | / - \ | / - \ | / done

## Package Plan ##
```

```
  environment location: /usr/local

  added / updated specs:
    - pyfmi==2.7.4


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    assimulo-3.2.9             |   py37h7fe24a9_0         2.6 MB  cond
a-forge
    ca-certificates-2022.9.24  |       ha878542_0         150 KB  cond
a-forge
    certifi-2022.9.24          |     pyhd8ed1ab_0         155 KB  cond
a-forge
    conda-22.9.0               |   py37h89c1867_1         960 KB  cond
a-forge
    fmilib-2.2.3               |       he1b5a44_0         532 KB  cond
a-forge
    gmp-6.2.1                  |       h58526e2_0         806 KB  cond
a-forge
    icu-68.2                   |       h9c3ff4c_0        13.1 MB  cond
a-forge
    libblas-3.9.0              |15_linux64_openblas          12 KB  co
nda-forge
    libcblas-3.9.0             |15_linux64_openblas          12 KB  co
nda-forge
    libgfortran-ng-12.2.0      |      h69a702a_19          22 KB  cond
a-forge
    libgfortran5-12.2.0        |      h337968e_19         1.8 MB  cond
a-forge
    libiconv-1.17              |       h166bdaf_0         1.4 MB  cond
a-forge
    liblapack-3.9.0            |15_linux64_openblas          12 KB  co
nda-forge
    libopenblas-0.3.20         |pthreads_h78a6416_0        10.1 MB  co
nda-forge
    libxml2-2.9.12             |       h72842e0_0         772 KB  cond
a-forge
    libxslt-1.1.33             |       h15afd5d_2         522 KB  cond
a-forge
    lxml-4.8.0                 |   py37h540881e_2         1.4 MB  cond
a-forge
    metis-5.1.0                |    h58526e2_1006         4.1 MB  cond
a-forge
    mpfr-4.1.0                 |       h9202a9a_1         2.6 MB  cond
a-forge
    numpy-1.21.6               |   py37h976b520_0         6.1 MB  cond
a-forge
    openssl-1.1.1o             |       h166bdaf_0         2.1 MB  cond
a-forge
    pyfmi-2.7.4                |   py37h161383b_0        12.4 MB  cond
a-forge
    python_abi-3.7             |          2_cp37m           4 KB  cond
a-forge
    scipy-1.7.3                |   py37hf2a6cf1_0        21.8 MB  cond
a-forge
    suitesparse-5.10.1         |       h9e50725_1         2.4 MB  cond
a-forge
    sundials-5.8.0             |       h558c624_0         1.0 MB  cond
a-forge
    tbb-2021.5.0               |       h924138e_1         1.9 MB  cond
```

```
a-forge
    ------------------------------------------------------------

                                           Total:        88.5 MB

The following NEW packages will be INSTALLED:

  assimulo           conda-forge/linux-64::assimulo-3.2.9-py37h7fe24a9
_0 None
  fmilib             conda-forge/linux-64::fmilib-2.2.3-he1b5a44_0 Non
e
  gmp                conda-forge/linux-64::gmp-6.2.1-h58526e2_0 None
  icu                conda-forge/linux-64::icu-68.2-h9c3ff4c_0 None
  libblas            conda-forge/linux-64::libblas-3.9.0-15_linux64_op
enblas None
  libcblas           conda-forge/linux-64::libcblas-3.9.0-15_linux64_o
penblas None
  libgfortran-ng     conda-forge/linux-64::libgfortran-ng-12.2.0-h69a7
02a_19 None
  libgfortran5       conda-forge/linux-64::libgfortran5-12.2.0-h337968
e_19 None
  libiconv           conda-forge/linux-64::libiconv-1.17-h166bdaf_0 No
ne
  liblapack          conda-forge/linux-64::liblapack-3.9.0-15_linux64_
openblas None
  libopenblas        conda-forge/linux-64::libopenblas-0.3.20-pthreads
_h78a6416_0 None
  libxml2            conda-forge/linux-64::libxml2-2.9.12-h72842e0_0 N
one
  libxslt            conda-forge/linux-64::libxslt-1.1.33-h15afd5d_2 N
one
  lxml               conda-forge/linux-64::lxml-4.8.0-py37h540881e_2 N
one
  metis              conda-forge/linux-64::metis-5.1.0-h58526e2_1006 N
one
  mpfr               conda-forge/linux-64::mpfr-4.1.0-h9202a9a_1 None
  numpy              conda-forge/linux-64::numpy-1.21.6-py37h976b520_0
None
  pyfmi              conda-forge/linux-64::pyfmi-2.7.4-py37h161383b_0
None
  python_abi         conda-forge/linux-64::python_abi-3.7-2_cp37m None
  scipy              conda-forge/linux-64::scipy-1.7.3-py37hf2a6cf1_0
None
  suitesparse        conda-forge/linux-64::suitesparse-5.10.1-h9e50725
_1 None
  sundials           conda-forge/linux-64::sundials-5.8.0-h558c624_0 N
one
  tbb                conda-forge/linux-64::tbb-2021.5.0-h924138e_1 Non
e

The following packages will be UPDATED:

  conda              pkgs/main::conda-22.9.0-py37h06a4308_0 --> conda-
forge::conda-22.9.0-py37h89c1867_1 None

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

  ca-certificates    pkgs/main::ca-certificates-2022.10.11~ --> conda-
forge::ca-certificates-2022.9.24-ha878542_0 None
  certifi            pkgs/main/linux-64::certifi-2022.9.24~ --> conda-
forge/noarch::certifi-2022.9.24-pyhd8ed1ab_0 None
  openssl              pkgs/main::openssl-1.1.1s-h7f8727e_0 --> conda-
forge::openssl-1.1.1o-h166bdaf_0 None
```

```
Downloading and Extracting Packages
openssl-1.1.1o       | 2.1 MB    | : 100% 1.0/1 [00:00<00:00,  1.61it/
s]
icu-68.2             | 13.1 MB   | : 100% 1.0/1 [00:02<00:00,  2.94s/i
t]
numpy-1.21.6         | 6.1 MB    | : 100% 1.0/1 [00:01<00:00,  1.96s/i
t]
sundials-5.8.0       | 1.0 MB    | : 100% 1.0/1 [00:00<00:00,  2.31it/
s]
gmp-6.2.1            | 806 KB    | : 100% 1.0/1 [00:00<00:00,  3.79it/
s]
libgfortran5-12.2.0  | 1.8 MB    | : 100% 1.0/1 [00:00<00:00,  2.15it/
s]
libxslt-1.1.33       | 522 KB    | : 100% 1.0/1 [00:00<00:00,  3.83it/
s]
mpfr-4.1.0           | 2.6 MB    | : 100% 1.0/1 [00:00<00:00,  1.57it/
s]
libopenblas-0.3.20   | 10.1 MB   | : 100% 1.0/1 [00:02<00:00,  2.57s/i
t]
libblas-3.9.0        | 12 KB     | : 100% 1.0/1 [00:00<00:00, 17.01it/
s]
pyfmi-2.7.4          | 12.4 MB   | : 100% 1.0/1 [00:02<00:00,  2.43s/i
t]
python_abi-3.7       | 4 KB      | : 100% 1.0/1 [00:00<00:00, 17.19it/
s]
suitesparse-5.10.1   | 2.4 MB    | : 100% 1.0/1 [00:00<00:00,  1.30it/
s]
libcblas-3.9.0       | 12 KB     | : 100% 1.0/1 [00:00<00:00, 19.04it/
s]
certifi-2022.9.24    | 155 KB    | : 100% 1.0/1 [00:00<00:00,  8.47it/
s]
libxml2-2.9.12       | 772 KB    | : 100% 1.0/1 [00:00<00:00,  4.29it/
s]
fmilib-2.2.3         | 532 KB    | : 100% 1.0/1 [00:00<00:00,  4.09it/
s]
libgfortran-ng-12.2. | 22 KB     | : 100% 1.0/1 [00:00<00:00, 14.70it/
s]
conda-22.9.0         | 960 KB    | : 100% 1.0/1 [00:00<00:00,  2.34it/
s]
assimulo-3.2.9       | 2.6 MB    | : 100% 1.0/1 [00:00<00:00,  1.24it/
s]
libiconv-1.17        | 1.4 MB    | : 100% 1.0/1 [00:00<00:00,  3.49it/
s]
metis-5.1.0          | 4.1 MB    | : 100% 1.0/1 [00:01<00:00,  1.17s/i
t]
tbb-2021.5.0         | 1.9 MB    | : 100% 1.0/1 [00:00<00:00,  1.90it/
s]
lxml-4.8.0           | 1.4 MB    | : 100% 1.0/1 [00:00<00:00,  2.30it/
s]
scipy-1.7.3          | 21.8 MB   | : 100% 1.0/1 [00:07<00:00,  7.59s/i
t]
liblapack-3.9.0      | 12 KB     | : 100% 1.0/1 [00:00<00:00, 21.79it/
s]
ca-certificates-2022 | 150 KB    | : 100% 1.0/1 [00:00<00:00, 15.45it/
s]
Preparing transaction: \ | / done
Verifying transaction: \ | / - \ | / done
Executing transaction: \ | / - \ | / - \ | / - \ | / - \ | / - \ done
Retrieving notices: ...working... done
```

In [7]:

```
!conda install numpy=1.19.1 --yes # Need to downgrade numpy
```

```
Collecting package metadata (current_repodata.json): - \ | / - \ | / d
```

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

## Package Plan ##

  environment location: /usr/local

  added / updated specs:
    - numpy=1.19.1


The following packages will be downloaded:

    package                    |            build
    ---------------------------|-----------------
    blas-1.0                   |         openblas          46 KB
    numpy-1.19.1               |   py37h30dfecb_0          21 KB
    numpy-base-1.19.1          |   py37h75fe3a5_0         4.1 MB
    ------------------------------------------------------------
                                           Total:         4.2 MB

The following NEW packages will be INSTALLED:

  blas               pkgs/main/linux-64::blas-1.0-openblas None
  numpy-base         pkgs/main/linux-64::numpy-base-1.19.1-py37h75fe3a
5_0 None

The following packages will be UPDATED:

  ca-certificates    conda-forge::ca-certificates-2022.9.2~ --> pkgs/m
ain::ca-certificates-2022.10.11-h06a4308_0 None
  openssl            conda-forge::openssl-1.1.1o-h166bdaf_0 --> pkgs/m
ain::openssl-1.1.1s-h7f8727e_0 None

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

  certifi            conda-forge/noarch::certifi-2022.9.24~ --> pkgs/m
ain/linux-64::certifi-2022.9.24-py37h06a4308_0 None
  conda              conda-forge::conda-22.9.0-py37h89c186~ --> pkgs/m
ain::conda-22.9.0-py37h06a4308_0 None
  numpy              conda-forge::numpy-1.21.6-py37h976b52~ --> pkgs/m
ain::numpy-1.19.1-py37h30dfecb_0 None



Downloading and Extracting Packages
blas-1.0             | 46 KB     | : 100% 1.0/1 [00:00<00:00,  6.99it/
s]
numpy-1.19.1         | 21 KB     | : 100% 1.0/1 [00:00<00:00, 10.21it/
s]
numpy-base-1.19.1    | 4.1 MB    | : 100% 1.0/1 [00:00<00:00,  2.43it/
s]
Preparing transaction: - done
Verifying transaction: | / - \ done
Executing transaction: / - \ | done
Retrieving notices: ...working... done
```

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

- FMU - BPL_TEST2_Batch_linux_jm_cs.fmu
- Setup-file - BPL_TEST2_Batch_explore.py

In [8]:
```
# Filter out DepracationWarnings for 'np.float as alias' is needed - w
import warnings
warnings.filterwarnings("ignore")
```

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

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 SLSQP 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 estimated and the purpose seems to only address smaller examples. Therefore we here define a no possibility to include parameter changes to the compiled model that should not be Python function evaluation() that facilitate the formulation of the parameter estimation and bring flexibility to choice of optimization method.

In [11]:
```
run -i BPL_TEST2_Batch_explore.py
```

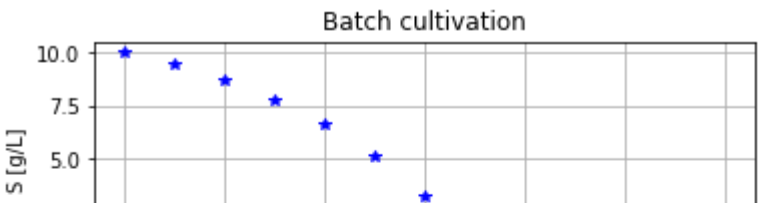
```
Linux - run FMU pre-comiled JModelica 2.4

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 s
imulation
 - describe()  - describe culture, broth, parameters, variables with v
alues / units

Note that both disp() and describe() takes values from the last simula
tion

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

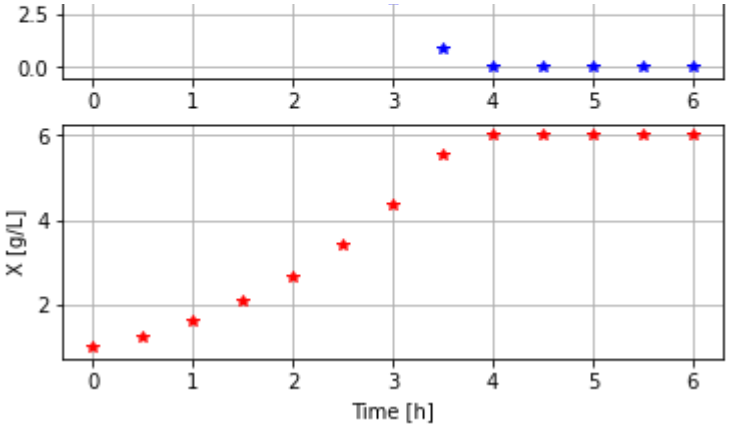
In [12]:
```
# Adjust the size of diagrams
plt.rcParams['figure.figsize'] = [15/2.54, 12/2.54]
```

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_0=1.0, VS_0=10, VX_0=1.0)
newplot(plotType='Demo_2')
opts['ncp'] = 12
simu(simulationTime)
```





In [15]:

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

Out[15]:

	time	X	S
0	0.0	1.000000	1.000000e+01
1	0.5	1.280773	9.438453e+00
2	1.0	1.640079	8.719842e+00
3	1.5	2.099615	7.800770e+00
4	2.0	2.686770	6.626459e+00
5	2.5	3.435479	5.129043e+00
6	3.0	4.385325	3.229350e+00
7	3.5	5.559252	8.814967e-01
8	4.0	6.000000	1.048673e-08
9	4.5	6.000000	-6.547559e-11
10	5.0	6.000000	6.182144e-11
11	5.5	6.000000	-4.234324e-12
12	6.0	6.000000	-1.961610e-13

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.

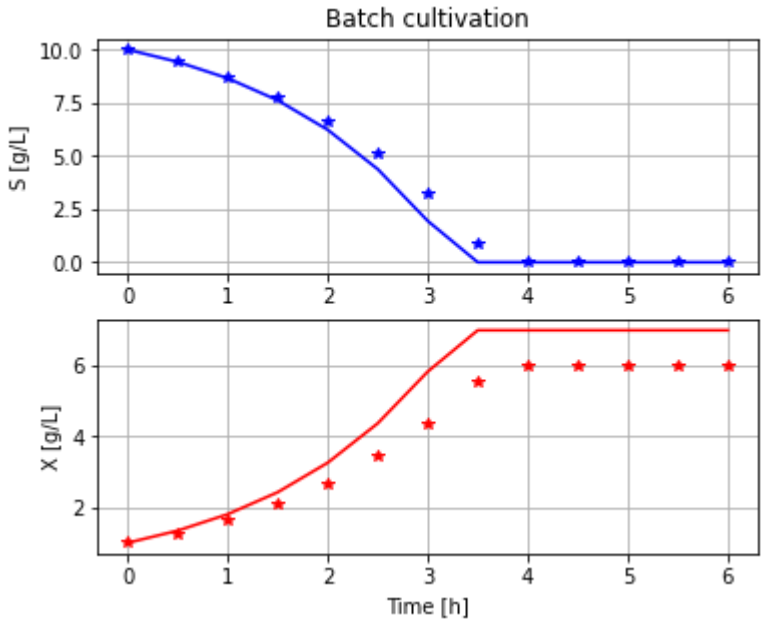
Simulation with these nominal parameter set and compare with data give an idea of who well the model fit data.

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))]
```

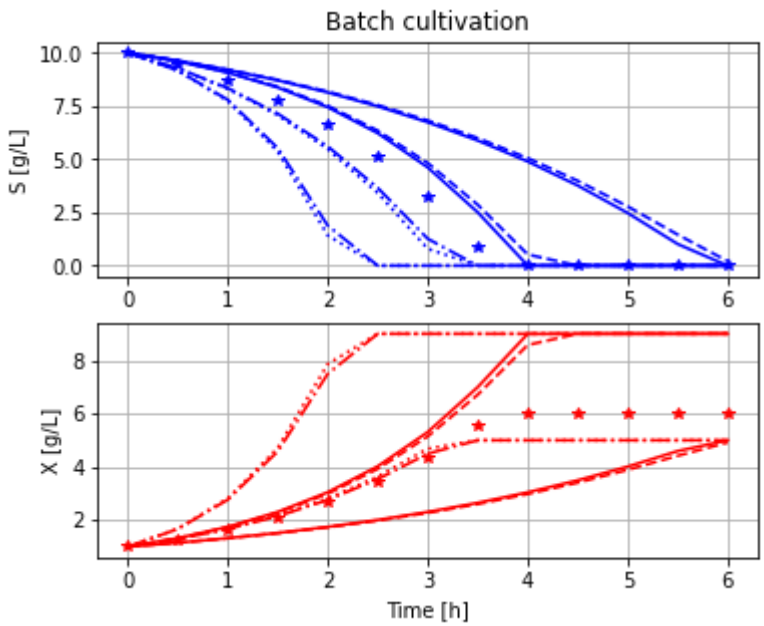
In [18]:

```
# 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 [19]:

```
# 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]. Since we has chosen to work with bounds on the parameters to be estimated there are only three methods to choose between. Here the method Sequential Least SQuares Programming SLSQP is chosen.

Note that we in the definition of evaluation() make use of PyFMI-functions to administrate the simulation parameters as well as running it, instead of using the simplified simu() function we are used to.

In [20]:
```
# Optimization routine import
import scipy.optimize
```

In [21]:
```
# Parameters to be estimated using parDict names and their bounds
extra_args = (parEstim, data, fmu_model, simulationTime, parDict, parL
```

In [22]:
```
# Modified evaluation function tailored for Python optimization algori
def evaluation(x, parEstim, data=data, fmu_model=fmu_model, simulation
               parDict=parDict, parLocation=parLocation):
    """The parameter list is tailored for scipy optimization algorithm
       where the first parameter x is an array with parameters that ar
       and evalauted and parEstim is a list of the names of these para

    # Load model
    global model
    if model is None:
        model = load_fmu(fmu_model)
    model.reset()

    # Change parameters and initial values from default
    for i, p in enumerate(parEstim): model.set(parLocation[p], x[i])
    for p in set(parDict)-set(parEstim): model.set(parLocation[p], par

    # Simulation options
    opts = model.simulate_options()
    opts['ncp'] = 12
    opts['result_handling'] = 'memory'
    opts['silent_mode'] = True

    # Simulate
    sim_res = model.simulate(start_time=0.0, final_time=simulationTime

    # Calculate loss function V
    V={}
```

Give feedback