

EOS — A HEP Program for Flavor Physics

User Manual

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version 0.2

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How to read this manual

To improve readability, the following concepts or entities discussed in this manual are highlighted.

shell specific Shell commands are monospaced-lowercase-and-grayed. Environment variables are \$ALL_CAPS_DOLLAR_PREFIXED.

```
echo "Example commands are boxed with a gray background."
# Comments are prefixed with a hash mark.
```

OS specific File names are light-blue, and /directories/end/with/a/slash//. Package names try to follow the original typesetting and are **green and bold**.

```
File contents are boxed with a light-blue background.
```

EOS specific Obserservables, options and parameters are orange and adhere to a syntax defined later in this manual. Classes are CamelCaseNoUnderscores. Methods are (almost always) lower_case_with_underscores.

```
print('Source code is boxed with a light orange back ground.')
# Source code listings have line numbers.
```

Software Documentation

1. Installation

The following instructions explain how to install **EOS** from source on a Linux-based operating system, such as Debian or Ubuntu, ¹ or MacOS X.

1.1. Installing the dependencies

1.1.1. Overview

The dependencies can be roughly categorized as either system software, Python-related software, or scientific software.

EOS requires the following system software:

g++ the GNU C++ compiler, in version 4.8.1 or higher;

autoconf the GNU tool for creating configure scripts, in version 2.69 or higher;

automake the GNU tool for creating makefiles, in version 1.14.1 or higher;

libtool the GNU tool for generic library support, in version 2.4.2 or higher;

pkg-config the freedesktop.org library helper, in version 0.28 or higher;

BOOST the BOOST C++ libraries (sub-libraries **boost-filesystem** and **boost-system**);

yaml-cpp a C++ YAML parser and interpreter library.

The Phython [1] interface to **EOS** requires the additional software:

python3 python3 interpreter in version 3.5 or higher, and required header files;

BOOST the BOOST C++ library **boost-python** for interfacing Python and C++;

h5py the Python interface to HDF5;

matplotlib the Python plotting library;

scipy the Python scientific library;

PyYAML the Python YAML parser and emitter library.

We recommend you install the above packages via your system's software management system.

EOS requires the following scientific software:

GSL the GNU Scientific Library [2], in version 1.16 or higher;

¹Other flavors of Linux will work as well, however, note that we will exclusively use package names as they appear in the Debian/Ubuntu apt databases.

HDF5 the Hierarchical Data Format version 5 (HDF5) [3], in version 1.8.11 or higher;

FFTW3 the C subroutine library for computing the discrete Fourier transform;

Minuit2 the physics analysis tool for function minimization, in version 5.28.00 or higher.

The optional (and highly recommended) Population Monte Carlo (PMC) sampling algorithm requires:

```
pmclib a free implementation of said algorithm [4], in version 1.01 or higher.
```

We recommend you install the above packages via your system's software management system, except for **pmclib** and **Minuit2** in particular cases discussed below.

1.1.2. Linux: Installing the dependencies with APT (Debian, Ubuntu)

You can install the prerequisite software with the **apt** package management system on any Debian or Ubuntu system as follows:

```
# for the 'System Software'
apt-get install g++ autoconf automake libtool pkg-config libboost-filesystem-dev \
    libboost-system-dev libyaml-cpp-dev
# for the 'Python Software'
apt-get install python3-dev libboost-python-dev python3-h5py python3-matplotlib python3-scipy \
    python3-yaml
# for the 'Scientific Software'
apt-get install libgs10-dev libhdf5-serial-dev libfftw3-dev
```

Do not install **Minuit2** via **APT**, since there is presently a bug in the Debian/Ubuntu packages for **Minuit2**, which prevents linking.

There are pre-built binary package files for **pmclib** and **Minuit2** available for the Ubuntu long-term-support varieties Xenial and Bionic via the Packagecloud web service. To use the EOS third-party repository, create a new file <code>eos.list</code> within the directory <code>/etc/apt/sources.list.d/</code> with the following contents:

```
deb https://packagecloud.io/eos/eos/ubuntu/ DIST main deb-src https://packagecloud.io/eos/eos/ubuntu/ DIST main
```

where you must replace DIST with either xenial or bionic, depending on your version of Ubuntu. Add our repository's GPG key by running

```
curl -L "https://packagecloud.io/eos/eos/gpgkey" 2> /dev/null | apt-key add - &>/dev/null
```

You can then install the binary packages through

```
apt-get update apt-get install minuit2 libpmc
```

You can then proceed with the EOS installation as documented in section 1.2.

1.1.3. Linux: Installing Minuit2 and pmclib from source

To install **Minuit2** from source, you need to disable the automatic support for OpenMP. Execute the following commands:

```
mkdir /tmp/Minuit2
pushd /tmp/Minuit2
wget http://www.cern.ch/mathlibs/sw/5_28_00/Minuit2/Minuit2-5.28.00.tar.gz
tar zxf Minuit2-5.28.00.tar.gz
pushd Minuit2-5.28.00
./configure --prefix=/opt/pkgs/Minuit2-5.28.00 --disable-openmp
```

```
make all sudo make install popd popd rm -R /tmp/Minuit2
```

Installation of **pmclib** for **EOS**'s purposes requires some modifications to the source code to make it compatible with C++. Execute the following commands:

```
mkdir /tmp/libpmc
pushd /tmp/libpmc
wget http://www2.iap.fr/users/kilbinge/CosmoPMC/pmclib v1.01.tar.gz
tar zxf pmclib_v1.01.tar.gz
pushd pmclib_v1.01
./waf configure --m64 --prefix=/opt/pkgs/pmclib-1.01
./waf
sudo ./waf install
sudo find /opt/pkgs/pmclib-1.01/include -name "*.h" \
   -exec sed -i \
   -e 's/#include "errorlist\.h"/#include <pmctools\/errorlist.h>/' \
   -e 's/#include "io\.h"/#include <pmctools\/io.h>/'
   -e 's/#include "mvdens\.h"/#include <pmctools\/mvdens.h>/' \
    -e 's/#include "maths\.h"/#include <pmctools\/maths.h>/' \
   -e 's/#include "maths_base\.h"/#include <pmctools\/maths_base.h>/' \
   {} \;
sudo sed -i \
   -e 's/^double fmin(double/\/\/\&/' \
   -e 's/^double fmax(double/\/\
   /opt/pkgs/pmclib-1.01/include/pmctools/maths.h
popd
rm -R /tmp/libpmc
```

Note: The waf build script used by **pmclib** is written in Python2. On systems that use Python3 as the default interpreter, you will see an error message similar to the following:

```
./waf configure --m64 --prefix=/opt/pkgs/pmclib-1.01
/tmp/src/libpmc/pmclib_v1.01/wscript: error: Traceback (most recent call last):
File \
    "/tmp/src/libpmc/pmclib_v1.01/.waf3-1.5.17-496be6959d6e0cd406d5f087856c4d79/wafadmin/Utils.py", \
    line 198, in load_module
    exec(compile(code,file_path,'exec'),module.__dict__)
File "/tmp/src/libpmc/pmclib_v1.01/wscript", line 130
    except Exception,e:
SyntaxError: invalid syntax
```

You can fixed this problem by replacing python with python2 in the very first line of the file waf in the top-level **pmclib** directory.

You can then proceed with the EOS installation as documented in section 1.2.

1.1.4. MacOSX: Installing the Dependencies with Homebrew and PyPi

You can install most of the prerequisite software via **Homebrew**. You will need to make **Homebrew** aware of **EOS**' third-party repository as follows:

```
brew tap eos/eos
```

To install the packages, execute the following commands:

```
# for the 'System Software'
brew install autoconf automake libtool pkg-config boost yaml-cpp
# for the 'Python Software'
brew install python3 boost-python3
# for the 'Scientific Software'
brew install gsl hdf5 minuit2 pmclib
```

Now you can use the pip3 command² to install the remaining packages from the **PyPi** package index:

```
pip3 install h5py matplotlib scipy PyYAML
```

You can then proceed with the EOS installation as documented in section 1.2.

1.2. Installing EOS

You can obtain the most recent version of EOS is available from Github ³. To download it for the first time, clone the repository via

```
git clone -o eos -b master https://github.com/eos/eos.git
```

You must first create all the necessary build scripts via

```
cd eos ./autogen.bash
```

You must specify where **EOS** will be installed by setting the \$PREFIX environment variable.

1. If you are administrating the computer on which you install EOS, you may choose any prefix. We recommend /usr/local/:

```
export PREFIX=/usr/local
```

We strongly discourage using /usr/, which avoids conflicts with your operating system's package management software.

2. If you are not administrating the computer, you must install EOS into a directory below your home directory or below any other directory for which you have the needed permissions. We recommend \$HOME/.local/:

```
export PREFIX=$HOME/.local/
```

Configuration

Next, you must configure the **EOS** build using the configure script.

- 1. If you want to use the **EOS** Python interface you must pass the --enable-python option to configure. The default is --disable-python.
- 2. If you want to use the **EOS** PMC algorithm you must pass the --enable-pmc option to configure. The default is --disable-pmc. If you installed **pmclib** from source to a non-standard location, you must specify its installation prefix by passing on --with-pmc=PMC-INSTALLATION-PREFIX.
- 3. If you want to use **ROOT**'s internal copy of Minuit2 you must pass --with-minuit2=root to configure.
- 4. Otherwise, if you have installed **Minuit2** from source to a non-standard location you must specify its installation prefix by passing on --with-minuit2=MINUIT2-INSTALLATION-PREFIX.

²Due to problems with the **Python 3** installation provided by Mac OS X, we strongly recommend to use the **Homebrew** provided pip3 instead via /usr/local/bin/pip3 .

³http://github.com/eos/eos

The recommended configuration is achieved using

```
./configure \
--prefix=$PREFIX \
--enable-python \
--enable-pmc
```

If the configure script finds any problems with your system, it will complain loudly.

Building and installing

After successful configuration, build EOS using

```
make -j all
```

The -j option instructs make to use all available processors to parallelize the build process. We strongly recommend testing the build by executing

```
make -j check VERBOSE=1
```

within the build directory. Please contact the authors if any test fails by opening an issue in the official **EOS** Github repository. If all tests pass, install **EOS** using

```
make install # Use 'sudo make install' if you install e.g. to '/usr/local' # or a similarly privileged directory
```

If you installed **EOS** to a non-standard location (i.e.not /usr/local/), to use it from the command line you must set up some environment variable. For **BASH**, which is the default Debian/Ubuntu shell, add the following lines to \$HOME/.bash_profile:

```
export PATH+=":$PREFIX/bin"
# uncomment the following line for Python support
#export PYTHONPATH+=":$PREFIX/lib/python3.5/site-packages"
```

The last line should be uncommented only if you built **EOS** with Python support. Note that <code>python3.5</code> piece must be replaced by the appropriate Python version with which **EOS** was built. You can determine the correct value using

```
python3 -c "import sys; print('python{0}.{1}'.format(sys.version_info[0], sys.version_info[1]))"
```

1.2.1. MacOS X short cuts

For users

The most recent development version of **EOS** (and all of its dependencies) can also be installed automatically using **Homebrew**:

```
brew tap eos/eos
brew install --HEAD eos
```

For developers

If you intend to make changes to the **EOS** source code you can still use **Homebrew**. First, you should clone the **EOS** repository into your home directory. We suggest

```
mkdir -p ~/Repositories/eos
cd ~/Repositories/eos
git clone https://github.com/eos/eos.git -b master
# make and commit your changes
```

1. Installation

To setup your local for use with **Homebrew** you must "tap" the **EOS** "formula" as usual, and then edit it.

```
brew tap eos/eos
brew edit eos
```

Change the line starting with head to look as follows:

```
head "/Users/USERNAME/Repositories/eos/.git", :branch => "master", :using => :git
```

where USERNAME is your username. You can determine it via whoami. Proceed to install the modified **EOS** version via brew install --HEAD eos. To reinstall **EOS** after further changes to the source code use brew reinstall --HEAD eos.

Note: Only changes that have been committed to the master branch of your local clone of the **EOS** repository will be used for the installation.

2. Usage

EOS has been authored with several use cases in mind.

- The evaluation of observables and further theoretical quantities in the field of flavor physics. EOS
 aspires to produce theory estimates of publication quality, and has produced such estimates in
 the past.
- 2. The inference of parameters from experimental observations. For this task, **EOS** defaults to the Bayesian framework of parameter inference.
- 3. The production of toy events for a variety of flavor-physics-related processes using Monte Carlo methods.

In the remainder of this chapter we document the usage of the existing **EOS** clients and scripts, to carry out tasks corresponding to the above use cases. We assume further that only the built-in observables, physics models and experimental constraints are used. The necessary steps to extend EOS with new observables, physics models or constraints is discussed in chapter 4.

2.1. Browsing the List of Parameters, Observables and Constraints

EOS has understands parameters, observables, options, kinematic variables, and constraints. Parameters, observables and constraints share a common naming scheme, in order to allow categorize these quantities more readily. The naming scheme is as follows: each name can be decomposed into a prefix (before the :: separator), an optional tag (after the optional separator), and the short name (between the separators); e.g.:

Here K^* indicated the association with the K^* meson, a_1_para is the short name for this object, and the tag is present and reads 1GeV.

Parameters are scalar floating-point-valued inputs. They are real-valued numbers that can be set to arbitrarily at run time. The full list of parameters known to EOS as well as their default values and ranges can be browsed by running <code>eos-list-parameters</code>.

Observables are **EOS**-internal functions that take a set of parameters and return a single (real-valued) number. These functions take a set of kinematic variables as their arguments. They include true observables in the physical sense (e.g. a branching ratio) but also pseudo observables such as hadronic form factors. A full list of observables known to EOS can be listed by running <code>eos-list-observables</code>.

Options are used to modify the behavior of an observable at run time. Universal examples include changing the physics model (via model) and changing form factor parametrization (via form-factors). However, generally their names are specific to a single observable. There is presently no way to list all possible options that pertain to a given observable.

2. Usage

Kinematic variables are used to provide numerical inputs to an observable that can be changed on a per-observable level. As such, the names of kinematic variables are specific to each observable. The required kinematic variables for each observable can be looked up using the eos-list-observables client

Constraints represent individual likelihood functions, either of an experimental measurement or a theoretical prediction. The list of built-in constraints is available through <code>eos-list-constraints</code>.

2.2. Evaluating Observables

Observables can be evaluated using eos-evaluate. It accepts the following command line arguments:

--kinematics NAME VALUE

Within the scope of the next observable, declare a new kinematic variable with name NAME and numerical value VALUE.

```
--range NAME MIN MAX POINTS
```

Within the scope of the next observable, declare a new kinematic variable with name $\frac{NAME}{NAME}$. Subdivide the interval $\frac{MIN}{NAME}$ in $\frac{NAME}{NAME}$ subintervals, and evaluate the observable at each subinterval boundary.

Note: More than one --range command can be issued per observable, but only one --range command per kinematic variable.

```
--observable NAME
```

Add a new observable with name NAME to the list of observables that shall be evaluated. All previously issued --kinematics and --range arguments apply, and will be used by the new observable. The kinematics will be reset (i.e., all kinematic variables will be removed) in anticipation of the next --observable argument.

```
--vary NAME
```

Estimate the uncertainty based on variation of the parameter NAME, as if the parameter was distributed like a univariate Gaussian.

```
--budget NAME
```

Create a new uncertainty budget, which encompasses all the subsequently issued --vary commands (until the issue of a new --budget command). By default, the delta budget always exists, and encompasses all variations.

As an example, we use the evaluation of the q^2 -integrated branching ratio $\mathcal{B}(\bar{B}^0 \to \pi^+ \mu^- \bar{\nu}_{\mu})$, which is addressable as B->pilnu::BR. For this example, we use the integration range

$$0\,\mathrm{GeV}^2 \le q^2 \le 12\,\mathrm{GeV}^2\,.$$

Further, we use the BCL2008 [5] parametrization of the $\bar{B}\to\pi$ form factor, as well as the Wolfenstein parametrization of the CKM matrix. The latter is achieved by choosing the physics model SM. By default, **EOS** uses the most recent results of the UTfit collaboration's fit of the CKM Wolfenstein

parameter to data on tree-level decays. In this example, we evaluate the observable and estimate parametric uncertainties based on the naive expectation of Gaussian uncertainty propagation. We classify two budgets of parametric uncertainties: one for uncertainties pertaining to the form factors (labeled 'FF'), and one for uncertainties pertaining to the CKM matrix elements (labeled 'CKM'). Our intentions translate to the following call to eos-evaluate:

The above call yields the following output:

```
# B->pilnu::BR: form-factors=BCL2008,l=mu

# s_min s_max central FF_min FF_max CKM_min CKM_max delta_min delta_max

0 12 0.000106816 3.00927e-05 1.46426e-05 9.14007e-06 9.70515e-06 3.14501e-05 1.75669e-05

(-29.4434% / +16.446%)
```

The output of calls to eos-evaluate is structured as follows:

- The first row names the observable at hand, as well as all active options.
- The second row contains column headers in the order:
 - kinematics variables.
 - the upper and lower uncertainty estimates for each individual uncertainty budget,
 - the total upper and lower uncertainty estimates.
- The third row contains the result as described by the above columns. In addition, at the end of the row the relative total uncertainties are given in parentheses.

The above structure repeats itself for every observable, as well as for each variation point of the kinematic variables as described by occurring --range arguments.

2.3. Producing Random Parameter Samples

For all the previously mentioned use cases (observable evaluation, Bayesian parameter inference, and production of pseudo events) one requires to draw random samples from some arbitrary Probability Density Function (PDF) $P(\vec{\theta})$. When using **EOS**, these random samples can be produced from Markov-Chain Monte Carlo (MCMC) random walks, using the Metropolis-Hastings algorithm, by calls to the eos-sample-mcmc client. In a second step, refined samples or samples for a very complicated setup, can be obtained from an algorithm described in Ref. [6]. This algorithm uses an adaptive importance sampling called Population Monte Carlo (PMC), implemented within the client eos-sample-pmc, and requires a prior run of eos-sample-mcmc for initialization.

The follow command-line arguments are common to the eos-sample-mcmc and eos-sample-pmc clients, as well as further clients described in subsequent sections:

```
--scan NAME --prior flat MIN MAX
--scan NAME [ABSMIN ABSMAX] --prior gaussian MIN CENTRAL MAX
--nuisance [...]
```

These arguments add a parameter to the statistical analysis, with either a flat or a gaussian prior. If ABSMIN and ABSMAX are specified, the prior will be cropped to this absolute interval. The --scan and --nuisance arguments work identically, with one exception: --nuisance declares the associated parameter as a nuisance parameter, which is flagged in the HDF5 output. The sampling algorithm treats nuisance parameters in the same way as scan parameters.

```
--constraint NAME
```

The named constraint from the internal database will be used as part of the likelihood. The functional form of the likelihood, details such as correlations, and the required options for the observables used will be automatically looked up. In order to browse the entries of the database, use the <code>eos-list-constraints</code> client.

```
--fix NAME VALUE
```

The value of parameter NAME will be set to the supplied VALUE, and thus potentially deviate from its default value.

The eos-sample-mcmc client further accepts the following arguments:

```
--seed [time|VALUE]
```

This argument sets the seed value for the Random Number Generator (RNG). Setting the seed to a fixed numerical VALUE ensures being able to reproduce the results. This is important for publication-quality usage of the client. If time is specified, the RNG is seeded with an integer value based on the current time.

```
--prerun-min VALUE
```

For the prerun phase of the sampling algorithm, set the minimum number of steps to VALUE.

```
--prerun-max VALUE
```

For the prerun phase of the sampling algorithm, set the maximum number of steps to VALUE.

```
--prerun-update VALUE
```

For the prerun phase of the sampling algorithm, force an adaptation of the Markov chain's proposal function to its environment after every VALUE steps.

```
--store-prerun [0|1]
```

Either disable or enable storing of the prerun samples to the output file.

```
--output FILENAME
```

Use the file FILENAME to store the output, using the HDF5 file format. The resulting HDF5 file follows the EOS-MCMC format, and can be accessed using, e.g., the eos.data.MCMCDataFile Python class.

The eos-sample-pmc client additionally accepts the following command-line arguments:

--seed [time|VALUE]

This argument sets the seed value for the RNG. Setting the seed to a fixed numerical VALUE ensures being able to reproduce the results. This is important for publication-quality usage of the client. If time is specified, the RNG is seeded with an interger value based on the current time.

```
--hc-target-ncomponents N
```

When creating mixture components, create N components per existing MC group.

```
--hc-patch-length LENGTH
```

When clustering a group's MCs onto the mixture components, cut the chains into patches of LENGTH samples each.

```
--hc-skip-initial FRACTION
```

Skip the first FRACTION of all MCMC samples in the clustering step.

Note: FRACTION must be a decimal number between 0 and 1.

```
--pmc-initialize-from-file HDF5FILE
```

Use the samples from a MCMC HDF5 output file HDF5FILE as generated with eos-sample-mcmc, in order to initialize the mixture density of the initial PMC step.

```
--pmc-group-by-r-value R
```

When forming groups of MCs from the initialization file, only add a chain to an existing group if the chain's R-value is less than R; create a new group otherwise.

```
--pmc-samples-per-component N
```

Set the number $\,\mathbb{N}\,$ of samples that will be drawn per component and per update step of the PMC run.

```
--pmc-final-samples N
```

Set the number $\ \mathbb{N}$ of samples that will be drawn for the final step, i.e.: after the PMC updates have converged.

```
--pmc-relative-std-deviation-over-last-step STD STEPS
```

If both perplexity and ESS have a standard deviation less than STD over the last STEPS updates, declare convergence.

```
--pmc-ignore-ess [0|1]
```

Set whether convergence of the PMC updates shall be determined from the effective sample size (ESS) *in addition* to the perplexity.

Default: Use the ESS.

```
--output FILENAME
```

Use the file FILENAME to store the output, using the HDF5 file format. The resulting HDF5 file follows the EOS-PMC structure, and can be read using the eos.data.PMCDataFile Python class.

As an example, we define the a-priori PDF for a study of the decay $\bar{B} \to \pi^+ \mu^- \bar{\nu}_{\mu}$. For the CKM Wolfenstein parameters, we use

```
\begin{split} \lambda &= 0.22535 \pm 0.00065 \,, \quad A = 0.807 \pm 0.020 \,, \\ \bar{\rho} &= 0.128 \pm 0.055 \,, \qquad \quad \bar{\eta} = 0.375 \pm 0.060 \,. \end{split}
```

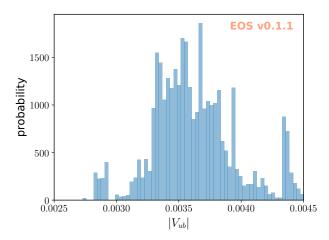
For the a-priori PDF, we use uniform distributions for the BCL2008 [5] parameters for the $B\to\pi$ form factor $f_+^{B\pi}$. However, we construct a likelihood from the results of a recent study (IKMvD2016 [7]) of the form factor $f_+^{B\pi}(q^2)$ within Light-Cone Sum Rules (LCSRs). We now intend to draw random numbers from the posterior PDF using EOS' adaptive Metropolis-Hasting algorithm. During its prerun phase, the algorithm adapts the chains' proposal functions. As a consequence, the prerun samples will in general *not* be distributed according to the posterior PDF. With a subequent PMC sampling run in mind, we should demand at least 500 steps. In this simple problem, the Markov chains converge (the prerun finishes) after a few thousand iterations; the adaption process should be executed after every 500 steps.

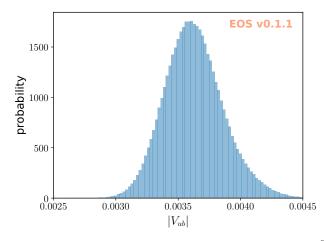
Our intentions translate to the following call to eos-sample-mcmc:

```
eos-sample-mcmc \
   --global-option model CKMScan \
   --global-option form-factors BCL2008 \
   --constraint "B->pi::f_+@IKMvD-2014" \
   --constraint "B^O->pi^+lnu::BR@BaBar-2010B" \
   --constraint "B^0->pi^+lnu::BR@Belle-2010A" \
   --constraint "B^0->pi^+lnu::BR@BaBar-2012D" \
   --constraint "B^0->pi^+lnu::BR@Belle-2013A" \
   --prerun-min 500 \
--prerun-max 7500 \
   --prerun-update 500 \
   --prerun-only
   --output /tmp/mcmc_prerun_btopi+ff.hdf5
    --chunks 10 \
   --chunk-size
                  1000 \
```

Optionally, if the prerun converges, the client can be used to perform a main run, in which the proposal functions will be kept static. For such these main run samples, we wish for a total of 10^4 , which we artifically decompose into 10 chunks with 1000 samples each. While the sampling at hand will be quite quick, sampling of computationally expensive functions should be done with small chunks so that the progress of the computations can be monitored. The require options for these intentation are shown above with a leading hash mark. Also, for a main run, the --prerun-only flag would need to be removed.

We use the above call to eos-sample-mcmc in order to initialize a PMC run. We wish for 4 mixture components per MC group, and to skip 20% of the MCMC samples as part of the burn in. MC groups will be created based on an R-value [8] threshold of 1.5. For each update, 500 samples per mixture component shall be drawn, in order to produce 10^6 samples in the final step. Convergence shall be declared upon a standard deviation for the perplexity only, of 0.05 over the last 4 update steps. The call then reads:





- (a) Histogram of the marginal posterior of $|V_{ub}|$, using 4×7500 samples. Despite the poor quality of these samples, they can be used to initialize the PMC run as described in the text.
- (b) Histogram of the marginal posterior of $|V_{ub}|$, using 10^6 samples.

Figure 2.1.: Histograms of the parameter of interest $|V_{ub}|$ in the two example fits as described in section 2.3, and plotted using the eos-plot-1d client; see section 2.7 for details.

```
--scan "B->pi::b_+^2@BCL2008"
                                -2.0
                                                --prior flat \
--constraint "B->pi::f_+@IKMvD-2014"
--constraint "B^O->pi^+lnu::BR@BaBar-2010B"
--constraint "B^O->pi^+lnu::BR@Belle-2010A"
 -constraint "B^O->pi^+lnu::BR@BaBar-2012D"
--constraint "B^0->pi^+lnu::BR@Belle-2013A" \
--pmc-initialize-from-file /tmp/mcmc_prerun_btopi+ff.hdf5 \setminus
--hc-target-ncomponents 4 \
--hc-skip-initial 0.2 \
--pmc-samples-per-component 500 \
 -pmc-group-by-r-value 1.5 \
--pmc-final-samples 1000000 \setminus
--pmc-ignore-ess 1 \
--pmc-relative-std-deviation-over-last-steps 0.05 4 \
--output /tmp/pmc_monolithic_btopi+ff.hdf5
```

Both clients output copious amounts diagnostic data to the standard output, which include

- all information about the prior and the likelihood as specified on the command line (both clients);
- information about the convergence of the Markov chains within the parameter space, based on the *R*-value criterion [8] (MCMC only);
- information about the convergence of the PMC run based on the perplexity and effective sampling size (PMC only).

We display the outcome of both the MCMC (prerun) sampling as well as the PMC sampling steps in figure 2.1.

2.4. Merging Markov Chains from multiple files

To run multiple Markov chains in parallel, one may use a compute cluster and submit independent jobs, each of which creates its own output file with one or more chains inside. To initialize PMC, it is necessary to have all Markov chains in a single HDF5 file. This is where eos-merge-mcmc comes into play. It allows one to merge chains from multiple files into a single HDF5 file and optionally to apply a

cut such that chains that got stuck in irrelevant local modes in the prerun can be filtered out. Note that chains both from the prerun and main run are copied into the output file. eos-merge-mcmc accepts the following command-line arguments:

```
Any number of input files created by eos-sample-mcmc
```

Skip chains whose maximum log posterior in the prerun is below the cut-off.

```
--input-file-list LIST
```

List input files in a text file, one file per line. If other input files are passed directly on the command line, then those take precedence but all files will be merged.

```
--output FILENAME
```

--cut-off NUMBER

The name of the output file in which the chains are stored.

2.5. Finding the Mode of a Probability Density

The mode, best-fit point, or simply the most-likely value, of some PDF $P(\vec{\theta})$ is regularly searched for in physics analyses. EOS supplies the client <code>eos-find-mode</code>, which accepts the common set of arguments describing the PDF as already discussed for the <code>eos-sample-mcmc</code> and <code>eos-sample-pmc</code> clients, see section 2.3 for further information. In addition, it accepts the following command-line arguments:

```
--starting-point { VALUE1 VALUE2 ... VALUEN }
```

Set the starting point for the maximization of the PDF $P(\vec{\theta})$ at $\theta = (VALUE1, ..., VALUEN)$.

```
--max-iterations INTEGER
```

The optimization algorithm is allowed to run at maximum NUMBER iterations.

```
--target-precision NUMBER
```

Attempt to determine the mode up to an uncertainty of NUMBER.

```
--output FILENAME
```

Write a YAML file with name FILENAME that contains the information of the mode in a machine-readable format.

In order to illustrate the client's usage, we use the same example as discussed in section 2.3. The corresponding call then reads:

The output starts with same diagnostic information on the composition of prior and likelihood as for the sampling clients. The results are displayed in the last few lines, including

- the starting point for the mode-finding process;
- · the coordinates of the best-fit point; and
- the log-posterior at the best-fit point.

```
# Starting optimization at ( 0.0035 0.31 0 0 )

# Found maximum at:

# ( 3.568778e-03 2.661032e-01 -2.670912e+00 2.231637e-02 )

# value = -3.101594e+02
```

2.6. Bayesian Uncertainty Propagation

EOS presently supports two ways to propagate theory uncertainties in the framework of Bayesian statistics: First, by using prior PDFs that describes the nuisance parameters; second, by using samples from a posterior PDF that have been obtained from running either eos-sample-mcmc or eos-sample-pmc. It accepts the following command-line arguments:

```
--vary NAME --prior flat MIN MAX
--vary NAME [ABSMIN ABSMAX] --prior gaussian MIN CENTRAL MAX
```

These arguments add a parameter to the statistical analysis, with either a flat or a Gaussian prior. If ABSMIN and ABSMAX are specified, the prior will be cropped to this absolute interval.

```
--fix NAME VALUE
```

Fix parameter to a certain value. Use this to change default values for parameters that are not varied.

```
--kinematics NAME VALUE
```

Within the scope of the next observable, declare a new kinematic variable with name NAME and numerical value VALUE.

```
--observable NAME
```

Add a new observable with name NAME to the list of observables that shall be evaluated. All previously issued --kinematics and --range arguments apply, and will be used by the new obervable. The kinematics will be reset (i.e., all kinematic variables will be removed) in anticipation of the next --observable argument.

```
--global-option NAME VALUE
```

Set an option to a string value that applies to all following observables.

```
--samples NUMBER
```

Sets the number of samples that shall be produced per observable and worker thread.

```
--workers NUMBER
```

Sets the number of worker threads. Default: 4.

--parallel [0|1]

Activate multithreaded evaluation. Default: 1.

```
--mcmc-input HDF5FILE BEGIN END
```

Use the samples at index BEGIN up to index END from each chain in the file HDF5FILE. If both preruns and main runs are present in the file, preference is give to the main run. To use all samples, use BEGIN=0 and choose a value for END equal to or larger than the actual length of any chain in the file.

Note: The file must have been produced by the eos-sample-mcmc client.

Note: If you have the HDF5 commandline tools available, use h51s -r HDF5FILE to see the number and length of the chains.

```
--mcmc-prefer-prerun [0|1]
```

Override the default setting to take samples from the prerun instead of the main run in case both are present in the <code>HDF5FILE</code>. Default: 0.

```
--pmc-input HDF5FILE BEGIN END
```

Use the samples at index BEGIN up to index END from a named data set in the file HDF5FILE.

Note: The file must have been produced by the eos-sample-pmc client.

```
--pmc-sample-directory NAME
```

Use the named data set within the file specified with <code>--pmc-input</code>. Valid names are <code>/data/X</code>, where X stands for either <code>initial</code>, <code>final</code>, or all numbers describing existing update steps that were carried out in the PMC run.

Note: You should use /data/final unless you are debuging the PMC algorithm.

```
--output NAME
```

Set the output file name.

```
--store-parameters [0|1]
```

Store the parameter samples drawn from the prior into the output file. Has no effect with --mcmc-input or --pmc-input. Default: 0.

```
--seed VALUE
```

Change the random number seed for generating parameter samples. Has no effect with --mcmc-input or --pmc-input. By default a fixed seed is chosen corresponding to VALUE=0. To get different samples on each invocation, use VALUE=time.

As an example of the first way, we would like to predict the branching ratio for the decay $B^- \to \tau^- \bar{\nu}_\tau$. This prediction involves two parameters: First, the absolute value of V_{ub} ; and second, the value of the B-meson decay constant f_B . For the former, we choose the HFAG average of the inclusive determination $|V_{ub}|=(4.45\pm0.26)\cdot10^{-3}$ [9], while for the latter we use the FLAG average $f_B=0.188\pm0.007\,\mathrm{GeV}$ [10]. Our intention translates to the following call to eos-propagate-uncertainty:

As an exmple of the second way, we would like to use samples from the posterior PDF as obtained in section 2.3 in order to predict the branching ratio of the differential decay $\bar{B}^0 \to \pi e^- \bar{\nu}_e$, at various points in the kinematic range as the decay to muons described previously. Our intention translates to the following call to eos-propagate-uncertainty:

```
eos-propagate-uncertainty \
           -kinematics s 0.00 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
         --kinematics s 0.25 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
        --kinematics s 0.50 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
         --kinematics s 0.75 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
         --kinematics s 1.00 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
        --kinematics s 1.50 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
        --kinematics s 2.00 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan" --kinematics s 2.50 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
        --kine \verb| matrics s | 3.00 | --observable | \verb| "B--pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan" | leading to the content of the co
         --kinematics s 3.50 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
        --kinematics s 4.00 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
         --kinematics s 6.00 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
        --kinematics s 7.00 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan" --kinematics s 8.00 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
         --kinematics s 9.00 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
         --kinematics s 10.00 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
         --kinematics s 11.00 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan"
         --kinematics s 12.00 --observable "B->pilnu::dBR/ds;l=e,form-factors=BCL2008,model=CKMScan" \
         --pmc-input /tmp/pmc_monolithic_btopi+ff.hdf5 0 10000 \
         --pmc-sample-directory "/data/final/
         --output /tmp/unc_btopilnu.hdf5
```

For both ways, the samples of the predictive distributions within the HDF5 files can be accessed using the eos.data.UncertaintyDataFile Python class.

2.7. Plotting Random Samples

Once random samples have been obtained from either a posterior PDF (e.g. as described in section 2.3) or a predictive PDF (e.g. as described in section 2.6), a visual inspection of the samples is the next step. EOS provides scripts for this purpose, which plot histograms of either a marginalized 1D (eos-plot-1d) or heatmaps of 2D (eos-plot-2d) PDFs. Both scripts presently detect the output format by inspection of the resepective HDF5 file name. Files containing MCMC samples should be prefixed with mcmc_, while PMC sample files should be prefixed with pmc_monolithic_. Files containing samples from the uncertainty propagation should be prefixed with unc_.

The eos-plot-1d produces a 1D histogram of the samples for one parameter. It accepts the following arguments:

HDF5FILE

The name of the HDF5 input file whose samples shall be plotted.

VAR

The name of the variable (either a Parameter or an Observable) whose density function shall be plotted.

PDFFILE

The name of the PDF output file, into which the plot shall be saved.

```
--xmin XMIN, --xmax XMAX
```

When specified, limit the plot range to the interval XMIN to XMAX. The default values are taken from the description of the parameter within the HDF5 input file.

```
--kde [0|1]
```

When enabled, plots a univariate Kernel Density Estimate of the probability density based on the available samples.

--kde-bandwidth KDEBANDWIDTH

When specified, multiplies the automatically determined KDE bandwidth parameter with KDEBANDWIDTH.

The eos-plot-2d produces a 2D heatmap of the samples for two parameters. It accepts the following arguments

HDF5FILE

The name of the HDF5 input file whose samples shall be plotted.

XIDX

The numerical index for the parameter that shall be plotted on the x acis. XIDX starts with zero

YIDX

The numerical index for the parameter that shall be plotted on the y acis. YIDX starts with zero

PDFFILE

The name of the PDF output file, into which the plot shall be saved.

```
--xmin XMIN, --xmax XMAX
```

When specified, limit the plot range on the x axis to the interval XMIN to XMAX. The default values are taken from the description of the parameter within the HDF5 input file.

```
--ymin YMIN, --ymax YMAX
```

When specified, limit the plot range on the y axis to the interval YMIN to YMAX. The default values are taken from the description of the parameter within the HDF5 input file.

3. Library Interface

The rationale behind several of the design decisions of the **EOS** libraries are explained in section 3.1. We document the core set of classes in section 3.2.

3.1. Design

To fulfill its intended use cases, the EOS libraries are designed by abiding to the follwing principles.

First, scalar quantities are treated as parameters. These include

- experimental inputs, such as particle masses and lifetimes;
- theoretically motivated quantities, such as quark masses (e.g.in the MS scheme) and the Wolfenstein parameters of the CKM matrix.

It is therefore straightforward to change a parameter's role from one analysis to the next; e.g.from being a nuisance parameter when producing theory estimates, to being a parameter of interest when inferring knowedlge from experimental data. To differentiate between the various parameters, a naming scheme is put in place:

where the meta variables convey the following meaning:

NAMESPACE A short description of the context in which the parameter should be interpreted.

Possible namespaces include, but are not limited to: mass, decay-constants,

CKM, and others.

ID A descriptive handle for the parameter in its namespace.

TAG A forther pices of information that allows to distinguish between parameters with

the same ID.

Second, quantities that exhibit a functional dependence on either a parameter or a kinematic variable are treated as plugins: An interface is created that allows implementing more than one realization of the respective function. The actual implementations of this interface are then accesible via a factory method. Each implementation of a plugin can depend on its own subset of parameters. For clarity, we use one of the hadronic form factor as an example. Consider the $B \to \pi$ vector form factor $f_+^{B\pi}$. One possible parametrization of this form factor has been proposed in [5] (denotes as BCL2008). It is achieved in terms of three parameters:

• the normalization $f_+^{B\pi}(0)$, and

¹A good example for such a modular design is found within the scope of hadronic matrix elements, in particular hadronic form factors.

• two shape parameters $b_1^{B\pi,+}$ and $b_2^{B\pi,+}$.

This parametrization is implemented within **EOS** as one of several options for a $B \to \pi$ form factor parametrization. The relevant **EOS** parameters are contained in the namespace B->pi, and tagged for the BCL2008 plugin:

$$B \rightarrow pi::f_+(0)BCL2008$$
, $B \rightarrow pi::b_+^1BCL2008$, and $B \rightarrow pi::b_+^2BCL2008$. (3.2)

This removes the risk of namespace collisions among the various plugins' parameters. Observables that depend on the the $B \to \pi$ form factors can be implemented by relying on the form factors interface, and leave the concrete parametrization to be a run-time option with name form-factors. The BCL2008 parametrization can be selected by passing form-factors=BCL2008 to the observable.

Third, data is only copied when explicitly requested. Copy constructors yield another object that points to the same underlying data. This is achieved through extensive use of the *Private Implementation* design pattern.² To make an independent copy, the **EOS** classes provide the clone() method.

3.2. Core Classes

At the core of the EOS API there are four classes:

Parameters which contains the whole set of Parameter known to EOS

Kinematics which contains the set of kinematic variables specific to one instance of Observable

Options which contains the set of options specific to one instance of Observable

which encapsulates the numerical implemention of a single (pseudo-)observable quantity.

3.2.1. Class Parameters

Implemented as a dictionary, with keys of type std:string and values of type Parameter. The default set of parameters is loaded from the **EOS**-supplied YAML files. It can be loaded by using the static Parameters::Defaults() method. Using the copy construtor does not yield an independent copy; instead the second object uses the underlying data of the initial instance. To obtain an independent copy with the same values as the present one, use the clone() method.

```
Parameters paramA = Parameters::Defaults();
Parameters paramB(paramA);

ObservablePtr obsA = Observable::make("A", paramA, Kinematics{ }, Options{ });
ObservablePtr obsB = Observable::make("A", paramB, Kinematics{ }, Options{ });
```

You can access individual parameters via the array subscript operator. It takes a class QualifiedName object as its key, which can be created implicitly from std::string or const char *. You can also iterate over all parameters via the begin() and end() methods. In both cases, the underlying objects are of class Parameter, which provides access to the current value via the evaluate() method.

²See https://cpppatterns.com/patterns/pimpl.html.

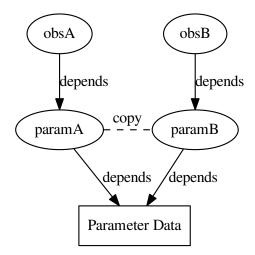


Figure 3.1.: Diagrammatic illustration that multiple observables can depend on the very same instance of Parameters.

3.2.2. Class Kinematics

The class Kinematics is a dictionary from std::string-valued keys to KinematicVariable-valued entries. Upon construction of an observable, a suitable instance of kinematics is bound to that observable. Acces to individual kinematic variables occurs through the array subscript operator. The class is used for the run-time construction of observables. For this purpose, the variable names apply only to a single observable and are not explicitly namespaced.

3.2.3. Class Options

The class Options is a dictionary from std::string-valued keys to std::string-valued entries. Upon construction of an observable, a suitable instance of Options is bound to that observable. The underlying class's constructor queries the options, and select the appropriate run-time behaviour.

Helper classes are available for repeated options-related task, e.g. the class SwitchOption.

3.2.4. Class Observable

The class Observable is an abstract base class. To create a new observable object, you must use the static Observable::make() factory method. It requires three arguments:

- a class QualifiedName object n;
- · a class Parameters object p; and
- · a class Kinematics object k; and
- an class Options object o.

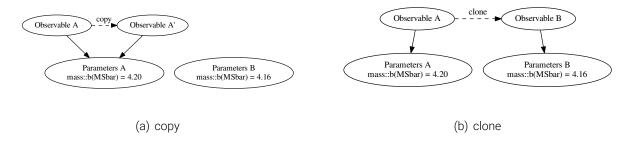


Figure 3.2.: Diagrammatic illustration of the differences between copying an instance of Observable via the copy-constructor, and cloning the observable via the clone method

To allow for more compact code, **EOS**' internal observables are not implemented as individual classes. Instead, related observables are bundled together into one class. Individual observable classes are then created using the template <...> class ConcreteObservable. We refer to section 4.2 for details on how to extend **EOS** with the implementation of a new observable.

Note: Any changes to the Options object o after construction of the observable do not affect the observable.

Note: All users of Observable must also support cloning. This allows to easily parallelize algorithms acting on Observable.

4. Extending EOS

We discuss the three most common cases of extending **EOS**, by adding either a new parameter, a new observable, or a new measurement. For extensions that do not fall in these categories please contact the main authors, who will be happy to discuss your work with you. The most efficient way to contribute new code or modifications to **EOS** is via a pull request in the main Github repository.¹

4.1. How to add a new parameter

Parameters are stored in YAML files below eos/parameters/, including the default values and range, as well as metadata and the origin thereof. Each file contains key-to-value maps:

- Keys starting and ending with an @ sign are considered to be metadata pertaining to the entire file.
- All other keys declare a new parameter.

The values in this map are the definitions of a parameters, and are also structured as maps. Valid parameter definitions must include all of the following entries:

central the default central value;

min the minimal value for the default range;

max the maximal value for the default range.

Optional entries include:

comment a comment on the purpose;

latex the LaTeX command for the display;

unit the unit in which the parameter is expressed.

Example

We introduce two new parameters: mass::X@Example, and decay-constant::X@Example, standing in for the mass and decay constant of a hypothetical particle X. We add the file eos/parameters/x.yaml with contents:

```
'mass::X@Example' :
    central: +1.0
    min: +0.5
    max: +1.5
    unit: 'GeV'
    latex: '$M_X$'
    comment: 'The mass of the unmotivated X particle'

'decay-constant::X@Example' :
    central: +0.10
```

¹ https://github.com/eos/eos

```
min: +0.09

max: +0.11

unit: 'GeV'

latex: '$f_X$'

comment: 'The decay constant of the unmotivated X particle'
```

4.2. How to add a new observable

An Observable is implemented in EOS as follows:

• The numerical code is implemented as the method double P::o(...) const, where P is the underlying class, and the dots stand in for any number of const double & arguments, including zero. The class P must inherit from class ParameterUser. It must have one constructor accepting a class Parameters and a class Options instance in that order. Schematically:

```
#include <eos/utils/parameters.hh>
#include <eos/utils/options.hh>

class P:
    public ParameterUser
{
        P(const Parameters \&, const Options \&);
        ~P();

        double observable_without_kinematics() const;
        double observable_with_one_kinematic_variable(const double &) const;
};
```

• The method or methods are then associated with their names within the file eos/observable.cc within the free-standing function make_observable_entries(). Within the existing map, new entries are created through a call to make_observable(...). For a regular observable the arguments are in order: the name of the observable; the pointer to its method; and the tuple of std::strings that names the kinematic variables in the order the method expects them. Schematically:

4.3. How to add a new constraint

Constraints are stored in YAML files below <code>eos/constraints/</code>. New constraints can be added to an existing file, or to an entirely new file. Each file contains key-to-value maps in which the top-level keys declare a new constraint. The values in this map are the definitions of a constraint, and are also structured as maps. Valid constraint definitions must at least include a <code>type</code> entry that governs the functional form of the associated likelihood. **EOS** understands the following types of constraints:

- Amoroso,
- · Gaussian,

- MultivariateGaussian,
- MultivariateGaussian(Covariance).

4.3.1. Type Amoroso

Type Amoroso uses a likelihood arising from the PDF of the Amoroso distribution [11], a four-parameter distribution. It is useful for the modeling of upper limits on as-of-yet undiscovered decays at given probabilities. For example, the upper limits on the decay $B_s \to \mu^+\mu^-$ by the LHCb experiment prior to the discovery of this decay are modeled using the Amoroso type of likelihood. The following keys are required in the description of the constraint:

observable the qualified name for an Observable or a Parameter;

kinematics the map representation of the kinematic variables pertaining to the observable;

options the map representation of the options pertaining to the observable;

physical-limit the physical lower bound on the observable;

theta the θ parameter of the Amoroso distribution;

alpha the α parameter of the Amoroso distribution;

beta the β parameter of the Amoroso distribution;

We strongly recommend contacting the **EOS** authors before adding your own constraint of type Amoroso.

4.3.2. Type Gaussian

Type Gaussian uses a univariate Gaussian or normally-distributed likelihood. The following keys are required in the description of the constraint:

observable the qualified name of an Observable or a Parameter;

kinematics the map representation of the kinematic variables pertaining to the observable;

options the map representation of the options pertaining to the observable;

mean the mean of the distribution:

sigma-stat the map representation with keys hi and lo for the upper and lower statistical uncertainty of the distribution, respectively;

sigma-sys the same as sigma-stat, but for the systematic uncertainty;

dof the degrees of freedom associated with this observation (should default to 1).

By default the uncertainties are symmetrized, and statistical and systematical uncertainties are added in quadrature.

4.3.3. Type MultivariateGaussian

Type MultivariateGaussian uses a multivariate Gaussian likelihood, parametrized in terms of its mode and correlation matrix. The following keys are required in the description of the constraint:

dim the dimensionality of the multivariate distribution;

observable the list of size dim of qualified names for either Observables or Parameters;

kinematics the list of size dim of map representations of the kinematic variables pertaining to each observable;

options servable; the list of size dim of map representations of the options pertaining to each ob-

mean the list of size dim describing the mean of the distribution;

sigma-stat-hi the list of size dim for the upper statistical uncertainty of the distribution;

sigma-stat-lo the list of size dim for the lower statistical uncertainty of the distribution;

correlations the matrix of size $\dim \times \dim$ for the statistical correlations;

sigma-sys the list of size dim for the systematic uncertainty;

dof the degrees of freedom associated with this observation (should default to dim).

By default the statistical and systematical uncertainties are added in quadrature, and the larger of the upper and lower uncertainties are chosen as the standard deviation. The covariance matrix Σ_{ij} is then computed from the variances σ_i and the correlation matrix ρ_{ij} as

$$\Sigma_{ij} = \sigma_i \sigma_j \rho_{ij} \,. \tag{4.1}$$

4.3.4. Type MultivariateGaussian(Covariance)

Type MultivariateGaussian(Covariance) uses a multivariate Gaussian likelihood, parametrized in terms of its mode and covariance matrix. The following keys are required in the description of the constraint:

dim the dimensionality of the multivariate distribution;

observable the list of size dim of qualified names for either Observables or Parameters;

kinematics the list of size dim of map representations of the kinematic variables pertaining to each observable:

options the list of size dim of map representations of the options pertaining to each observable;

mean the list of size dim describing the mean of the distribution;

covariance the matrix of size $\dim \times \dim$ for the covariance of the distribution;

dof the degrees of freedom associated with this observation (should default to dim).

Example

We introduce a constraint to correlate the new parameters mass::X@Example, and decay-constant::X@Example from section 4.1. The correlation is fixed at 50%, and the means and standard deviations reflect the previous one. We add the file eos/constraints/x.yaml with contents:

```
X::mass+decay-constant@Example:
    type: MultivariateGaussian
    dim: 2
    observables: ['mass::X@Example', 'decay-constant::X@Example']
    kinematics: [{}, {}]
    options: [{}, {}]
    means: [1.0, 0.1]
    covariance: [[0.25, 2.5e-3], [2.5e-3, 1.0e-4]]
    dof: 2
```

Physics

5. Effective Field Theories

The electro-weak decays of hadrons (mesons and baryons) with masses much smaller than the electro-weak scale of order of the W-boson mass, m_W , can be efficiently described using effective field theories (EFT) in the spirit of the well-known Fermi theory of the β -decay. This comprises practically all hadrons containing light quarks q=(u,d,s,c,b). In this context, specific flavour-changing higher-dimensional (dim>4) operators arise in the standard model (SM) and it's extensions, accompanied by effective couplings (Wilson coefficients) giving rise to the generic structure of the effective Lagrangian

$$\mathcal{L}_{\text{EFT}} = \mathcal{L}_{\text{QCD} \times \text{QED}}(\text{light particles}) + \sum_{i} \mathcal{C}_{i}(\mu)\mathcal{O}_{i} + \text{h.c.} + \dots$$
 (5.1)

The first term describes the $SU(3)_c \times U(1)_{\rm em}$ gauge interactions of all light quarks, q, and leptons, $\ell=(e,\,\mu,\,\tau)$, with QCD and QED gauge bosons. The second part are the aforementioned operators \mathcal{O}_i and effective couplings \mathcal{C}_i , where the latter depend on a factorization scale $\mu_{\rm low}$ that is usually of the order of the mass of the decaying hadron. The operators are composed out of light degrees of freedom, i.e. fermions q and ℓ , as well as $SU(3)_c$ and $U(1)_{\rm em}$ gauge bosons. Beyond the SM, it is conceivable that in principle additional light degrees of freedom exist, which however must have escaped direct detection so far. The Wilson coefficients are suppressed by inverse powers of the electroweak scale or some new physics scale, depending on the dimension of their operators. Finally, the dots denote higher-dimensional operators that have been neglected. In practical applications, assuming the SM, they are suppressed at least by $m_b^2/m_W^2 \sim 0.004$, where m_b denotes the bottom-quark mass.

The EFT framework is sufficient to describe interactions at and below the scale μ_{low} , including hadronic binding effects due to strong interactions as well as electro-magnetic virtual and real corrections to observables. The implementation of according observables in EOS is thus based on universal EFT Lagrangians. All respective short-distance interactions above μ_{low} are fixed by the structure of the operators and the values of the Wilson coefficients. In the spirit of Fermi, the according Wilson coefficients can be viewed as unknowns to be determined from experiment. This so-called *model-independent* approach implies the independence of all Wilson coefficients and correlation among observables arise from the assumption of which operators are included, i.e. have non-vanishing Wilson coefficients at the scale μ_{low} (or some other).

The latter point is important in view of operator mixing (under QCD and QED), which is governed by the anomalous dimension matrices (ADM) of the involved operators. In the case of operator mixing, vanishing Wilson coefficients at some scale μ_0 can become non-zero at some other scale μ_1 , depending on their mixing and the initial conditions of Wilson coefficients involved in the mixing. This is summarized by the general solution of the renormalisation group equation (RGE)

$$C_i(\mu_1) = \sum_j [U(\mu_1, \mu_0)]_{ij} C_j(\mu_0).$$
(5.2)

The evolution matrix U depends on the ADM's of the operators, the strong and electro-magnetic couplings, α_s and α_e respectively, and their respective RG-functions (beta-functions). Throughout Wilson coefficients and couplings are $\overline{\rm MS}$ -renormalized quantities.

In the following we collect the conventions of the effective theories implemented in EOS for hadron decays based on quark transitions

$$b \to (d, s),$$
 (5.3)

For an introduction to the topic, the reader is referred to the exhaustive review articles [12, 13]. The following abbreviations will be often used below for products of elements of the CKM quark mixing matrix appearing in b-quark decays

$$\lambda_U^{(D)} = V_{Ub}V_{UD}^*, \qquad D = (d, s), \qquad U = (u, c, t).$$
 (5.4)

5.1. $|\Delta B| = |\Delta S| = 1$

In this section we summarize the convention of the EFT for $|\Delta B|=|\Delta S|=1$ decays covering transitions

$$\begin{array}{ll} b \to s + (\bar{u}u,\,\bar{c}c) & \text{current-current}\,, \\ b \to s + \bar{q}q & \text{QCD \& QED penguin}\,, \\ b \to s + (\gamma,\,\text{gluon}) & \text{electro- \& chromo-magnetic dipole}\,, \\ b \to s + (\bar{\ell}\ell,\,\bar{\nu}\nu) & \text{semi-leptonic}\,, \end{array}$$

where the classification corresponds to the origin of the operators from decoupling W and Z bosons and the top quark in the SM. The basis contains several blocks that are however related via operator mixing and renders the RGE of the Wilson coefficients non-trivial. The results for $|\Delta B| = |\Delta D| = 1$ transitions are obtained by the replacement $s \to d$.

We start with the operators generated in the SM, where the initial Wilson coefficients and ADM's are known at several orders in perturbation theory. The most appropriate choice of basis for higher order QCD calculations of ADM's was given in [14, 15] with according extension for QED corrections in [16, 17]. The Lagrangian

$$\mathcal{L}_{\text{EFT}} = \mathcal{L}_{\text{QCD} \times \text{QED}}(q; \, \ell) + \frac{4G_F}{\sqrt{2}} \lambda_u^{(s)} \sum_{i=1}^2 \mathcal{C}_i (\mathcal{O}_i^c - \mathcal{O}_i^u)$$

$$+ \frac{4G_F}{\sqrt{2}} \lambda_t^{(s)} \left[\sum_{i=1}^2 \mathcal{C}_i \mathcal{O}_i^c + \sum_{i=3}^{10} \mathcal{C}_i \mathcal{O}_i + \sum_{i=3}^6 \mathcal{C}_{iQ} \mathcal{O}_{iQ} + \mathcal{C}_b \mathcal{O}_b \right] + \text{h.c.} .$$

$$(5.5)$$

incorporates unitarity of the CKM matrix $\lambda_u^{(s)} + \lambda_c^{(s)} + \lambda_t^{(s)} = 0$. All Wilson coefficients \mathcal{C}_i are evaluated at $\mu_{\text{low}} \sim m_b$. The up-quark sector $\sim \lambda_u^{(s)}$ is doubly-Cabibbo suppressed for $b \to s$ transitions and leads to tiny CP-asymmetries in the SM.

The current-current (U = u, c) operators are defined as

$$\mathcal{O}_1^U = (\bar{s}\gamma_\mu P_L T^a U)(\bar{U}\gamma^\mu P_L T^a b), \quad \mathcal{O}_2^U = (\bar{s}\gamma_\mu P_L U)(\bar{U}\gamma^\mu P_L b), \tag{5.6}$$

which arise already at tree-level from decoupling the W-boson in $b \to s + (\bar{u}u, \bar{c}c)$ and mix into all other operators, except the semi-leptonic \mathcal{O}_{10} . Here and below $P_{L,R} = (1 \mp \gamma_5)/2$ denote chirality projectors. The QCD-penguin operators are

$$\mathcal{O}_{3} = (\bar{s}\gamma_{\mu}P_{L}b)\sum_{q}(\bar{q}\gamma^{\mu}q), \qquad \mathcal{O}_{5} = (\bar{s}\gamma_{\mu\nu\rho}P_{L}b)\sum_{q}(\bar{q}\gamma^{\mu\nu\rho}q),
\mathcal{O}_{4} = (\bar{s}\gamma_{\mu}P_{L}T^{a}b)\sum_{q}(\bar{q}\gamma^{\mu}T^{a}q), \quad \mathcal{O}_{6} = (\bar{s}\gamma_{\mu\nu\rho}P_{L}T^{a}b)\sum_{q}(\bar{q}\gamma^{\mu\nu\rho}T^{a}q),$$
(5.7)

where the sum extends over all $q=(u,\,d,\,s,\,c,\,b)$ and T^a are the generators of $SU(3)_c$. Products of several gamma matrices have been abbreviated $\gamma^{\mu\nu\rho}\equiv\gamma^\mu\gamma^\nu\gamma^\rho$. Analogous QED-penguin operators are defined as

$$\mathcal{O}_{3Q} = (\bar{s}\gamma_{\mu}P_{L}b) \sum_{q} Q_{q}(\bar{q}\gamma^{\mu}q) , \qquad \mathcal{O}_{5Q} = (\bar{s}\gamma_{\mu\nu\rho}P_{L}b) \sum_{q} Q_{q}(\bar{q}\gamma^{\mu\nu\rho}q) ,
\mathcal{O}_{4Q} = (\bar{s}\gamma_{\mu}P_{L}T^{a}b) \sum_{q} Q_{q}(\bar{q}\gamma^{\mu}T^{a}q) , \quad \mathcal{O}_{6Q} = (\bar{s}\gamma_{\mu\nu\rho}P_{L}T^{a}b) \sum_{q} Q_{q}(\bar{q}\gamma^{\mu\nu\rho}T^{a}q) ,$$
(5.8)

where ${\cal Q}_q$ denotes the quark charges as multiples of e. Further, an additional operator has to be considered

$$\mathcal{O}_b = -\frac{1}{3} (\bar{s}\gamma_\mu P_L b) (\bar{b}\gamma^\mu b) + \frac{1}{12} (\bar{s}\gamma_{\mu\nu\rho} P_L b) (\bar{b}\gamma^{\mu\nu\rho} b), \qquad (5.9)$$

receiving contributions from electro-weak boxes. In four dimension it would correspond to $(\bar{s}\gamma_{\mu}P_Lb)(\bar{b}\gamma^{\mu}P_Lb)$, however the above form allows to avoid traces with γ_5 to all orders in QCD.

The electro- and chromo-magnetic dipole operators

$$\tilde{\mathcal{O}}_7 = \frac{e}{g_s^2} [\bar{s}\sigma^{\mu\nu}(\overline{m}_b P_R + \overline{m}_s P_L)b] F_{\mu\nu} , \qquad \tilde{\mathcal{O}}_8 = \frac{1}{g_s} [\bar{s}\sigma^{\mu\nu}(\overline{m}_b P_R + \overline{m}_s P_L)T^a b] G^a_{\mu\nu} , \qquad (5.10)$$

receive contributions from on-shell photon and gluon penguins. The appearing quark masses are renormalized in the $\overline{\rm MS}$ scheme.

In the SM there are two semi-leptonic operators

$$\tilde{\mathcal{O}}_{9}^{\ell} = \frac{e^2}{g_s^2} (\bar{s}\gamma_{\mu} P_L b)(\bar{\ell}\gamma^{\mu}\ell), \qquad \qquad \tilde{\mathcal{O}}_{10}^{\ell} = \frac{e^2}{g_s^2} (\bar{s}\gamma_{\mu} P_L b)(\bar{\ell}\gamma^{\mu}\gamma_5\ell), \qquad (5.11)$$

describing $b \to s + \bar{\ell}\ell$ transitions. In this case the lepton charge Q_ℓ has been pulled into the definition of the Wilson coefficient.

note definition of evanescent operators, without whom ADM's and initial Wilson coefficients are meaningless ...

For the tilde operators the normalization to $(4\pi/g_s)^2$, the QCD coupling, has been chosen for practical reasons such that the leading SM 1-loop correction to the initial Wilson coefficients counts formally as a strong correction rather then an electro-magnetic one. The initial Wilson coefficients are known up to NNLO in QCD and NLO in EW corrections

$$C_i(\mu_0) = \dots {(5.12)}$$

 $(a_i \equiv \alpha_i/(4\pi))$ For practical applications, however, we use operators without a tilde, which are related via

$$\mathcal{O}_i = \frac{g_s^2}{(4\pi)^2} \,\tilde{\mathcal{O}}_i \,. \tag{5.13}$$

The full basis of semi-leptonic operators is spanned by $\mathcal{O}_{9,10}$ as above, and additionally

$$\mathcal{O}_{9'}^{\ell} = \frac{e^2}{(4\pi)^2} (\bar{s}\gamma_{\mu} P_R b) (\bar{\ell}\gamma^{\mu}\ell) , \qquad \qquad \mathcal{O}_{10'}^{\ell} = \frac{e^2}{(4\pi)^2} (\bar{s}\gamma_{\mu} P_R b) (\bar{\ell}\gamma^{\mu}\gamma_5\ell) , \qquad (5.14)$$

$$\mathcal{O}_{S}^{\ell} = \frac{e^{2}}{(4\pi)^{2}} (\bar{s}P_{R}b)(\bar{\ell}\ell), \qquad \qquad \mathcal{O}_{P}^{\ell} = \frac{e^{2}}{(4\pi)^{2}} (\bar{s}P_{R}b)(\bar{\ell}\gamma_{5}\ell), \qquad (5.15)$$

$$\mathcal{O}_{S'}^{\ell} = \frac{e^2}{(4\pi)^2} (\bar{s}P_L b)(\bar{\ell}\ell), \qquad \qquad \mathcal{O}_{P'}^{\ell} = \frac{e^2}{(4\pi)^2} (\bar{s}P_L b)(\bar{\ell}\gamma_5\ell), \qquad (5.16)$$

$$\mathcal{O}_{T}^{\ell} = \frac{e^{2}}{(4\pi)^{2}} (\bar{s}\sigma_{\mu\nu}b)(\bar{\ell}\sigma^{\mu\nu}\ell) , \qquad \qquad \mathcal{O}_{T5}^{\ell} = \frac{e^{2}}{(4\pi)^{2}} (\bar{s}\sigma_{\mu\nu}b)(\bar{\ell}\sigma^{\mu\nu}\gamma_{5}\ell) . \qquad (5.17)$$

Quantity	Qualified Name		
	i = 7, 7'		
$\overline{\operatorname{Re} C_i(\mu_b)}$	b->s::Re{c <i>i</i> }		
$\operatorname{Im} C_i(\mu_b)$	$\texttt{b->s}::\texttt{Im}\{\texttt{c}i\}$		
i=9,9',1	10, 10', S, S', P, P', T, T5		
$\operatorname{Re} \mathcal{C}_i^{(\ell)}(\mu_b)$	b->s $\ell\ell$::Re{ci}		
$\operatorname{Im} \mathcal{C}_i^{(\ell)}(\mu_b)$	$\texttt{b->s}\ell\ell : \texttt{Im}\{\texttt{c}i\}$		
	$i = 1 \dots 6, 8, 8'$		
$\overline{C_i(\mu_b)}$	b->s::ci		

Table 5.1.: Naming scheme for the $|\Delta B| = |\Delta S| = 1$ operators.

For studies of NP effects in these operators the values of the respective Wilson coefficients can be changed within the EOS code at run time. For the changed to take effect, the observables must be constructed with the option model set to WilsonScan. In that case, the coefficients \mathcal{C}_i with $i \in \{7,7',9,9',10,10',S,S',P,P',T,T5\}$ are treated as complex-valued parameters. Since EOS parameters are real-valued only, this implies that real and imaginary part of these coefficients can be adjusted separately. The coefficients \mathcal{C}_jU with $j=\{1,2\}$ are presently U-flavour-universal, and are simply considered as two independent coefficients \mathcal{C}_j . The coefficients with $j=\{1,\ldots 6,8\}$ are treated as real-valued parameters. The naming scheme for these coefficients is listed in table 5.1.

5.2.
$$|\Delta B| = |\Delta U| = 1$$

The Lagrangian reads:

$$\mathcal{L}_{\text{EFT}} = \mathcal{L}_{\text{QCD} \times \text{QED}}(q; \, \ell) - \frac{4G_F}{\sqrt{2}} V_{ub}^{\text{eff}} \left[\sum_{X} C_X \mathcal{O}_X \right] \,. \tag{5.18}$$

Note the change of sign compared to the journal version of [18], which has a wrong but inconsequential global factor of -1. The operators are defined as

$$\mathcal{O}_{V,L(R)} \equiv \left[\bar{u} \gamma^{\mu} P_{L(R)} b \right] \left[\bar{\ell} \gamma_{\mu} P_{L} \nu_{\ell} \right] ,
\mathcal{O}_{S,L(R)} \equiv \left[\bar{u} P_{L(R)} b \right] \left[\bar{\ell} P_{L} \nu_{\ell} \right] ,
\mathcal{O}_{T} \equiv \left[\bar{u} \sigma^{\mu \nu} b \right] \left[\bar{\ell} \sigma_{\mu \nu} P_{L} \nu_{\ell} \right] .$$
(5.19)

5.3.
$$|\Delta B| = |\Delta C| = 1$$

The Lagrangian reads:

$$\mathcal{L}_{\text{EFT}} = \mathcal{L}_{\text{QCD} \times \text{QED}}(q; \, \ell) - \frac{4G_F}{\sqrt{2}} V_{cb}^{\text{eff}} \left[\sum_{X} \mathcal{C}_X \mathcal{O}_X \right] \,. \tag{5.20}$$

5.3.
$$|\Delta B| = |\Delta C| = 1$$

Note the change of sign compared to the journal version of [18], which has a wrong but inconsequential global factor of -1. The operators are defined as

$$\mathcal{O}_{V,L(R)} \equiv \left[\bar{c} \gamma^{\mu} P_{L(R)} b \right] \left[\bar{\ell} \gamma_{\mu} P_{L} \nu_{\ell} \right] ,
\mathcal{O}_{S,L(R)} \equiv \left[\bar{c} P_{L(R)} b \right] \left[\bar{\ell} P_{L} \nu_{\ell} \right] ,
\mathcal{O}_{T} \equiv \left[\bar{c} \sigma^{\mu \nu} b \right] \left[\bar{\ell} \sigma_{\mu \nu} P_{L} \nu_{\ell} \right] .$$
(5.21)

A. List of default parameters

The complete list of default parameters is given in this appendix, in a series of tables.

Qualified Name	Parameter Description
b->s::c1	???
b->s::c2	???
b->s::c3	????
b->s::c4	????
b->s::c5	????
b->s::c6	???
b->s::Re{c7}	???
b->s::Im{c7}	???
b->s::c8	????
b->see::Re{c9}	???
b->see::Im{c9}	???
b->see::Re{c10}	???
b->see::Im{c10}	???
b->smumu::Re{c9}	????
b->smumu::Im{c9}	???
b->smumu::Re{c10}	???
b->smumu::Im{c10}	???
b->s::Re{c7'}	???
b->s::Im{c7'}	???
b->s::c8'	???
b->see::Re{c9'}	???
b->see::Im{c9'}	???
b->see::Re{c10'}	???
b->see::Im{c10'}	????
b->smumu::Re{c9'}	???
b->smumu::Im{c9'}	???
b->smumu::Re{c10'}	????
b->smumu::Im{c10'}	????
b->see::Re{cS}	????
b->see::Im{cS}	???
b->see::Re{cS'}	???
b->see::Im{cS'}	???
b->see::Re{cP}	???
b->see::Im{cP}	???
b->see::Re{cP'}	???

A. List of default parameters

b->see::Im{cP'}	???
b->see::Re{cT}	???
b->see::Im{cT}	???
b->see::Re{cT5}	???
b->see::Im{cT5}	???
b->smumu::Re{cS}	???
b->smumu::Im{cS}	???
b->smumu::Re{cS'}	???
b->smumu::Im{cS'}	???
b->smumu::Re{cP}	???
b->smumu::Im{cP}	???
b->smumu::Re{cP'}	???
b->smumu::Im{cP'}	???
b->smumu::Re{cT}	???
b->smumu::Im{cT}	???
b->smumu::Re{cT5}	????
b->smumu::Im{cT5}	????

Table A.2.: The list of parameters describing the b->sqqbar,gamma,ll Wilson coefficients. See the EOS manual for their physical definitions.

Qualified Name	Parameter	Description
HQET::lambda_1	λ_1	cf. [ALGH2001], Table 2, p. 13
HQET::lambda_2	λ_2	cf. [ALGH2001], Table 2, p. 13
B->B::mu_pi^2@1GeV	$\mu_\pi^2(1{\sf GeV})$	cf. [BBMU2003], Eq. (19), p. 9
B->B::mu_G^2@1GeV	$\mu_G^2(1{\rm GeV})$	cf. [BBMU2003], Eq. (17), p. 9
B->B::rho_D^3@1GeV	$ ho_D^3(1{\sf GeV})$	cf. [BBMU2003], between Eqs. (19),(20),
		p. 9
B->B::rho_LS^3@1GeV	$ ho_{LS}^3(1{\rm GeV})$	cf. [BBMU2003], Eq. (20), p. 9
Lambda_b->Lambda_b::mu_pi^2@1GeV	$\mu_\pi^2(1{\sf GeV})$	cf. [MvD2015]
Lambda_b->Lambda_b::rho_D^3@1GeV	$\rho_D^3(1{\rm GeV})$	cf. [MvD2015]

Table A.4.: The list of hadronic forward matrix elements of operators arising in the heavy quark expansion. For the matrix elements $\mu_{\pi,G}^2$ and similar, see [MTU2010] for the definition.

Qualified Name	Parameter	Description
CKM::A	A_{CKM}	The Wolfenstein CKM parameter A
CKM::lambda	λ_{CKM}	The Wolfenstein CKM parameter λ
CKM::rhobar	ar hoCKM	The Wolfenstein CKM parameter $ar ho$

CKM::etabar	$ar{\eta}_{CKM}$ Th	e Wolfenstein CKM parameter $ar{\eta}$
CKM::abs(V_ud)	$ V_{ud} $	
<pre>CKM::arg(V_ud)</pre>	$\operatorname{arg} V_{ud}$	
<pre>CKM::abs(V_us)</pre>	$ V_{us} $	
<pre>CKM::arg(V_us)</pre>	$\operatorname{arg} V_{us}$	
CKM::abs(V_ub)	$ V_{ub} $	
<pre>CKM::arg(V_ub)</pre>	$\operatorname{arg} V_{ub}$	
<pre>CKM::abs(V_cd)</pre>	$ V_{cd} $	
<pre>CKM::arg(V_cd)</pre>	$\operatorname{arg} V_{cd}$	
<pre>CKM::abs(V_cs)</pre>	$ V_{cs} $	
<pre>CKM::arg(V_cs)</pre>	$\operatorname{arg} V_{cs}$	
<pre>CKM::abs(V_cb)</pre>	$ V_{cb} $	
<pre>CKM::arg(V_cb)</pre>	$\operatorname{arg} V_{cb}$	
<pre>CKM::abs(V_td)</pre>	$ V_{td} $	
<pre>CKM::arg(V_td)</pre>	$\operatorname{arg} V_{td}$	
<pre>CKM::abs(V_ts)</pre>	$ V_{ts} $	
<pre>CKM::arg(V_ts)</pre>	$\operatorname{arg} V_{ts}$	
<pre>CKM::abs(V_tb)</pre>	$ V_{tb} $	
CKM::arg(V_tb)	$\operatorname{arg} V_{tb}$	

Table A.6.: The list of parameters describing the CKM matrix. For the Wolfenstein parameters of the CKM matrix see e.g. [UTFIT2013] for their definition.

Acronyms

HDF5 Hierarchical Data Format version 5. 4, 12, 13

LCSR Light-Cone Sum Rule. 14

MCMC Markov-Chain Monte Carlo. 11, 12

PDF Probability Density Function. 11, 14, 16, 27

PMC Population Monte Carlo. 4, 6, 13

RNG Random Number Generator. 12, 13

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