

Developing the OpenTURNS documentation

Joseph MURÉ - EDF R&D February 14th-17th 2022

OpenTURNS Consortium

1

A few words about the development infrastructure (1/2)

Versioning system

- Git is a software versioning and a revision control system started by Linus
 Torvalds. It is used for the sources of the platform, the documentation, as well as
 for the development of modules.
- GitHub is a web-based hosting service for version control using Git. GitHub provides a bug tracker, pull requests (GitLab equivalent: merge requests), continuous integration, and other features.

Official repository and forks

The official repository of the library is https://github.com/openturns/openturns.

- All developers have a fork of that repository to host their development branches.
- Only the integrator (and a backup) has write access to the official repository.
- Modules are not part of the library, but some of them are maintained by the
 consortium: their repositories are hosted at https://github.com/openturns and
 they have the same development process as the library.
- Other modules are hosted elsewhere and do not need to follow the same development process.

2

A few words about the development infrastructure (2/2)

Structure of the library repository

The repository of the library contains source code for the C++ library, the Python interface and the documentation. Its layout is quite standard:

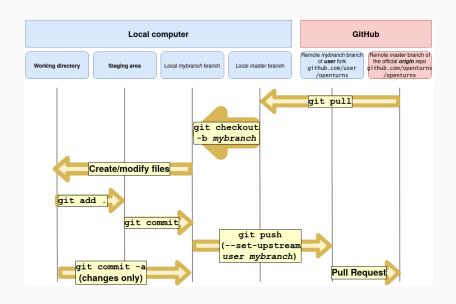
- A master branch that stores the source code of the upcoming version of the platform. The rule is to have only source code that passes all tests.
- Branches for stable versions and tags for releases and release candidates.
- Development branches are part of contributor forks.
- Development branches are merged with master via pull requests.
- At least 2 reviewers must approve the PR, and unanimity is required.

Continuous integration

OpenTURNS makes extensive use of online continuous integration providers to test the library throughout the development process. Currently the following services are used to test the library:

- CircleCI: Linux and MinGW
- GitHub Actions: macOS and Windows

OpenTURNS development workflow



4

Overview of the OpenTURNS documentation

The OpenTURNS documentation is built using the Python Sphinx package.

One of the Continuous Integration machines (CircleCl build-linux) produces the documentation and publishes it online. Several versions are online:

- The version corresponding to the current release has <u>latest</u> in its URL: https://openturns.github.io/openturns/latest/
- The version corresponding to the master branch has master in its URL: https://openturns.github.io/openturns/master/
- Older versions are accessible with the version number: https://openturns.github.io/openturns/1.17/

If you spot a mistake, make sure you are looking at master before correcting!

The built-in search engine distinguishes between 3 main sections:

- Examples
- API (user manual)
- Theory

You may also want to check out:

- Contribute (developer guide)
- Common use cases (added in 2020)

Outline

1. Theory

2. Examples

3. API (user manual)

4. Tips and tricks

Looking up the source file of a theory page

Let us consider the Using QQ-plot to compare two samples page:

https://openturns.github.io/openturns/master/theory/data_analysis/qqplot_graph.html

All Theory files are RST and the URL fits the source folder structure, so the relevant source file is: python/doc/theory/data_analysis/qqplot_graph.rst

There are great RST and Sphinx cheatsheet available, but here are the basics:

- A page can be indexed as page_name by writing .. _page_name: at the top.
- Because of this, that page can be linked to from anywhere in the doc with :ref:'page_name'
- Titles are underlined (the number of underlining characters must match the title).
- Inline math is LATEX code with \$a=b\$ replaced with :math: 'a=b'.
- Display math is LATEX code with \$\$a=b\$\$ replaced with
 - . math::
 - a = b
- Macros are defined in python/doc/math_notations.sty
- Try to use notations consistent with other theory pages.
- The bibliography can be found at python/doc/bibliography.rst

Adding a new theory page

Code of the main table of contents (python/doc/theory/theory.rst):

```
1 .. theory:
  =====
  Theory
  The theoretical documentation.
  This contains an in-depth description of all algorithms.
9
  .. toctree::
      :maxdepth: 2
      data_analysis/data_analysis.rst
      probabilistic_modeling/probabilistic_modeling.rst
14
      meta_modeling/meta_modeling.rst
16
      reliability_sensitivity/reliability_sensitivity.rst
      numerical_methods/numerical_methods.rst
```

Table of contents of subdirectories are essentially the same.

What holds for the Theory section also mostly holds for the Contribute (developer guide) and Common use cases sections.

Outline

1. Theory

2. Examples

3. API (user manual)

4. Tips and tricks

Looking up the source Python script of an example

The Examples section is produced by Sphinx-gallery, a Sphinx extension.

Let us consider the Kriging with an isotropic covariance function example:

https://openturns.github.io/openturns/master/auto_meta_modeling/kriging_metamodel/plot_kriging_isotropic.html

Example source files are Python scripts. The URL is still linked to the the source folder structure, but the auto_part is a Sphinx-gallery artifact. Its source file is:

python/doc/examples/meta_modeling/kriging_metamodel/
plot_kriging_isotropic.py

- Use # %% to start a new cell.
- Write Python code as you normally would.
- Write text as RST code, but each RST line must start with #.
- A cell can contain both RST and Python code, but RST must come first.
- RST rules are the same as in the Theory section.
- A blank line interrupts RST code and switches to Python. For the remainder of the cell, lines starting with # are simply interpreted as Python comments.
- By default, the first image is used as thumbnail picture. To use e.g. the third:
 # sphinx_gallery_thumbnail_number = 3 (ideally right above the plot code)

Adding a new example

- Normally, you should not need to change python/doc/examples/examples.rst.
- Every subfolder has a README.txt file, which is actually an RST file that only
 contains a label for hypertext links and the subsection title.
- All source Python scripts are automatically detected and used to build HTML examples and the corresponding thumbnails, provided their name follows the plot_xxx.py template.
- No need to index the files, just put them in the appropriate subfolder.
- You can use the docstring at the start of the file not only to write the title of the
 example, but also the introductory text. This docstring is the only part of the
 script that is interpreted as RST code without a # at the start of every line.
- Hypertext links help users connect various aspects of the library:
 - :class:'~openturns.ClassName' to link to the API doc of a class.
 - :meth: '~openturns.ClassName.method' to link to the API doc of a class method.
 - :ref:'_theory_page' to link to a Theory doc page using its RST label.
 - :doc: '/auto_category/subcategory/plot_xxx' (no .py) to link to another example.
- Python scripts should be properly formatted according to the PEP8.
 Use Black to format them automatically if needed.
- Examples should combine several classes in order to do something useful.

Examples section: write interesting English (1/2)

In the Examples section, the English content should be an interesting explanation of the Python content.

Do not write:

```
# %%
2 # Draw the function
3
4 n = 10000
5 sampleX = im.distributionX.getSample(n)
6 sampleY = im.model(sampleX)
7 [...]
8 plotXvsY(sampleX, sampleY)
```

Examples section: write interesting English (2/2)

Write instead:

```
1 # %%
2 # In the next cell, we create a large sample of the input random
3 # vector and evaluate the corresponding output from the physical
4 # model. We then create a function which takes the input and output
    samples as input argument and creates a grid of scatter plots.
6
7 n = 10000
8 sampleX = im.distributionX.getSample(n)
9 sampleY = im.model(sampleX)
10 [...]
plotXvsY(sampleX, sampleY)
13 # %%
14 # We see that the variance of the output is mostly sensitive to the
15 # first variable :math: 'X 1'.
16 # The variance of the output is not sensitive to the third
17 # variable, since the conditional variance is zero.
```

Outline

1. Theory

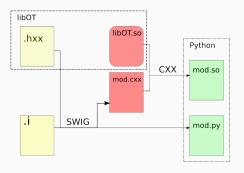
2. Examples

3. API (user manual)

4. Tips and tricks

SWIG: Simplified Wrapper and Interface Generator

A tool to link C/C++ libraries with script languages SWIG parses the library headers (.hxx) and swig interface files (.i) to generate the corresponding module source that must be compiled to produce a binary Python module.



Python docstrings are written in _doc.i.in files which supplement the SWIG .i files.

These docstrings are then read by Sphinx to build the API doc section.

Looking up the sources of docstrings

Let us consider the LinearCombinationFunction class and its source file: https://openturns.github.io/openturns/master/user_manual/_generated/openturns.LinearCombinationFunction.html python/src/LinearCombinationFunction_doc.i.in

- Docstring sources are in src rather than doc because they are part of the library.
- A docstring is just a string "...": double quotes are thus forbidden inside, use
 '...' instead (not to be confused with '...' as in :math:'...'). Do not put
 any whitespace between the opening " and the first docstring character, nor
 between the last docstring character and the closing ".
- Docstrings follow Numpydoc style. RST rules remain the same.
- Example code lines start with >>> and are run during Python tests! If you call
 print, you need to specify the expected output or the test will fail.
- Numerical values can differ slightly between platforms. To prevent CI failures, you
 may replace the last digits with an ellipsis: 0.34023... instead of 0.3402362897
- Class inheritance extends to docstrings: LinearCombinationFunction inherits all
 its method docstrings from FunctionImplementation: look for the docstrings in
 python/src/FunctionImplementation_doc.i.in.
- FunctionImplementation has no HTML page, although it has many docstrings.
 Instead, those docstrings are used to produce the HTML file of Function. This holds for almost all Interface/Implementation couples.

Docstrings of a new class and/or method: SWIG part

To get the docstrings to appear in the Python library, you need to act on python/src:

- Create a docstring file MyClass_doc.i.in
- Declare the class docstring: %feature("docstring") OT::MyClass
- Declare a method docstring: "feature("docstring") OT::MyClass::myMethod
- Two ways are available to actually create the docstring:
 - 1. Write the docstring between double-quotes right under the declaration.
- For a new class, do not forget to declare:
 - the docstrings in MyClass.i: %include MyClass_doc.i
 - \bullet the class in the appropriate ${\tt xxx_module.i} : {\tt %include MyClass.i}$
 - the class and its docstrings in the appropriate xxx_module section of CMakeLists.txt: MyClass.i MyClass_doc.i.in
- For a new Interface/Implementation couple, define the docstrings in XxxImplementation_doc.i.in with "define to be able to reuse them in the Interface docstrings file Xxx_doc.i.in: see Function_doc.i.in and FunctionImplementation_doc.i.in for example.

Docstrings of a new class: Sphinx part

Sphinx looks at $python/doc/user_manual$ for the structure of the API documentation.

For example, LinearCombinationFunction is referenced in python/doc/user_manual/functions.rst

To get your new class to appear in the HTML API doc section:

- Find the RST file of the appropriate subsection.
- Insert the name of your class where you want it to appear.
- Make sure it uses the correct template, otherwise use the :template: directive.

Templates are found in the python/doc/_templates folder. The main templates are:

- class.rst_t
- classWithPlot.rst_t

If you want to use classWithPlot.rst_t, you need to provide the code to generate the graph at the top of the page. For example, LinearCombinationFunction runs the code in python/doc/pyplots/LinearCombinationFunction.py.

Note that the plot code can be downloaded from the API doc page itself by clicking on "Source code".

API example: always document the most significant method

In the API documentation, the most significant method should have an example within the main section, at the top of the help page. This main example should document the *flagship* of the class, that is, the most significant method(s) of the class.

For example, one of the main features of the LinearEnumerateFunction class is its evaluation operator, which is why the first example is:

```
1 >>> import openturns as ot
2 >>> enumerateFunction = ot.LinearEnumerateFunction(2, 0.5)
3 >>> for i in range(10):
4 >>> print(enumerateFunction(i))
```

Constrast with examples from the Examples section, which combine several classes in order to do useful Uncertainty Quantification.

Summary of the previous parts

Two tools are involved in the creation of the documentation.

Sphinx:

- Theory files: python/doc/theory
- Example files: python/doc/examples
- API tables of contents: python/doc/user_manual
- API plots: python/doc/pyplots
- Math notations are defined in python/doc/math_notations.sty

SWIG:

API docstrings: *_doc.i.in files in python/src

Docstrings are in python/src because they are part of the Python library and not only the HTML documentation.

Outline

1. Theory

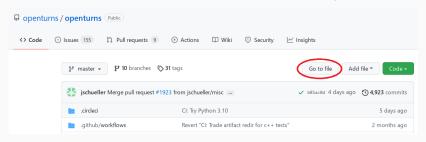
2. Examples

3. API (user manual)

4. Tips and tricks

Quickly find the appropriate source file

The GitHub "Go to file" button does wonders to find the source file you need.



- API: simply type the class name.
- Examples: scroll down to "Download Python source code" for the script name.
- Theory: click on "Show source", the exact .rst file name appears in the URL.

Write clear commit messages: examples

1 Create a quick start example for points and samples

Add new ResourceMap keys for Mesh checking

```
4 as the method might be costly.
1 Doc: Fix keyword in graph example
3 Closes #1742
 Fixed GaussianNonLinearCalibration
The estimation of distribution of the observations error was
4 incorrect. It was created using a zero mean to compute the Cholesky
5 factor of its (known) covariance matrix in order to compute the
6 residual function, but was not updated once the residual function
7 was known.
9 Closes #1529
```

3 We add a new RM key for mesh checking. Default value is set to False

Write clear commit messages: the rules

- First line: a title of 50 characters or less.
- Second line: blank
- Next lines: body of the message with unlimited length.
- If your commit closes an issue, use one of the following keywords in the body:

```
• Close #....
• Closes #....
• Fix #....
• Fixes #....
• Solve #....
• Solves #....
```

Some text editors like Vim use syntax coloring to help you remember these rules.

Closing keywords are recognized by GitHub: when your commit enters the master branch, the corresponding issue is automatically closed.

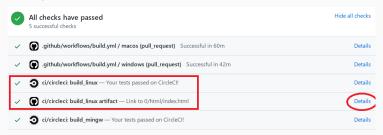
Remember to also use these keywords in the first message of your pull request, so that GitHub registers the PR as fixing the issue.

The first message of the PR should summarize the changes made by the commits of the PR.

Tip for reviewers: always look at the HTML output, not the source file!

CircleCl build_linux builds the doc in addition to the library when a PR is submitted.

For easy access, click on the "Details" link of the build_linux artifact "check".



- The build_linux artifact pseudo-check "succeeds" if, and only if, the build_linux check succeds. This means that a test failure could cause a red cross to appear in front of both of them, even though the doc was actually successfully generated.
- If the person submitting the Pull Request has CircleCl set up on their fork, then
 the build_linux artifact link is always broken regardless of whether or not the
 doc was successfully built. You can still access it through the "Artifacts" tab in
 CircleCl after clicking on the build_linux "Details" link.

Build the documentation with the library

Pass the following option to CMake in order to build the doc with the library:

-DSPHINX_FLAGS="-j6" (to build with 6 cores)

Pass the following option to CMake in order to not build the doc:

-DUSE_SPHINX=OFF

Building the doc takes a while if you build from scratch. It is much shorter afterwards.

Quick patch to the doc (1/2)

You can patch the doc directly from GitHub:

- Go to the master branch of the official repository: https://github.com/openturns/openturns
- 2. Find the file you want to edit (with "Go to file" for example).
- 3. Click on the pencil button.



- 4. Make your change and click on "*Preview changes*" to make sure you have not made any mistake.
- Scroll down to write the title (with 50 characters or fewer) and the body of your commit message. You cannot edit more than one file in a GitHub commit.
- 6. Click on "Propose changes" to:
 - Create a new patch-1 (or more) branch on your fork.
 - Validate the commit.

Quick patch to the doc (2/2)

- 7. GitHub will ask if you want to create a Pull Request. If you accept, you are done!
- 8. If you want to add more commits to your newly created branch, close the tab.
- 9. Go to your fork and select the patch-1 (for example) branch from the menu.
- 10. Edit a file as before and create a new commit.
- 11. After you have created all the commits you want, create a Pull Request.

Advantage of this method:

• Do everything remotely. No need to worry about local/remote branches.

Drawbacks of this method:

- Only one file can be changed per commit.
- No way to inspect the HTML output before pushing.

Build select parts of the documentation without the library with docfast.py

The Python script utils/docfast.py can build selected parts of the library and only requires OpenTURNS to be installed, not necessarily compiled.

Prerequisites: python 3.8+, sphinx, sphinx-gallery, numpydoc, openturns, matplotlib.

- \$ docfast.py build-sphinxonly smirnov_test.rst plot_smoothing_mixture.py
 - build-sphinxonly is the name of the build folder: HTML output files will be stored in build-sphinxonly/install
 - smirnov_test.rst is the source file of the Kolmogorov-Smirnov two samples test theory page.
 - plot_smoothing_mixture.py is the source file of the Bandwidth sensitivity in kernel smoothing example.

Advantages of this method:

- Fast: the command above only builds one example and one theory page.
- Does not require a full compilation environment.

Drawbacks of this method:

- If the installed version of OpenTURNS is older than master, examples relying on new classes or methods will fail.
- Since it does not use SWIG, how can it deal with docstrings?

Docstring handling with docfast.py

- Recall: docstring source files are stored in python/src as _doc.i.in files.
- Sphinx does not deal with them: that is part of SWIG's job.
- In a normal build, SWIG creates the Python library with the docstrings.
- Sphinx reads the docstrings in the Python library, not its source files.

Since Sphinx reads the docstrings of the installed OpenTURNS Python library, docstring.py attempts to patch them with the changes made to the python/src/*_doc.i.in source files.

By default, it relies on git diff: this only takes unstaged changes into account. You can pass an additional argument to git diff with the --diff option:

\$ docfast.py --diff master ... uses git diff master instead.

Regardless, to tell docfast.py which API page(s) it needs to build, you need to pass the name of a file from python/doc/user_manual. They are RST table of content files.

\$ docfast.py [--diff master] functions.rst plot_smoothing_mixture.py Unfortunately, docstring patches can fail in various ways.

To disable them and build from the installed docstrings, use the --nodiff option:

\$ docfast.py --nodiff functions.rst plot_smoothing_mixture.py