SIMPA

version 0.1.0

CAMI (Computer Assisted Medical Interventions), DKFZ, Heidelberg

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Contents

Welcome to the SIMPA documentation!

README

The Simulation and Image Processing for Photoacoustic Imaging (SIMPA) toolkit.

SIMPA Install Instructions

These install instructions are made under the assumption that you have access to the phabricator simpa project. When you are reading these instructions there is a 99% chance that is the case (or someone send these instructions to you).

So, for the 1% of you: Please also follow steps 1 - 3:

1. `git clone https://phabricator.mitk.org/source/simpa.git`
2. `git checkout master`
3. `git pull`

Now open a python instance in the 'simpa' folder that you have just downloaded. Make sure that you have your preferred virtual environment activated

1. `cd simpa`
2. `python -m setup.py build install`
3. Test if the installation worked by using `python` followed by `import simpa` then `exit()`

If no error messages arise, you are now setup to use simpa in your project.

Building the documentation

When the installation went fine and you want to make sure that you have the latest documentation you should do the following steps in a command line:

1. Navigate to the `simpa` source directory (same level where the setup.py is in)
2. Execute the command `sphinx-build -b pdf -a simpa_documentation/src simpa_documentation`
3. Find the PDF file in `simpa_documentation/simpa_documantation.pdf`

External Tools installation instructions

mcx (Optical Forward Model)

Either download suitable executables or build yourself from the following sources: http://mcx.space/

k-Wave (Acoustic Forward Model)

Please follow the following steps and use the k-Wave install instructions for further (and much better) guidance under http://www.k-wave.org/!

1. Install MATLAB with the core and parallel computing toolboxes activated at the minimum.
2. Download the kWave toolbox
3. Add the kWave toolbox base bath to the toolbox paths in MATLAB
4. If wanted: Download the CPP and CUDA binary files and place them inthe k-Wave/binaries folder
5. Note down the system path to the `matlab` executable file.

On MATLAB r2020a or newer there is a bug when using the GPU binaries with kWave. Please follow these instructions http://www.k-wave.org/forum/topic/error-reading-h5-files-when-using-binaries to fix this bug.

MITK

Overview

The main use case for the simpa framework is the simulation of photoacoustic images. However, it can also be used for image processing.

Simulating photoacoustic images

A basic example on how to use simpa in you project to run an optical forward simulation is given in the samples/minimal_optical_simulation.py file.

Performance profiling

Do you wish to know which parts of the simulation pipeline cost the most amount of time? If that is the case then you can use the following commands to profile the execution of your simulation script. You simply need to replace the `myscript` name with your script name.

```
python -m cProfile -o myscript.cprof myscript.py
```

```
pyprof2calltree -k -i myscript.cprof
```

Developer Guide

Dear SIMPA developers, Dear person who wants to contribute to the SIMPA toolkit,

First of all: Thank you for your participation and help! It is much appreciated! This Guide is meant to be used as a collection of How-To's to contribute to the framework. In case you have any questions, do not hesitate to get in touch with the members of the core development team:

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Janek M. Groehl (janek.grohl@cruk.cam.ac.uk)

How to contribute

The SIMPA code is written and maintained on a closed repository that is hosted on a server of the German Cancer Research Center. The current master branch of the repository is open source and mirrored on github.

To contribute to SIMPA, please fork the SIMPA github repository and create a pull request with a branch containing your suggested changes. The core team developers will then review the suggested changes and integrate these into the code base.

Please see the github guidelines for creating pull requests: https://docs.github.com/en/github/collaborating-with-issues-and-pull-requests/about-pull-requests

Coding style

When writing code for SIMPA, please use the PEP 8 python coding conventions (https://www.python.org/dev/peps/pep-0008/) and consider to use the following structures in your code in order to make a new developer or someone external always know exactly what to expect.

- Classnames are written in camel-case notation `ClassName`
- Function names are written in small letter with _ as the delimiter `function_name`
- Function parameters are always annotated with their type `arg1: type = default`
- Only use primitive types as defaults. If a non-primitive type is used, then the default should be `None` and the parameter should be initialized in the beginning of a function.
- A single line of code should not be longer than 120 characters.
- Functions should follow the following simple structure:

  1. Input validation (arguments all not `None`, correct type, and acceptable value ranges?)
  2. Processing (clean handling of errors that might occur)
  3. Output generation (sanity checking of the output before handing it off to the caller)

Documenting your code

Only documented code will appear in the sphinx generated documentation.

A class should be documented using the following syntax:

```
class ClassName(Superclass):
    """
    Explain how the class is used and what it does.
    """
```

For functions, a lot of extra attributes can be added to the documentation:

```
def function_name(self, arg1:type = default, arg2:type = default) -> return_type:
    """
    Explain how the function is used and what it does.

    :param arg1: type, value range, Null acceptable?
    :param arg2: type, value range, Null acceptable?
    :returns: type, value range, does it return Null?
    :raises ExceptionType: explain when and why this exception is raised
    """
```

Adding literature absorption spectra

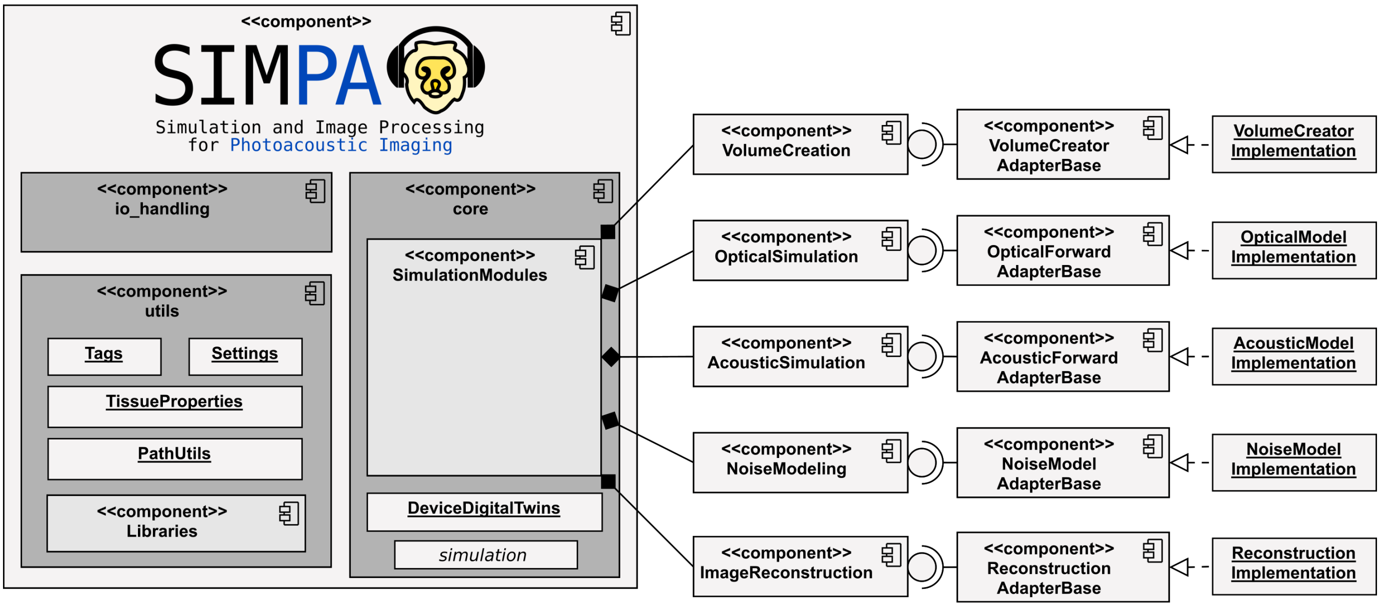
The central point, where absorption spectra are collected and handled is in `simpa.utils.libraries.spectra_library.py`. The file comprises the class `AbsorptionSpectrumLibrary`, in which the new absorption spectra can be added using the following two steps:

1. In the beginning of the class, there is a bunch of constants that define spectra using the `AbsorptionSpectrum` class. Add a new constant here: `NEW_SPECTRUM = AbsorptionSpectrum(absorber_name, wavelengths, absorptions)`. By convention, the naming of the constant should be the same as the `absorber_name` field. The `wavelengths` and `absorptions` arrays must be of the same length and contain corresponding values.
2. In the `__init__` method of the `AbsorptionSpectrumLibrary` class, the class constants are added to an internal list. This has the benefit of enabling the Library class to be iterable. Add your newly added constant field to the list here.

3. Your absorption spectrum is now usable throughout all of simpa and is accessible using the `SPECTRAL_LIBRARY` sngleton that can be imported using `from simpa.utils import SPECTRAL_LIBRARY`.

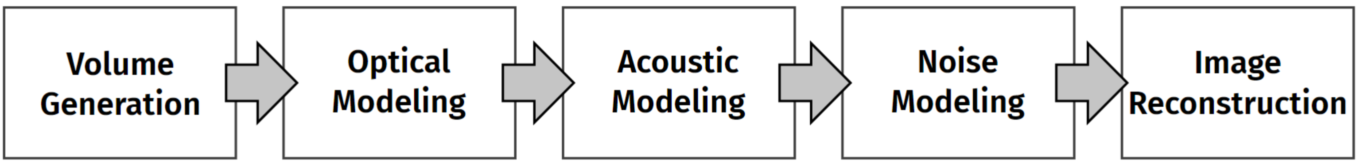
Class references

This component diagram shows the three principle modules of the SIMPA toolkit and gives an insight into their constituents. The core is concerned with providing interfaces for the simulation tools, while the utils module contains many scripts and classes to facilitate the use of the simulation pipeline.



Module: core

The purpose of the core module is to provide interfaces that facilitate the integration of toolboxes and code for photoacoustic modeling into a single continuous pipeline:



Volume creation

class `simpa.core.volume_creation.`**`VolumeCreatorBase`**

Use this class to define your own volume creation adapter.

abstract **`create_simulation_volume`** **(**`settings: simpa.utils.settings_generator.Settings`**)** → dict

This method will be called to create a simulation volume. @param settings:

Optical forward modeling

class `simpa.core.optical_simulation.`**`OpticalForwardAdapterBase`**

Use this class as a base for implementations of optical forward models.

abstract **`forward_model`** **(**`absorption_cm`, `scattering_cm`, `anisotropy`, `settings`**)**

A deriving class needs to implement this method according to its model.

Parameters:

- **absorption_cm** – Absorption in units of per centimeter
- **scattering_cm** – Scattering in units of per centimeter
- **anisotropy** – Dimensionless scattering anisotropy
- **settings** – Setting dictionary

Returns: Fluence in units of J/cm^2

`simulate (optical_properties_path, settings)`

Call this method to invoke the simulation process.

A adapter that implements the forward_model method, will take optical properties of absorption, scattering, and scattering anisotropy as input and return the light fluence as output.

Parameters:

- **optical_properties_path** – path to a .npz file that contains the following tags: Tags.PROPERTY_ABSORPTION_PER_CM -> contains the optical absorptions in units of one per centimeter Tags.PROPERTY_SCATTERING_PER_CM -> contains the optical scattering in units of one per centimeter Tags.PROPERTY_ANISOTROPY -> contains the dimensionless optical scattering anisotropy
- **settings** –

Returns:

Acoustic forward modeling

`simpa.core.acoustic_simulation.acoustic_modelling.run_acoustic_forward_model (settings)`

This method is the entry method for running an acoustic forward model. It is invoked in the *simpa.core.simulation.simulate* method, but can also be called individually for the purposes of performing acoustic forward modeling only or in a different context.

The concrete will be chosen based on the:

```
Tags.ACOUSTIC_MODEL
```

tag in the settings dictionary.

Parameters: **settings** – The settings dictionary containing key-value pairs that determine the simulation. Here, it must contain the Tags.ACOUSTIC_MODEL tag and any tags that might be required by the specific acoustic model.

Raises: **AssertionError** – an assertion error is raised if the Tags.ACOUSTIC_MODEL tag is not given or points to an unknown acoustic forward model.

Returns: returns the path to the simulated data within the saved HDF5 container.

class `simpa.core.acoustic_simulation.AcousticForwardAdapterBase`

This class should be used as a base for implementations of acoustic forward models.

abstract `forward_model (settings)` → numpy.ndarray

This method performs the acoustic forward modeling given the initial pressure distribution and the acoustic tissue properties contained in the settings file. A deriving class needs to implement this method according to its model.

Parameters: **settings** – Setting dictionary

Returns: time series pressure data

`simulate (settings)` → numpy.ndarray

Call this method to invoke the simulation process.

Parameters: **settings** – the settings dictionary containing all simulation parameters.

Returns: a numpy array containing the time series pressure data per detection element

k-Wave

class `simpa.core.acoustic_simulation.k_wave_adapter.`**`KwaveAcousticForwardModel`**

The KwaveAcousticForwardModel adapter enables acoustic simulations to be run with the k-wave MATLAB toolbox. k-Wave is a free toolbox (http://www.k-wave.org/) developed by Bradley Treeby and Ben Cox (University College London) and Jiri Jaros (Brno University of Technology).

In order to use this toolbox, MATLAB needs to be installed on your system and the path to the MATLAB binary needs to be specified in the settings dictionary.

In order to use the toolbox from with SIMPA, a number of parameters have to be specified in the settings dictionary:

```
The initial pressure distribution:
    Tags.OPTICAL_MODEL_INITIAL_PRESSURE
Acoustic tissue properties:
    Tags.PROPERTY_SPEED_OF_SOUND
    Tags.PROPERTY_DENSITY
    Tags.PROPERTY_ALPHA_COEFF
The digital twin of the imaging device:
    Tags.DIGITAL_DEVICE
Other parameters:
    Tags.PERFORM_UPSAMPLING
    Tags.SPACING_MM
    Tags.UPSCALE_FACTOR
    Tags.MEDIUM_ALPHA_POWER
    Tags.GPU
    Tags.PMLInside
    Tags.PMLAlpha
    Tags.PlotPML
    Tags.RECORDMOVIE
    Tags.MOVIENAME
    Tags.ACOUSTIC_LOG_SCALE
    Tags.SENSOR_DIRECTIVITY_PATTERN
```

Many of these will be set automatically by SIMPA, but you may use the simpa.utils.settings_generator convenience methods to generate settings files that contain sensible defaults for these parameters.

Please also refer to the simpa_examples scripts to see how the settings file can be parametrized successfully.

`forward_model`(`settings`) → numpy.ndarray

This method performs the acoustic forward modeling given the initial pressure distribution and the acoustic tissue properties contained in the settings file. A deriving class needs to implement this method according to its model.

Parameters: **settings** – Setting dictionary

Returns: time series pressure data

Noise modeling

class `simpa.core.noise_simulation.`**`GaussianNoiseModel`**

This class is reponsible to apply an additive gaussian noise to the input data.

`apply_noise_model`(`data`, `settings`)

Parameters:

- **data** –
- **settings** –

Returns:

Image reconstruction

Digital device twins

At every step along the forward simulation, knowledge of the photoacoustic device that is used for the measurements is needed. This is important to reflect characteristic artefacts and challenges for the respective device.

To this end, we have included digital twins of commonly used devices into the SIMPA core.

MSOT Acuity Echo

class `simpa.core.device_digital_twins.msot_devices.`**`MSOTAcuityEcho`**

TODO

`adjust_simulation_volume_and_settings` **(**`global_settings: simpa.utils.settings_generator.Settings`**)**

In case that the PAI device needs space for the arrangement of detectors or illuminators in the volume, this method will update the volume accordingly.

`check_settings_prerequisites` **(**`global_settings: simpa.utils.settings_generator.Settings`**)** → bool

It might be that certain device geometries need a certain dimensionality of the simulated PAI volume, or that it required the existence of certain Tags in the global global_settings. To this end, a PAI device should use this method to inform the user about a mismatch of the desired device and throw a ValueError if that is the case.

Raises: **ValueError** – raises a value error if the prerequisites are not matched.

Returns: True if the prerequisites are met.

`get_detector_element_orientations` **(**`global_settings: simpa.utils.settings_generator.Settings`**)**

TODO

`get_detector_element_positions_accounting_for_device_position_mm` **(**`global_settings: simpa.utils.settings_generator.Settings`**)**

TODO

`get_detector_element_positions_base_mm` **()**

TODO

`get_illuminator_definition` **(**`global_settings: simpa.utils.settings_generator.Settings`**)**

TODO

RSOM Explorer P50

class `simpa.core.device_digital_twins.rsom_device.`**`RSOMExplorerP50`**`(element_spacing_mm=0.02)`

This class represents an approximation of the Raster-scanning Optoacoustic Mesoscopy (RSOM) device built by iThera Medical (Munich, Germany). Please refer to the companie’s website for more information (https://www.ithera-medical.com/products/rsom-explorer-p50/).

Since simulating thousands of individual forward modeling steps to obtain a single raster-scanned image is computationally not feasible, we approximate the process with a device design that has detection elements across the entire field of view. Because of this limitation we also need to approximate the light source with a homogeneous illumination across the field of view.

The digital device is modeled based on the reported specifications of the RSOM Explorer P50 system. Technical details of the system can be found in the dissertation of Mathias Schwarz (https://mediatum.ub.tum.de/doc/1324031/1324031.pdf) and you can find more details on use cases of the device in the following literature sources:

Yew, Yik Weng, et al. “Raster-scanning optoacoustic mesoscopy (RSOM) imaging as an objective disease severity tool in atopic dermatitis patients.” Journal of the American Academy of Dermatology (2020).
Hindelang, B., et al. “Non■invasive imaging in dermatology and the unique potential of raster■scan optoacoustic mesoscopy.” Journal of the European Academy of Dermatology and Venereology 33.6 (2019): 1051-1061.

adjust_simulation_volume_and_settings (global_settings: simpa.utils.settings_generator.Settings)
In case that the PAI device needs space for the arrangement of detectors or illuminators in the volume, this method will update the volume accordingly.

check_settings_prerequisites (global_settings: simpa.utils.settings_generator.Settings) → bool
It might be that certain device geometries need a certain dimensionality of the simulated PAI volume, or that it required the existence of certain Tags in the global global_settings. To this end, a PAI device should use this method to inform the user about a mismatch of the desired device and throw a ValueError if that is the case.

Raises: **ValueError** – raises a value error if the prerequisites are not matched.

Returns: True if the prerequisites are met.

get_detector_element_orientations (global_settings: simpa.utils.settings_generator.Settings)
TODO

get_detector_element_positions_accounting_for_device_position_mm (global_settings: simpa.utils.settings_generator.Settings)
TODO

get_detector_element_positions_base_mm ()
TODO

get_illuminator_definition (global_settings: simpa.utils.settings_generator.Settings)
TODO

Module: utils

The utils module contains several general-purpose utility functions whose purpose it is to facilitate the use of SIMPA. The most important of these is the Tags class, which defines the strings and data types that have to be used for the keys and values of the settings dictionary.

class simpa.utils.tags.**Tags**
This class contains all ‘Tags’ for the use in the settings dictionary.

BACKGROUND = *'Background'*
ADHERE_TO_DEFORMATION default is True

DIGITAL_DEVICE_POSITION = *('digital_device_position', (<class 'list'>, <class 'tuple'>, <class 'numpy.ndarray'>))*
Optical model settings

MAX_DEFORMATION_MM = *'max_deformation'*
Structure Settings

MEDIUM_TEMPERATURE_CELCIUS = *('medium_temperature', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))*
Volume Creation Settings

PROPERTY_SEGMENTATION = *'seg'*
We define PROPERTY_GRUNEISEN_PARAMETER to contain all wavelength-independent constituents of the PA signal. This means that it contains the percentage of absorbed light converted into heat. Naturally, one could make an argument that this should not be the case, however, it simplifies the usage of this tool.

RECONSTRUCTION_MODE_FULL = *'full'*
Upsampling settings

STRUCTURE_DIRECTION = *('structure_direction', (<class 'list'>, <class 'tuple'>, <class 'numpy.ndarray'>))*
Digital Device Twin Settings

TIME_REVEARSAL_SCRIPT_LOCATION = *('time_revearsal_script_location', <class 'str'>)*
Acoustic model settings

UNITS_PRESSURE = *'newton_per_meters_squared'*
IO settings

class simpa.utils.constants.**SaveFilePaths**
The save file paths specify the path of a specific data structure in the dictionary of the simpa output hdf5. All of these paths have to be used like: SaveFilePaths.PATH.format(Tags.UPSAMPLED_DATA or Tags.ORIGINAL_DATA, wavelength)

class simpa.utils.constants.**SegmentationClasses**
The segmentation classes define which “tissue types” are modelled in the simulation volumes.

simpa.utils.deformation_manager.**create_deformation_settings** (bounds_mm, maximum_z_elevation_mm=1, filter_sigma=1, cosine_scaling_factor=4)
FIXME

simpa.utils.deformation_manager.**get_functional_from_deformation_settings** (deformation_settings: dict)
FIXME

class simpa.utils.settings_generator.**Settings** (dictionary: dict = None)

simpa.utils.calculate.**calculate_gruneisen_parameter_from_temperature** (temperature_in_celcius)
This function returns the dimensionless gruneisen parameter based on a heuristic formula that was determined experimentally:

```
@book{wang2012biomedical,
    title={Biomedical optics: principles and imaging},
    author={Wang, Lihong V and Wu, Hsin-i},
    year={2012},
    publisher={John Wiley \& Sons}
}
```

Parameters: **temperature_in_celcius** – the temperature in degrees celcius

Returns: a floating point number, if temperature_in_celcius is a number or a float array, if temperature_in_celcius is an array

simpa.utils.calculate.**calculate_oxygenation** (molecule_list)

Returns: an oxygenation value between 0 and 1 if possible, or None, if not computable.

simpa.utils.calculate.**create_spline_for_range** (xmin_mm=0, xmax_mm=10, maximum_y_elevation_mm=1, spacing=0.1)
Creates a functional that simulates distortion along the y position between the minimum and maximum x positions. The elevation can never be smaller than 0 or bigger than maximum_y_elevation_mm.

Parameters:

- **xmin_mm** – the minimum x axis value the return functional is defined in
- **xmax_mm** – the maximum x axis value the return functional is defined in
- **maximum_y_elevation_mm** – the maximum y axis value the return functional will yield

Returns: a functional that describes a distortion field along the y axis

simpa.utils.calculate.**randomize_uniform** (min_value: float, max_value: float) returns a uniformly drawn random number in [min_value, max_value[

Parameters:
- **min_value** – minimum value
- **max_value** – maximum value

Returns: random number in [min_value, max_value[

class `simpa.utils.tissue_properties.`**`TissueProperties`**

Libraries

Another important aspect of the utils class is the libraries that are being provided. These contain compilations of literature values for the acoustic and optical properties of commonly used tissue.

class `simpa.utils.libraries.molecule_library.`**`MolecularComposition`**`(segmentation_type=None, molecular_composition_settings=None)`

`update_internal_properties` **()**
FIXME

class `simpa.utils.libraries.literature_values.`**`MorphologicalTissueProperties`**
This class contains a listing of morphological tissue parameters as reported in literature. The listing is not the result of a meta analysis, but rather uses the best fitting paper at the time pf implementation. Each of the fields is annotated with a literature reference or a descriptions of how the particular values were derived for tissue modelling.

class `simpa.utils.libraries.literature_values.`**`OpticalTissueProperties`**
This class contains a listing of optical tissue parameters as reported in literature. The listing is not the result of a meta analysis, but rather uses the best fitting paper at the time pf implementation. Each of the fields is annotated with a literature reference or a descriptions of how the particular values were derived for tissue modelling.

class `simpa.utils.libraries.literature_values.`**`StandardProperties`**
This class contains a listing of default parameters that can be used. These values are sensible default values but are generally not backed up by proper scientific references, or are rather specific for internal use cases.

class `simpa.utils.libraries.spectra_library.`**`AbsorptionSpectrum`**`(spectrum_name: str, wavelengths: numpy.ndarray, absorption_per_centimeter: numpy.ndarray)`
An instance of this class represents the absorption spectrum over wavelength for a particular

`get_absorption_for_wavelength` **(**`wavelength: int`**)** → float

Parameters: **wavelength** – the wavelength to retrieve a optical absorption value for [cm^{-1}]. Must be an integer value between the minimum and maximum wavelength.

Returns: the best matching linearly interpolated absorption value for the given wavelength.

`get_absorption_over_wavelength` **()**

Returns: numpy array with the available wavelengths and the corresponding absorption properties

`simpa.utils.libraries.spectra_library.`**`view_absorption_spectra`**`(save_path=None)`
Opens a matplotlib plot and visualizes the available absorption spectra.

Parameters: **save_path** – If not None, then the figure will be saved as a png file to the destination.

class `simpa.utils.libraries.tissue_library.`**`MolecularCompositionGenerator`**
The MolecularCompositionGenerator is a helper class to facilitate the creation of a MolecularComposition instance.

class `simpa.utils.libraries.tissue_library.`**`TissueLibrary`**
TODO

blood_arterial ()

Returns: a settings dictionary containing all min and max parameters fitting for full blood.

blood_generic (oxygenation=None**)**

Returns: a settings dictionary containing all min and max parameters fitting for full blood.

blood_venous ()

Returns: a settings dictionary containing all min and max parameters fitting for full blood.

bone ()

Returns: a settings dictionary containing all min and max parameters fitting for full blood.

constant (mua, mus, g**)**
TODO

dermis (background_oxy=0.5**)**

Returns: a settings dictionary containing all min and max parameters fitting for dermis tissue.

epidermis ()

Returns: a settings dictionary containing all min and max parameters fitting for epidermis tissue.

get_blood_volume_fractions (total_blood_volume_fraction, oxygenation**)**
TODO

muscle (background_oxy=0.5**)**

Returns: a settings dictionary containing all min and max parameters fitting for generic background tissue.

subcutaneous_fat (background_oxy=0.5**)**

Returns: a settings dictionary containing all min and max parameters fitting for subcutaneous fat tissue.

class simpa.utils.libraries.structure_library.**Background** (global_settings: simpa.utils.settings_generator.Settings, background_settings: simpa.utils.settings_generator.Settings = None)

to_settings () → dict
TODO :return : A tuple containing the settings key and the needed entries

class simpa.utils.libraries.structure_library.**CircularTubularStructure** (global_settings: simpa.utils.settings_generator.Settings, single_structure_settings: simpa.utils.settings_generator.Settings = None)

to_settings ()
TODO :return : A tuple containing the settings key and the needed entries

class simpa.utils.libraries.structure_library.**EllipticalTubularStructure** (global_settings: simpa.utils.settings_generator.Settings, single_structure_settings: simpa.utils.settings_generator.Settings = None)

to_settings ()
TODO :return : A tuple containing the settings key and the needed entries

class `simpa.utils.libraries.structure_library.`**`GeometricalStructure`** `(global_settings: simpa.utils.settings_generator.Settings, single_structure_settings: simpa.utils.settings_generator.Settings = None)`

TODO

abstract **`to_settings`** **()** → simpa.utils.settings_generator.Settings

TODO :return : A tuple containing the settings key and the needed entries

class `simpa.utils.libraries.structure_library.`**`HorizontalLayerStructure`** `(global_settings: simpa.utils.settings_generator.Settings, single_structure_settings: simpa.utils.settings_generator.Settings = None)`

`to_settings` **()**

TODO :return : A tuple containing the settings key and the needed entries

class `simpa.utils.libraries.structure_library.`**`ParallelepipedStructure`** `(global_settings: simpa.utils.settings_generator.Settings, single_structure_settings: simpa.utils.settings_generator.Settings = None)`

This class currently has no partial volume effects implemented. TODO

`to_settings` **()**

TODO :return : A tuple containing the settings key and the needed entries

class `simpa.utils.libraries.structure_library.`**`RectangularCuboidStructure`** `(global_settings: simpa.utils.settings_generator.Settings, single_structure_settings: simpa.utils.settings_generator.Settings = None)`

`to_settings` **()**

TODO :return : A tuple containing the settings key and the needed entries

class `simpa.utils.libraries.structure_library.`**`SphericalStructure`** `(global_settings: simpa.utils.settings_generator.Settings, single_structure_settings: simpa.utils.settings_generator.Settings = None)`

`to_settings` **()**

TODO :return : A tuple containing the settings key and the needed entries

class `simpa.utils.libraries.structure_library.`**`Structures`** `(settings: simpa.utils.settings_generator.Settings)`

TODO

class `simpa.utils.libraries.structure_library.`**`VesselStructure`** `(global_settings: simpa.utils.settings_generator.Settings, single_structure_settings: simpa.utils.settings_generator.Settings = None)`

`to_settings` **()**

TODO :return : A tuple containing the settings key and the needed entries

Module: io_handling

`simpa.io_handling.io_hdf5.`**`load_hdf5`** `(file_path, file_dictionary_path='/')`

Loads a dictionary from an hdf5 file.

Parameters:
- **file_path** – Path of the file to load the dictionary from.
- **file_dictionary_path** – Path in dictionary structure of hdf5 file to lo the dictionary in.

Returns: Dictionary

`simpa.io_handling.io_hdf5.`**`save_hdf5`** `(dictionary: dict, file_path: str, file_dictionary_path: str = '/', file_compression: str = None)`

Saves a dictionary with arbitrary content to an hdf5-file with given filepath.

Parameters:

- **dictionary** – Dictionary to save.
- **file_path** – Path of the file to save the dictionary in.
- **file_dictionary_path** – Path in dictionary structure of existing hdf5 file to store the dictionary in.
- **file_compression** – possible file compression for the hdf5 output file. Values are: gzip, lzf and szip.

Returns: `Null`

Examples

Performing a complete forward simulation with acoustic modeling, optical modeling, as well as image reconstruction

The file can be found in simpa_examples/minimal_optical_simulation.py:

```
from simpa.utils import Tags, TISSUE_LIBRARY

from simpa.core.simulation import simulate
from simpa.utils.settings_generator import Settings
from simpa.utils.libraries.structure_library import HorizontalLayerStructure
import numpy as np

# TODO change these paths to the desired executable and save folder
SAVE_PATH = "D:/save/"
MCX_BINARY_PATH = "D:/bin/Release/mcx.exe"

VOLUME_TRANSDUCER_DIM_IN_MM = 75
VOLUME_PLANAR_DIM_IN_MM = 20
VOLUME_HEIGHT_IN_MM = 25
SPACING = 0.15
RANDOM_SEED = 4711


def create_example_tissue():
    """
    This is a very simple example script of how to create a tissue definition.
    It contains a muscular background, an epidermis layer on top of the muscles
    and a blood vessel.
    """
    background_dictionary = Settings()
    background_dictionary[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.muscle()
    background_dictionary[Tags.STRUCTURE_TYPE] = Tags.BACKGROUND

    muscle_dictionary = Settings()
    muscle_dictionary[Tags.PRIORITY] = 1
    muscle_dictionary[Tags.STRUCTURE_START_MM] = [0, 0, 0]
    muscle_dictionary[Tags.STRUCTURE_END_MM] = [0, 0, 100]
    muscle_dictionary[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.muscle()
    muscle_dictionary[Tags.CONSIDER_PARTIAL_VOLUME] = True
    muscle_dictionary[Tags.ADHERE_TO_DEFORMATION] = True
    muscle_dictionary[Tags.STRUCTURE_TYPE] = Tags.HORIZONTAL_LAYER_STRUCTURE

    vessel_1_dictionary = Settings()
    vessel_1_dictionary[Tags.PRIORITY] = 3
    vessel_1_dictionary[Tags.STRUCTURE_START_MM] = [VOLUME_TRANSDUCER_DIM_IN_MM/2,
```

```
                                                        0, 10]
    vessel_1_dictionary[Tags.STRUCTURE_END_MM] = [VOLUME_TRANSDUCER_DIM_IN_MM/2, VOLUME_PLAN
    vessel_1_dictionary[Tags.STRUCTURE_RADIUS_MM] = 3
    vessel_1_dictionary[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.blood_generic()
    vessel_1_dictionary[Tags.CONSIDER_PARTIAL_VOLUME] = True
    vessel_1_dictionary[Tags.STRUCTURE_TYPE] = Tags.CIRCULAR_TUBULAR_STRUCTURE

    epidermis_dictionary = Settings()
    epidermis_dictionary[Tags.PRIORITY] = 8
    epidermis_dictionary[Tags.STRUCTURE_START_MM] = [0, 0, 0]
    epidermis_dictionary[Tags.STRUCTURE_END_MM] = [0, 0, 1]
    epidermis_dictionary[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.epidermis()
    epidermis_dictionary[Tags.CONSIDER_PARTIAL_VOLUME] = True
    epidermis_dictionary[Tags.ADHERE_TO_DEFORMATION] = True
    epidermis_dictionary[Tags.STRUCTURE_TYPE] = Tags.HORIZONTAL_LAYER_STRUCTURE

    tissue_dict = Settings()
    tissue_dict[Tags.BACKGROUND] = background_dictionary
    tissue_dict["muscle"] = muscle_dictionary
    tissue_dict["epidermis"] = epidermis_dictionary
    tissue_dict["vessel_1"] = vessel_1_dictionary
    return tissue_dict

# Seed the numpy random configuration prior to creating the global_settings file in
# order to ensure that the same volume
# is generated with the same random seed every time.

np.random.seed(RANDOM_SEED)

settings = {
    # These parameters set the general propeties of the simulated volume
    Tags.RANDOM_SEED: RANDOM_SEED,
    Tags.VOLUME_NAME: "CompletePipelineTestMSOT_"+str(RANDOM_SEED),
    Tags.SIMULATION_PATH: SAVE_PATH,
    Tags.SPACING_MM: SPACING,
    Tags.DIM_VOLUME_Z_MM: VOLUME_HEIGHT_IN_MM,
    Tags.DIM_VOLUME_X_MM: VOLUME_TRANSDUCER_DIM_IN_MM,
    Tags.DIM_VOLUME_Y_MM: VOLUME_PLANAR_DIM_IN_MM,
    Tags.VOLUME_CREATOR: Tags.VOLUME_CREATOR_VERSATILE,
    Tags.SIMULATE_DEFORMED_LAYERS: True,
    # Tags.DEFORMED_LAYERS_SETTINGS: create_deformation_settings([[0, VOLUME_TRANSDUCER_DIM_
    #                                                             [0, VOLUME_PLANAR_DIM_IN_MM
    #                                                             maximum_z_elevation_mm=10,
    #                                                             filter_sigma=0,
    #                                                             cosine_scaling_factor=1),

    # Simulation Device
    Tags.DIGITAL_DEVICE: Tags.DIGITAL_DEVICE_MSOT,

    # The following parameters set the optical forward model
    Tags.RUN_OPTICAL_MODEL: True,
    Tags.WAVELENGTHS: [700],
    Tags.OPTICAL_MODEL_NUMBER_PHOTONS: 1e7,
    Tags.OPTICAL_MODEL_BINARY_PATH: MCX_BINARY_PATH,
    Tags.OPTICAL_MODEL: Tags.OPTICAL_MODEL_MCX,
    Tags.ILLUMINATION_TYPE: Tags.ILLUMINATION_TYPE_MSOT_ACUITY_ECHO,
    Tags.LASER_PULSE_ENERGY_IN_MILLIJOULE: 50,

    # The following parameters tell the script that we do not want any extra
    # modelling steps
```

```
    Tags.RUN_ACOUSTIC_MODEL: True,
    Tags.ACOUSTIC_SIMULATION_3D: False,
    Tags.ACOUSTIC_MODEL: Tags.ACOUSTIC_MODEL_K_WAVE,
    Tags.ACOUSTIC_MODEL_BINARY_PATH: "C:/Program Files/MATLAB/R2020b/bin/matlab.exe",
    Tags.ACOUSTIC_MODEL_SCRIPT_LOCATION: "C:/simpa/simpa/core/acoustic_simulation",
    Tags.GPU: True,

    Tags.MEDIUM_ALPHA_POWER: 1.05,

    Tags.SENSOR_RECORD: "p",
    # Tags.SENSOR_DIRECTIVITY_PATTERN: "pressure",

    Tags.PMLInside: False,
    Tags.PMLSize: [31, 32],
    Tags.PMLAlpha: 1.5,
    Tags.PlotPML: False,
    Tags.RECORDMOVIE: False,
    Tags.MOVIENAME: "visualization_log",
    Tags.ACOUSTIC_LOG_SCALE: True,

    Tags.APPLY_NOISE_MODEL: False,
    Tags.SIMULATION_EXTRACT_FIELD_OF_VIEW: True,

    Tags.PERFORM_IMAGE_RECONSTRUCTION: True,
    Tags.RECONSTRUCTION_ALGORITHM: Tags.RECONSTRUCTION_ALGORITHM_BACKPROJECTION
}
settings = Settings(settings)
# global_settings[Tags.SIMULATE_DEFORMED_LAYERS] = True
np.random.seed(RANDOM_SEED)

settings[Tags.STRUCTURES] = create_example_tissue()
print("Simulating ", RANDOM_SEED)
import time
timer = time.time()
simulate(settings)
print("Needed", time.time()-timer, "seconds")
print("Simulating ", RANDOM_SEED, "[Done]")
```

Reading the HDF5 simulation output

The file can be found in simpa_examples/access_saved_PAI_data.py:

```
from simpa.io_handling import load_hdf5, save_hdf5
import matplotlib.pyplot as plt
import matplotlib as mpl
import numpy as np
from simpa.utils import SegmentationClasses, Tags
from simpa.utils.settings_generator import Settings

values = []
names = []

for string in SegmentationClasses.__dict__:
    if string[0:2] != "__":
        values.append(SegmentationClasses.__dict__[string])
        names.append(string)

values = np.asarray(values)
names = np.asarray(names)
sort_indexes = np.argsort(values)
```

```
values = values[sort_indexes]
names = names[sort_indexes]

colors = [list(np.random.random(3)) for _ in range(len(names))]
cmap = mpl.colors.LinearSegmentedColormap.from_list(
    'Custom cmap', colors, len(names))

PATH = "D:/save/LNetOpticalForward_planar_0.hdf5"
WAVELENGTH = 532

file = load_hdf5(PATH)
settings = Settings(file["settings"])

fluence = (file['simulations']['original_data']['optical_forward_model_output']
           [str(WAVELENGTH)]['fluence'])
initial_pressure = (file['simulations']['original_data']
                    ['optical_forward_model_output']
                    [str(WAVELENGTH)]['initial_pressure'])
absorption = (file['simulations']['original_data']['simulation_properties']
              [str(WAVELENGTH)]['mua'])

segmentation = (file['simulations']['original_data']['simulation_properties']
              [str(WAVELENGTH)]['seg'])

reconstruction = None
speed_of_sound = None
if Tags.PERFORM_IMAGE_RECONSTRUCTION in settings and settings[Tags.PERFORM_IMAGE_RECONSTRUCT
    time_series = np.squeeze(
        file["simulations"]["original_data"]["time_series_data"][str(WAVELENGTH)]["time_seri
    reconstruction = np.squeeze(
            file["simulations"]["original_data"]["reconstructed_data"][str(WAVELENGTH)]["rec

    speed_of_sound = file['simulations']['original_data']['simulation_properties'][str(WAVEL

reconstruction = reconstruction.T

shape = np.shape(reconstruction)

x_pos = int(shape[0]/2)
y_pos = int(shape[1]/2)
z_pos = int(shape[2]/2)

plt.figure()
plt.subplot(161)
plt.imshow(np.fliplr(np.rot90(reconstruction[x_pos, :, :], -1)))
plt.subplot(162)
plt.imshow(np.rot90(np.log10(initial_pressure[x_pos, :, :]), -1))
plt.subplot(163)
plt.imshow(np.fliplr(np.rot90(reconstruction[:, y_pos, :], -1)))
plt.subplot(164)
plt.imshow(np.rot90(np.log10(initial_pressure[:, y_pos, :]), -1))
plt.subplot(165)
plt.imshow(np.fliplr(np.rot90(reconstruction[:, :, z_pos], -1)))
plt.subplot(166)
plt.imshow(np.rot90(np.log10(initial_pressure[:, :, z_pos]), -3))
plt.show()
exit()

if Tags.PERFORM_IMAGE_RECONSTRUCTION in settings and settings[Tags.PERFORM_IMAGE_RECONSTRUCT
    if len(shape) > 2:
```

```
        plt.figure()
        plt.subplot(141)
        plt.imshow(np.rot90(np.log10(np.log10(time_series[:, :]-np.min(time_series))), -1),
        plt.subplot(142)
        plt.imshow(np.rot90((reconstruction[:, y_pos, :]), -2))
        plt.subplot(143)
        plt.imshow(np.rot90(np.log10(initial_pressure[:, y_pos, :]), -1))
        plt.subplot(144)
        plt.imshow(np.rot90(segmentation[:, y_pos, :], -1), vmin=values[0], vmax=values[-1],
        plt.show()
    else:
        plt.figure()
        plt.subplot(141)
        plt.imshow(np.rot90((reconstruction[:, :]), -1))
        plt.subplot(142)
        plt.imshow(np.rot90((speed_of_sound), -1))
        plt.subplot(143)
        plt.imshow(np.rot90(np.log10(initial_pressure), -1))
        plt.subplot(144)
        plt.imshow(np.rot90(segmentation, -1), vmin=values[0], vmax=values[-1], cmap=cmap)
        plt.show()
else:
    if len(shape) > 2:
        plt.figure()
        plt.subplot(241)
        plt.title("Fluence")
        plt.imshow(np.rot90((fluence[x_pos, :, :]), -1))
        plt.subplot(242)
        plt.title("Absorption")
        plt.imshow(np.rot90(np.log10(absorption[x_pos, :, :]), -1))
        plt.subplot(243)
        plt.title("Initial Pressure")
        plt.imshow(np.rot90(np.log10(initial_pressure[x_pos, :, :]), -1))
        plt.subplot(244)
        plt.title("Segmentation")
        plt.imshow(np.rot90(segmentation[x_pos, :, :], -1), vmin=values[0], vmax=values[-1],
        cbar = plt.colorbar(ticks=values)
        cbar.ax.set_yticklabels(names)
        plt.subplot(245)
        plt.imshow(np.rot90(fluence[:, y_pos, :], -1))
        plt.subplot(246)
        plt.imshow(np.rot90(np.log10(absorption[:, y_pos, :]), -1))
        plt.subplot(247)
        plt.imshow(np.rot90(np.log10(initial_pressure[:, y_pos, :]), -1))
        plt.subplot(248)
        plt.imshow(np.rot90(segmentation[:, y_pos, :], -1), vmin=values[0], vmax=values[-1],
        cbar = plt.colorbar(ticks=values)
        cbar.ax.set_yticklabels(names)
        plt.show()
    else:
        plt.figure()
        plt.subplot(141)
        plt.imshow(np.rot90(np.log10(fluence), -1))
        plt.subplot(142)
        plt.imshow(np.rot90(np.log10(absorption), -1))
        plt.subplot(143)
        plt.imshow(np.rot90(np.log10(initial_pressure), -1))
        plt.subplot(144)
        plt.imshow(np.rot90(segmentation, -1))
        plt.show()
```

Defining custom tissue structures and properties

The file can be found in simpa_examples/create_custom_tissues.py:

```
from simpa.utils import MolecularCompositionGenerator
from simpa.utils import MOLECULE_LIBRARY
from simpa.utils import Molecule
from simpa.utils import AbsorptionSpectrum
import numpy as np


def create_custom_absorber():
    wavelengths = np.linspace(200, 1500, 100)
    absorber = AbsorptionSpectrum(spectrum_name="random absorber",
                                  wavelengths=wavelengths,
                                  absorption_per_centimeter=np.random.random(
                                      np.shape(wavelengths)))
    return absorber


def create_custom_chromophore(volume_fraction: float = 1.0):
    chromophore = Molecule(
            spectrum=create_custom_absorber(),
            volume_fraction=volume_fraction,
            mus500=40.0,
            b_mie=1.1,
            f_ray=0.9,
            anisotropy=0.9
        )
    return chromophore


def create_custom_tissue_type():

    # First create an instance of a TissueSettingsGenerator
    tissue_settings_generator = MolecularCompositionGenerator()

    water_volume_fraction = 0.4
    bvf = 0.5
    oxy = 0.4

    # Then append chromophores that you want
    tissue_settings_generator.append(key="oxyhemoglobin", value=
                        MOLECULE_LIBRARY.oxyhemoglobin(oxy * bvf))
    tissue_settings_generator.append(key="deoxyhemoglobin", value=
                        MOLECULE_LIBRARY.deoxyhemoglobin(oxy * bvf))
    tissue_settings_generator.append(key="water", value=
                        MOLECULE_LIBRARY.water(water_volume_fraction))
    tissue_settings_generator.append(key="custom", value=
                        create_custom_chromophore(0.1))

    return tissue_settings_generator.get_settings()
```

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