# **SIMPA**

# version 0.4.0

CAMI (Computer Assisted Medical Interventions), DKFZ, Heidelberg and Cancer Research UK, Cambridge Institute (CRUK CI)

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## Welcome to the SIMPA documentation!



Simulation and Image Processing for Photoacoustic Imaging

## **README**

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

## **SIMPA Install Instructions**

You can install simpa with pip. Simply run:

pip install simpa

For a manual installation from the code, please follow steps 1 - 3:

- 1. git clone https://github.com/CAMI-DKFZ/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. pip install -r requirements.txt
- 3. python -m setup.py install
- 4. 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.

You also need to manually install the pytorch library to use all features of SIMPA. To this end, use the pytorch website tool to figure out which version to install: https://pytorch.org/get-started/locally/

## **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/

In order to obtain access to all custom sources that we implemented, please build mcx yourself from the following mcx Github fork: https://www.github.com/jgroehl/mcx

For the installation, please follow the instructions from the original repository. Please note that there might be compatiblity issues using mcx-cl with the MCX Adapter as this use case is not being tested and supported by the SIMPA developers.

## 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
- 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.

## **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.

## Path Management

As a pipelining tool that serves as a communication layer between different numerical forward models and processing tools, SIMPA needs to be configured with the paths to these tools on your local hard drive. To this end, we have implemented the PathManager class that you can import to your project using from simpa.utils import PathManager. The PathManager looks for a path\_config.env file (just like the one we provided in the simpa examples) in the following places in this order:

- The optional path you give the PathManager
- 2. Your \$HOME\$ directory
- 3. The current working directory
- 4. The SIMPA home directory path

## How to contribute

Please find a more detailed description of how to contribute as well as code style references in our developer\_guide.md

The SIMPA code is written and maintained on a closed git repository that is hosted on a server of the German Cancer Research Center (DKFZ), Heidelberg, Germany and changes to the develop or master branch are mirrored on Github. As such, only the current master and develop branch of the repository are open source.

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 make sure that you have included unit tests for your code and that all previous tests still run through.

There is a regular SIMPA status meeting every Friday on even calendar weeks at 10:00 CET/CEST and you are very welcome to participate and raise any issues or suggest new features. You can join the meeting using the following link:

https://meet.google.com/rze-bxej-cvj

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

## 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:

Kris K. Dreher (k.dreher@dkfz-heidelberg.de)

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 and changes to the develop or master branch are mirrored on Github (https://github.com/CAMI-DKFZ/simpa/). As such, only the current master and develop branch of the repository are open source.

To make us aware of an issue, please create an issue on the SIMPA github repository.

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.

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There is a regular SIMPA status meeting every Friday on even calendar weeks at 10:00 CET/CEST and you are very welcome to participate and raise any issues or suggest new features. You can obtain the meeting links from the core developer team. We also have a Slack workspace that you can join if you are interested to contribute.

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 using 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 collected and handled central point, where absorption spectra are 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 <u>\_\_init\_\_</u> 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 description details 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.

```
simpa.core.simulation.simulate (settings)
```

This method constitutes the staring point for the simulation pipeline of the SIMPA toolkit. It calls all relevant and wanted simulation modules in the following pre-determined order:

```
def simulation(settings):
    for wavelength in settings[Tags.WAVELENGTHS]:

    simulation_data = volume_creator.create_simulation_volumes(settings)
    if optical_simulation in settings:
        optical_model.simulate(simulation_data, settings)
    if acoustic_simulation in settings:
        acoustic_model.simulate(simulation_data, settings)
    if noise_simulation in settings:
        noise_model.simulate(simulation_data, settings)
    if image_reconstruction in settings:
        reconstruction_model.simulate(simulation_data, settings)

io_handler.save_hdf5(simulation_data, settings)
```

**Parameters:** settings – settings dictionary containing the simulation instructions **Returns:** list with the save paths of the simulated data within the HDF5 file.

## Volume creation

The core contribution of the SIMPA toolkit is the creation of in silico tissue-mimicking phantoms. This feature is represented by the volume\_creation module, that two main volume creation modules:

- Model-based creation of volumes using a set of rules
- Segmentation-based creation of volumes

Module: utils

Model-based volume creation

Segmentation-based volume creation

Optical forward modelling

mcx integration

Acoustic forward modelling

k-Wave integration

Image reconstruction

**Backprojection** 

Delay-Multiply-And-Sum (DMAS)

signed Delay-Multiply-And-Sum (sDMAS)

Time Reversal

## **Processing Components**

Noise Models

# 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. Additionally, we have included detection geometries and illumination geometries that can be used to create custom photoacoustic devices for simulation.

**Detection Geometries** 

**Illumination Geometries** 

Models of real world devices

## 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.

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 vield

**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]

```
simpa.utils.calculate.rotation (angles)
```

Rotation matrix around the x-, y-, and z-axis with angles [theta\_x, theta\_y, theta\_z].

**Parameters:** angles – Angles through which the matrix is supposed to rotate in the form of [theta\_x,

theta\_y, theta\_z].

Returns: rotation matrix

simpa.utils.calculate.rotation\_x (theta)

Rotation matrix around the x-axis with angle theta.

**Parameters:** theta – Angle through which the matrix is supposed to rotate.

Returns: rotation matrix

simpa.utils.calculate.rotation\_y (theta)

Rotation matrix around the y-axis with angle theta.

**Parameters:** theta – Angle through which the matrix is supposed to rotate.

**Returns:** rotation matrix

simpa.utils.calculate.rotation\_z (theta)

Rotation matrix around the z-axis with angle theta.

**Parameters:** theta – Angle through which the matrix is supposed to rotate.

**Returns:** rotation matrix

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

simpa.utils.dict\_path\_manager.generate\_dict\_path (settings, data\_field, wavelength: (<class 'int'>, <class 'float'>) = None, upsampled\_data: bool = None) → Str

Generates a path within an hdf5 file in the SIMPA convention

## Parameters:

- settings SIMPA Settings dictionary.
- data\_field Data field that is supposed to be stored in an hdf5 file.
- wavelength Wavelength of the current simulation.
- upsampled\_data If True, data\_field will be stored in the "upsampled\_data" section of the hdf5 file.

**Returns:** String which defines the path to the data\_field.

## class simpa.utils.tags.Tags

This class contains all 'Tags' for the use in the settings dictionary as well as strings that are used in SIMPA as naming conventions. Every Tag that is intended to be used as a key in the settings dictionary is represented by a tuple. The first element of the tuple is a string that corresponds to the name of the Tag. The second element of the tuple is a data type or a tuple of data types. The values that are assigned to the keys in the settings should match these data types. Their usage within the SIMPA package is divided in "SIMPA package", "module X", "adapter Y", "class Z" and "naming convention".

ACOUSTIC\_LOG\_SCALE = ('acoustic\_log\_scale', (<class 'bool'>, <class 'bool'>, <class 'numpy.bool\_'>))

If True, the movie of the kwave simulation will be recorded in a log scale.

Usage: adapter KwaveAcousticForwardModel

ACOUSTIC\_MODEL = ('acoustic\_model', <class 'str'>)

Choice of the used acoustic model. Usage: module acoustic simulation

ACOUSTIC\_MODEL\_BINARY\_PATH = ('acoustic\_model\_binary\_path', <class 'str'>)

Absolute path of the location of the acoustic forward model binary.

Usage: module optical\_simulation

## ACOUSTIC MODEL K WAVE = 'kwave'

Corresponds to the kwave simulaiton.

Usage: module acoustic simulation, naming convention

#### ACOUSTIC\_MODEL\_OUTPUT\_NAME = 'acoustic\_forward\_model\_output'

Name of the acoustic forward model output field in the SIMPA output file.

Usage: naming convention

ACOUSTIC\_MODEL\_SCRIPT\_LOCATION = ('acoustic\_model\_script\_location', <class 'str'>)

Absolute path of the location of the acoustic\_simulation folder in the SIMPA core module.

Usage: module acoustic\_simulation

## ACOUSTIC MODEL TEST = 'simpa tests'

Corresponds to an adapter for testing purposes only.

Usage: module acoustic simulation, naming convention

## ACOUSTIC\_SIMULATION\_3D = ('acoustic\_simulation\_3d', <class 'bool'>)

If True, simulates the acoustic forward model in 3D.

Usage: SIMPA package

## ADHERE\_TO\_DEFORMATION = ('adhere\_to\_deformation', <class 'bool'>)

If True, a structure will be shifted according to the deformation.

Usage: adapter versatile\_volume\_creation

## APPLY\_NOISE\_MODEL = ('apply\_noise\_model', <class 'bool'>)

If True, the simulation will apply a noise model.

Usage: module core (simulate.py)

## BACKGROUND = 'Background'

Corresponds to the name of a structure.

Usage: adapter versatile\_volume\_creation, naming convention

## CIRCULAR\_TUBULAR\_STRUCTURE = 'CircularTubularStructure'

Corresponds to the CircularTubularStructure in the structure\_library.

Usage: module volume\_creation, naming\_convention

## CONSIDER\_PARTIAL\_VOLUME = ('consider\_partial\_volume', <class 'bool'>)

If True, the structure will be generated with its edges only occupying a partial volume of the voxel.

Usage: adapter versatile\_volume\_creation

## CROP\_IMAGE = ('crop\_image', <class 'bool'>)

If True, the PA image cropped in the image processing.

Usage: module process

## CROP\_POWER\_OF\_TWO = ('crop\_power\_of\_two', <class 'bool'>)

If True, the PA image cropped to the shape as the nearest power of two in the image processing.

Usage: module process

## **DEFORMATION\_X\_COORDINATES\_MM** = 'deformation\_x\_coordinates'

Mesh that defines the x coordinates of the deformation.

Usage: adapter versatile volume creation, naming convention

## **DEFORMATION\_Y\_COORDINATES\_MM** = 'deformation\_y\_coordinates'

Mesh that defines the y coordinates of the deformation.

Usage: adapter versatile\_volume\_creation, naming convention

## **DEFORMATION\_Z\_ELEVATIONS\_MM** = 'deformation\_z\_elevation'

Mesh that defines the z coordinates of the deformation.

Usage: adapter versatile volume creation, naming convention

## DEFORMED\_LAYERS\_SETTINGS = ('deformed\_layers\_settings', <class 'dict'>)

Settings that contain the functional which defines the deformation of the layers.

Usage: adapter versatile\_volume\_creation

## DIGITAL\_DEVICE = ('digital\_device', <class 'str'>)

Digital device that is chosen as illumination source and detector for the simulation.

Usage: SIMPA package

## DIGITAL\_DEVICE\_MSOT = 'digital\_device\_msot'

Corresponds to the MSOTAcuityEcho device.

Usage: SIMPA package, naming convention

# DIGITAL\_DEVICE\_POSITION = ('digital\_device\_position', (<class 'list'>, <class 'tuple'>, <class 'numpy.ndarray'>))

Position in [x, y, z] coordinates of the device in the generated volume.

Usage: SIMPA package

## DIGITAL\_DEVICE\_RSOM = 'digital\_device\_rsom'

Corresponds to the RSOMExplorerP50 device. Usage: SIMPA package, naming convention

DIM\_VOLUME\_X\_MM = ('volume\_x\_dim\_mm', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>))
Extent of the x-axis of the generated volume.

Usage: SIMPA package

DIM\_VOLUME\_Y\_MM = ('volume\_y\_dim\_mm', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))
Extent of the y-axis of the generated volume.

Usage: SIMPA package

DIM\_VOLUME\_Z\_MM = ('volume\_z\_dim\_mm', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))
Extent of the z-axis of the generated volume.

Usage: SIMPA package

## DL\_MODEL\_PATH = ('dl\_model\_path', <class 'str'>)

Absolute path to the deep learning model used for the deep learning upsampling.

Usage: module process

## **ELLIPTICAL\_TUBULAR\_STRUCTURE** = 'EllipticalTubularStructure'

Corresponds to the EllipticalTubularStructure in the structure library.

Usage: module volume\_creation, naming\_convention

## GPU = ('gpu', (<class 'bool'>, <class 'bool'>, <class 'numpy.bool\_'>))

If True, uses all available gpu options of the used modules.

Usage: SIMPA package

## HORIZONTAL\_LAYER\_STRUCTURE = 'HorizontalLayerStructure'

Corresponds to the HorizontalLayerStructure in the structure\_library.

Usage: module volume\_creation, naming\_convention

## ILLUMINATION\_DIRECTION = ('illumination\_direction', (<class 'list'>, <class 'tuple'>, <class 'numpy.ndarray'>))

Direction of the photon source as [x, y, z] vector used in mcx.

Usage: module optical modelling, adapter mcx adapter

## ILLUMINATION\_PARAM1 = ('illumination\_param1', (<class 'list'>, <class 'tuple'>, <class 'numpy.ndarray'>))

First parameter group of the specified illumination type as [x, y, z, w] vector used in mcx.

Usage: module optical\_modelling, adapter mcx\_adapter

## ${\tt ILLUMINATION\_PARAM2} = ('illumination\_param2', (<class 'list'>, <class 'tuple'>, <class 'numpy.ndarray'>))$

Second parameter group of the specified illumination type as [x, y, z, w] vector used in mcx.

Usage: module optical\_modelling, adapter mcx\_adapter

## **ILLUMINATION\_POSITION** = ('illumination\_position', (<class 'list'>, <class 'tuple'>, <class 'numpy.ndarray'>))

Position of the photon source in [x, y, z] coordinates used in mcx.

Usage: module optical\_modelling, adapter mcx\_adapter

## ILLUMINATION\_TYPE = ('optical\_model\_illumination\_type', <class 'str'>)

Type of the illumination geometry used in mcx.

Usage: module optical\_modelling, adapter mcx\_adapter

## ILLUMINATION\_TYPE\_DISK = 'disk'

Corresponds to disk source in mcx.

Usage: adapter mcx\_adapter, naming convention

## ILLUMINATION\_TYPE\_DKFZ\_PAUS = 'pasetup'

Corresponds to pasetup source in mcx. The geometrical definition is described in:

Usage: adapter mcx\_adapter, naming convention

#### ILLUMINATION TYPE FOURIER = 'fourier'

Corresponds to fourier source in mcx.

Usage: adapter mcx\_adapter, naming convention

#### ILLUMINATION TYPE FOURIER X = 'fourierx'

Corresponds to fourierx source in mcx.

Usage: adapter mcx\_adapter, naming convention

## ILLUMINATION\_TYPE\_FOURIER\_X\_2D = 'fourierx2d'

Corresponds to fourierx2d source in mcx.

Usage: adapter mcx\_adapter, naming convention

## ILLUMINATION TYPE GAUSSIAN = 'qaussian'

Corresponds to gaussian source in mcx.

Usage: adapter mcx\_adapter, naming convention

## ILLUMINATION\_TYPE\_MSOT\_ACUITY\_ECHO = 'msot\_acuity\_echo'

Corresponds to msot\_acuity\_echo source in mcx. The device is manufactured by iThera Medical, Munich, Germany (https://www.ithera-medical.com/products/msot-acuity/).

Usage: adapter mcx\_adapter, naming convention

## ILLUMINATION\_TYPE\_PATTERN = 'pattern'

Corresponds to pattern source in mcx.

Usage: adapter mcx\_adapter, naming convention

## ILLUMINATION\_TYPE\_PATTERN\_3D = 'pattern3d'

Corresponds to pattern3d source in mcx.

Usage: adapter mcx\_adapter, naming convention

## ILLUMINATION\_TYPE\_PENCIL = 'pencil'

Corresponds to pencil source in mcx.

Usage: adapter mcx\_adapter, naming convention

#### ILLUMINATION TYPE PENCILARRAY = 'pencilarray'

Corresponds to pencilarray source in mcx.

Usage: adapter mcx\_adapter, naming convention

## ILLUMINATION\_TYPE\_PLANAR = 'planar'

Corresponds to planar source in mcx.

Usage: adapter mcx\_adapter, naming convention

## ILLUMINATION TYPE RING = 'ring'

Corresponds to ring source in mcx.

Usage: adapter mcx\_adapter, naming convention

## ILLUMINATION\_TYPE\_SLIT = 'slit'

Corresponds to slit source in mcx.

Usage: adapter mcx adapter, naming convention

## INPUT\_SEGMENTATION\_VOLUME = ('input\_segmentation\_volume', <class 'numpy.ndarray'>)

Array that defines a segmented volume.

Usage: adapter segmentation\_based\_volume\_creator

# K\_WAVE\_SPECIFIC\_DT = ('dt\_acoustic\_sim', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>)) Temporal resolution of kwave.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter

# K\_WAVE\_SPECIFIC\_NT = ('Nt\_acoustic\_sim', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Total time steps simulated by kwave.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter

LASER\_PULSE\_ENERGY\_IN\_MILLIJOULE = ('laser\_pulse\_energy\_in\_millijoule', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>, <class 'list'>, <class 'range'>, <class 'tuple'>, <class 'numpy.ndarray'>))

Laser pulse energy used in the optical simulation.

Usage: module optical\_simulation

## MAX\_DEFORMATION\_MM = 'max\_deformation'

Maximum deformation in z-direction.

Usage: adapter versatile\_volume\_creation, naming convention

**MEDIUM\_TEMPERATURE\_CELCIUS** = ('medium\_temperature', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Temperature of the simulated volume.

Usage: module noise\_simulation

## MOLECULE\_COMPOSITION = ('molecule\_composition', <class 'list'>)

List that contains all the molecules within a structure.

Usage: module volume\_creation

## MOVIENAME = ('movie\_name', <class 'str'>)

Name of the movie recorded by kwave.

Usage: adapter KwaveAcousticForwardModel

## NOISE\_MEAN = ('noise\_mean', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Mean of the gaussian noise model used in the noise modelling.

Usage: module noise\_simulation

## NOISE\_MODEL = ('noise\_model', <class 'str'>)

Choice of the noise model.

Usage: module noise\_simulation

## NOISE\_MODEL\_GAUSSIAN = 'noise\_model\_gaussian'

Corresponds to a gaussian noise model.

Usage: module noise\_simulation

## NOISE\_MODEL\_PATH = ('noise\_model\_path', <class 'str'>)

Absolute path of a .csv file with an experimentally recorded noise model.

Usage: module noise\_simulation

## NOISE\_STD = ('noise\_std', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Standard deviation of the gaussian noise model used in the noise modelling.

Usage: module noise simulation

## OPTICAL\_MODEL = ('optical\_model', <class 'str'>)

Choice of the used optical model.

Usage: module optical\_simulation

#### OPTICAL MODEL BINARY PATH = ('optical model binary path', <class 'str'>)

Absolute path of the location of the optical forward model binary.

Usage: module optical\_simulation

## OPTICAL\_MODEL\_FLUENCE = 'fluence'

Name of the optical forward model output fluence field in the SIMPA output file.

Usage: naming convention

# OPTICAL\_MODEL\_ILLUMINATION\_GEOMETRY\_XML\_FILE = ('optical\_model\_illumination\_geometry\_xml\_file', <class 'str'>)

Absolute path of the location of the optical forward model illumination geometry.

Usage: module optical\_simulation

## OPTICAL\_MODEL\_INITIAL\_PRESSURE = 'initial\_pressure'

Name of the optical forward model output initial pressure field in the SIMPA output file.

Usage: naming convention

## OPTICAL\_MODEL\_MCX = 'mcx'

Corresponds to the mcx simulation.

Usage: module optical\_simulation, naming convention

#### OPTICAL\_MODEL\_MCXYZ = 'mcxyz'

Corresponds to the mcxyz simulation.

Usage: module optical\_simulation, naming convention

OPTICAL\_MODEL\_NUMBER\_PHOTONS = ('optical\_model\_number\_of\_photons', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Number of photons used in the optical simulation.

Usage: module optical\_simulation

## OPTICAL\_MODEL\_OUTPUT\_NAME = 'optical\_forward\_model\_output'

Name of the optical forward model output field in the SIMPA output file.

Usage: naming convention

## OPTICAL\_MODEL\_TEST = 'simpa\_tests'

Corresponds to an adapter for testing purposes only.

Usage: module optical\_simulation, naming convention

## OPTICAL\_MODEL\_UNITS = 'units'

Name of the optical forward model output units field in the SIMPA output file.

Usage: naming convention

#### ORIGINAL\_DATA = 'original\_data'

Name of the simulation outputs as original data in the SIMPA output file.

Usage: naming convention

## PARALLELEPIPED\_STRUCTURE = 'ParallelepipedStructure'

Corresponds to the ParallelepipedStructure in the structure library.

Usage: module volume\_creation, naming\_convention

PERFORM\_IMAGE\_RECONSTRUCTION = ('perform\_image\_reconstruction', (<class 'bool'>, <class 'bool'>, <class 'numpy.bool '>))

If True, the simulation will run the image reconstruction.

Usage: module core (simulate.py)

## PERFORM UPSAMPLING = ('sample', <class 'bool'>)

If True, the PA image upsampled in the image processing.

Usage: module process

## PMLAlpha = ('pml\_alpha', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Alpha coefficient of the "perfectly matched layer" (PML) around the simulated volume in kwave.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

## PMLInside = ('pml\_inside', (<class 'bool'>, <class 'bool'>, <class 'numpy.bool\_'>))

If True, the "perfectly matched layer" (PML) in kwave is located inside the volume.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

## PMLSize = ('pml\_size', (<class 'list'>, <class 'tuple'>, <class 'numpy.ndarray'>))

Size of the "perfectly matched layer" (PML) around the simulated volume in kwave.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

## PRIORITY = ('priority', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>))

Number that corresponds to a priority of the assigned structure. If another structure occupies the same voxel in a volume, the structure with a higher priority will be preferred.

Usage: adapter versatile\_volume\_creator

#### PROPERTY ABSORPTION PER CM = 'mua'

Optical absorption of the generated volume/structure in 1/cm.

Usage: SIMPA package, naming convention

## PROPERTY ALPHA COEFF = 'alpha coeff'

Acoustic attenuation of kwave of the generated volume/structure in dB/cm/MHz.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

# PROPERTY\_ALPHA\_POWER = ('medium\_alpha\_power', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Exponent of the exponential acoustic attenuation law of kwave.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

## PROPERTY\_ANISOTROPY = 'g'

Optical scattering anisotropy of the generated volume/structure.

Usage: SIMPA package, naming convention

## PROPERTY\_DENSITY = 'density'

Density of the generated volume/structure in kg/m³.

Usage: SIMPA package, naming convention

## PROPERTY\_DIRECTIVITY\_ANGLE = 'directivity\_angle'

Directionality of the sensors in kwave of the used PA device.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

## PROPERTY\_GRUNEISEN\_PARAMETER = 'gamma'

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.

Usage: SIMPA package, naming convention

## PROPERTY\_OXYGENATION = 'oxy'

Oxygenation of the generated volume/structure.

Usage: SIMPA package, naming convention

## PROPERTY\_SCATTERING\_PER\_CM = 'mus'

Optical scattering (NOT REDUCED SCATTERING mus'! mus'=mus\*(1-g) ) of the generated volume/structure in 1/cm.

Usage: SIMPA package, naming convention

## PROPERTY\_SEGMENTATION = 'seg'

Segmentation of the generated volume/structure.

Usage: SIMPA package, naming convention

## PROPERTY SENSOR MASK = 'sensor mask'

Sensor mask of kwave of the used PA device.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

## PROPERTY\_SPEED\_OF\_SOUND = 'SOS'

Speed of sound of the generated volume/structure in m/s.

Usage: SIMPA package, naming convention

## PlotPML = ('plot pml', (<class 'bool'>, <class 'bool'>, <class 'numpy.bool '>))

If True, the "perfectly matched layer" (PML) around the simulated volume in kwave is plotted.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

## RANDOM\_SEED = ('random\_seed', (<class 'int'>, <class 'numpy.integer'>))

Random seed for numpy and torch.

Usage: SIMPA package

## RECONSTRUCTED\_DATA = 'reconstructed\_data'

Name of the reconstructed data field in the SIMPA output file.

Usage: naming convention

## RECONSTRUCTED\_DATA\_NOISE = 'reconstructed\_data\_noise'

Name of the reconstructed data with applied noise field in the SIMPA output file.

Usage: naming convention

## **RECONSTRUCTION\_ALGORITHM** = ('reconstruction\_algorithm', <class 'str'>)

Choice of the used reconstruction algorithm.

Usage: module image\_reconstruction

#### RECONSTRUCTION ALGORITHM BACKPROJECTION = 'backprojection'

Corresponds to the reconstruction algorithm Backprojection with BackprojectionAdapter.

Usage: module image\_reconstruction, naming convention

## RECONSTRUCTION ALGORITHM DAS = 'DAS'

Corresponds to the reconstruction algorithm DAS with the MitkBeamformingAdapter.

Usage: module image\_reconstruction, naming convention

## RECONSTRUCTION ALGORITHM DMAS = 'DMAS'

Corresponds to the reconstruction algorithm DMAS with the MitkBeamformingAdapter.

Usage: module image\_reconstruction, naming convention

#### RECONSTRUCTION ALGORITHM SDMAS = 'SDMAS'

Corresponds to the reconstruction algorithm sDMAS with the MitkBeamformingAdapter.

Usage: module image\_reconstruction, naming convention

## RECONSTRUCTION\_ALGORITHM\_TEST = 'TEST'

Corresponds to an adapter for testing purposes only.

Usage: module image\_reconstruction, naming convention

## RECONSTRUCTION\_ALGORITHM\_TIME\_REVERSAL = 'time\_reversal'

Corresponds to the reconstruction algorithm Time Reversal with TimeReversalAdapter.

Usage: module image reconstruction, naming convention

## RECONSTRUCTION\_BMODE\_METHOD = ('reconstruction\_bmode\_method', <class 'str'>)

Choice of the B-Mode method used in the Mitk Beamforming.

Usage: adapter MitkBeamformingAdapter

## RECONSTRUCTION\_BMODE\_METHOD\_ABS = 'Abs'

Corresponds to the absolute value as the B-Mode method used in the Mitk Beamforming.

Usage: adapter MitkBeamformingAdapter, naming convention

## RECONSTRUCTION BMODE METHOD HILBERT TRANSFORM = 'EnvelopeDetection'

Corresponds to the Hilbert transform as the B-Mode method used in the Mitk Beamforming.

Usage: adapter MitkBeamformingAdapter, naming convention

# **RECONSTRUCTION\_INVERSE\_CRIME** = ('reconstruction\_inverse\_crime', (<class 'bool'>, <class 'bool'>, <class 'numpy.bool '>))

If True, the Time Reversal reconstruction will commit the "inverse crime".

Usage: TimeReversalAdapter

## RECONSTRUCTION MITK BINARY PATH = ('reconstruction mitk binary path', <class 'str'>)

Absolute path to the Mitk Beamforming script.

Usage: adapter MitkBeamformingAdapter

## RECONSTRUCTION\_MITK\_SETTINGS\_XML = ('reconstruction\_mitk\_settings\_xml', <class 'str'>)

Absolute path to the Mitk Beamforming script settings.

Usage: adapter MitkBeamformingAdapter

## RECONSTRUCTION\_MODE = ('reconstruction\_mode', <class 'str'>)

Choice of the reconstruction mode used in the Backprojection.

Usage: adapter BackprojectionAdapter

## RECONSTRUCTION\_MODE\_DIFFERENTIAL = 'differential'

Corresponds to the differential mode used in the Backprojection.

Usage: adapter BackprojectionAdapter, naming\_convention

## RECONSTRUCTION\_MODE\_FULL = 'full'

Corresponds to the full mode used in the Backprojection.

Usage: adapter BackprojectionAdapter, naming\_convention

#### RECONSTRUCTION MODE PRESSURE = 'pressure'

Corresponds to the pressure mode used in the Backprojection.

Usage: adapter BackprojectionAdapter, naming\_convention

## **RECONSTRUCTION\_OUTPUT\_NAME** = ('reconstruction\_result', <class 'str'>)

Absolute path of the image reconstruction result.

Usage: adapter MitkBeamformingAdapter

## RECORDMOVIE = ('record\_movie', (<class 'bool'>, <class 'bool'>, <class 'numpy.bool\_'>))

If True, a movie of the kwave simulation will be recorded.

Usage: adapter KwaveAcousticForwardModel

## RECTANGULAR\_CUBOID\_STRUCTURE = 'RectangularCuboidStructure'

Corresponds to the RectangularCuboidStructure in the structure\_library.

Usage: module volume\_creation, naming\_convention

## RUN\_ACOUSTIC\_MODEL = ('run\_acoustic\_forward\_model', (<class 'bool'>, <class 'bool'>, <class 'numpy.bool\_'>))

If True, the simulation will run the acoustic forward model.

Usage: module core (simulate.py)

## RUN\_OPTICAL\_MODEL = ('run\_optical\_forward\_model', <class 'bool'>)

If True, the simulation will run the optical forward model.

Usage: module core (simulate.py)

## SEGMENTATION\_CLASS\_MAPPING = ('segmentation\_class\_mapping', <class 'dict'>)

Mapping that assigns every class in the INPUT\_SEGMENTATION\_VOLUME a MOLECULE\_COMPOSITION.

Usage: adapter segmentation\_based\_volume\_creator

# SENSOR\_BANDWIDTH\_PERCENT = ('sensor\_bandwidth', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Sensor bandwidth in kwave.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

# SENSOR\_CENTER\_FREQUENCY\_HZ = ('sensor\_center\_frequency', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>,)

Sensor center frequency in kwave.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

## SENSOR\_CONCAVE = 'concave'

Indicates that the geometry of the used PA device in the Mitk Beamforming is concave.

Usage: adapter MitkBeamformingAdapter, naming convention

## SENSOR DIRECTIVITY PATTERN = 'sensor directivity pattern'

Sensor directivity pattern of the sensor in kwave. Default should be "pressure".

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

# SENSOR\_DIRECTIVITY\_SIZE\_M = ('sensor\_directivity\_size', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Size of each detector element in kwave.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

#### SENSOR LINEAR = 'linear'

Indicates that the geometry of the used PA device in the Mitk Beamforming is linear.

Usage: adapter MitkBeamformingAdapter, naming convention

## SENSOR\_NUM\_ELEMENTS = ('sensor\_num\_elements', (<class 'int'>, <class 'numpy.integer'>))

Number of detector elements for kwave if no device was selected.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

## SENSOR\_NUM\_USED\_ELEMENTS = ('sensor\_num\_used\_elements', (<class 'int'>, <class 'numpy.integer'>))

Number of detector elements that fit into the generated volume if the dimensions and/or spacing of the generated volume were not highly resolved enough to be sufficient for the selected PA device.

Usage: module acoustic simulation, naming convention

## SENSOR\_RADIUS\_MM = 'sensor\_radius\_mm'

Radius of a concave geometry of the used PA device in the Mitk Beamforming.

Usage: adapter MitkBeamformingAdapter, naming convention

## SENSOR\_RECORD = ('sensor\_record', <class 'str'>)

Sensor Record mode of the sensor in kwave. Default should be "p".

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

# SENSOR\_SAMPLING\_RATE\_MHZ = ('sensor\_sampling\_rate\_mhz', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Sampling rate of the used PA device.

Usage: adapter KwaveAcousticForwardModel, adapter TimeReversalAdapter, naming convention

## **SETTINGS** = 'settings'

Location of the simulation settings in the SIMPA output file.

Usage: naming convention

## SETTINGS\_JSON = ('settings\_json', (<class 'bool'>, <class 'numpy.bool\_'>))

If True, the SIMPA settings are saved in a .json file.

Usage: SIMPA package

## SETTINGS\_JSON\_PATH = ('settings\_json\_path', <class 'str'>)

Absolute path to a .json file if SETTINGS\_JSON is set to True. Usage: SIMPA package

## SIMPA\_OUTPUT\_NAME = 'simpa\_output.hdf5'

Default filename of the SIMPA output if not specified otherwise.

Usage: SIMPA package, naming convention

## SIMPA OUTPUT PATH = ('simpa output path', <class 'str'>)

Default path of the SIMPA output if not specified otherwise.

Usage: SIMPA package

## SIMULATE\_DEFORMED\_LAYERS = ('simulate\_deformed\_layers', <class 'bool'>)

If True, the horizontal layers are deformed according to the DEFORMED\_LAYERS\_SETTINGS.

Usage: adapter versatile\_volume\_creation

## **SIMULATIONS** = 'simulations'

Location of the simulation outputs in the SIMPA output file.

Usage: naming convention

## SIMULATION\_EXTRACT\_FIELD\_OF\_VIEW = ('extract\_field\_of\_view', <class 'bool'>)

If True, converts a 3D volume to a 2D volume by extracting the middle slice along the y-axis.

Usage: SIMPA package

## **SIMULATION\_PATH** = ('simulation\_path', <class 'str'>)

Absolute path to the folder where the SIMPA output is saved.

Usage: SIMPA package

#### SIMULATION PROPERTIES = 'simulation properties'

Location of the simulation properties in the SIMPA output file.

Usage: naming convention

SPACING\_MM = ('voxel\_spacing\_mm', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Isotropic extent of one voxels in mm in the generated volume.

Usage: SIMPA package

## SPHERICAL\_STRUCTURE = 'SphericalStructure'

Corresponds to the SphericalStructure in the structure\_library.

Usage: module volume\_creation, naming\_convention

## **STRUCTURES** = ('structures', <class 'dict'>)

Settings dictionary which contains all the structures that should be generated inside the volume.

Usage: module volume\_creation

**STRUCTURE\_BIFURCATION\_LENGTH\_MM** = ('structure\_bifurcation\_length\_mm', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Length after which a VesselStructure will bifurcate.

Usage: adapter versatile\_volume\_creation, class VesselStructure

STRUCTURE\_CURVATURE\_FACTOR = ('structure\_curvature\_factor', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>,)

Factor that determines how strongly a vessel tree is curved.

Usage: adapter versatile\_volume\_creation, class VesselStructure

## STRUCTURE\_DIRECTION = ('structure\_direction', (<class 'list'>, <class 'tuple'>, <class 'numpy.ndarray'>))

Direction as [x, y, z] vector starting from STRUCTURE\_START\_MM in which the vessel will grow.

Usage: adapter versatile\_volume\_creation, class VesselStructure

**STRUCTURE\_ECCENTRICITY** = ('structure\_excentricity', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>, <class 'numpy.ndarray'>))

Eccentricity of the structure.

Usage: adapter versatile\_volume\_creation, class EllipticalTubularStructure

## STRUCTURE\_END\_MM = ('structure\_end', (<class 'list'>, <class 'tuple'>, <class 'numpy.ndarray'>))

Ending of the structure as [x, y, z] coordinates in the generated volume.

Usage: adapter versatile\_volume\_creation, class GeometricalStructure

STRUCTURE\_FIRST\_EDGE\_MM = ('structure\_first\_edge\_mm', (<class 'list'>, <class 'tuple'>, <class
'numpy.ndarray'>))

Edge of the structure as [x, y, z] vector starting from STRUCTURE\_START\_MM in the generated volume.

Usage: adapter versatile\_volume\_creation, class ParallelepipedStructure

STRUCTURE\_RADIUS\_MM = ('structure\_radius', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'numpy.ndarray'>))

Radius of the structure.

Usage: adapter versatile\_volume\_creation, class GeometricalStructure

**STRUCTURE\_RADIUS\_VARIATION\_FACTOR** = ('structure\_radius\_variation\_factor', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Factor that determines how strongly a the radius of vessel tree varies.

Usage: adapter versatile volume creation, class VesselStructure

STRUCTURE\_SECOND\_EDGE\_MM = ('structure\_second\_edge\_mm', (<class 'list'>, <class 'tuple'>, <class 'numpy.ndarray'>))

Edge of the structure as [x, y, z] vector starting from STRUCTURE\_START\_MM in the generated volume.

Usage: adapter versatile\_volume\_creation, class ParallelepipedStructure

## STRUCTURE\_SEGMENTATION\_TYPE = 'structure\_segmentation\_type'

Defines the structure segmentation type to one segmentation type in SegmentationClasses.

Usage: module volume creation, naming convention

STRUCTURE\_START\_MM = ('structure\_start', (<class 'list'>, <class 'tuple'>, <class 'numpy.ndarray'>))

Beginning of the structure as [x, y, z] coordinates in the generated volume.

Usage: adapter versatile\_volume\_creation, class GeometricalStructure

STRUCTURE\_THIRD\_EDGE\_MM = ('structure\_third\_edge\_mm', (<class 'list'>, <class 'tuple'>, <class 'numpy.ndarray'>))

Edge of the structure as [x, y, z] vector starting from STRUCTURE\_START\_MM in the generated volume.

Usage: adapter versatile\_volume\_creation, class ParallelepipedStructure

#### **STRUCTURE TYPE** = ('structure type', <class 'str'>)

Defines the structure type to one structure in the structure library.

Usage: module volume\_creation

STRUCTURE\_X\_EXTENT\_MM = ('structure\_x\_extent\_mm', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

X-extent of the structure in the generated volume.

Usage: adapter versatile\_volume\_creation, class RectangularCuboidStructure

STRUCTURE\_Y\_EXTENT\_MM = ('structure\_y\_extent\_mm', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Y-extent of the structure in the generated volume.

Usage: adapter versatile\_volume\_creation, class RectangularCuboidStructure

STRUCTURE\_Z\_EXTENT\_MM = ('structure\_z\_extent\_mm', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>, <class 'float'>))

Z-extent of the structure in the generated volume.

Usage: adapter versatile\_volume\_creation, class RectangularCuboidStructure

## TIME\_REVEARSAL\_SCRIPT\_LOCATION = ('time\_revearsal\_script\_location', <class 'str'>)

Absolute path of the location of the image\_reconstruction folder in the SIMPA core module.

Usage: adapter TimeReversalAdapter

## TIME\_SERIES\_DATA = 'time\_series\_data'

Name of the time series data field in the SIMPA output file.

Usage: naming convention

## TIME\_SERIES\_DATA\_NOISE = 'time\_series\_data\_noise'

Name of the time series data with applied noise field in the SIMPA output file.

Usage: naming convention

## TIME\_STEP = ('time\_step', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>))

Temporal resolution of mcx.

Usage: adapter mcx adapter

## TISSUE\_PROPERTIES\_OUPUT\_NAME = 'properties'

Name of the simulation properties field in the SIMPA output file.

Usage: naming convention

## TOTAL\_TIME = ('total\_time', (<class 'int'>, <class 'numpy.integer'>, <class 'float'>))

Total simulated time in mcx.

Usage: adapter mcx\_adapter

## **UNITS\_ARBITRARY** = 'arbitrary\_unity'

Define arbitrary units if no units were given in the settings.

Usage: module optical\_simulation, naming convention

## UNITS\_PRESSURE = 'newton\_per\_meters\_squared'

Standard units used in the SIMPA framework.

Usage: module optical\_simulation, naming convention

#### **UPSAMPLED** DATA = 'upsampled data'

Name of the simulation outputs as upsampled data in the SIMPA output file.

Usage: naming convention

## UPSAMPLING\_METHOD = ('upsampling\_method', <class 'str'>)

Choice of the upsampling method used in the image processing.

Usage: module process

#### UPSAMPLING METHOD BILINEAR = 'bilinear'

Corresponds to the bilinear upsampling method used in the image processing.

Usage: module process, naming concention

## UPSAMPLING\_METHOD\_DEEP\_LEARNING = 'deeplearning'

Corresponds to deep learning as the upsampling method used in the image processing.

Usage: module process, naming concention

## UPSAMPLING\_METHOD\_LANCZOS2 = 'lanczos2'

Corresponds to lanczos with kernel size 2 as the upsampling method used in the image processing.

Usage: module process, naming concention

## UPSAMPLING\_METHOD\_LANCZOS3 = 'lanczos3'

Corresponds to lanczos with kernel size 3 as the upsampling method used in the image processing.

Usage: module process, naming concention

## UPSAMPLING\_METHOD\_NEAREST\_NEIGHBOUR = 'nearestneighbour'

Corresponds to nearest neighbour as the upsampling method used in the image processing.

Usage: module process, naming concention

## UPSAMPLING\_SCRIPT = ('upsampling\_script', <class 'str'>)

Name of the upsampling script used for the lanczos upsampling.

Usage: module process

## UPSAMPLING\_SCRIPT\_LOCATION = ('upsampling\_script\_location', <class 'str'>)

Absolute path to the upsampling script used for the lanczos upsampling.

Usage: module process

# UPSCALE\_FACTOR = ('upscale\_factor', (<class 'int'>, <class 'float'>, <class 'numpy.int64'>, <class 'numpy.float64'>))

Upscale factor of the upsampling in the image processing.

Usage: module process

#### VESSEL STRUCTURE = 'VesselStructure'

Corresponds to the VesselStructure in the structure\_library.

Usage: module volume\_creation, naming\_convention

## VOLUME\_CREATOR = ('volume\_creator', <class 'str'>)

Choice of the volume creator adapter.

Usage: module volume creation, module device digital twins

## VOLUME\_CREATOR\_SEGMENTATION\_BASED = 'volume\_creator\_segmentation\_based'

Corresponds to the SegmentationBasedVolumeCreator.

Usage: module volume\_creation, naming convention

#### **VOLUME CREATOR VERSATILE = 'volume creator versatile'**

Corresponds to the ModelBasedVolumeCreator.

Usage: module volume\_creation, naming convention

## **VOLUME\_NAME** = ('volume\_name', <class 'str'>)

Name of the SIMPA output file.

Usage: SIMPA package

**WAVELENGTH** = ('wavelength', (<class 'int'>, <class 'numpy.integer'>))

Single wavelength used for the current simulation.

Usage: SIMPA package

WAVELENGTHS = ('wavelengths', (<class 'list'>, <class 'range'>, <class 'tuple'>, <class 'numpy.ndarray'>))

Iterable of all the wavelengths used for the simulation.

Usage: SIMPA package

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.

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

 $\texttt{get\_absorption\_for\_wavelength}$  (wavelength: int)  $\rightarrow$  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.

 ${\it class} \ {\tt simpa.utils.libraries.tissue\_library.} \textbf{MolecularCompositionGenerator}$ 

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
simpa.utils.settings\_generator.Settings,
simpa.utils.settings\_generator.Settings = None)
(global\_settings:
background\_settings:

Defines a background that fills the whole simulation volume. It is always given the priority of 0 so that other structures can overwrite it when necessary. Example usage:

background\_dictionary = Settings() background\_dictionary[Tags.MOLECULE\_COMPOSITION] = TISSUE\_LIBRARY.constant(0.1, 100.0, 0.9) background\_dictionary[Tags.STRUCTURE\_TYPE] = Tags.BACKGROUND

#### get enclosed indices ()

Gets indices of the voxels that are either entirely or partially occupied by the GeometricalStructure. :return: mask for a numpy array

```
get_params_from_settings (single_structure_settings)
```

Gets all the parameters required for the specific GeometricalStructure. :param single\_structure\_settings: Settings which describe the specific GeometricalStructure. :return: Tuple of parameters

## to\_settings () $\rightarrow$ dict

Creates a Settings dictionary which contains all the parameters needed to create the same GeometricalStructure again. :return : A tuple containing the settings key and the needed entries

Defines a circular tube which is defined by a start and end point as well as a radius. This structure implements partial volume effects. The tube can be set to adhere to a deformation defined by the simpa.utils.deformation\_manager. The start and end points of the tube will then be shifted along the z-axis accordingly. Example usage:

# single\_structure\_settings initialization structure = Settings()

```
structure[Tags.PRIORITY] = 9 structure[Tags.STRUCTURE_START_MM] = [50, 0, 50] structure[Tags.STRUCTURE_END_MM] = [50, 100, 50] structure[Tags.STRUCTURE_RADIUS_MM] = 5 structure[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.blood() structure[Tags.CONSIDER_PARTIAL_VOLUME] = True structure[Tags.ADHERE_TO_DEFORMATION] = True structure[Tags.STRUCTURE_TYPE] = Tags.CIRCULAR_TUBULAR_STRUCTURE
```

## get\_enclosed\_indices()

Gets indices of the voxels that are either entirely or partially occupied by the GeometricalStructure. :return: mask for a numpy array

## get\_params\_from\_settings (single\_structure\_settings)

Gets all the parameters required for the specific GeometricalStructure. :param single\_structure\_settings: Settings which describe the specific GeometricalStructure. :return: Tuple of parameters

#### to\_settings()

Creates a Settings dictionary which contains all the parameters needed to create the same GeometricalStructure again. :return : A tuple containing the settings key and the needed entries

Defines a elliptical tube which is defined by a start and end point as well as a radius and an eccentricity. The elliptical geometry corresponds to a circular tube of the specified radius which is compressed along the z-axis until it reaches the specified eccentricity under the assumption of a constant volume. This structure implements partial volume effects. The tube can be set to adhere to a deformation defined by the simpa.utils.deformation\_manager. The start and end points of the tube will then be shifted along the z-axis accordingly. Example usage:

```
# single_structure_settings initialization structure = Settings()
```

```
structure[Tags.PRIORITY] = 9 structure[Tags.STRUCTURE_START_MM] = [50, 0, 50] structure[Tags.STRUCTURE_END_MM] = [50, 100, 50] structure[Tags.STRUCTURE_RADIUS_MM] = 5 structure[Tags.STRUCTURE_ECCENTRICITY] = 0.8 structure[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.blood() structure[Tags.CONSIDER_PARTIAL_VOLUME] = True structure[Tags.ADHERE_TO_DEFORMATION] = True structure[Tags.STRUCTURE_TYPE] = Tags.ELLIPTICAL_TUBULAR_STRUCTURE
```

#### get enclosed indices ()

Gets indices of the voxels that are either entirely or partially occupied by the GeometricalStructure. :return: mask for a numpy array

## get\_params\_from\_settings (single\_structure\_settings)

Gets all the parameters required for the specific GeometricalStructure. :param single\_structure\_settings: Settings which describe the specific GeometricalStructure. :return: Tuple of parameters

## to settings ()

Creates a Settings dictionary which contains all the parameters needed to create the same GeometricalStructure again. :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, simpa.utils.settings_generator.Settings = None)
```

Base class for all model-based structures for ModelBasedVolumeCreator. A GeometricalStructure has an internal representation of its own geometry. This is represented by self.geometrical\_volume which is a 3D array that

defines for every voxel within the simulation volume if it is enclosed in the GeometricalStructure or if it is outside. Most of the GeometricalStructures implement a partial volume effect. So if a voxel has the value 1, it is completely enclosed by the GeometricalStructure. If a voxel has a value between 0 and 1, that fraction of the volume is occupied by the GeometricalStructure. If a voxel has the value 0, it is outside of the GeometricalStructure.

## fill\_internal\_volume()

Fills self.geometrical\_volume of the GeometricalStructure.

## abstract get\_enclosed\_indices ()

Gets indices of the voxels that are either entirely or partially occupied by the GeometricalStructure. :return: mask for a numpy array

## abstract get\_params\_from\_settings (single\_structure\_settings)

Gets all the parameters required for the specific GeometricalStructure. :param single\_structure\_settings: Settings which describe the specific GeometricalStructure. :return: Tuple of parameters

## properties\_for\_wavelength (wavelength) → simpa.utils.tissue\_properties.TissueProperties

Returns the values corresponding to each optical/acoustic property used in SIMPA. :param wavelength: Wavelength of the queried properties :return: optical/acoustic properties

## **abstract** to\_settings () → simpa.utils.settings\_generator.Settings

Creates a Settings dictionary which contains all the parameters needed to create the same GeometricalStructure again. :return : A tuple containing the settings key and the needed entries

Defines a Layer structure which spans the xy-plane in the SIMPA axis convention. The thickness of the layer is defined along the z-axis. This layer can be deformed by the simpa.utils.deformation\_manager. Example usage:

```
# single_structure_settings initialization structure = Settings()
```

```
structure[Tags.PRIORITY] = 10 structure[Tags.STRUCTURE_START_MM] = [0, 0, 0] structure[Tags.STRUCTURE_END_MM] = [0, 0, 100] structure[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.epidermis() structure[Tags.CONSIDER_PARTIAL_VOLUME] = True structure[Tags.ADHERE_TO_DEFORMATION] = True structure[Tags.STRUCTURE_TYPE] = Tags.HORIZONTAL_LAYER_STRUCTURE
```

## get\_enclosed\_indices()

Gets indices of the voxels that are either entirely or partially occupied by the GeometricalStructure. :return: mask for a numpy array

## get\_params\_from\_settings (single\_structure\_settings)

Gets all the parameters required for the specific GeometricalStructure. :param single\_structure\_settings: Settings which describe the specific GeometricalStructure. :return: Tuple of parameters

## to\_settings()

Creates a Settings dictionary which contains all the parameters needed to create the same GeometricalStructure again. :return : A tuple containing the settings key and the needed entries

Defines a parallelepiped which is defined by a start point and three edge vectors which originate from the start point. This structure currently does not implement partial volume effects. Example usage:

```
# single_structure_settings initialization structure = Settings()
```

```
structure[Tags.PRIORITY]
                                 structure[Tags.STRUCTURE_START_MM]
                            9
                                                                            [25,
                                                                                  25,
                                                                                        25]
                        =
structure[Tags.STRUCTURE_FIRST_EDGE_MM]
                                                                                         1]
                                                                [5,
                                                                             1,
structure[Tags.STRUCTURE_SECOND_EDGE_MM]
                                                                 [1,
                                                                                         1]
structure[Tags.STRUCTURE_THIRD_EDGE_MM] = [1, 1, 5] structure[Tags.MOLECULE_COMPOSITION] =
TISSUE_LIBRARY.muscle() structure[Tags.STRUCTURE_TYPE] = Tags.PARALLELEPIPED_STRUCTURE
```

#### get enclosed indices ()

Gets indices of the voxels that are either entirely or partially occupied by the GeometricalStructure. :return: mask for a numpy array

## get\_params\_from\_settings (single\_structure\_settings)

Gets all the parameters required for the specific GeometricalStructure. :param single\_structure\_settings: Settings which describe the specific GeometricalStructure. :return: Tuple of parameters

## to\_settings()

Creates a Settings dictionary which contains all the parameters needed to create the same GeometricalStructure again. :return : A tuple containing the settings key and the needed entries

Defines a rectangular cuboid (box) which is defined by a start point its extent along the x-, y-, and z-axis. This structure implements partial volume effects. The box can be set to adhere to a deformation defined by the simpa.utils.deformation\_manager. The start point of the box will then be shifted along the z-axis accordingly. Example usage:

# single\_structure\_settings initialization structure = Settings()

```
structure[Tags.PRIORITY] = 9 structure[Tags.STRUCTURE_START_MM] = [25, 25, 25] structure[Tags.STRUCTURE_X_EXTENT_MM] = 40 structure[Tags.STRUCTURE_Y_EXTENT_MM] = 50 structure[Tags.STRUCTURE_Z_EXTENT_MM] = 60 structure[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.muscle() structure[Tags.CONSIDER_PARTIAL_VOLUME] = True structure[Tags.ADHERE_TO_DEFORMATION] = True structure[Tags.STRUCTURE_TYPE] = Tags.RECTANGULAR_CUBOID_STRUCTURE
```

#### get\_enclosed\_indices ()

Gets indices of the voxels that are either entirely or partially occupied by the GeometricalStructure. :return: mask for a numpy array

## get\_params\_from\_settings (single\_structure\_settings)

Gets all the parameters required for the specific GeometricalStructure. :param single\_structure\_settings: Settings which describe the specific GeometricalStructure. :return: Tuple of parameters

#### to settings ()

Creates a Settings dictionary which contains all the parameters needed to create the same GeometricalStructure again. :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, simple_structure_settings:
simpa.utils.settings generator.Settings = None)
```

Defines a sphere which is defined by a start point and a radius. This structure implements partial volume effects. The sphere can be set to adhere to a deformation defined by the simpa.utils.deformation\_manager. The start point of the sphere will then be shifted along the z-axis accordingly. Example usage:

```
# single_structure_settings initialization structure = Settings()
```

```
structure[Tags.PRIORITY] = 9 structure[Tags.STRUCTURE_START_MM] = [50, 50, 50] structure[Tags.STRUCTURE_RADIUS_MM] = 10 structure[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.blood() structure[Tags.CONSIDER_PARTIAL_VOLUME] = True structure[Tags.ADHERE_TO_DEFORMATION] = True structure[Tags.STRUCTURE_TYPE] = Tags.SPHERICAL_STRUCTURE
```

## get\_enclosed\_indices()

Gets indices of the voxels that are either entirely or partially occupied by the GeometricalStructure. :return: mask for a numpy array

```
get_params_from_settings (single_structure_settings)
```

Gets all the parameters required for the specific GeometricalStructure. :param single\_structure\_settings: Settings which describe the specific GeometricalStructure. :return: Tuple of parameters

#### to\_settings()

Creates a Settings dictionary which contains all the parameters needed to create the same GeometricalStructure again. :return: A tuple containing the settings key and the needed entries

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

Defines a vessel tree that is generated randomly in the simulation volume. The generation process begins at the start with a specified radius. The vessel grows roughly in the specified direction. The deviation is specified by the curvature factor. Furthermore, the radius of the vessel can vary depending on the specified radius variation factor. The bifurcation length defines how long a vessel can get until it will bifurcate. This structure implements partial volume effects. Example usage:

# single\_structure\_settings initialization structure\_settings = Settings()

```
structure_settings[Tags.PRIORITY] = 10 structure_settings[Tags.STRUCTURE_START_MM] = [50, 0, 50]
structure_settings[Tags.STRUCTURE_DIRECTION]
                                                                  [0,
                                                                              1,
                                                                                          0]
structure_settings[Tags.STRUCTURE_RADIUS_MM]
                                                                                           4
structure_settings[Tags.STRUCTURE_CURVATURE_FACTOR]
                                                                                        0.05
structure_settings[Tags.STRUCTURE_RADIUS_VARIATION_FACTOR]
                                                                                           1
structure_settings[Tags.STRUCTURE_BIFURCATION_LENGTH_MM]
                                                                                          70
structure_settings[Tags.MOLECULE_COMPOSITION]
                                                                     TISSUE_LIBRARY.blood()
structure_settings[Tags.CONSIDER_PARTIAL_VOLUME]
                                                                                        True
structure_settings[Tags.STRUCTURE_TYPE] = Tags.VESSEL_STRUCTURE
```

## fill\_internal\_volume()

Fills self.geometrical\_volume of the GeometricalStructure.

## get\_enclosed\_indices()

Gets indices of the voxels that are either entirely or partially occupied by the GeometricalStructure. :return: mask for a numpy array

```
get_params_from_settings (single_structure_settings)
```

Gets all the parameters required for the specific GeometricalStructure. :param single\_structure\_settings: Settings which describe the specific GeometricalStructure. :return: Tuple of parameters

## to\_settings()

Creates a Settings dictionary which contains all the parameters needed to create the same GeometricalStructure again. :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

```
class simpa.io_handling.serialization.SIMPAJSONSerializer
   TODO

   default (_object: object)
      TODO

class simpa.io_handling.serialization.SIMPASerializer
   TODO

serialize (_object: object)
```

## Module: log

# **Examples**

## Performing an optical forward simulation

The file can be found in simpa\_examples/minimal\_optical\_simulation.py:

```
SPDX-FileCopyrightText: 2021 Computer Assisted Medical Interventions Group, DKFZ
SPDX-FileCopyrightText: 2021 VISION Lab, Cancer Research UK Cambridge Institute (CRUK CI)
SPDX-License-Identifier: MIT
from simpa.utils import Tags, TISSUE_LIBRARY
from simpa.core.simulation import simulate
from simpa.utils.settings import Settings
from simpa.visualisation.matplotlib_data_visualisation import visualise_data
from simpa.core.device_digital_twins import *
import numpy as np
from simpa.core import VolumeCreationModelModelBasedAdapter, OpticalForwardModelMcxAdapter,
    GaussianNoiseProcessingComponent
from simpa.utils.path_manager import PathManager
# FIXME temporary workaround for newest Intel architectures
import os
os.environ["KMP_DUPLICATE_LIB_OK"] = "TRUE"
# TODO: Please make sure that a valid path_config.env file is located in your home directory
  point to the correct file in the PathManager().
path_manager = PathManager()
VOLUME_TRANSDUCER_DIM_IN_MM = 60
VOLUME_PLANAR_DIM_IN_MM = 30
VOLUME_HEIGHT_IN_MM = 60
SPACING = 0.5
```

```
RANDOM_SEED = 471
VOLUME_NAME = "MyVolumeName_"+str(RANDOM_SEED)
# If VISUALIZE is set to True, the simulation result will be plotted
VISUALIZE = True
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.constant(1e-4, 1e-4, 0
    background_dictionary[Tags.STRUCTURE_TYPE] = Tags.BACKGROUND
    muscle dictionary = Settings()
    muscle_dictionary[Tags.PRIORITY] = 1
    muscle_dictionary[Tags.STRUCTURE_START_MM] = [0, 0, 10]
    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,
                                                     VOLUME_HEIGHT_IN_MM/2]
    vessel_1_dictionary[Tags.STRUCTURE_END_MM] = [VOLUME_TRANSDUCER_DIM_IN_MM/2,
                                                   VOLUME_HEIGHT_IN_MM/2]
    vessel_1_dictionary[Tags.STRUCTURE_RADIUS_MM] = 3
    vessel_1_dictionary[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.blood()
    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, 9]
    epidermis_dictionary[Tags.STRUCTURE_END_MM] = [0, 0, 10]
    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)
```

```
general_settings = {
    # These parameters set the general propeties of the simulated volume
    Tags.RANDOM_SEED: RANDOM_SEED,
    Tags.VOLUME_NAME: VOLUME_NAME,
    Tags.SIMULATION_PATH: path_manager.get_hdf5_file_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.WAVELENGTHS: [798],
    Tags.DIGITAL_DEVICE_POSITION: [VOLUME_TRANSDUCER_DIM_IN_MM/2,
                                   VOLUME_PLANAR_DIM_IN_MM/2,
    Tags.LOAD AND SAVE HDF5 FILE AT THE END OF SIMULATION TO MINIMISE FILESIZE: True
}
settings = Settings(general_settings)
settings.set_volume_creation_settings({
    Tags.SIMULATE_DEFORMED_LAYERS: True,
    Tags.STRUCTURES: create_example_tissue()
})
settings.set_optical_settings({
    Tags.OPTICAL_MODEL_NUMBER_PHOTONS: 1e7,
    Tags.OPTICAL_MODEL_BINARY_PATH: path_manager.get_mcx_binary_path(),
    Tags.OPTICAL_MODEL: Tags.OPTICAL_MODEL_MCX,
    Tags.ILLUMINATION_TYPE: Tags.ILLUMINATION_TYPE_PENCIL,
    Tags.LASER_PULSE_ENERGY_IN_MILLIJOULE: 50
})
settings["noise_model_1"] = {
    Tags.NOISE_MEAN: 1.0,
    Tags.NOISE_STD: 0.1,
    Tags.NOISE_MODE: Tags.NOISE_MODE_MULTIPLICATIVE,
    Tags.DATA_FIELD: Tags.OPTICAL_MODEL_INITIAL_PRESSURE,
    Tags.NOISE_NON_NEGATIVITY_CONSTRAINT: True
}
pipeline = [
    VolumeCreationModelModelBasedAdapter(settings),
    OpticalForwardModelMcxAdapter(settings),
    GaussianNoiseProcessingComponent(settings, "noise_model_1")
class ExampleDeviceSlitIlluminationLinearDetector(PhotoacousticDevice):
    This class represents a digital twin of a PA device with a slit as illumination next to
    def ___init___(self):
        super().__init__(device_position_mm=np.asarray([VOLUME_TRANSDUCER_DIM_IN_MM/2,
                                                         VOLUME_PLANAR_DIM_IN_MM/2, 0]))
        self.set_detection_geometry(LinearArrayDetectionGeometry())
        self.add_illumination_geometry(SlitIlluminationGeometry(slit_vector_mm=[20, 0, 0],
                                                                 direction_vector_mm=[0, 0, 5
device = ExampleDeviceSlitIlluminationLinearDetector()
simulate(pipeline, settings, device)
```

```
if Tags.WAVELENGTH in settings:
   WAVELENGTH = settings[Tags.WAVELENGTH]
else:
    WAVELENGTH = 700
if VISUALIZE:
    visualise_data(path_manager.get_hdf5_file_save_path() + "/" + VOLUME_NAME + ".hdf5", WAV
                   log_scale=True)
```

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

The file can be found in simpa\_examples/optical\_and\_acoustic\_simulation.py:

```
SPDX-FileCopyrightText: 2021 Computer Assisted Medical Interventions Group, DKFZ
SPDX-FileCopyrightText: 2021 VISION Lab, Cancer Research UK Cambridge Institute (CRUK CI)
SPDX-License-Identifier: MIT
from simpa.utils import Tags, TISSUE_LIBRARY
from simpa.core.simulation import simulate
from simpa.utils.settings import Settings
from simpa.visualisation.matplotlib_data_visualisation import visualise_data
import numpy as np
from simpa.utils.path_manager import PathManager
from simpa.core import ImageReconstructionModuleDelayAndSumAdapter, GaussianNoiseProcessingConstructionModuleDelayAndSumAdapter, GaussianConstructionModuleDelayAndSumAdapter, Gauss
        OpticalForwardModelMcxAdapter, AcousticForwardModelKWaveAdapter, VolumeCreationModelMode
        FieldOfViewCroppingProcessingComponent, ImageReconstructionModuleSignedDelayMultiplyAndS
        ReconstructionModuleTimeReversalAdapter
from simpa.core.device_digital_twins import MSOTAcuityEcho
from simpa.core.device_digital_twins import LinearArrayDetectionGeometry, SlitIlluminationGe
# FIXME temporary workaround for newest Intel architectures
import os
os.environ["KMP_DUPLICATE_LIB_OK"] = "TRUE"
VOLUME TRANSDUCER DIM IN MM = 75
VOLUME_PLANAR_DIM_IN_MM = 20
VOLUME_HEIGHT_IN_MM = 25
SPACING = 0.25
RANDOM\_SEED = 4711
# TODO: Please make sure that a valid path_config.env file is located in your home directory
    point to the correct file in the PathManager().
path_manager = PathManager()
# If VISUALIZE is set to True, the simulation result will be plotted
VISUALIZE = True
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.constant(1e-10, 1e-10,
    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.constant(0.05, 100, 0.9)
    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 + 5,
                                                     0, 10]
    vessel_1_dictionary[Tags.STRUCTURE_END_MM] = [VOLUME_TRANSDUCER_DIM_IN_MM/2 + 5, VOLUME_
    vessel_1_dictionary[Tags.STRUCTURE_RADIUS_MM] = 3
    vessel_1_dictionary[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.blood()
    vessel_1_dictionary[Tags.CONSIDER_PARTIAL_VOLUME] = True
    vessel_1_dictionary[Tags.STRUCTURE_TYPE] = Tags.CIRCULAR_TUBULAR_STRUCTURE
    vessel_2_dictionary = Settings()
    vessel_2_dictionary[Tags.PRIORITY] = 3
    vessel_2_dictionary[Tags.STRUCTURE_START_MM] = [VOLUME_TRANSDUCER_DIM_IN_MM/2 -10,
                                                     0, 5]
    vessel_2_dictionary[Tags.STRUCTURE_END_MM] = [VOLUME_TRANSDUCER_DIM_IN_MM/2 -10, VOLUME_
    vessel_2_dictionary[Tags.STRUCTURE_RADIUS_MM] = 2
    vessel_2_dictionary[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.blood()
    vessel_2_dictionary[Tags.CONSIDER_PARTIAL_VOLUME] = True
    vessel_2_dictionary[Tags.STRUCTURE_TYPE] = Tags.CIRCULAR_TUBULAR_STRUCTURE
    epidermis_dictionary = Settings()
    epidermis_dictionary[Tags.PRIORITY] = 8
    epidermis_dictionary[Tags.STRUCTURE_START_MM] = [0, 0, 1]
    epidermis_dictionary[Tags.STRUCTURE_END_MM] = [0, 0, 1.1]
    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
    tissue_dict["vessel_2"] = vessel_2_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)
VOLUME_NAME = "CompletePipelineTestMSOT_"+str(RANDOM_SEED)
general_settings = {
```

```
# These parameters set the general properties of the simulated volume
            Tags.RANDOM_SEED: RANDOM_SEED,
            Tags.VOLUME_NAME: "CompletePipelineTestMSOT_" + str(RANDOM_SEED),
            Tags.SIMULATION_PATH: path_manager.get_hdf5_file_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.GPU: True,
            # The following parameters set the optical forward model
            Tags.WAVELENGTHS: [700]
settings = Settings(general_settings)
np.random.seed(RANDOM_SEED)
settings.set volume creation settings({
    Tags.STRUCTURES: create_example_tissue(),
    Tags.SIMULATE_DEFORMED_LAYERS: True
})
settings.set_optical_settings({
    Tags.OPTICAL_MODEL_NUMBER_PHOTONS: 1e7,
    Tags.OPTICAL_MODEL_BINARY_PATH: path_manager.get_mcx_binary_path(),
    Tags.ILLUMINATION_TYPE: Tags.ILLUMINATION_TYPE_MSOT_ACUITY_ECHO,
    Tags.LASER_PULSE_ENERGY_IN_MILLIJOULE: 50,
    Tags.MCX_ASSUMED_ANISOTROPY: 0.9,
})
settings.set_acoustic_settings({
    Tags.ACOUSTIC_SIMULATION_3D: False,
    Tags.ACOUSTIC_MODEL_BINARY_PATH: path_manager.get_matlab_binary_path(),
    Tags.PROPERTY_ALPHA_POWER: 1.05,
    Tags.SENSOR_RECORD: "p",
    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
})
settings.set_reconstruction_settings({
    Tags.RECONSTRUCTION_PERFORM_BANDPASS_FILTERING: False,
    Tags.ACOUSTIC_MODEL_BINARY_PATH: path_manager.get_matlab_binary_path(),
    # Tags.ACOUSTIC_SIMULATION_3D: True,
    Tags.PROPERTY_ALPHA_POWER: 1.05,
    Tags.TUKEY_WINDOW_ALPHA: 0.5,
    Tags.BANDPASS_CUTOFF_LOWPASS: int(8e6),
    Tags.BANDPASS_CUTOFF_HIGHPASS: int(0.1e6),
    Tags.RECONSTRUCTION_BMODE_AFTER_RECONSTRUCTION: True,
    Tags.RECONSTRUCTION_BMODE_METHOD: Tags.RECONSTRUCTION_BMODE_METHOD_HILBERT_TRANSFORM,
    Tags.RECONSTRUCTION_APODIZATION_METHOD: Tags.RECONSTRUCTION_APODIZATION_BOX,
    Tags.RECONSTRUCTION_MODE: Tags.RECONSTRUCTION_MODE_DIFFERENTIAL,
    Tags.SENSOR_RECORD: "p",
    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
})
settings["noise initial pressure"] = {
    Tags.NOISE_MEAN: 1,
    Tags.NOISE_STD: 0.01,
    Tags.NOISE_MODE: Tags.NOISE_MODE_MULTIPLICATIVE,
    Tags.DATA_FIELD: Tags.OPTICAL_MODEL_INITIAL_PRESSURE,
    Tags.NOISE_NON_NEGATIVITY_CONSTRAINT: True
}
settings["noise time series"] = {
    Tags.NOISE_STD: 1,
    Tags.NOISE_MODE: Tags.NOISE_MODE_ADDITIVE,
    Tags.DATA_FIELD: Tags.TIME_SERIES_DATA
# TODO: For the device choice, uncomment the undesired device
device = MSOTAcuityEcho(device_position_mm=np.array([VOLUME_TRANSDUCER_DIM_IN_MM/2,
                                                      VOLUME_PLANAR_DIM_IN_MM/2,
device.update_settings_for_use_of_model_based_volume_creator(settings)
# device = PhotoacousticDevice(device_position_mm=np.array([VOLUME_TRANSDUCER_DIM_IN_MM/2,
#
                                                             VOLUME_PLANAR_DIM_IN_MM/2,
#
                                                             0]))
# device.set_detection_geometry(LinearArrayDetectionGeometry(device_position_mm=device.devic
# device.add_illumination_geometry(SlitIlluminationGeometry(slit_vector_mm=[50, 0, 0]))
SIMUATION_PIPELINE = [
    VolumeCreationModelModelBasedAdapter(settings),
    OpticalForwardModelMcxAdapter(settings),
    GaussianNoiseProcessingComponent(settings, "noise_initial_pressure"),
    AcousticForwardModelKWaveAdapter(settings),
    GaussianNoiseProcessingComponent(settings, "noise_time_series"),
    ReconstructionModuleTimeReversalAdapter(settings),
simulate(SIMUATION_PIPELINE, settings, device)
if Tags.WAVELENGTH in settings:
    WAVELENGTH = settings[Tags.WAVELENGTH]
else:
    WAVELENGTH = 700
if VISUALIZE:
    visualise_data(path_manager.get_hdf5_file_save_path() + "/" + VOLUME_NAME + ".hdf5", WAV
                   show_time_series_data=True,
                   show_initial_pressure=True,
                   show_absorption=False,
                   show_segmentation_map=False,
                   show_tissue_density=False,
                   show_reconstructed_data=True,
                   show_fluence=False,
                   log_scale=False)
```

# Defining custom tissue structures and properties

The file can be found in simpa\_examples/create\_custom\_tissues.py:

```
SPDX-FileCopyrightText: 2021 Computer Assisted Medical Interventions Group, DKFZ
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from simpa.utils import MolecularCompositionGenerator
from simpa.utils import MOLECULE_LIBRARY
from simpa.utils import Molecule
from simpa.utils import Spectrum
from simpa.utils.libraries.spectra_library import ScatteringSpectrumLibrary, AnisotropySpect
import numpy as np
def create_custom_absorber():
    wavelengths = np.linspace(200, 1500, 100)
    absorber = Spectrum(spectrum_name="random absorber",
                        wavelengths=wavelengths,
                        values=np.random.random(
                                      np.shape(wavelengths)))
    return absorber
def create_custom_chromophore(volume_fraction: float = 1.0):
    chromophore = Molecule(
            absorption_spectrum=create_custom_absorber(),
            volume_fraction=volume_fraction,
            scattering_spectrum=ScatteringSpectrumLibrary.CONSTANT_SCATTERING_ARBITRARY(40.0
            anisotropy_spectrum=AnisotropySpectrumLibrary.CONSTANT_ANISOTROPY_ARBITRARY(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
    blood_volume_fraction = 0.5
    custom_chromophore_volume_fraction = 0.1
    # The volume fraction within every tissue type should sum up to 1.
    oxygenation = 0.4
    # Then append chromophores that you want
    tissue_settings_generator.append(key="oxyhemoglobin",
                                     value=MOLECULE_LIBRARY.oxyhemoglobin(oxygenation * bloc
    tissue_settings_generator.append(key="deoxyhemoglobin",
                                     value=MOLECULE_LIBRARY.deoxyhemoglobin((1 - oxygenation
    tissue_settings_generator.append(key="water",
                                     value=MOLECULE_LIBRARY.water(water_volume_fraction))
    tissue_settings_generator.append(key="custom",
                                     value=create_custom_chromophore(custom_chromophore_volu
    return tissue_settings_generator
```

# Defining a custom digital device twin class

The file can be found in simpa\_examples/create\_a\_custom\_digital\_device\_twin.py:

```
SPDX-FileCopyrightText: 2021 Computer Assisted Medical Interventions Group, DKFZ
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SPDX-License-Identifier: MIT
# FIXME temporary workaround for newest Intel architectures
import os
os.environ["KMP_DUPLICATE_LIB_OK"] = "TRUE"
from simpa.core.device_digital_twins.digital_device_twin_base import PhotoacousticDevice
from simpa.core.device_digital_twins.devices.illumination_geometries.slit_illumination_import
from simpa.core.device_digital_twins.devices.detection_geometries.linear_array import Linear
from simpa.utils import Settings, Tags
import numpy as np
class ExampleDeviceSlitIlluminationLinearDetector(PhotoacousticDevice):
    This class represents a digital twin of a PA device with a slit as illumination next to
    def ___init___(self):
        super().__init__()
        self.set_detection_geometry(LinearArrayDetectionGeometry())
        self.add_illumination_geometry(SlitIlluminationGeometry())
if __name__ == "__main__":
    device = ExampleDeviceSlitIlluminationLinearDetector()
    settings = Settings()
    settings[Tags.DIM_VOLUME_X_MM] = 20
    settings[Tags.DIM_VOLUME_Y_MM] = 50
    settings[Tags.DIM VOLUME Z MM] = 20
    settings[Tags.SPACING_MM] = 0.5
    settings[Tags.STRUCTURES] = {}
    x_dim = int(round(settings[Tags.DIM_VOLUME_X_MM]/settings[Tags.SPACING_MM]))
    z_dim = int(round(settings[Tags.DIM_VOLUME_Z_MM]/settings[Tags.SPACING_MM]))
    positions = device.get detection geometry().get detector element positions accounting for
    detector_elements = device.get_detection_geometry().get_detector_element_orientations(gl
    positions = np.round(positions/settings[Tags.SPACING_MM]).astype(int)
    import matplotlib.pyplot as plt
    plt.scatter(positions[:, 0], positions[:, 2])
    plt.quiver(positions[:, 0], positions[:, 2], detector_elements[:, 0], detector_elements[
    plt.show()
```

# **Defining custom tissue types**

The file can be found in simpa\_examples/create\_custom\_tissues.py:

```
"""

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```

```
.....
from simpa.utils import MolecularCompositionGenerator
from simpa.utils import MOLECULE_LIBRARY
from simpa.utils import Molecule
from simpa.utils import Spectrum
from simpa.utils.libraries.spectra_library import ScatteringSpectrumLibrary, AnisotropySpect
import numpy as np
def create custom absorber():
    wavelengths = np.linspace(200, 1500, 100)
    absorber = Spectrum(spectrum_name="random absorber",
                        wavelengths=wavelengths,
                        values=np.random.random(
                                      np.shape(wavelengths)))
    return absorber
def create_custom_chromophore(volume_fraction: float = 1.0):
    chromophore = Molecule(
            absorption_spectrum=create_custom_absorber(),
            volume_fraction=volume_fraction,
            scattering_spectrum=ScatteringSpectrumLibrary.CONSTANT_SCATTERING_ARBITRARY(40.0
            anisotropy_spectrum=AnisotropySpectrumLibrary.CONSTANT_ANISOTROPY_ARBITRARY(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
    blood_volume_fraction = 0.5
    custom_chromophore_volume_fraction = 0.1
    # The volume fraction within every tissue type should sum up to 1.
    oxygenation = 0.4
    # Then append chromophores that you want
    tissue_settings_generator.append(key="oxyhemoglobin",
                                     value=MOLECULE_LIBRARY.oxyhemoglobin(oxygenation * bloc
    tissue_settings_generator.append(key="deoxyhemoglobin",
                                     value=MOLECULE_LIBRARY.deoxyhemoglobin((1 - oxygenation
    tissue_settings_generator.append(key="water",
                                     value=MOLECULE_LIBRARY.water(water_volume_fraction))
    tissue_settings_generator.append(key="custom",
                                     value=create_custom_chromophore(custom_chromophore_volu-
    return tissue_settings_generator
```

# Load a segmentation mask and use it to simulate

The file can be found in simpa\_examples/segmentation\_loader.py:

```
"""

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```

```
SPDX-License-Identifier: MIT
from simpa.core.simulation import simulate
from simpa.utils.settings import Settings
from simpa.utils import Tags, SegmentationClasses
import numpy as np
from skimage.data import shepp_logan_phantom
from simpa.utils.libraries.tissue_library import TISSUE_LIBRARY
from simpa.utils.libraries.molecule_library import MOLECULE_LIBRARY
from simpa.utils.libraries.tissue_library import MolecularCompositionGenerator
from simpa.visualisation.matplotlib_data_visualisation import visualise_data
from scipy.ndimage import zoom
from simpa.utils.path_manager import PathManager
from simpa.core.device digital twins import RSOMExplorerP50
from simpa.core import VolumeCreationModuleSegmentationBasedAdapter, OpticalForwardModelMcxA
# FIXME temporary workaround for newest Intel architectures
import os
os.environ["KMP_DUPLICATE_LIB_OK"] = "TRUE"
# If VISUALIZE is set to True, the simulation result will be plotted
VISUALIZE = True
# TODO: Please make sure that a valid path_config.env file is located in your home directory
  point to the correct file in the PathManager().
path_manager = PathManager()
target_spacing = 1.0
label_mask = shepp_logan_phantom()
label_mask = np.digitize(label_mask, bins=np.linspace(0.0, 1.0, 11), right=True)
label_mask = np.reshape(label_mask, (400, 1, 400))
input_spacing = 0.2
segmentation_volume_tiled = np.tile(label_mask, (1, 128, 1))
segmentation_volume_mask = np.round(zoom(segmentation_volume_tiled, input_spacing/target_space)
                                         order=0)).astype(int)
def segmention_class_mapping():
    ret_dict = dict()
    ret_dict[0] = TISSUE_LIBRARY.heavy_water()
    ret_dict[1] = TISSUE_LIBRARY.blood()
    ret_dict[2] = TISSUE_LIBRARY.epidermis()
    ret_dict[3] = TISSUE_LIBRARY.muscle()
    ret_dict[4] = TISSUE_LIBRARY.mediprene()
    ret_dict[5] = TISSUE_LIBRARY.ultrasound_gel()
    ret_dict[6] = TISSUE_LIBRARY.heavy_water()
    ret_dict[7] = (MolecularCompositionGenerator()
                   .append(MOLECULE_LIBRARY.oxyhemoglobin(0.01))
                   .append(MOLECULE_LIBRARY.deoxyhemoglobin(0.01))
                   .append(MOLECULE_LIBRARY.water(0.98))
                   .get_molecular_composition(SegmentationClasses.COUPLING_ARTIFACT))
    ret_dict[8] = TISSUE_LIBRARY.heavy_water()
    ret_dict[9] = TISSUE_LIBRARY.heavy_water()
    ret_dict[10] = TISSUE_LIBRARY.heavy_water()
    return ret_dict
```

```
settings = Settings()
settings[Tags.SIMULATION_PATH] = path_manager.get_hdf5_file_save_path()
settings[Tags.VOLUME_NAME] = "SegmentationTest"
settings[Tags.RANDOM_SEED] = 1234
settings[Tags.WAVELENGTHS] = [700]
settings[Tags.SPACING_MM] = target_spacing
settings[Tags.DIM_VOLUME_X_MM] = 400 / (target_spacing / input_spacing)
settings[Tags.DIM_VOLUME_Y_MM] = 128 / (target_spacing / input_spacing)
settings[Tags.DIM_VOLUME_Z_MM] = 400 / (target_spacing / input_spacing)
settings.set_volume_creation_settings({
    Tags.INPUT_SEGMENTATION_VOLUME: segmentation_volume_mask,
    Tags.SEGMENTATION_CLASS_MAPPING: segmention_class_mapping(),
})
settings.set optical settings({
    Tags.OPTICAL_MODEL_NUMBER_PHOTONS: 1e7,
    Tags.OPTICAL_MODEL_BINARY_PATH: path_manager.get_mcx_binary_path(),
    Tags.ILLUMINATION_TYPE: Tags.ILLUMINATION_TYPE_MSOT_ACUITY_ECHO,
    Tags.LASER_PULSE_ENERGY_IN_MILLIJOULE: 50,
})
pipeline = [
    VolumeCreationModuleSegmentationBasedAdapter(settings),
    OpticalForwardModelMcxAdapter(settings)
simulate(pipeline, settings, RSOMExplorerP50(element_spacing_mm=1.0))
if Tags.WAVELENGTH in settings:
    WAVELENGTH = settings[Tags.WAVELENGTH]
else:
    WAVELENGTH = 700
if VISUALIZE:
    visualise_data(path_manager.get_hdf5_file_save_path() + "/" + "SegmentationTest" + ".hdf
```

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