# SIMPA

# version 0.2.0

**CAMI (Computer Assisted Medical Interventions), DKFZ, Heidelberg** 

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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

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

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

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

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

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

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

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/

# k-Wave (Acoustic Forward Model)

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

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

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

# **MITK**

# **Overview**

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

# Simulating photoacoustic images

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

# Performance profiling

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

```
python -m cProfile -o myscript.cprof myscript.py
pyprof2calltree -k -i myscript.cprof
```

# **Developer Guide**

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

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

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. The current master branch of the repository is open source and mirrored on github.

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

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

# **Coding style**

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

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

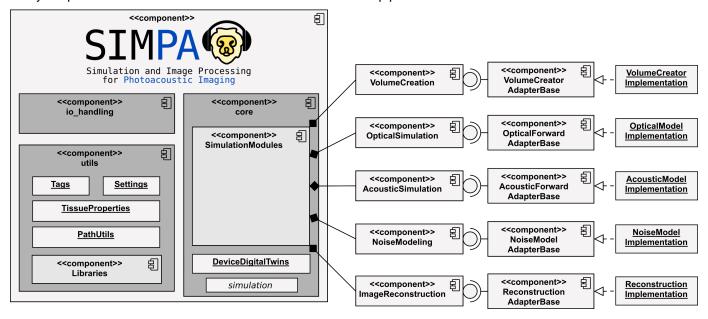
handled central point, where absorption spectra are collected and in The simpa.utils.libraries.spectra\_library.py. file comprises the class AbsorptionSpectrumLibrary, in which the new absorption spectra can be added using the following two steps:

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



# Module: core

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



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

class simpa.core.volume\_creation.VolumeCreatorBase

Use this class to define your own volume creation adapter.

abstract create\_simulation\_volume (settings: simpa.utils.settings\_generator.Settings)  $\rightarrow$  dict

This method will be called to create a simulation volume.

**Parameters:** settings – the settings dictionary containing the simulation instructions.

```
simpa.core.volume_creation.volume_creation.run_volume_creation (global_settings:
simpa.utils.settings_generator.Settings)
```

This method is the main entry point of volume creation for the SIMPA framework. It uses the Tags.VOLUME\_CREATOR tag to determine which of the volume creators should be used to create the simulation phantom.

Parameters: global\_settings – the settings dictionary that contains the simulation instructions

# Model-based volume creation

class simpa.core.volume\_creation.versatile\_volume\_creator.ModelBasedVolumeCreator
The model-based volume creator uses a set of rules how to generate structures to create a simulation volume.
These structures are added to the dictionary and later combined by the algorithm:

```
# Initialise settings dictionaries
simulation_settings = Settings()
all_structures = Settings()
structure = Settings()
# Definition of en example structure.
# The concrete structure parameters will change depending on the
# structure type
structure[Tags.PRIORITY] = 1
structure[Tags.STRUCTURE_START_MM] = [0, 0, 0]
structure[Tags.STRUCTURE_END_MM] = [0, 0, 100]
structure[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.muscle()
structure[Tags.CONSIDER_PARTIAL_VOLUME] = True
structure[Tags.ADHERE_TO_DEFORMATION] = True
structure[Tags.STRUCTURE_TYPE] = Tags.HORIZONTAL_LAYER_STRUCTURE
all_structures["arbitrary_identifier"] = structure
simulation_settings[Tags.STRUCTURES] = all_structures
# Define further simulation settings
 . . .
simulate(simulation_settings)
```

```
{\tt create\_simulation\_volume~(settings)} \rightarrow {\sf dict}
```

This method creates a in silico respresentation of a tissue as described in the settings file that is given.

Parameters: settings - a dictionary containing all relevant Tags for the simulation to be able to

instantiate a tissue.

Returns: a path to a npz file containing characteristics of the simulated volume: absorption,

scattering, anisotropy, oxygenation, and a segmentation mask. All of these are given as

3d numpy arrays.

# Segmentation-based volume creation

class simpa.core.volume\_creation.segmentation\_based\_volume\_creator.SegmentationBasedVol
umeCreator

This volume creator expects a np.ndarray to be in the settigs under the Tags.INPUT\_SEGMENTATION\_VOLUME tag and uses this array together with a SegmentationClass mapping which is a dict defined in the settings under Tags.SEGMENTATION\_CLASS\_MAPPING.

With this, an even greater utility is warranted.

 $create\_simulation\_volume$  (settings: simpa.utils.settings\_generator.Settings)  $\rightarrow$  dict This method will be called to create a simulation volume.

**Parameters:** settings – the settings dictionary containing the simulation instructions.

# Optical forward modeling

simpa.core.optical\_simulation.optical\_modelling.run\_optical\_forward\_model (settings)
This method is the main entry point for running optical forward simulations with the SIMPA toolkit. It is important, that the Tags.OPTICAL\_MODEL tag is set in the settings dictionary, as well as any tags that have to be present for the specific model.

class simpa.core.optical\_simulation.OpticalForwardAdapterBase
 Use this class as a base for implementations of optical forward models.

**abstract** forward\_model (absorption\_cm, scattering\_cm, anisotropy, settings)
A deriving class needs to implement this method according to its model.

### Parameters:

- absorption\_cm Absorption in units of per centimeter
- scattering\_cm Scattering in units of per centimeter
- anisotropy Dimensionless scattering anisotropy
- settings Setting dictionary

Returns: Fluence in units of J/cm^2

simulate (optical\_properties\_path, settings)

Call this method to invoke the simulation process.

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

### Parameters:

- optical\_properties\_path path to a .npz file that contains the following tags: Tags.PROPERTY\_ABSORPTION\_PER\_CM -> contains the optical absorptions in units of one per centimeter Tags.PROPERTY\_SCATTERING\_PER\_CM -> contains the optical scattering in units of one per centimeter Tags.PROPERTY\_ANISOTROPY -> contains the dimensionless optical scattering anisotropy
- settings -

### Returns:

simpa.core.optical\_simulation.illumination\_definition.define\_illumination(settings, nx, ny, nz)

This method creates a dictionary that represents the illumination geometry in a way that it can be used with the respective illumination framework.

### Parameters:

- settings The settings file containing the simulation instructions
- nx number of voxels along the x dimension of the volume
- ny number of voxels along the y dimension of the volume
- nz number of voxels along the z dimension of the volume

simpa.core.optical\_simulation.illumination\_definition.define\_illumination\_mcx (settings, nx, ny, nz)  $\rightarrow$  dict

This method creates a dictionary that contains tags as they are expected for the mcx simulation tool to represent the illumination geometry.

#### Parameters:

- settings The settings file containing the simulation instructions
- nx number of voxels along the x dimension of the volume
- ny number of voxels along the y dimension of the volume
- nz number of voxels along the z dimension of the volume

# mcx integration

class simpa.core.optical\_simulation.mcx\_adapter.McxAdapter

This class implements a bridge to the mcx framework to integrate mcx into SIMPA. MCX is a GPU-enabled Monte-Carlo model simulation of photon transport in tissue:

Fang, Qianqian, and David A. Boas. "Monte Carlo simulation of photon migration in 3D turbid media accelerated by graphics processing units."

Optics express 17.22 (2009): 20178-20190.

**forward\_model** (absorption\_cm, scattering\_cm, anisotropy, settings) A deriving class needs to implement this method according to its model.

### Parameters:

- absorption cm Absorption in units of per centimeter
- scattering\_cm Scattering in units of per centimeter
- anisotropy Dimensionless scattering anisotropy
- settings Setting dictionary

Returns: Fluence in units of J/cm^2

# Acoustic forward modeling

simpa.core.acoustic\_simulation.acoustic\_modelling.run\_acoustic\_forward\_model (settings)
This method is the entry method for running an acoustic forward model. It is invoked in the simpa.core.simulation.simulate method, but can also be called individually for the purposes of performing acoustic forward modeling only or in a different context.

The concrete will be chosen based on the:

Tags.ACOUSTIC\_MODEL

tag in the settings dictionary.

Parameters: settings – The settings dictionary containing key-value pairs that determine the simulation.

Here, it must contain the Tags.ACOUSTIC\_MODEL tag and any tags that might be required

by the specific acoustic model.

Raises: AssertionError – an assertion error is raised if the Tags.ACOUSTIC\_MODEL tag is not

given or points to an unknown acoustic forward model.

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

class simpa.core.acoustic\_simulation.AcousticForwardAdapterBase

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

# abstract forward\_model (settings) → numpy.ndarray

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

**Parameters:** settings – Setting dictionary Returns: time series pressure data

**simulate** (settings) → numpy.ndarray

Call this method to invoke the simulation process.

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

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

# k-Wave integration

class simpa.core.acoustic\_simulation.k\_wave\_adapter.KwaveAcousticForwardModel

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

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

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

```
The initial pressure distribution:
    Tags.OPTICAL MODEL INITIAL PRESSURE
Acoustic tissue properties:
    Tags.PROPERTY_SPEED_OF_SOUND
    Tags.PROPERTY DENSITY
    Tags.PROPERTY_ALPHA_COEFF
The digital twin of the imaging device:
    Tags.DIGITAL_DEVICE
Other parameters:
    Tags.PERFORM_UPSAMPLING
    Tags.SPACING_MM
    Tags.UPSCALE_FACTOR
    Tags.PROPERTY ALPHA POWER
    Tags.GPU
    Tags.PMLInside
    Tags.PMLAlpha
    Tags.PlotPML
    Tags.RECORDMOVIE
    Tags.MOVIENAME
    Tags.ACOUSTIC LOG SCALE
    Tags.SENSOR_DIRECTIVITY_PATTERN
```

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

Please also refer to the simpa\_examples scripts to see how the settings file can be parametrized successfully.

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

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

**Parameters:** settings – Setting dictionary Returns: time series pressure data

# Noise modeling

simpa.core.noise\_simulation.noise\_modelling.apply\_noise\_model\_to\_time\_series\_data
(settings, acoustic\_model\_result\_path)

This is the primary method for performing noise pertubation of data.

The noise model can be activated using the Tags.NOISE\_MODEL and Tags.APPLY\_NOISE\_MODEL tags.

### Parameters:

- settings the settings dictionary containing the simulation instructions
- acoustic\_model\_result\_path path where the data is within the HDF5 file.

#### Returns:

class simpa.core.noise\_simulation.GaussianNoiseModel

The purpose of the GaussianNoiseModel class is to apply an additive gaussian noise to the input data.

The mean and standard deviation of the model can be defined either by using the Tags.NOISE\_MEAN and Tags.NOISE\_STD tags, but they can also be set using a pandas dataframe that contains mean and standard deviation of noise for different wavelengths and temperatures. This can be done using the Tags.NOISE\_MODEL\_PATH tag.

```
apply_noise_model (time_series_data, settings)
```

Applies the defined noise model to the input time series data.

#### Parameters:

- time\_series\_data the data the noise should be applied to.
- settings the settings dictionary that contains the simulation instructions.

**Returns:** a numpy array of the same shape as the input data.

```
class simpa.core.noise_simulation.NoiseModelAdapterBase
```

This class functions as a base class that can be used to easily define different noise models by extending the apply\_noise\_model function.

abstract apply\_noise\_model (time\_series\_data: numpy.ndarray, settings: dict) -numpy.ndarray

Applies the defined noise model to the input time series data.

#### Parameters:

- time\_series\_data the data the noise should be applied to.
- settings the settings dictionary that contains the simulation instructions.

Returns: a numpy array of the same shape as the input data.

# Image reconstruction

```
simpa.core.image_reconstruction.reconstruction_modelling.perform_reconstruction (settings: dict) \rightarrow str
```

This method is the main entry point to perform image reconstruction using the SIMPA toolkit. All information necessary for the respective reconstruction method must be contained in the settings dictionary.

**Parameters:** settings – a dictionary containing key-value pairs with simulation instructions.

**Returns:** the path to the result data in the written HDF5 file.

```
class simpa.core.image_reconstruction.ReconstructionAdapterBase
TODO
```

```
abstract reconstruction_algorithm (time_series_sensor_data, settings)
```

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

Parameters:

• time\_series\_sensor\_data - the time series sensor data

• settings - Setting dictionary

**Returns:** a reconstructed photoacoustic image

simulate (settings)

Parameters: settings –

Returns:

# **Backprojection**

class simpa.core.image\_reconstruction.BackprojectionAdapter.BackprojectionAdapter
SIMPA provides a pytorch-based implementations of the universal backprojection algorithm:

Xu, Minghua, and Lihong V. Wang. "Universal back-projection algorithm for photoacoustic computed tomography." Physical Review E 71.1 (2005): 016706.

In case a CUDA-capable device is available on the system, the backprojection algorithm will be computed on the GPU, otherwise, the code will be run on the CPU.

Depending on the reconstruction mode (Tags.RECONSTRUCTION\_MODE), the image reconstruction will be performed using the time series pressure (Tags.RECONSTRUCTION\_MODE\_PRESSURE), the derivative of the time series pressure (Tags.RECONSTRUCTION\_MODE\_DIFFERENTIAL), or a combination (Tags.RECONSTRUCTION\_MODE\_FULL).

backprojection3D\_torch (time\_series\_data, speed\_of\_sound\_m, target\_dim\_m, resolution\_m,
sensor\_positions\_m, sampling\_frequency\_Hz, mode=None)

The implementation of the actual algorithm.

### Parameters:

- **time\_series\_data** The time series pressure data with the shape [num\_samples, num\_detectors]
- speed\_of\_sound\_m The speed of sound in meters
- target\_dim\_m The target dimension of the reconstruction volume in meters
- resolution\_m The target resolution of the reconstruction volume in meters
- sensor\_positions\_m The sensor positions in meters. Must be num\_detector elements.
- sampling\_frequency\_Hz The sampling frequency of the device in Hertz
- mode The reconstruction mode. Depending on the reconstruction mode (Tags.RECONSTRUCTION\_MODE), the image reconstruction will be performed using the time series pressure (Tags.RECONSTRUCTION\_MODE\_PRESSURE), the derivative of the time series pressure (Tags.RECONSTRUCTION\_MODE\_DIFFERENTIAL), or a combination (Tags.RECONSTRUCTION MODE FULL).

**Returns:** a numpy array containing the reconstructed volume.

reconstruction\_algorithm (time\_series\_sensor\_data, settings)
A deriving class needs to implement this method according to its model.

### Parameters:

- time\_series\_sensor\_data the time series sensor data
- settings Setting dictionary

**Returns:** a reconstructed photoacoustic image

# Time Revearsal

class simpa.core.image reconstruction.TimeReversalAdapter.TimeReversalAdapter

The time reversal adapter includes the time reversal reconstruction algorithm implemented by the k-Wave toolkit into SIMPA.

Time reversal reconstruction uses the time series data and computes the forward simulation model backwards in time:

```
Treeby, Bradley E., Edward Z. Zhang, and Benjamin T. Cox. "Photoacoustic tomography in absorbing acoustic media using time reversal." Inverse Problems 26.11 (2010): 115003.
```

### Static get\_acoustic\_properties (global\_settings: dict, input\_data: dict)

This method extracts the acoustic tissue properties from the settings dictionary and amends the information to the input\_data.

#### Parameters:

- **global\_settings** the settings dictionary containing key value pairs with the simulation instructions.
- input\_data a dictionary containing the information needed for time reversal.

reconstruction\_algorithm (time\_series\_sensor\_data, settings)

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

**Parameters:** 

- time\_series\_sensor\_data the time series sensor data
- settings Setting dictionary

**Returns:** a reconstructed photoacoustic image

# Digital device twins

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

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

# **MSOT Acuity Echo**

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

This class represents a digital twin of the MSOT Acuity Echo, manufactured by iThera Medical, Munich, Germany (https://www.ithera-medical.com/products/msot-acuity/). It is based on the real specifications of the device, but due to the limitations of the possibilities how to represent a device in the software frameworks, constitutes only an approximation.

Some important publications that showcase the use cases of the MSOT Acuity and Acuity Echo device are:

```
Regensburger, Adrian P., et al. "Detection of collagens by multispectral optoacoustic tomography as an imaging biomarker for Duchenne muscular dystrophy."

Nature Medicine 25.12 (2019): 1905-1915.
```

Knieling, Ferdinand, et al. "Multispectral Optoacoustic Tomography for Assessment of Crohn's Disease Activity."

The New England journal of medicine 376.13 (2017): 1292.

# adjust\_simulation\_volume\_and\_settings

(global\_settings:

simpa.utils.settings\_generator.Settings)

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

```
check_settings_prerequisites
```

(global\_settings:

simpa.utils.settings\_generator.Settings $) \rightarrow bool$ 

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

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

Returns: True if the prerequisites are met, False if they are not met, but no exception has been

raised.

# get\_detector\_element\_orientations

(global\_settings:

simpa.utils.settings\_generator.Settings) → numpy.ndarray

This method yields a normalised orientation vector for each detection element. The length of this vector is the same as the one obtained via the position methods:

```
get_detector_element_positions_base_mm
get_detector_element_positions_accounting_for_device_position_mm
```

Returns: a numpy array that contains normalised orientation vectors for each detection element

```
get_detector_element_positions_accounting_for_device_position_mm
simpa.utils.settings_generator.Settings) → numpy.ndarray
Similar to:
get_detector_element_positions_base_mm
(global_settings:
get_detector_element_positions_base_mm
```

```
This method returns the check to positions of the detection elements relative to the device position in the image.
```

This method returns the absolute positions of the detection elements relative to the device position in the imaged volume, where the device position is defined by the following tag:

```
Tags.DIGITAL_DEVICE_POSITION
```

Returns: A numpy array containing the coordinates of the detection elements

```
get_detector_element_positions_base_mm () → numpy.ndarray
```

Defines the abstract positions of the detection elements in an arbitraty coordinate system. Typically, the center of the field of view is defined as the origin.

To obtain the positions in an interpretable coordinate system, please use the other method:

```
get_detector_element_positions_accounting_for_device_position_mm
```

**Returns:** A numpy array containing the position vestors of the detection elements.

get\_illuminator\_definition (global\_settings: simpa.utils.settings\_generator.Settings)
Defines the illumination geometry of the device in the settings dictionary.

# **RSOM Explorer P50**

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

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

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

```
Yew, Yik Weng, et al. "Raster-scanning optoacoustic mesoscopy (RSOM) imaging as an objective disease severity tool in atopic dermatitis patients."
```

```
Journal of the American Academy of Dermatology (2020).

Hindelang, B., et al. "Non-invasive imaging in dermatology and the unique potential of raster-scan optoacoustic mesoscopy."

Journal of the European Academy of Dermatology and Venereology 33.6 (2019): 1051-1061.
```

# adjust\_simulation\_volume\_and\_settings

(global\_settings:

simpa.utils.settings\_generator.Settings)

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

## check\_settings\_prerequisites

(global\_settings:

simpa.utils.settings\_generator.Settings) → bool

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

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

Returns: True if the prerequisites are met, False if they are not met, but no exception has been

raised.

# get\_detector\_element\_orientations

(global\_settings:

simpa.utils.settings\_generator.Settings)

This method yields a normalised orientation vector for each detection element. The length of this vector is the same as the one obtained via the position methods:

```
get_detector_element_positions_base_mm
get_detector_element_positions_accounting_for_device_position_mm
```

Returns: a numpy array that contains normalised orientation vectors for each detection element

get\_detector\_element\_positions\_accounting\_for\_device\_position\_mm (global\_settings:
simpa.utils.settings\_generator.Settings)

Similar to:

```
get_detector_element_positions_base_mm
```

This method returns the absolute positions of the detection elements relative to the device position in the imaged volume, where the device position is defined by the following tag:

```
Tags.DIGITAL_DEVICE_POSITION
```

**Returns:** A numpy array containing the coordinates of the detection elements

# get\_detector\_element\_positions\_base\_mm ()

Defines the abstract positions of the detection elements in an arbitraty coordinate system. Typically, the center of the field of view is defined as the origin.

To obtain the positions in an interpretable coordinate system, please use the other method:

```
get_detector_element_positions_accounting_for_device_position_mm
```

**Returns:** A numpy array containing the position vestors of the detection elements.

get\_illuminator\_definition (global\_settings: simpa.utils.settings\_generator.Settings)
Defines the illumination geometry of the device in the settings dictionary.

# Module: utils

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

class simpa.utils.tags.Tags

This class contains all 'Tags' for the use in the settings dictionary 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'>, <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'>)) 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

# 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 = 'gaussian'

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'>)

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

# PMLA1pha = ('pml\_alpha', (<class 'int'>, <class 'numpy.integer'>, <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\_ison', (<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'>))

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'>, <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'>), <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'>), <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.int32'>, <class
'numpy.float64'>))

Upscale factor of the upsampling in the image processing.

Usage: module process

# **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.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)

Module: utils

### **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.settings_generator.Settings (dictionary: dict = None)
```

The Settings class is a dictionary that contains all relevant settings for running a simulation in the SIMPA toolkit. It includes an automatic sanity check for input parameters using the simpa.utils.Tags class. Usage: Seetings({Tags.KEY1: value1, Tags.KEY2: value2, ...})

Usage. Seelings({Tags.NETT. valueT, Tags.NETZ. valueZ, ...})

add\_acoustic\_properties (run\_acoustic\_model: bool = None, acoustic\_model: str = None,
acoustic\_simulation\_3D: bool = None, speed\_of\_sound: (<class 'int'>, <class 'float'>)
= None, density: (<class 'int'>, <class 'float'>) = None)

Helper function that adds minimal acoustic properties required for running an optical forward model in SIMPA to an existing Settings inplace.

#### Parameters:

- run\_acoustic\_model If True, the simulation will run the acoustic forward model.
- acoustic\_model Choice of the used acoustic model.
- acoustic\_simulation\_3D If True, simulates the acoustic forward model in 3D.
- speed\_of\_sound Speed of sound of the generated volume/structure in m/s.
- density Density of the generated volume/structure in kg/m³.

add\_minimal\_meta\_information (volume\_name: str = None, simulation\_path: str = None,
random\_seed: int = None, spacing: float = None, volume\_dim\_x: (<class 'int'>, <class
'float'>) = None, volume\_dim\_y: (<class 'int'>, <class 'float'>) = None, volume\_dim\_z:
(<class 'int'>, <class 'float'>) = None)

Helper function that adds minimal meta information required for running a simulation in SIMPA to an existing Settings inplace.

### Parameters:

- volume name Name of the SIMPA output file.
- simulation\_path Absolute path to the folder where the SIMPA output is saved.
- random seed Random seed for numpy and torch.
- **spacing** Isotropic extent of one voxels in mm in the generated volume.
- **volume** dim x Extent of the x-axis of the generated volume.
- volume\_dim\_y Extent of the y-axis of the generated volume.
- volume\_dim\_z Extent of the z-axis of the generated volume.

add\_minimal\_optical\_properties (run\_optical\_model: bool = None, wavelengths: list =
None, optical\_model: str = None, photon\_number: int = None, illumination\_type: str =
None, illumination\_position: list = None, illumination\_direction: list = None)

Helper function that adds minimal optical properties required for running an optical forward model in SIMPA to an existing Settings inplace.

#### Parameters:

- run\_optical\_model If True, the simulation will run the optical forward model.
- wavelengths Iterable of all the wavelengths used for the simulation.
- optical\_model Choice of the used optical model.
- **photon\_number** Number of photons used in the optical simulation.
- illumination\_type Type of the illumination geometry used in the optical simulation.
- illumination\_position Position of the photon source in [x, y, z] coordinates used in the optical

simulation. :param illumination\_direction: Direction of the photon source as [x, y, z] vector used in the optical simulation.

```
add_reconstruction_properties (perform_image_reconstruction: bool = None,
reconstruction_algorithm: str = None)
```

Helper function that adds minimal reconstruction properties required for running an optical forward model in SIMPA to an existing Settings inplace.

#### Parameters:

- perform\_image\_reconstruction If True, the simulation will run the image reconstruction.
- reconstruction\_algorithm Choice of the used reconstruction algorithm.

```
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

**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)
```

simpa.utils.calculate.calculate\_oxygenation (molecule\_list)

Creates a functional that simulates distortion along the y position between the minimum and maximum x positions. The elevation can never be smaller than 0 or bigger than maximum\_y\_elevation\_mm.

### Parameters:

- xmin mm the minimum x axis value the return functional is defined in
- xmax\_mm the maximum x axis value the return functional is defined in
- maximum\_y\_elevation\_mm the maximum y axis value the return functional will yield

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

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

### Parameters:

- min\_value minimum value
- max\_value maximum value

**Returns:** random number in [min\_value, max\_value]

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.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

get\_absorption\_for\_wavelength (wavelength: int) → float

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

an integer value between the minimum and maximum wavelength.

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

```
get_absorption_over_wavelength()
           Returns: numpy array with the available wavelengths and the corresponding absorption properties
simpa.utils.libraries.spectra_library.view_absorption_spectra (save_path=None)
 Opens a matplotlib plot and visualizes the available absorption spectra.
      Parameters: save_path – If not None, then the figure will be saved as a png file to the destination.
class simpa.utils.libraries.tissue_library.MolecularCompositionGenerator
 The MolecularCompositionGenerator is a helper class to facilitate the creation of a MolecularComposition
 instance.
class simpa.utils.libraries.tissue_library.TissueLibrary
 TODO
 blood_arterial()
                     a settings dictionary containing all min and max parameters fitting for full blood.
           Returns:
 blood_generic (oxygenation=None)
                     a settings dictionary containing all min and max parameters fitting for full blood.
           Returns:
 blood_venous()
                      a settings dictionary containing all min and max parameters fitting for full blood.
           Returns:
 bone ()
                      a settings dictionary containing all min and max parameters fitting for full blood.
           Returns:
 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)
                      a settings dictionary containing all min and max parameters fitting for generic background
           Returns:
                      tissue.
 subcutaneous_fat (background_oxy=0.5)
           Returns:
                      a settings dictionary containing all min and max parameters fitting for subcutaneous fat
                      tissue.
              simpa.utils.libraries.structure_library.Background
class
                                                                                     (global_settings:
simpa.utils.settings generator.Settings,
                                                                                background settings:
```

# get\_enclosed\_indices()

simpa.utils.settings\_generator.Settings = None)

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() → 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.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 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()

```
9
                                structure[Tags.STRUCTURE_START_MM]
structure[Tags.PRIORITY]
                                                                                    501
                       =
                                                                          [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] =
                            structure[Tags.CONSIDER_PARTIAL_VOLUME]
                                                                                   True
TISSUE LIBRARY.blood()
structure[Tags.ADHERE_TO_DEFORMATION]
                                                     structure[Tags.STRUCTURE_TYPE]
                                             True
                                       =
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

```
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) $\rightarrow$ 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

This class currently has no partial volume effects implemented. TODO

### 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.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

```
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.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

class simpa.utils.libraries.structure\_library.VesselStructure (global\_settings:
simpa.utils.settings\_generator.Settings, simple\_structure\_settings:
simpa.utils.settings\_generator.Settings = None)

### 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

# **Examples**

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

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

```
from simpa.utils import Tags, TISSUE_LIBRARY
from simpa.core.simulation import simulate
from simpa.utils.settings_generator import Settings
from simpa.utils.libraries.structure_library import HorizontalLayerStructure
import numpy as np
# TODO change these paths to the desired executable and save folder
SAVE_PATH = "D:/save/"
MCX_BINARY_PATH = "D:/bin/Release/mcx.exe"
VOLUME_TRANSDUCER_DIM_IN_MM = 75
VOLUME_PLANAR_DIM_IN_MM = 20
VOLUME_HEIGHT_IN_MM = 25
SPACING = 0.15
RANDOM_SEED = 4711
def create_example_tissue():
    This is a very simple example script of how to create a tissue definition.
    It contains a muscular background, an epidermis layer on top of the muscles
    and a blood vessel.
    background_dictionary = Settings()
    background dictionary[Tags.MOLECULE COMPOSITION] = TISSUE LIBRARY.muscle()
    background_dictionary[Tags.STRUCTURE_TYPE] = Tags.BACKGROUND
    muscle_dictionary = Settings()
    muscle_dictionary[Tags.PRIORITY] = 1
    muscle_dictionary[Tags.STRUCTURE_START_MM] = [0, 0, 0]
    muscle_dictionary[Tags.STRUCTURE_END_MM] = [0, 0, 100]
    muscle_dictionary[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.muscle()
    muscle_dictionary[Tags.CONSIDER_PARTIAL_VOLUME] = True
    muscle_dictionary[Tags.ADHERE_TO_DEFORMATION] = True
    muscle_dictionary[Tags.STRUCTURE_TYPE] = Tags.HORIZONTAL_LAYER_STRUCTURE
    vessel_1_dictionary = Settings()
    vessel_1_dictionary[Tags.PRIORITY] = 3
    vessel_1_dictionary[Tags.STRUCTURE_START_MM] = [VOLUME_TRANSDUCER_DIM_IN_MM/2,
                                                    0, 10]
    vessel_1_dictionary[Tags.STRUCTURE_END_MM] = [VOLUME_TRANSDUCER_DIM_IN_MM/2, VOLUME_PLAN
    vessel_1_dictionary[Tags.STRUCTURE_RADIUS_MM] = 3
    vessel_1_dictionary[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.blood_generic()
    vessel_1_dictionary[Tags.CONSIDER_PARTIAL_VOLUME] = True
    vessel_1_dictionary[Tags.STRUCTURE_TYPE] = Tags.CIRCULAR_TUBULAR_STRUCTURE
    epidermis_dictionary = Settings()
    epidermis_dictionary[Tags.PRIORITY] = 8
    epidermis_dictionary[Tags.STRUCTURE_START_MM] = [0, 0, 0]
    epidermis_dictionary[Tags.STRUCTURE_END_MM] = [0, 0, 1]
    epidermis_dictionary[Tags.MOLECULE_COMPOSITION] = TISSUE_LIBRARY.epidermis()
    epidermis_dictionary[Tags.CONSIDER_PARTIAL_VOLUME] = True
    epidermis_dictionary[Tags.ADHERE_TO_DEFORMATION] = True
    epidermis_dictionary[Tags.STRUCTURE_TYPE] = Tags.HORIZONTAL_LAYER_STRUCTURE
    tissue_dict = Settings()
    tissue_dict[Tags.BACKGROUND] = background_dictionary
    tissue_dict["muscle"] = muscle_dictionary
    tissue_dict["epidermis"] = epidermis_dictionary
```

```
tissue_dict["vessel_1"] = vessel_1_dictionary
    return tissue_dict
# Seed the numpy random configuration prior to creating the global_settings file in
# order to ensure that the same volume
# is generated with the same random seed every time.
np.random.seed(RANDOM_SEED)
settings = {
    # These parameters set the general propeties of the simulated volume
    Tags.RANDOM_SEED: RANDOM_SEED,
    Tags.VOLUME_NAME: "CompletePipelineTestMSOT_"+str(RANDOM_SEED),
    Tags.SIMULATION_PATH: SAVE_PATH,
    Tags.SPACING_MM: SPACING,
    Tags.DIM_VOLUME_Z_MM: VOLUME_HEIGHT_IN_MM,
    Tags.DIM_VOLUME_X_MM: VOLUME_TRANSDUCER_DIM_IN_MM,
    Tags.DIM VOLUME Y MM: VOLUME PLANAR DIM IN MM,
    Tags.VOLUME_CREATOR: Tags.VOLUME_CREATOR_VERSATILE,
    Tags.SIMULATE_DEFORMED_LAYERS: True,
    # Tags.DEFORMED_LAYERS_SETTINGS: create_deformation_settings([[0, VOLUME_TRANSDUCER_DIM_
                                                                  [0, VOLUME_PLANAR_DIM_IN_MM
    #
                                                                  maximum_z_elevation_mm=10,
    #
                                                                  filter_sigma=0,
                                                                  cosine_scaling_factor=1),
    # Simulation Device
    Tags.DIGITAL_DEVICE: Tags.DIGITAL_DEVICE_MSOT,
    # The following parameters set the optical forward model
    Tags.RUN_OPTICAL_MODEL: True,
    Tags.WAVELENGTHS: [700],
    Tags.OPTICAL_MODEL_NUMBER_PHOTONS: 1e7,
    Tags.OPTICAL_MODEL_BINARY_PATH: MCX_BINARY_PATH,
    Tags.OPTICAL_MODEL: Tags.OPTICAL_MODEL_MCX,
    Tags.ILLUMINATION_TYPE: Tags.ILLUMINATION_TYPE_MSOT_ACUITY_ECHO,
    Tags.LASER_PULSE_ENERGY_IN_MILLIJOULE: 50,
    # The following parameters tell the script that we do not want any extra
    # modelling steps
    Tags.RUN_ACOUSTIC_MODEL: True,
    Tags.ACOUSTIC_SIMULATION_3D: False,
    Tags.ACOUSTIC_MODEL: Tags.ACOUSTIC_MODEL_K_WAVE,
    Tags.ACOUSTIC_MODEL_BINARY_PATH: "C:/Program Files/MATLAB/R2020b/bin/matlab.exe",
    Tags.ACOUSTIC_MODEL_SCRIPT_LOCATION: "C:/simpa/simpa/core/acoustic_simulation",
    Tags.GPU: True,
    Tags.PROPERTY_ALPHA_POWER: 1.05,
    Tags.SENSOR_RECORD: "p",
    # Tags.SENSOR_DIRECTIVITY_PATTERN: "pressure",
    Tags.PMLInside: False,
    Tags.PMLSize: [31, 32],
    Tags.PMLAlpha: 1.5,
    Tags.PlotPML: False,
    Tags.RECORDMOVIE: False,
    Tags.MOVIENAME: "visualization_log",
    Tags.ACOUSTIC_LOG_SCALE: True,
```

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

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

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

# Reading the HDF5 simulation output

The file can be found in simpa\_examples/access\_saved\_PAI\_data.py:

```
from simpa.io_handling import load_hdf5, save_hdf5
import matplotlib.pyplot as plt
import matplotlib as mpl
import numpy as np
from simpa.utils import SegmentationClasses, Tags
from simpa.utils.settings_generator import Settings
values = []
names = []
for string in SegmentationClasses.__dict__:
    if string[0:2] != "___":
        values.append(SegmentationClasses.__dict__[string])
        names.append(string)
values = np.asarray(values)
names = np.asarray(names)
sort_indexes = np.argsort(values)
values = values[sort_indexes]
names = names[sort_indexes]
colors = [list(np.random.random(3)) for _ in range(len(names))]
cmap = mpl.colors.LinearSegmentedColormap.from_list(
    'Custom cmap', colors, len(names))
PATH = "D:/save/LNetOpticalForward_planar_0.hdf5"
WAVELENGTH = 532
file = load_hdf5(PATH)
settings = Settings(file["settings"])
fluence = (file['simulations']['original_data']['optical_forward_model_output']
           [str(WAVELENGTH)]['fluence'])
initial_pressure = (file['simulations']['original_data']
                    ['optical_forward_model_output']
                    [str(WAVELENGTH)]['initial_pressure'])
absorption = (file['simulations']['original_data']['simulation_properties']
              [str(WAVELENGTH)]['mua'])
```

```
segmentation = (file['simulations']['original_data']['simulation_properties']
              [str(WAVELENGTH)]['seg'])
reconstruction = None
speed of sound = None
if Tags.PERFORM_IMAGE_RECONSTRUCTION in settings and settings[Tags.PERFORM_IMAGE_RECONSTRUCT
    time_series = np.squeeze(
        file["simulations"]["original_data"]["time_series_data"][str(WAVELENGTH)]["time_seri
    reconstruction = np.squeeze(
            file["simulations"]["original_data"]["reconstructed_data"][str(WAVELENGTH)]["rec
    speed_of_sound = file['simulations']['original_data']['simulation_properties'][str(WAVEI
reconstruction = reconstruction.T
shape = np.shape(reconstruction)
x_pos = int(shape[0]/2)
y_pos = int(shape[1]/2)
z_pos = int(shape[2]/2)
plt.figure()
plt.subplot(161)
plt.imshow(np.fliplr(np.rot90(reconstruction[x_pos, :, :], -1)))
plt.subplot(162)
plt.imshow(np.rot90(np.log10(initial_pressure[x_pos, :, :]), -1))
plt.subplot(163)
plt.imshow(np.fliplr(np.rot90(reconstruction[:, y_pos, :], -1)))
plt.subplot(164)
plt.imshow(np.rot90(np.log10(initial_pressure[:, y_pos, :]), -1))
plt.subplot(165)
plt.imshow(np.fliplr(np.rot90(reconstruction[:, :, z_pos], -1)))
plt.subplot(166)
plt.imshow(np.rot90(np.log10(initial_pressure[:, :, z_pos]), -3))
plt.show()
exit()
if Tags.PERFORM_IMAGE_RECONSTRUCTION in settings and settings[Tags.PERFORM_IMAGE_RECONSTRUCT
    if len(shape) > 2:
        plt.figure()
        plt.subplot(141)
        plt.imshow(np.rot90(np.log10(np.log10(time_series[:, :]-np.min(time_series))), -1),
        plt.subplot(142)
        plt.imshow(np.rot90((reconstruction[:, y_pos, :]), -2))
        plt.imshow(np.rot90(np.log10(initial_pressure[:, y_pos, :]), -1))
        plt.subplot(144)
        plt.imshow(np.rot90(segmentation[:, y_pos, :], -1), vmin=values[0], vmax=values[-1],
        plt.show()
    else:
        plt.figure()
        plt.subplot(141)
        plt.imshow(np.rot90((reconstruction[:, :]), -1))
        plt.subplot(142)
        plt.imshow(np.rot90((speed_of_sound), -1))
        plt.subplot(143)
        plt.imshow(np.rot90(np.log10(initial_pressure), -1))
        plt.subplot(144)
        plt.imshow(np.rot90(segmentation, -1), vmin=values[0], vmax=values[-1], cmap=cmap)
```

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

# Defining custom tissue structures and properties

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

```
def create_custom_chromophore(volume_fraction: float = 1.0):
    chromophore = Molecule(
            spectrum=create_custom_absorber(),
            volume_fraction=volume_fraction,
            mus500=40.0,
            b mie=1.1,
            f_ray=0.9,
            anisotropy=0.9
   return chromophore
def create_custom_tissue_type():
    # First create an instance of a TissueSettingsGenerator
    tissue_settings_generator = MolecularCompositionGenerator()
    water_volume_fraction = 0.4
    bvf = 0.5
    oxy = 0.4
    # Then append chromophores that you want
    tissue_settings_generator.append(key="oxyhemoglobin", value=
                            MOLECULE_LIBRARY.oxyhemoglobin(oxy * bvf))
    tissue_settings_generator.append(key="deoxyhemoglobin", value=
                            MOLECULE_LIBRARY.deoxyhemoglobin(oxy * bvf))
    tissue_settings_generator.append(key="water", value=
                            MOLECULE_LIBRARY.water(water_volume_fraction))
    tissue_settings_generator.append(key="custom", value=
                            create_custom_chromophore(0.1))
    return_tissue_settings_generator.get_settings()
```

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