quanfima Documentation

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Contents

Quanfima (**qu**antitative **an**alysis of **fi**brous **ma**terials) is a collection of useful routines for morphological analysis and visualization of 2D/3D data from various areas of material science. The aim is to simplify the analysis process by providing functionality for frequently required tasks in the same place.

- Analysis of fibrous structures by tensor-based method in 2D / 3D datasets.
- Estimation of structure diameters in 2D / 3D by a ray-casting method.
- Counting of particles in 2D / 3D datasets and providing a detailed report in pandas.DataFrame format.
- Calculation of porosity measure for each material in 2D / 3D datasets.
- Visualization in 2D / 3D using matplotlib, visvis packages.

CHAPTER 1

User Guide

1.1 Overview

1.1.1 Requirements

- Python 2.7
- PyCUDA >= 2017.1.1
- Numpy >= 1.13
- SciPy >= 0.19
- scikit-image >= 0.12
- scikit-learn >= 0.18
- Pandas >= 0.19
- Matplotlib >= 2.0

1.1.2 Installation

The easiest way to install the latest version is by using pip:

```
$ pip install quanfima
```

You may also use Git to clone the repository and install it manually:

```
$ git clone https://github.com/rshkarin/quanfima.git
$ cd quanfima
$ python setup.py install
```

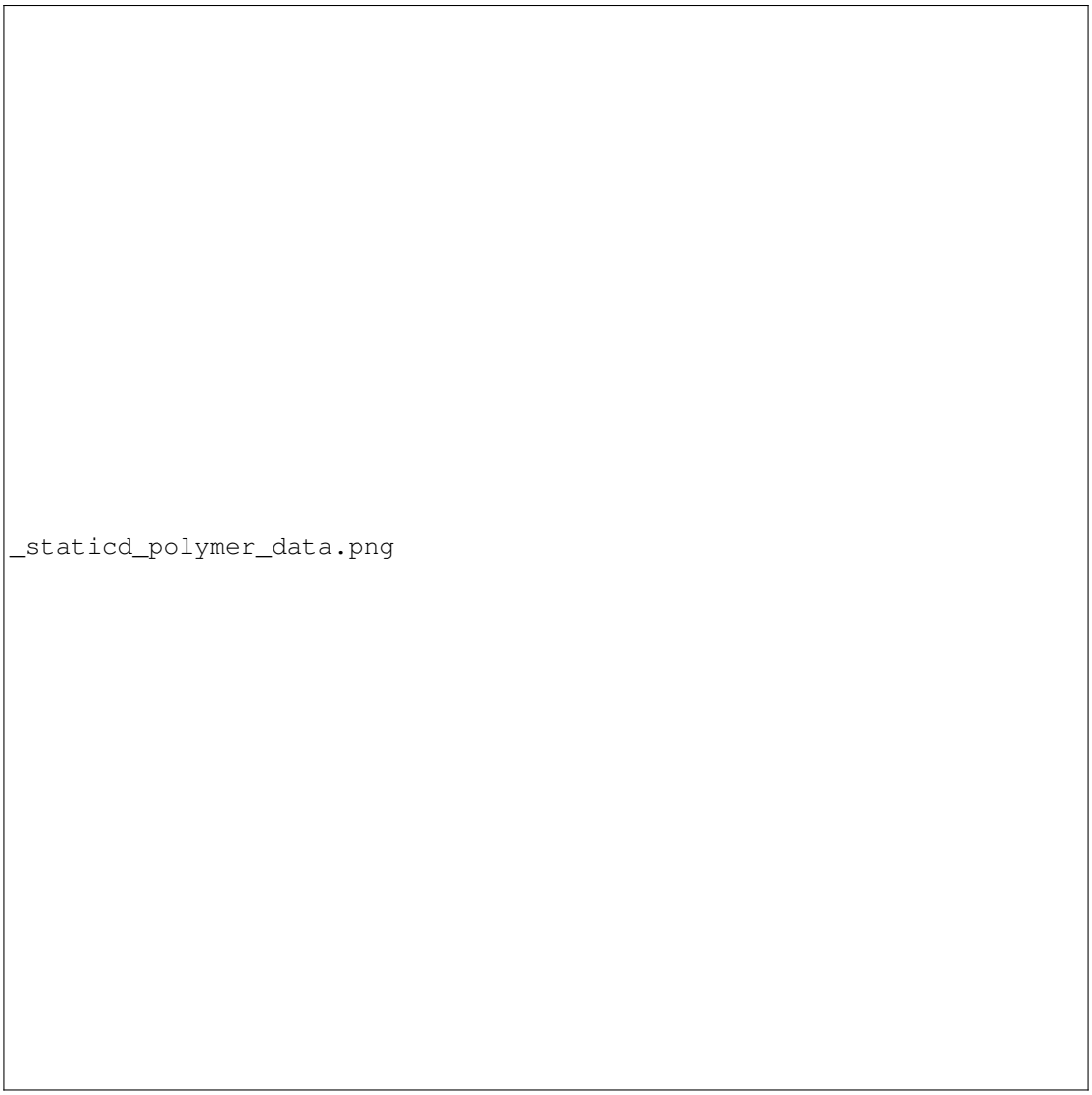
1.2 Quickstart

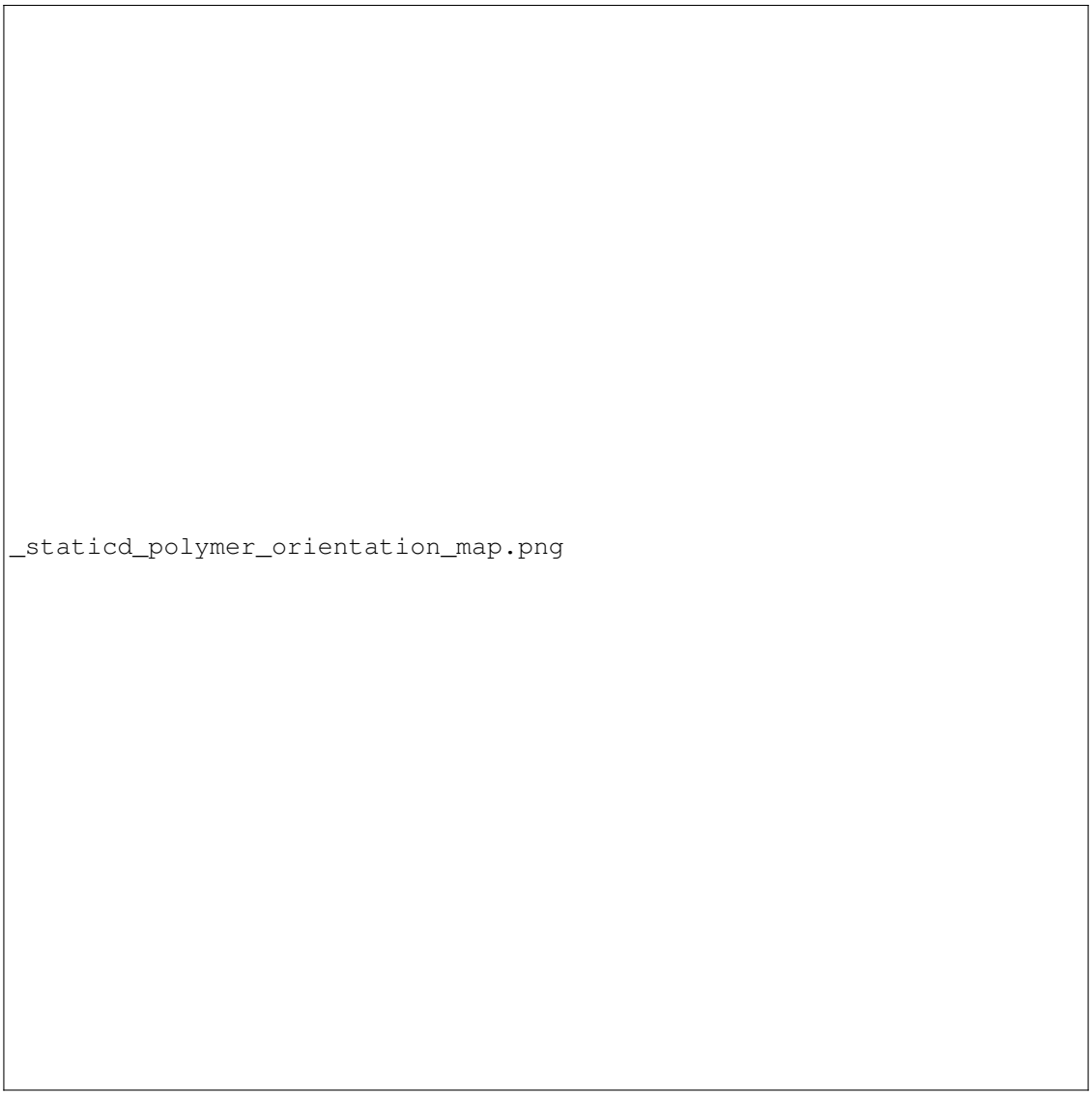
1.2.1 Analysis of fibrous 2D data

Open a grayscale image, perform segmentation, estimate porosity, analyze fiber orientation and diameters, and plot the results.

```
import numpy as np
from skimage import io, filters
from quanfima import morphology as mrph
from quanfima import visualization as vis
from quanfima import utils

img = io.imread('../../data/polymer_slice.tif')

th_val = filters.threshold_otsu(img)
img_seg = (img > th_val).astype(np.uint8)

# estiamte porosity
pr = mrph.calc_porosity(img_seg)
for k,v in pr.items():
  print 'Porosity ({}): {}'.format(k, v)

# prepare data and analyze fibers
data, skeleton, skeleton_thick = utils.prepare_data(img_seg)
cskel, fskel, omap, dmap, ovals, dvals = \
                    mrph.estimate_fiber_properties(data, skeleton)

# plot results
vis.plot_orientation_map(omap, fskel, min_label=u'0°', max_label=u'180°',
                         figsize=(10,10),
                         name='2d_polymer',
                         output_dir='../../data/results')
vis.plot_diameter_map(dmap, cskel, figsize=(10,10), cmap='gist_rainbow',
                      name='2d_polymer',
                      output_dir='../../data/results')
```

```
>> Porosity (Material 1): 0.845488888889
```


_staticd_polymer_data.png


_staticd_polymer_orientation_map.png

_staticd_polymer_diameter_map.png

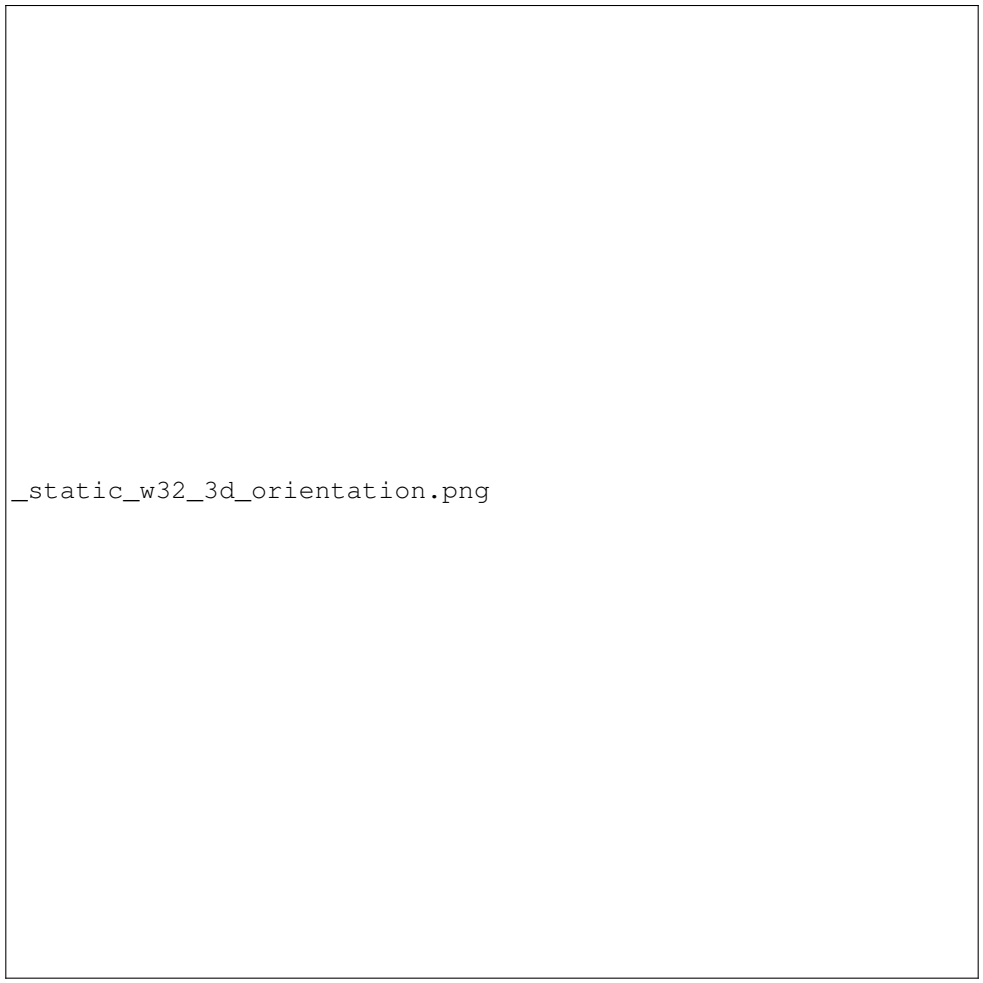
1.2.2 Analysis of 3D data of fibrous material

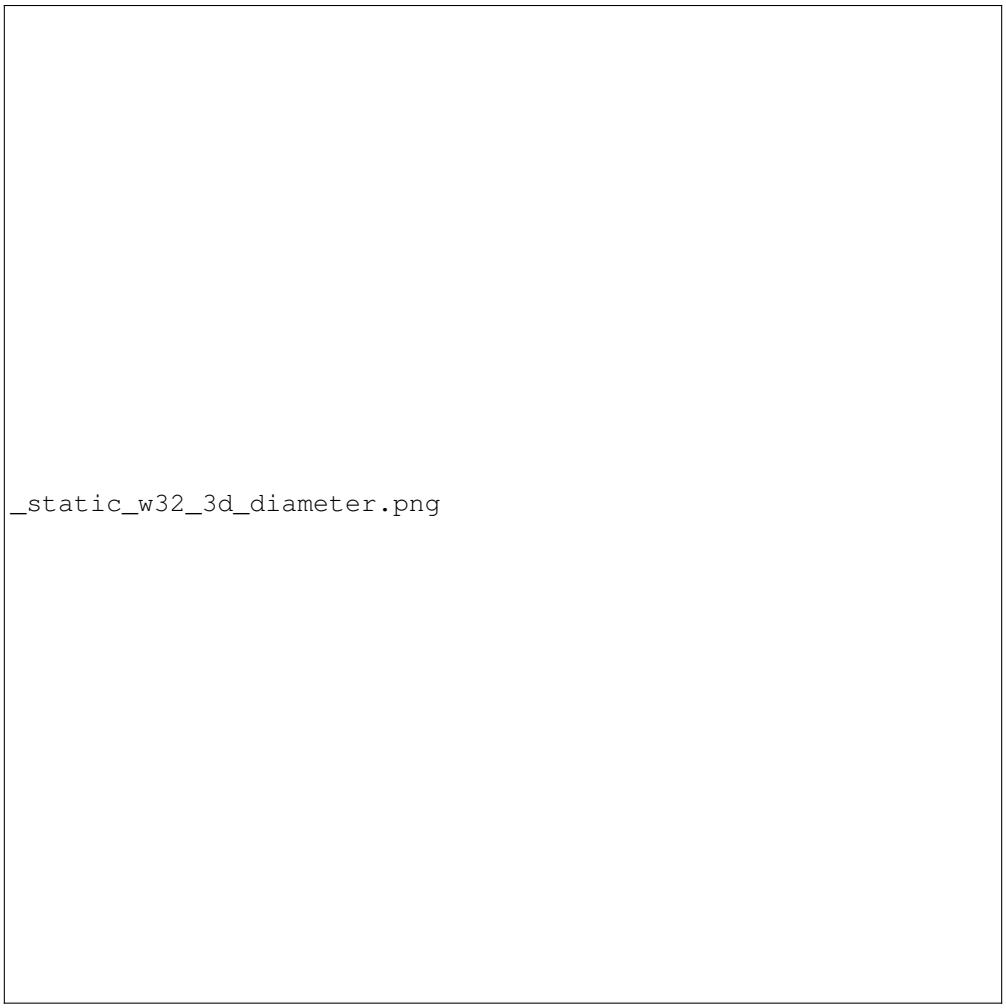
Open a micro-CT dataset, perform slice-wise segmentation, estimate porosity, analyze 3D fiber orientation and diameters, and visualize the results.

```
import numpy as np
from skimage import filters
from quanfima import morphology as mrph
from quanfima import visualization as vis
from quanfima import utils

data = np.memmap('../../data/polymer3d_8bit_128x128x128.raw',
                 shape=(128,128,128), dtype=np.uint8, mode='r')

data_seg = np.zeros_like(data, dtype=np.uint8)
for i in xrange(data_seg.shape[0]):
  th_val = filters.threshold_otsu(data[i])
  data_seg[i] = (data[i] > th_val).astype(np.uint8)
```

```
# estimate porosity
pr = mrph.calc_porosity(data_seg)
for k,v in pr.items():
  print 'Porosity ({}): {}'.format(k, v)

# prepare data and analyze fibers
pdata, pskel, pskel_thick = utils.prepare_data(data_seg)
oprops =  mrph.estimate_tensor_parallel('polymer_orientation_w32', pskel,
                                        pskel_thick, 32,
                                        '../../data/results')

odata = np.load(oprops['output_path']).item()
lat, azth, skel = odata['lat'], odata['azth'], odata['skeleton']

dprops = mrph.estimate_diameter_single_run('polymer_diameter',
                                           '../../data/results',
                                           pdata, skel, lat, azth)
dmtr = np.load(dprops['output_path']).item()['diameter']

# plot results
vis.plot_3d_orientation_map('polymer_w32', lat, azth,
                            output_dir='../../data/results',
                            camera_azth=40.47,
                            camera_elev=32.5,
                            camera_fov=35.0,
                            camera_loc=(40.85, 46.32, 28.85),
                            camera_zoom=0.005124)

vis.plot_3d_diameter_map('polymer_w32', dmtr,
                         output_dir='../../data/results',
                         measure_quantity='vox',
                         camera_azth=40.47,
                         camera_elev=32.5,
                         camera_fov=35.0,
                         camera_loc=(40.85, 46.32, 28.85),
                         camera_zoom=0.005124,
                         cb_x_offset=5,
                         width=620)
```

```
>> Porosity (Material 1): 0.855631351471
```


_static_w32_3d_orientation.png



1.2.3 Estimation of p-values

Estimate p-values between several groups of samples with corresponding measurements of some material's property.

```
import pandas as pd
from quanfima import utils

prop_vals = [174.93, 182.42, 194.61, 234.6, 229.73, 242.6, 38.78, 37.79,
             32.06, 14.81, 15.23, 13.84]
mat_groups = ['PCL_cl', 'PCL_cl', 'PCL_cl', 'PCL_wa', 'PCL_wa', 'PCL_wa',
              'PCL_SiHA_cl', 'PCL_SiHA_cl', 'PCL_SiHA_cl', 'PCL_SiHA_wa',
              'PCL_SiHA_wa', 'PCL_SiHA_wa']
df_elongation = pd.DataFrame({'elongation': prop_vals, 'type': mat_groups})

_, _ = utils.calculate_tukey_posthoc(df_elongation, 'elongation',
                                     name='samples_elongation',
                                     write=True,
                                     output_dir='../../data/results')
```

```
>> Tukey post-hoc (elongation)
>>     Multiple Comparison of Means - Tukey HSD,FWER=0.05
>> =====================================================
```

```
>>    group1      group2   meandiff  lower    upper   reject
>> ---------------------------------------------------------
>> PCL_SiHA_cl PCL_SiHA_wa -21.5833 -37.8384 -5.3282   True
>> PCL_SiHA_cl    PCL_cl   147.7767 131.5216 164.0318  True
>> PCL_SiHA_cl    PCL_wa   199.4333 183.1782 215.6884  True
>> PCL_SiHA_wa    PCL_cl    169.36  153.1049 185.6151  True
>> PCL_SiHA_wa    PCL_wa   221.0167 204.7616 237.2718  True
>>    PCL_cl      PCL_wa   51.6567  35.4016  67.9118   True
>> ---------------------------------------------------------
>> ['PCL_SiHA_cl' 'PCL_SiHA_wa' 'PCL_cl' 'PCL_wa']
>> PCL_SiHA_cl-PCL_SiHA_wa :  0.011919282004
>> PCL_SiHA_wa-PCL_cl :  0.001
>> PCL_SiHA_wa-PCL_wa :  0.001
>> PCL_cl-PCL_wa :  0.001
>> PCL_SiHA_cl-PCL_wa :  0.001
>> PCL_SiHA_cl-PCL_cl :  0.001
```

1.2.4 Simulate and count particles in 3D data

Count and estimate properties of particles in a generated dataset comprised of spheres of varying radius.

```
from quanfima import simulation
from quanfima import morphology as mrph

volume, diameter, _, _ = simulation.simulate_particles((512,512,512),
                                                       n_particles=1000)

stats, labeled_volume = mrph.object_counter(volume)
```

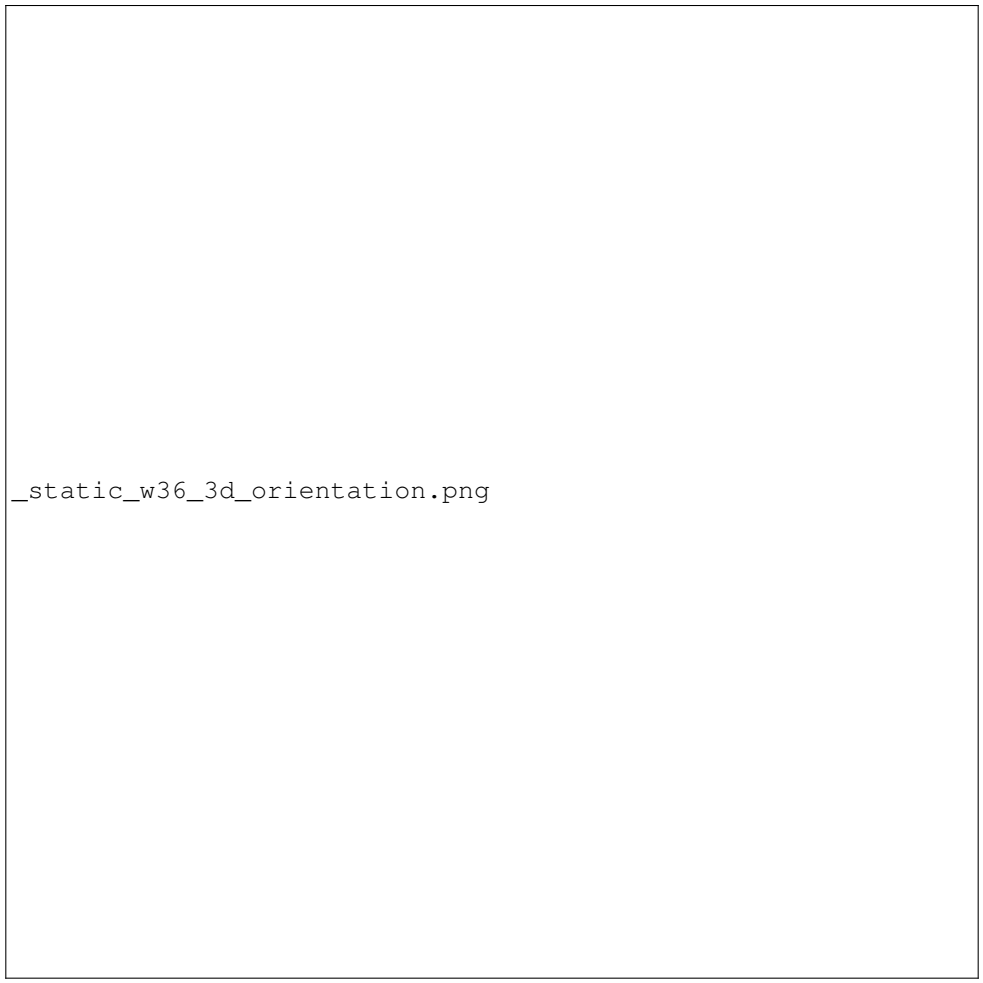
```
>>     Label      Area    Perimeter  Sphericity
>> 0     1.0   20479.0  2896.958728    1.249533
>> 1     2.0    5575.0  1184.028571    1.284158
>> 2     3.0   57777.0  5816.142853    1.242660
>> 3     4.0   17077.0  2545.194226    1.260001
>> 4     5.0    5575.0  1184.028571    1.284158
>> 5     6.0   65267.0  6348.926691    1.234752
>> ..    ...       ...          ...         ...
>> 791  792.0    2109.0   605.185858    1.314154
>> 792  793.0     257.0   134.225397    1.456369
>> 793  794.0     257.0   134.225397    1.456369
>> 794  795.0     123.0    78.627417    1.521179

>> [795 rows x 4 columns]
```

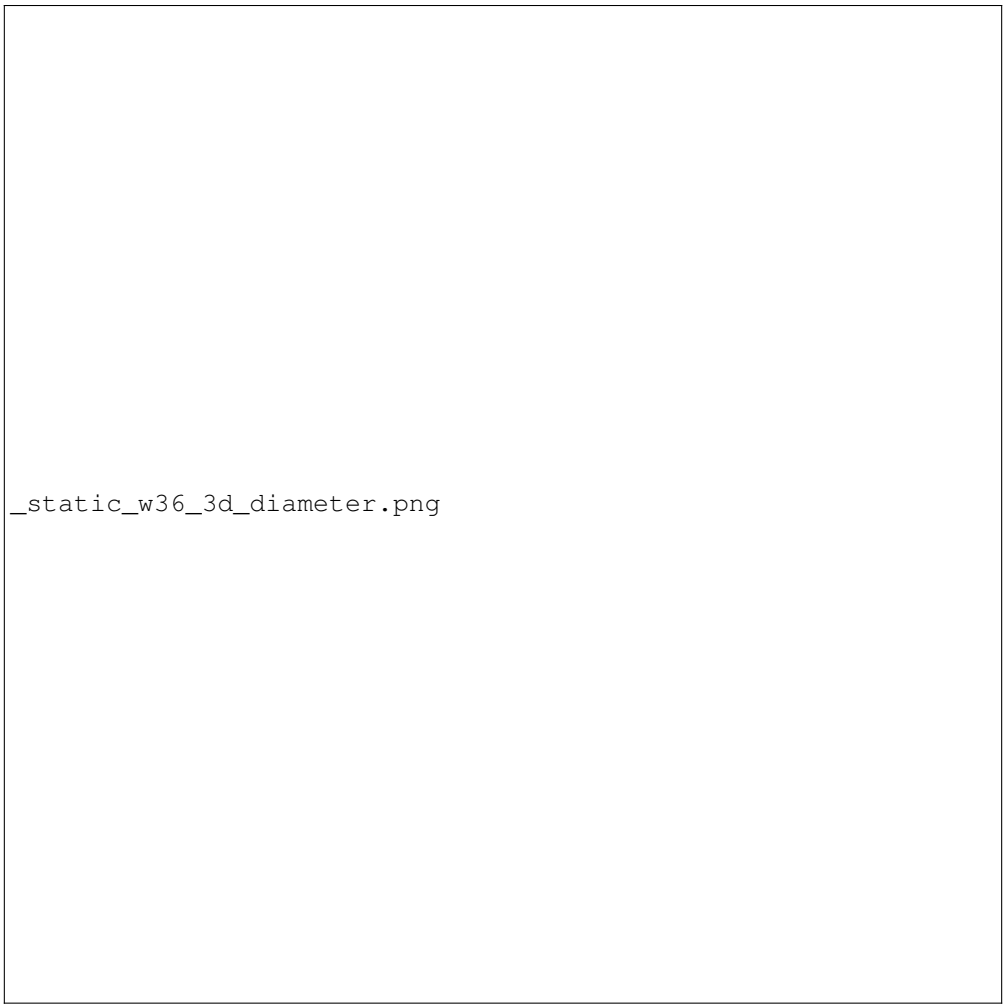
1.2.5 Simulate fibers and estimate properties

Simulate a 3D dataset containing some number of fibers, estimate their properties and visualize.

```
import numpy as np
from scipy import ndimage as ndi
from skimage import morphology
from quanfima import simulation
from quanfima import morphology as mrph
from quanfima import utils
```

```
from quanfima import visualization as vis

volume, lat_ref, azth_ref, diameter, _, _ = \
          simulation.simulate_fibers((128,128,128), n_fibers=30, max_fails=100,
                                     radius_lim=(2, 3), gap_lim=(3,5))
volume = volume.astype(np.uint8)
volume = ndi.binary_fill_holes(volume)
volume = ndi.median_filter(volume, footprint=morphology.ball(2))
lat_ref = ndi.median_filter(lat_ref, footprint=morphology.ball(2))
azth_ref = ndi.median_filter(azth_ref, footprint=morphology.ball(2))

# prepare data and analyze fibers
pdata, pskel, pskel_thick = utils.prepare_data(volume)
oprops =  mrph.estimate_tensor_parallel('dataset_orientation_w36',
                                        pskel, pskel_thick, 36,
                                        '../../data/results')

odata = np.load(oprops['output_path']).item()
lat, azth, skel = odata['lat'], odata['azth'], odata['skeleton']

dprops = mrph.estimate_diameter_single_run('dataset_diameter',
                                           '../../data/results',
                                           pdata, skel, lat, azth)
dmtr = np.load(dprops['output_path']).item()['diameter']

# plot results
vis.plot_3d_orientation_map('dataset_w36', lat, azth,
                            output_dir='../../data/results',
                            camera_azth=40.47,
                            camera_elev=32.5,
                            camera_fov=35.0,
                            camera_loc=(40.85, 46.32, 28.85),
                            camera_zoom=0.005124)

vis.plot_3d_diameter_map('dataset_w36', dmtr,
                         output_dir='../../data/results',
                         measure_quantity='vox',
                         camera_azth=40.47,
                         camera_elev=32.5,
                         camera_fov=35.0,
                         camera_loc=(40.85, 46.32, 28.85),
                         camera_zoom=0.005124,
                         cb_x_offset=5,
                         width=620)
```


_static_w36_3d_orientation.png



1.3 API reference

1.3.1 quanfima.morphology module

1.3.2 quanfima.simulation module

quanfima.simulation.**additive_noise**(*params*, *noise_lvl*, *smooth_lvl*, *use_median=True*, *median_rad=3*)

Contaminates datasets with a speficied additive Gaussian noise and smoothing level.

Contaminates the datasets (generated with *generate_datasets* function) with the specified level of additive Gaussian noise and smoothing, uneven illumination can be added by extracting *blobs* from *params* tuple with some other arguments.

params [tuple] Contains *name*, *dataset_path*, *blobs*, *output_dir* arguments passed from *generate_noised_data*.

noise_level [float] Indicates the standard deviations of noise.

smooth_level [float] Indicates the sigma value of Gaussian filter.

use_median [boolean] Specifies if the median filter should be applied after addition of noise.

median_rad [integer] Indicates the size of median filter.

datasets_props [dict] The dictionary containing the path to the reference dataset, the path to the contaminated dataset, the generated name, the SNR level, the precision, the recall and f1-score, and the level of noise and smoothing.

quanfima.simulation.**generate_blobs**(*volume_size*, *blob_size_fraction=0.1*, *transparency_ratio=0.5*, *sigma=90.0*)

Generates random blobs smoothed with Gaussian filter in a volume.

Generates several blobs of random size in a volume using function from scikit-image, which are subsequently smoothed with a Gaussian filter of a large sigma to imitate 3D uneven illumination of the volume.

volume_size [tuple] Indicates the size of the volume.

blob_size_fraction [float] Indicates the fraction of volume occupied by blobs.

transparency_ratio [float] Indicates the transparency of blobs in a range [0, 1].

sigma [float] Indicates the sigma of Gaussian filter.

blobs_smeared [ndarray] The volume with smoothed blobs of a specified transparency.

quanfima.simulation.**generate_datasets**(*volume_size=(512, 512, 512)*, *n_fibers=50*, *radius_lim=(4, 10)*, *length_lim=(0.2, 0.8)*, *gap_lim=(3, 10)*, *max_fails=100*, *median_rad=3*, *intersect=False*, *output_dir=None*, *params=None*)

Simulates speficied configurations of fibers and stores in a npy file.

Simulates a number of fiber configurations speficied in *params* with *n_fibers* of the radii and lengths in ranges *radius_lim* and *length_lim*, separated with gaps in a range of *gap_lim*. The simulation process stops if the number of attempts to generate a fiber exceeds *max_fails*.

volume_size [tuple] Indicates the size of the volume.

n_fibers [integer] Indicates the number of fibers to be generated.

radius_lim [tuple] Indicates the range of radii for fibers to be generated.

length_lim [tuple] Indicates the range of lengths for fibers to be generated.

gap_lim [tuple] Indicates the range of gaps separating the fibers from each other.

max_fails [integer] Indicates the maximum number of failures during the simulation process.

median_rad [integer] Indicates the radius of median filter to fill holes occured due to rounding of coordinates of the generated fibers.

intersect [boolean] Specifies if generated fibers can intersect.

output_dir [str] Indicates the path to the output folder where the data will be stored.

params [dict] Indicates the configurations of orientation of fibers to be generated.

out [dict] The dictionary of generated datasets of specified configurations.

quanfima.simulation.**generate_noised_data**(*datasets_path, noise_levels=[0.0, 0.15, 0.3], smooth_levels=[0.0, 1.0, 2.0], blobs=None, use_median=True, median_rad=3, output_dir=None, n_processes=9*)

Contaminates datasets with a speficied additive Gaussian noise and smoothing level.

Contaminates the datasets (generated with *generate_datasets* function) with the specified level of additive Gaussian noise and smoothing, uneven illumination can be added if *blobs* is provided. The contaminating process can be performed in a parallel *n_processes* processes.

datasets_path [str] Indicates the path to dataset.

noise_levels [array] Indicates the array of standard deviations of noise.

smooth_levels [array] Indicates the array of sigma values of Gaussian filter.

blobs [ndarray] Indicates the volume of uneven illumination generated by *generate_blobs*.

use_median [boolean] Specifies if the median filter should be applied after addition of noise.

median_rad [integer] Indicates the size of median filter.

output_dir [str] Indicates the path to the output folder where the data will be stored.

n_processes [integer] Indicates the number of parallel processes.

results [array of dicts] The array of dictionaries containing paths to contaminated datasets, and other properties.

quanfima.simulation.**generate_particle_dataset**(*volume_size=(512, 512, 512), n_particles=500, radius_lim=(4, 10), max_fails=100, output_dir=None*)

Simulates a speficied number of particles and stores complete dataset in a npy file.

volume_size [tuple] Indicates the size of the volume.

n_particles [integer] Indicates the number of particles to be generated.

radius_lim [tuple] Indicates the range of radii for particles to be generated.

max_fails [integer] Indicates the maximum number of failures during the simulation process.

output_dir [str] Indicates the path to the output folder where the data will be stored.

out [dict] The dictionary of generated dataset.

quanfima.simulation.**mkfiber**(*dims_size*, *length*, *radius*, *azth*, *lat*, *offset_xyz*)

Computes fiber coordinates and its length.

Computes a fiber of speficied *length*, *radius*, oriented under azimuth *azth* and latitude / elevation *lat* angles shifted to *offset_xyz* from the center of a volume of size *dims_size*.

dims_size [tuple] Indicates the size of the volume.

length [integer] Indicates the length of the simulated fiber.

radius [integer] Indicates the radius of the simulated fiber.

azth [float] Indicates the azimuth component of the orientation angles of the fiber in radians.

lat [float] Indicates the latitude / elevation component of the orientation angles of the fiber in radians.

offset_xyz [tuple] Indicates the offset from the center of the volume where the fiber will be generated.

fiber_pts, fiber_len [tuple of array and number] The array of fiber coordinates and the length.

quanfima.simulation.**random_in**(*rng*, *number=1*)

Returns a random value within a given range.

quanfima.simulation.**simulate_fibers**(*volume_shape*, *n_fibers=1*, *radius_lim=(4, 10)*, *length_lim=(0.2, 0.8)*, *lat_lim=(0, 3.141592653589793)*, *azth_lim=(0, 3.141592653589793)*, *gap_lim=(3, 10)*, *max_fails=10*, *max_len_loss=0.5*, *intersect=False*)

Simulates fibers in a volume.

Simulates *n_fibers* of the radii and lengths in ranges *radius_lim* and *length_lim*, oriented in a range of azimuth *azth_lim* and latitude elevation 'lat_lim' angles, separated with a gap in a range of *gap_lim*. The simulation process stops if the number of attempts to generate a fiber exceeds *max_fails*.

volume_shape [tuple] Indicates the size of the volume.

n_fibers [integer] Indicates the number of fibers to be generated.

radius_lim [tuple] Indicates the range of radii for fibers to be generated.

length_lim [tuple] Indicates the range of lengths for fibers to be generated.

lat_lim [tuple] Indicates the range of latitude / elevation component of the orientation angles of the fibers to be generated.

azth_lim [tuple] Indicates the range of azimuth component of the orientation angles of the fibers to be generated.

gap_lim [tuple] Indicates the range of gaps separating the fibers from each other.

max_fails [integer] Indicates the maximum number of failures during the simulation process.

max_len_loss [float] Indicates the maximum fraction of the generated fiber placed out of volume, exceeding which the fiber is counted as failed.

intersect [boolean] Specifies if generated fibers can intersect.

(volume, lat_ref, azth_ref, diameter, n_generated, elapsed_time) [tuple of arrays and numbers] The binary volume of generated fibers, the volumes of latitude / elevation and azimuth angles at every fiber point, the volume of diameters at every fibers point, the number of generated fibers and the simulation time.

quanfima.simulation.**simulate_particles**(*volume_shape*, *n_particles=1*, *radius_lim=(3, 30)*, *max_fails=10*)

Simulates particles in a volume.

Simulates *n_particles* of the radii in a range *radius_lim*. The simulation process stops if the number of attempts to generate a particle exceeds *max_fails*.

volume_shape [tuple] Indicates the size of the volume.

n_particles [integer] Indicates the number of particles to be generated.

radius_lim [tuple] Indicates the range of radii for particles to be generated.

max_fails [integer] Indicates the maximum number of failures during the simulation process.

(volume, diameter, n_generated, elapsed_time) [tuple of arrays and numbers] The binary volume of generated particles, the volume of diameters at every point of particles, the number of generated particles and the simulation time.

quanfima.simulation.**unpack_additive_noise**(*args*)

Unpack arguments and return result of *additive_noise* function.

1.3.3 quanfima.utils module

1.3.4 quanfima.visualization module

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