CristalX

Release 1.1.0

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GETTING STARTED

Global intro

CHAPTER

ONE

CRISTALX

Identification of individual grains in microscopic images

CristalX is a Python package that helps in the analysis of polycrystalline microstructures. Its name originates from the French word 'cristal', corresponding to the English word 'crystal'.

1.1 Features

- Image segmentation to identify the grains in a microstructure
- Analysis tools for the segmented image
- Explicit geometrical representation of the grains
- Interacting with meshes created on the microstructure
- Mapping fields between a mesh and the grid of DIC measurements
- Simulation tools for the inverse problem arising from a combined numerical-experimental method (in progress . . .)
- Visualization and data exchange

1.2 Getting help

1. Read the documentation.
2. Check the existing issues. They may already provide an answer to you question.
3. Open a new issue.

1.3 Contributing

Read the `docs/source/contributing.md` file.

1.4 Citing *CristalX*

We have an article freely available on SoftwareX, showing the background and the design of *CristalX*.

When using *CristalX* in scientific publications, please cite the following paper:

- Csati, Z.; Witz, J.-F.; Magnier, V.; Bartali, A. E.; Limodin, N. & Najjar, D. *CristalX: Facilitating simulations for experimentally obtained grain-based microstructures*. SoftwareX, **2021**, *14*, 100669

BibTeX entry:

```
@Article{Csati2021,
  author    = {Zoltan Csati and Jean-Fran{\c{c}}ois Witz and Vincent Magnier and
↪Ahmed El Bartali and Nathalie Limodin and Denis Najjar},
  journal   = {{SoftwareX}},
  title     = {{CristalX}: {F}acilitating simulations for experimentally obtained
↪grain-based microstructures},
  year      = {2021},
  month     = jun,
  pages     = {100669},
  volume    = {14},
  doi       = {10.1016/j.softx.2021.100669},
}
```

CHAPTER

TWO

INSTALLATION

CristalX is easy to install; you can get started in minutes.

2.1 Dependencies

CristalX is a written in pure Python, although it relies on packages that use other languages (mostly C and C++). However, it is not a problem from the user's perspective as no manual compilation is needed. Those who are interested can see the dependencies in the `environment.yml` file in the root directory.

Whether you install *CristalX* by *conda* or try it online, all but one dependency is installed. In a common workflow, that single missing dependency will not affect you. For details, see ...

2.2 Try it online

If you just want to get a taste of *CristalX*, you can try it online without installing anything.

Click here to jump to the root directory. Existing Jupyter notebooks are in the `notebooks/` directory. You can modify them and create new ones. If you directly want to open the main tutorial, which describes a real-world application, click here.

2.3 Install it locally

If you want more control (debugging, inspecting variables, etc.) over *CristalX* or if you wish to contribute to the project, it is recommended to install it on your machine.

2.3.1 Obtain the source

If you are a user of *CristalX*, the best is to get the latest release:

- download it from GitHub
- or clone it with Git:

```
git clone https://github.com/CsatiZoltan/CristalX.git
cd CristalX
git checkout v<version_number>
```

where `<version_number>` is the version you want to use. E.g. if you want to use version 1.0.1, you need to type `git checkout v1.0.1`. See the available tags, corresponding to the published releases, for the possibilities.

Note that in this case, you will be in a "detached HEAD" state, meaning that the HEAD does not point to a branch but to the specific tag. Any commit you make in this state will not be associated with a branch. Therefore, if you want to develop or contribute to *CristalX*, check out the *master* branch (see the next paragraph).

If you want to develop *CristalX* or simply want to have access to the latest features, you need to fetch the latest state:

- download it from GitHub
- or clone it with Git:

```
git clone https://github.com/CsatiZoltan/CristalX.git
```

2.3.2 Install with *conda*

All you need to have is the *conda* package manager. Open a terminal (or a command prompt if you are under Windows) in the root directory and type

```
conda env create -f environment.yml
```

CristalX has been installed to a separate environment, so you can safely work inside it. Activate that environment:

```
conda activate CristalX
```

Once you have finished working with *CristalX*, either close the terminal or type

```
conda deactivate
```

to return to your default *conda* environment.

If you want to uninstall *CristalX*, make sure that the `CristalX` conda environment is not active and then

```
conda env remove -n CristalX
```

When uninstalled, `conda env list` will not show it.

2.3.3 Install with *pip*

If you do not have *conda* or you prefer *pip*, you can also install *CristalX* by typing

```
pip install -r requirements.txt
```

assuming that you have Python installed. It is highly recommended that you first create a new virtual environment to make sure you do not break your Python installation. However, an important component of *CristalX* (functions that rely on *PythonOCC*) will **not** be installed if you choose *pip*. The reason for this is that *PythonOCC* is not (yet) available on PyPI.

CHAPTER

THREE

DOCUMENTATION

The documentation for *CristalX* is available both locally and online. It is generated by Sphinx and consists of the code documentation and the various guides (including the one you are currently reading). If you want to extend the documentation, please read the *corresponding section* in the Developer guide.

3.1 Local documentation

It resides in the `docs/` directory. Open a terminal there and type `make html`. The output will be written to `docs/build/`. Open `docs/build/html/index.html` to land on the home page of the documentation.

3.2 Online documentation

For every *push event*, the documentation is rebuilt by Read the Docs. The latest HTML version is available on https://cristalx.readthedocs.io/en/latest. Read the Docs is configured to build a PDF and EPUB output as well. All three formats can be downloaded for offline use if you click on the bottom of the left sidebar. For convenience, here are the direct links: HTML, PDF, EPUB.

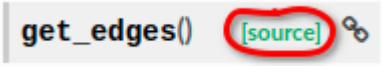
3.3 Using the HTML documentation

For browsing on a computer, the HTML documentation is the most convenient and feature-rich.

The side-bar on the left provides quick navigation.

Code example boxes have two toggle buttons. Clicking on the prompt button >>> hides the prompt and the output. If you then click on the copy icon next to it, you can copy the contents of the box, making it easy to try the code chunks in your Python environment.

A direct link can be obtained for most sections, including the code documentation, by moving the cursor to the right of the text and then clicking on the chain icon.

When browsing the API documentation and want to look at the implementation, you can easily access the source code by clicking on the `[source]` tag. 

CHAPTER

FOUR

HOW TO USE THE CODES

If you want to get to know the classes and functions, the best is to check the *API documentation*. Most components are amply documented and contain one or more examples. If you want to see them in action, check out our *workflow* for a real-world application. If you are curious about the underlying algorithms, consult with the *Algorithms* section.

4.1 Tutorials

The tutorials are available in two forms: Python scripts and Jupyter notebooks.

4.1.1 Python scripts

The scripts are intended to be run in batch mode. They need to be run in a specific order as the subsequent scripts rely on the output of the previous ones. These scripts are useful if you are already a bit familiar with *CristalX* or if you wish to adapt the scripts to your needs. Indeed, if you intend to extend the package, the safest way is to copy the relevant scripts and modify them. The scripts are named as `run_moduleName`, where `moduleName` is the name of the module in the `grains/` directory that the script mainly relies on. In some way, `run_moduleName` acts as a demonstration of what the `moduleName` module is used for. The scripts are meant to be run as modules, i.e. navigate to the root of the project and type

```
python -m scripts.moduleName
```

4.1.2 Jupyter notebooks

Almost the same workflow is available as a single Jupyter notebook, located at the `nootebooks/` directory. this allows you to interactively discover *CristalX* through an example. You can easily rerun parts of the code to see the effects of the parameters, and the rich output is embedded into the same document. If you are a novice Python user or just want to have a taste of *CristalX*, notebooks are the recommended way to get started.

4.2 Undo changes

When you experiment with *CristalX*, you will probably change parameter values. As the scripts communicate by reading and writing data, the original data that come with *CristalX* will be overwritten. There are multiple ways to undo the changes.

4.2.1 In Binder

As written in the *Installation instructions*, you can try *CristalX* online without the need to install anything on your computer. Then a separate virtual environment is created. Whatever changes you make there, they will not influence your local installation (if you have) or the data on the GitHub repository.

4.2.2 In a local installation

If you downloaded *CristalX* from GitHub, you can simply replace the new files with the original ones. In case you cloned *CristalX* with Git, you can easily discard the changes you make.

CHAPTER

FIVE

A DETAILED WORKFLOW

CristalX contains several modules that facilitate experimental and numerical works on polycrystalline microstructures. The usage of these modules is demonstrated on a complex example.

5.1 Problem formulation

Grain-based microstructures occur in nature but also develop during industrial processes. We are interested in how the size and the distribution of grains, and the material they are made up of influence the resistance of train wheels and axles to fatigue loading. The problem requires that

- the individual grains can be distinguished on a microscopic image
- a good quality mesh is generated on the microstructure
- the numerical solution obtained on this mesh can be compared to full-field measurements

The first two steps are discussed here.

5.2 Initial setup

First, we switch to the root directory of the project so that the package imports are consistent. Note that the relative path always works because the current directory in case of a Jupyter notebook is always the directory in which the notebook is.

[1]:
```
import os
os.chdir('../')
main_dir = os.path.abspath(os.curdir)
```

Let us set the directory that will hold our data.

[2]:
```
data_dir = os.path.abspath('data')
try:
    os.mkdir(data_dir)
except FileExistsError:
    pass
```

We now copy the necessary data files that come with *CristalX* into this freshly created directory.

[3]:
```
from os.path import join
from shutil import copy
selected_files = ['1.png', '1_cropped.png', 'splinegons.png', '1_mesh_extended.npz']
```

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```
for file in selected_files:
    copy(join('scripts/data', file), data_dir)
```

In interactive mode, debug information are displayed. They are not useful for presentation purposes as they pollute the rendered output. Similarly for runtime warnings.

[4]:
```
import logging
logging.basicConfig(level=logging.ERROR)
import warnings
warnings.simplefilter('ignore')
```

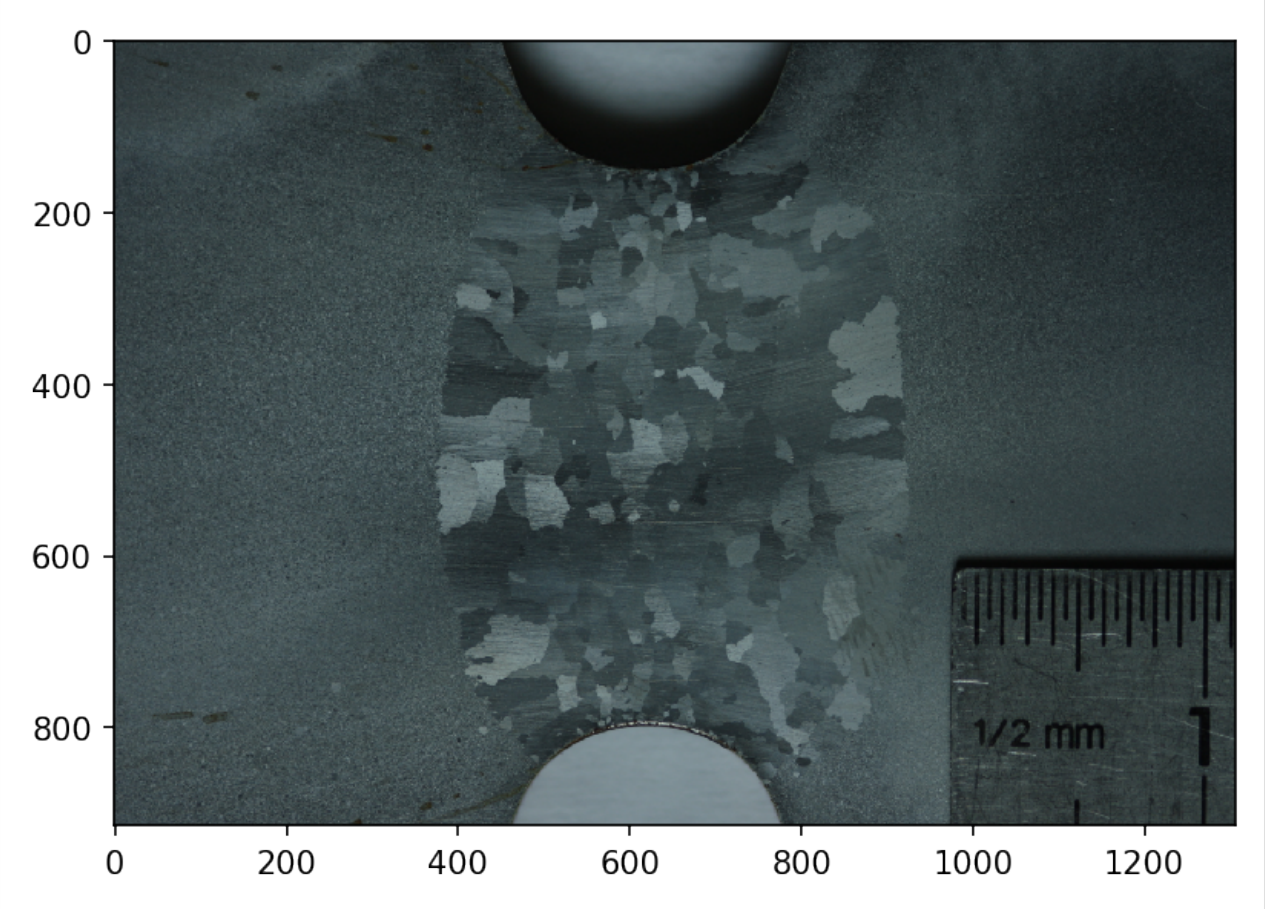
For the figures to be visible in this notebook, we define a utility function to scale them.

[5]:
```
import matplotlib.pyplot as plt
def scale_figure(dpi):
    plt.gcf().set_dpi(dpi)
```

5.3 Identify grains in a microstructure

The picture below was taken with a digital camera and shows the central part of a tensile specimen. In this section, we will identify the individual grains in the image.

[6]:
```
from skimage.io import imshow
imshow(join(data_dir, '1.png'))
scale_figure(150)
```



So that the surrounding region does not interfere with the segmentation, we will work on a cropped region.

[7]:
```
from skimage.io import imread
import numpy as np
image = join(data_dir, '1_cropped.png')
```

As you can see, the RGB image is represented as a 3D numpy array.

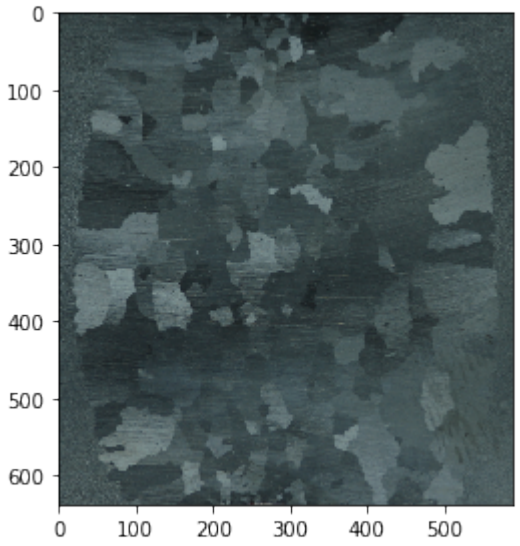
[8]:
```
image_as_matrix = imread(image)
type(image_as_matrix), image_as_matrix.shape
```

[8]:
```
(numpy.ndarray, (638, 589, 3))
```

However, you do not explicitly have to deal with this matrix as the `Segmentation` class will handle it.

The `Segmentation` class offers a set of methods to perform the consecutive steps of the segmentation workflow. We pass to the constructor the path to the image to be segmented. By default, the resulting images are shown at the end of each step. In batch mode, you probably want to set the `interactive_mode` optional parameter to `False`. But in this interactive document, we want to see the outputs.

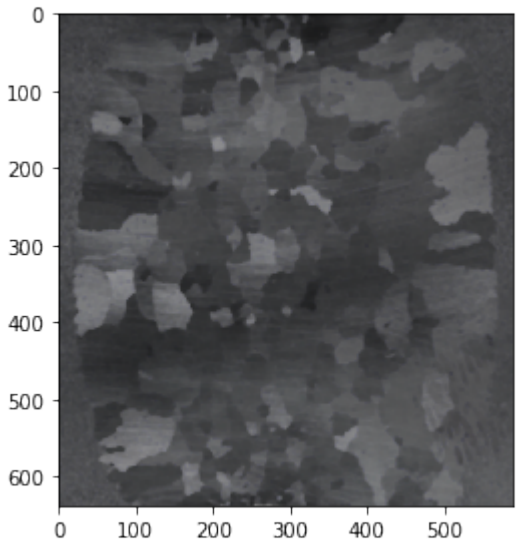
[9]:
```
from grains.segmentation import Segmentation
GS = Segmentation(image)
```




```
Image successfully loaded.
```

After the image has been loaded and stored in the `GS` object, we want to remove the noise. Since the interfaces among the grains are important for us, we use median filtering for smoothing as it preserves the contours. The smoothing is governed by the *window size*. The larger this number, the smoother the processed image is, and the higher the computational cost becomes.

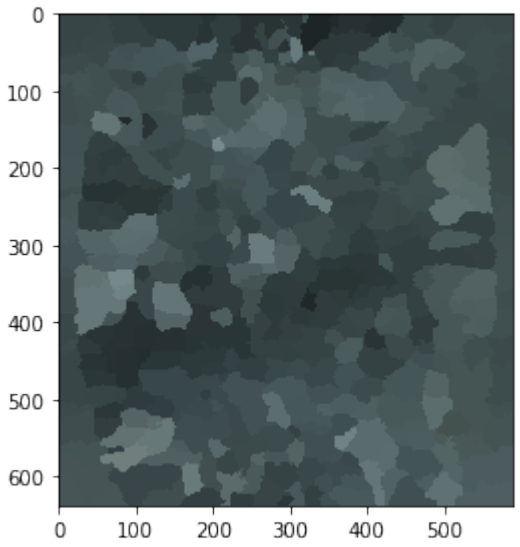
[10]:
```
filter_window_size = 5
filtered = GS.filter_image(filter_window_size)
```




```
Median filtering finished.
```

To improve the segmentation result later, we perform *superpixel segmentation* as an initial step. During this process, the image is subdivided into superpixels, groups of pixels that belong together based on colour, spatial distance or other properties. On this image, a superpixel algorithm called *Quick Shift* proved to be the best among the algorithms available in *scikit-image*.

[11]:
```
segmented = GS.initial_segmentation(filtered)
```




```
Quick shift segmentation finished. Number of segments: 421
```

The result is indeed a segmented (also called labelled) image. Distinct positive integers, called labels, are associated to groups of pixels in the labelled image and each pixel belongs to one and only one such group.

[12]:
```
segmented
```

[12]:
```
array([[  8,   8,   8, ...,   2,   2,   2],
       [  8,   8,   8, ...,   2,   2,   2],
       [  8,   8,   8, ...,   2,   2,   2],
       ...,
       [400, 400, 400, ..., 414, 414, 414],
       [400, 400, 400, ..., 414, 414, 414],
       [400, 400, 400, ..., 414, 414, 414]])
```

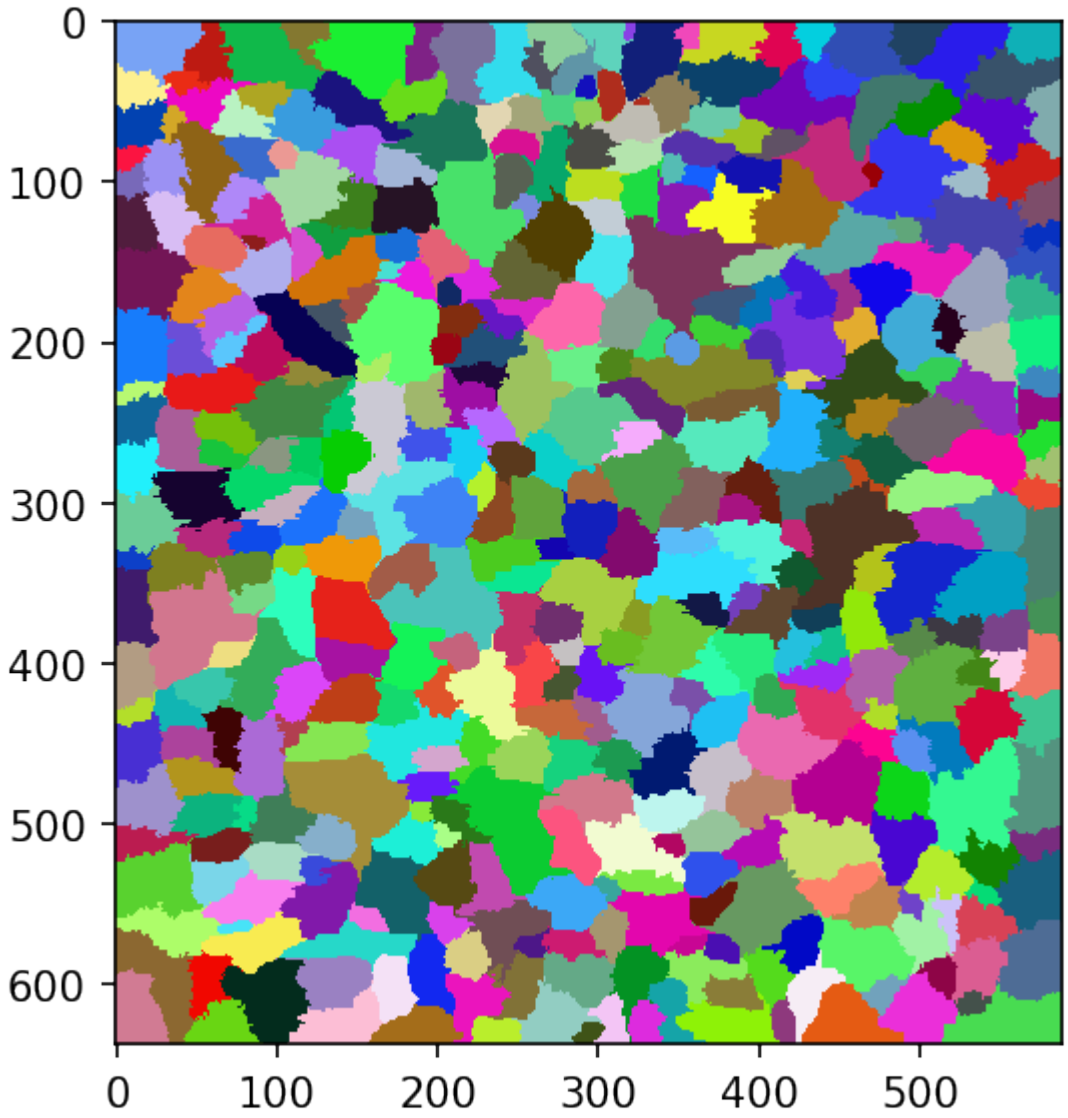
The segmented image has the same size as the original image, but it is not an RGB image any more.

[13]:
```
segmented.shape, image_as_matrix.shape
```

[13]:
```
((638, 589), (638, 589, 3))
```

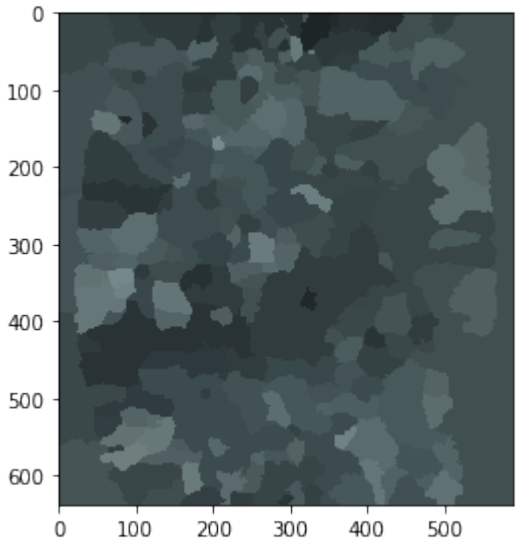
We can visualize a labelled image by associating different colours to the different labels.

[14]:
```
from skimage.color import label2rgb
from numpy.random import random
nlabel = len(np.unique(segmented))
imshow(label2rgb(segmented, colors=random((nlabel, 3))))
scale_figure(150)
```



As the superpixel segmentation in the previous step resulted in an oversegmented image, the region adjacency graph is constructed and used to merge some of the neighbouring superpixels based on their similarity with respect to mean colour. Regions connected by edges with smaller weights than a prescribed threshold are combined. As you can see, the number of supersegments decreases.

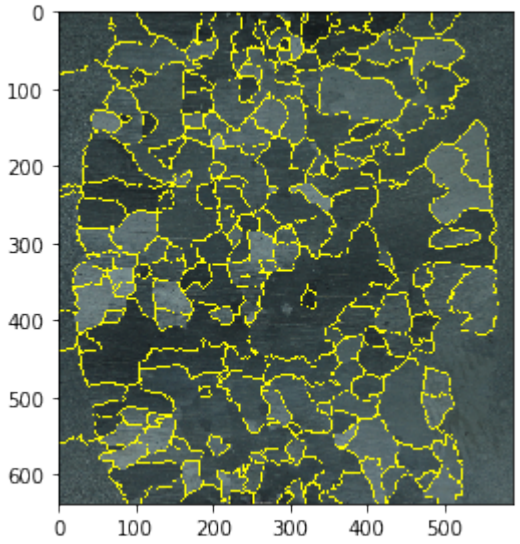
[15]:
```
cluster_merging_threshold = 7
reduced = GS.merge_clusters(segmented, threshold=cluster_merging_threshold)
```




```
Tiny clusters merged. Number of segments: 177
```

We need a few more steps before succesfully applying another segmentation technique to obtain the final segmented image. First, we detect the grain boundaries. They are shown superposed on the original image.

[16]:
```
boundary = GS.find_grain_boundaries(reduced)
```




```
Grain boundaries found.
```

The boundary image is a binary image in which the `True` values indicate the boundaries among the labelled regions.

[17]:
```
boundary
```

[17]:
```
array([[False, False, False, ..., False, False, False],
       [False, False, False, ..., False, False, False],
       [False, False, False, ..., False, False, False],
       ...,
       [False, False, False, ..., False, False, False],
```

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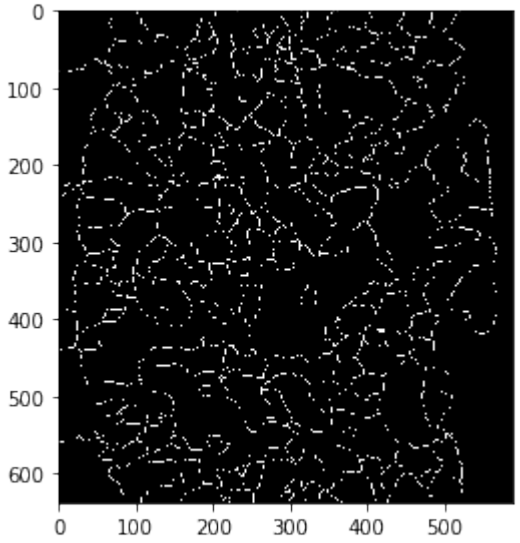
```
       [False, False, False, ..., False, False, False],
       [False, False, False, ..., False, False, False]])
```

The we use thinning on the grain boundary to obtain a single-pixel wide skeleton.

[18]:
```
skeleton = GS.create_skeleton(boundary)
```

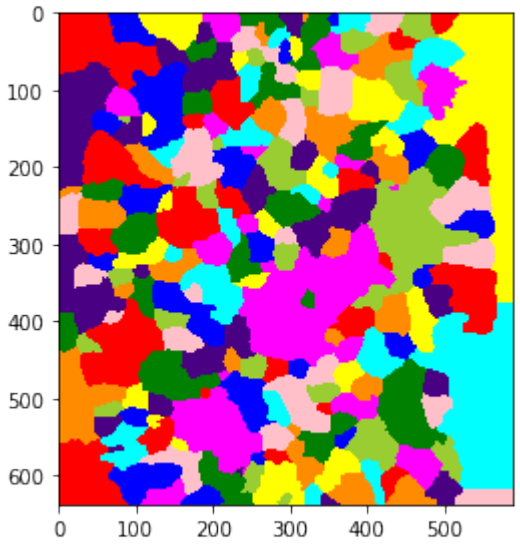



```
Skeleton constructed.
```

If the automatic segmentation carried out so far is not good enough, the user can manually edit the skeleton as a graph in ImagePy. The combination of the automatic segmentation with human supervision is a powerful way to achieve good results in a relatively short amount of time. Here, we stay with the automatic method.

To recover the segments again, we use *watershed segmentation* on the skeleton. Had it been directly applied on the original image, the result of the watershed segmentation would have been an oversegmented image due to the noises that act as local minima. The success of the watershed segmentation depends on how well the catchment basins are identified, which are the locations where the flooding starts. The so-called marker-based watershed segmentation methods rely on markers (computed automatically or given by the user), i.e. the location of the catchment basins, as inputs. In the `watershed_segmentation` method of the `Segmentation` class, various transformations are used to obtain a desirable outcome.

[19]:
```
watershed = GS.watershed_segmentation(skeleton)
```




```
Watershed segmentation finished. Number of segments: 247
```

To the left and to the right of the central zone, artificial "grains" appear. This is not a problem, they can either be merged, or left as it is and associate the same material to them.

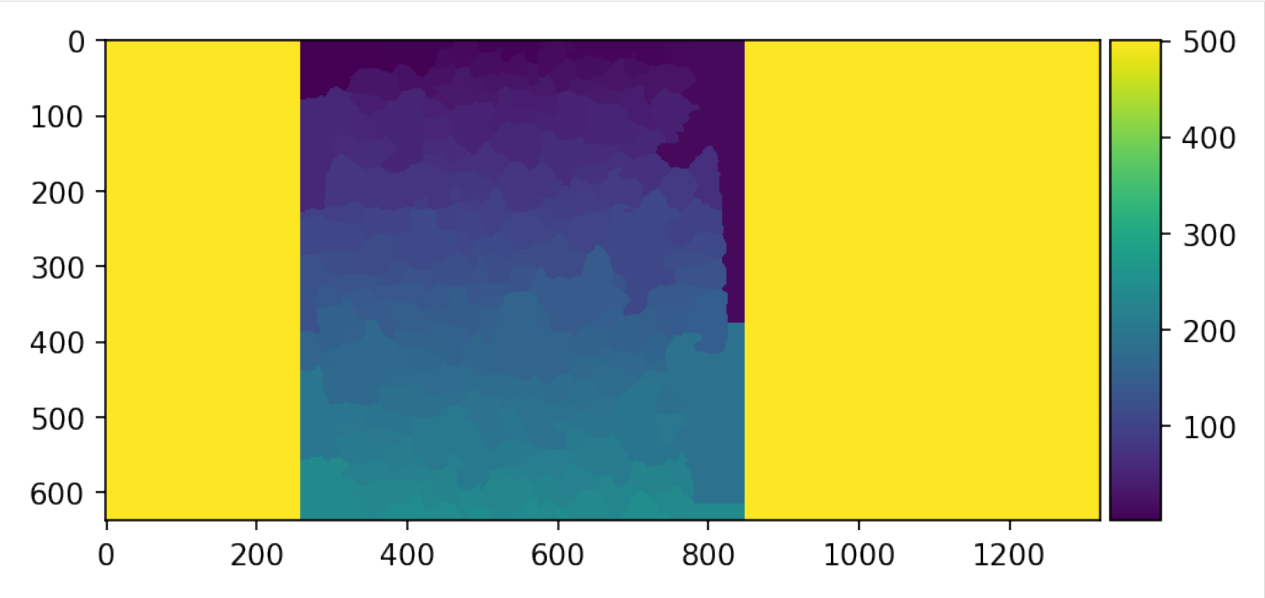
5.4 Extending the image domain

The segmented image corresponds to the recrystallized part of the specimen. When we perform the traction test numerically we need a larger domain, the boundary on which the boundary conditions are applied. The size of this extended domain does not have to match with the physical size of the tensile specimen, but it has to be sufficiently large so that the far-field boundary conditions do no not influence the deformation state in the central region.

As a first step, we extend the domain by padding the corresponding numpy array. Since we want to handle the added domains (grains) on the left and on the right as separate grains, we associate different labels to them. There are about 250 grains in the central region, so choosing labels 500 and 501 ensures that these regions have unique labels.

The extended domain is constructed in such a way that it matches the region of the DIC measurements. This will be useful when comparing the results of the simulation with the experimental data.

[20]:
```
from grains.simulation import change_domain
extended_image = change_domain(watershed, 0.4395, 0, 0, 0, 500)
extended_image = change_domain(extended_image, 0, 0.5568, 0, 0, 501)
imshow(extended_image)
scale_figure(150)
```



5.5 From image to geometry

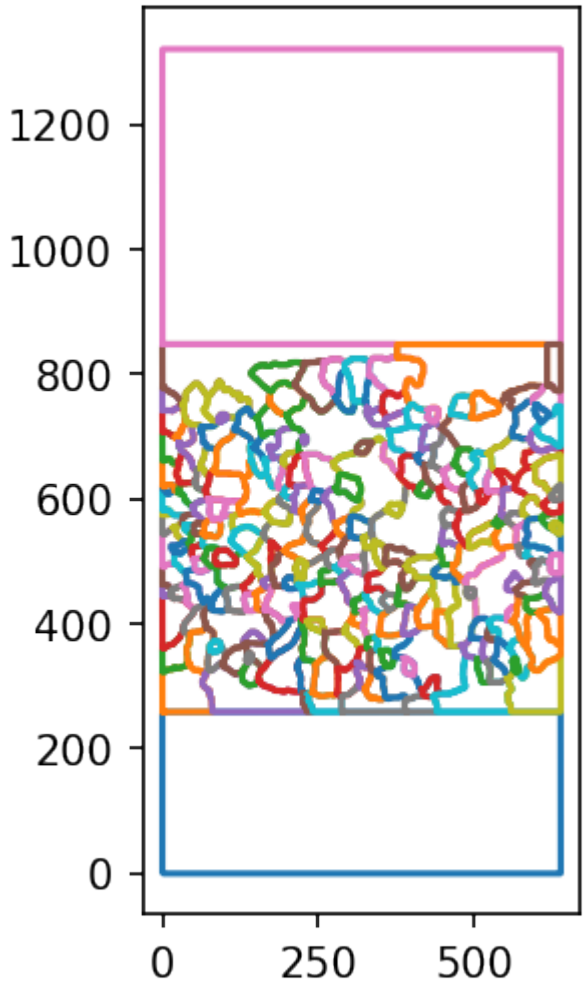
In this section, we show how to represent the grains as an explicit geometry. See our paper for the motivation.

For grain representation, we can choose between polygon and splinegon approximations. We will base the meshing on the splinegon representation, but the polygons are also shown. The high-level functions `polygonize` and `splinegonize` wrap all the important algorithms. You can see from the code below that they share similar function signature. The only difference is that the spline parameters can be provided to the `splinegonize` function.

[21]:
```
from grains.cad import polygonize, search_neighbor, splinegonize
polygons = polygonize(extended_image, search_neighbor(2, np.inf), connectivity=1)
splinegons, _ = splinegonize(extended_image, search_neighbor(2, np.inf),␣
↪connectivity=1, degree_min=3, degree_max=3, continuity='C0', tol=1)
```

Let us plot the grains. For polygons:

[22]:
```
from grains.cad import plot_polygons
plot_polygons(list(polygons.values()));
scale_figure(150)
```



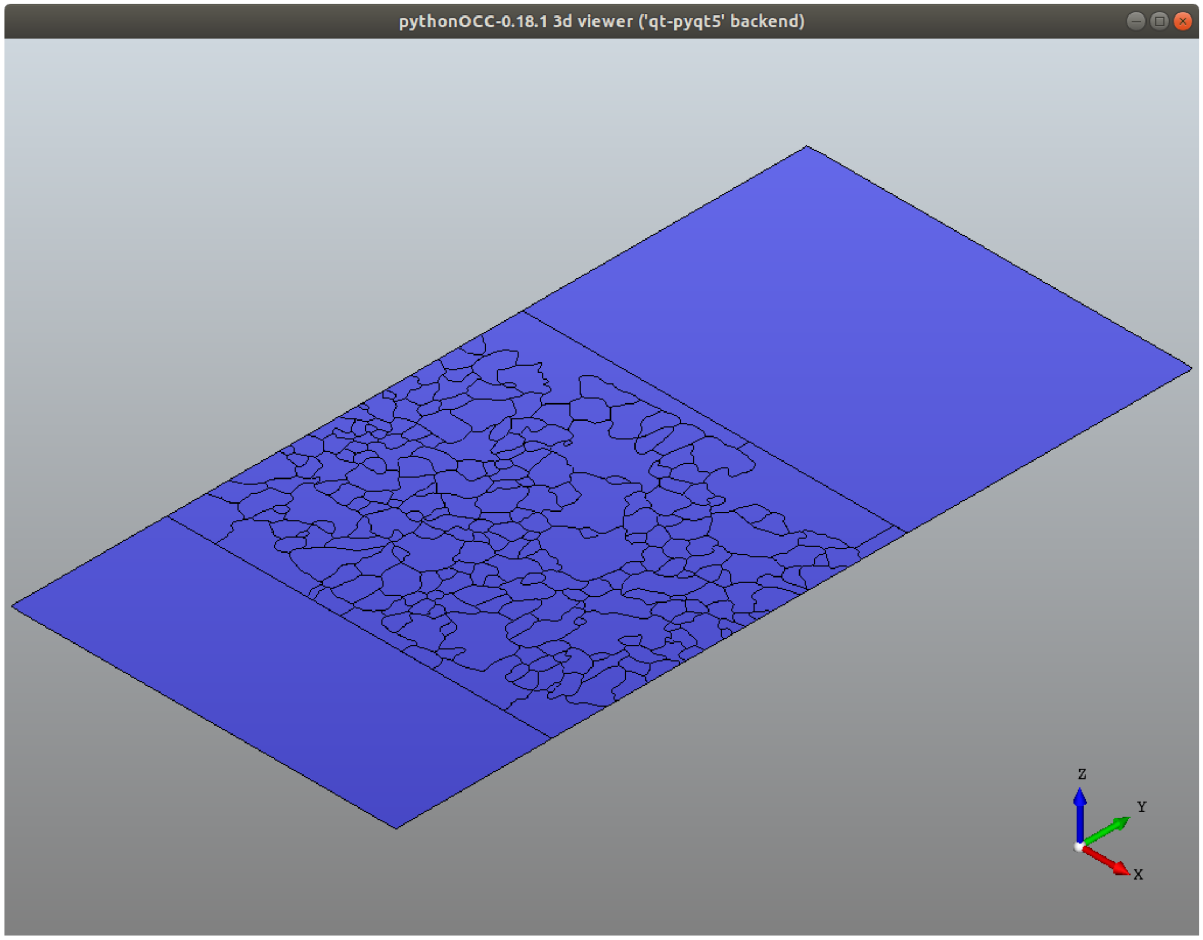
Plotting the spline surfaces will bring up a window.

[23]:
```
from grains.cad import plot_splinegons
from OCC.Display.SimpleGui import init_display
plot_splinegons(list(splinegons.values()), color=(0, 0, 1))
```

```
Layer manager created
Layer dimensions: 1024, 768
```

To allow reading this document statically, here is a screenshot of the window that popped up.

[24]:
```
fig, ax = plt.subplots(dpi=500)
imshow(join(data_dir, 'splinegons.png'), ax=ax)
ax.set_axis_off()
```



Once we have the spline surfaces, we write them to a STEP file. This allows us to edit the geometry in a CAD program and to generate a mesh for the grains.

[25]:
```
from grains.cad import regions2step
regions2step(list(splinegons.values()), join(data_dir, 'microstructure.stp'))
```

5.6 Repairing the geometry

For the sample microstructure, one grain was not identified, i.e. it contains a hole. The hole can be filled in by creating a new grain. We have a detailed guide on how to do this.

5.7 Mesh generation

The same guide linked in the previous section continues with the mesh generation. It happens that we constructed the conforming mesh in Salome, and then exported it to a .med file. Using the med module of *CristalX*, the triangular mesh cells for each grain and the boundary nodes have been extracted. We also have a tutorial on how to process a .med file.

5.8 Modifying the mesh

First, we obtain the mesh data that was saved using the `med` module.

[26]:
```
mesh_file = join(data_dir, '1_mesh_extended.npz')
with np.load(mesh_file, allow_pickle=True) as mesh:
    nodes = mesh['nodes']
    elements = mesh['elements']
    element_groups = mesh['element_groups']
    node_groups = mesh['node_groups']
# Retrieve groups, which were stored in dictionaries (https://stackoverflow.com/a/
↪40220343/4892892)
element_groups = element_groups.item()
node_groups = node_groups.item()
```

The array `elements` contains the label of the nodes in the mesh.

[27]:
```
elements
```

[27]:
```
array([[  603,   604,  4311],
       [  604,    19,   605],
       [  606,    18,  4312],
       ...,
       [13377, 13369, 13374],
       [13372, 13377, 13373],
       [13373, 13370, 13372]])
```

The array `nodes` holds the coordinates of each node of the mesh.

[28]:
```
nodes
```

[28]:
```
array([[2.50000000e-01, 2.59000000e+02],
       [8.00000000e+01, 2.59250000e+02],
       [2.31000000e+02, 2.59250000e+02],
       ...,
       [6.28062814e+02, 8.02235833e+02],
       [6.22855688e+02, 7.95968504e+02],
       [6.23756131e+02, 7.89612749e+02]])
```

The elements are available for each grain. For instance, grain 87 is labelled as *Face_87* and it contains the following elements.

[29]:
```
element_groups['Face_87']
```

[29]:
```
array([23231, 23232, 23233, 23234, 23235, 23236, 23237, 23238, 23239,
       23240, 23241, 23242, 23243, 23244, 23245])
```

We mentioned earlier that some grains are artefacts of the watershed segmentation. In other words, they are outside the recrystallized central region. Therefore, those grains along with the two extensions (that were given the labels 500

and 501) were merged in Salome and a single mesh was constructed on the merged region. That region contains the most elements.

[30]:
```
len(element_groups['homogeneous'])
```

[30]:
```
3718
```

To be able to prescribe boundary conditions later, the boundary nodes were also exported from Salome.

[31]:
```
node_groups
```

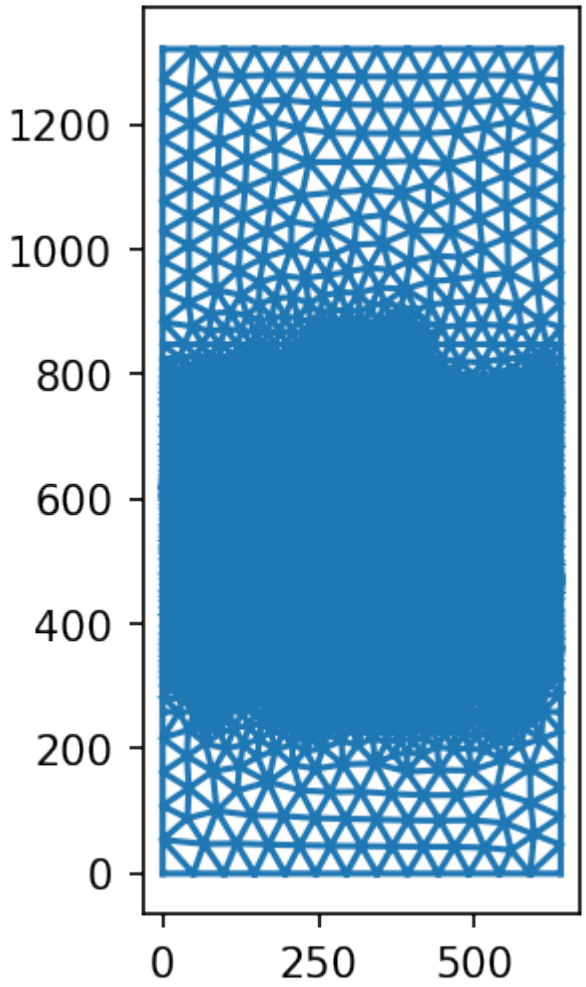
[31]:
```
{'bottom': array([   8,   14,  448,  452,  467,  468,  470,  471,  472,  474,  475,
         477,  478,  479,  480,  481,  482,  495,  496,  497,  498,  499,
         557,  558,  559,  560,  561,  562,  563,  564,  565, 3673, 3674,
        3675, 3676, 3706, 3707, 3708, 3839, 3840, 3841, 3842, 3851, 3852,
        3861, 3862, 3863, 3864, 3865, 3866, 3867, 3874, 3880, 3881, 3882,
        3883, 3884, 3885, 3886, 3887, 3888, 3895, 3896, 3897, 3914, 3915,
        3922, 3923, 3924, 3925, 3926, 3930, 3931, 3932, 3933, 3943, 3944,
        3945, 3951, 3952, 3953, 3954, 3955, 3956, 3957, 3958, 3959, 3960,
        3961, 3962, 3963, 3964], dtype=int32),
 'left': array([  9,  10, 483, 484, 485, 486, 487, 488, 489, 490, 491, 492, 493,
        494], dtype=int32),
 'right': array([ 15,  16, 545, 546, 547, 548, 549, 550, 551, 552, 553, 554, 555,
        556], dtype=int32),
 'top': array([   0,   11,   17,   20,   21,   25,   28,   33,   34,   36,   44,
          45,   46,   52,   61,   63,  541,  542,  543,  544,  594,  595,
         596,  597,  598,  599,  600,  601,  602,  609,  653,  654,  655,
         656,  673,  674,  675,  676,  677,  678,  679,  702,  703,  704,
         705,  706,  707,  724,  725,  749,  750,  751,  759,  760,  761,
         762,  763,  764,  812,  813,  814,  815,  816,  817,  827,  828,
         829,  830,  831,  832,  848,  849,  850,  851,  896,  897,  898,
         920,  921, 1637, 1638, 1639, 1640], dtype=int32)}
```

Handling all these data individually is tedious. Hence, we created a mesh class that bundles them and defines operations on them. The `TriMesh` class is an abstraction for a triangular mesh. First, we initialize it with the elements and the nodes that were loaded from the *1_mesh_extended.npz* file.

[32]:
```
from grains.geometry import TriMesh
mesh = TriMesh(nodes, elements)
```

The `TriMesh` class has several options to plot the mesh, for now we consider the default plotting.

[33]:
```
mesh.plot()
scale_figure(150)
```



Then the element and node sets are associated to the mesh object.

[34]:
```
# Associate the element and node groups to it
for group_name, elements in element_groups.items():
    mesh.create_cell_set(group_name, elements)
for group_name, nodes in node_groups.items():
    mesh.create_vertex_set(group_name, nodes)
```

Mesh-based discretization methods often presume that the node ordering within an element is counter-clockwise. To make sure this is the case, we explicitly enforce it.

[35]:
```
mesh.change_vertex_numbering('ccw', inplace=True);
```

The mesh was created on the geometry, which was constructed based on the image, i.e. in pixel units. For the simulation to be comparable with the experimental data (full-field measurement), the real size of the tensile speciment must be given. In the first image of this notebook, you can observe a ruler. With the help of it, we set the correspondance between the physical unit and the pixel unit: there are 29.55 pixels in 1 mm.

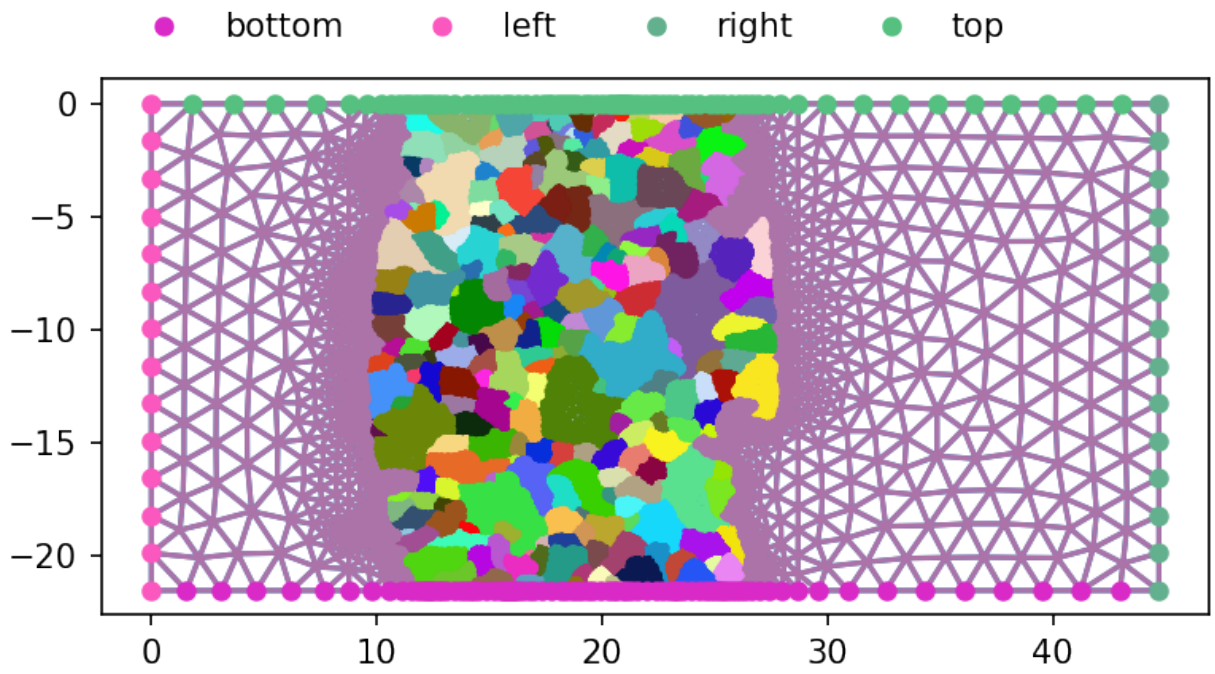
[36]:
```
mesh.scale(1/29.55, inplace=True);
```

For convenience, we rotate the specimen so that its axis is parallel to the horizontal tensile loading.

[37]:
```
from math import pi
mesh.rotate(-pi/2, inplace=True);
```

Let us check if this is what we wanted.

[38]:
```
mesh.plot(vertex_legends=True)
scale_figure(150)
```



We are satisfied with the resulting transformations, so let us save them.

[39]:
```
np.savez_compressed(join(data_dir, '1_mesh_extended_scaled.npz'),
                    nodes=mesh.vertices, elements=mesh.cells,
                    element_groups=mesh.cell_sets, node_groups=mesh.vertex_sets)
```

5.9 Conclusions

We successfully obtained a good quality mesh starting from an image.

In the near future, we will solve an inverse problem to identify characteristic parameters in the constitutive model. This optimization task requires the comparison of the numerical solution obtained on the mesh with the measured field values acquired through digital image correlation (DIC). Some of this work is already available in the `dic` and `simulation` modules.

This document is meant to serve as a global overview of what *CristalX* can be used for. Feel free to play with the parameters to investigate their effects. The functions and classes of *CristalX* provide many more functionalities. Browse the documentation to familiarize yourself with the details.

The initially created directory (`data/`) is now deleted.

[40]:
```
from shutil import rmtree
try:
    rmtree(data_dir)
except FileNotFoundError:
    pass
```

CHAPTER

SIX

GEOMETRY AND MESH PROCESSING IN SALOME

The *cad* module, as shown in the *Algorithms* section, allows to approximate a segmented image with planar spline surfaces (splinegons) and those surfaces can be written to a STEP file. Now, we demonstrate on the sample microstructure how to repair the geometry and generate a conforming mesh on the splinegons. All the manipulations are done in Salome 9.4.0.

6.1 Geometry

1. Import the geometry To import a STEP file (obtained by writing the splinegons into a STEP file), select the *Geometry* module and then *File -> Import -> STEP*.
2. Repair the geometry

   For the sample microstructure, one grain has not been identified, i.e. it contains a hole. To fill the hole, we perform the following steps (always select the object that was created the last time):

   1. *Repair -> Close Contour* and select the (in our sample) two boundary curves of the unidentified grain.
   2. *Repair -> Suppress Holes* and select the two boundary curves you selected in the previous step. Salome informs you that a face will be created in place of the hole.
   3. *Repair -> Limit tolerance* and set the tolerance to 1e-3.
   4. *Repair -> Sewing* and set 1e-2 for the tolerance.
3. Extract the grains We will need the mesh on each grain, therefore, we extract the grain faces by "exploding" the microstructure using *New Entity -> Explode*. In the dialog box, select the sewn geometry (end result of the geometry repairing workflow above) as *Main Object* and *Face* as *Sub-shapes Type*. Salome properly identifies the 250 sub-shapes, i.e. the grains.
4. Fix the "artificial" grains

   The sample microstructure describes the central part of a tensile specimen. However, to adhere to the Saint-Venant principle, the loading is exerted further from this central zone. Hence, we created long enough regions in the direction of the prescribed load by attaching two rectangular faces to the central region. These faces are not precise rectangles because the boundary of the microstructure does not consist of straight segments. Nevertheless, from now on, we will use the term rectangle to describe the extended region. To achieve perfect matching between the rectangle and the boundary of the microstructure, one side of the rectangle must contain the same lines as the boundary of the microstructure. The other three sides will be straight line segments.

   1. We want to extract the boundary lines of the microstructure. To do that, we explode the boundary grains into edges with *New Entity -> Explode*. The *Main Object* in the dialog box is a selected boundary grain, and the *Sub-shape Type* is *Edge*. Do this with all the boundary grains.
   2. Create the three sides of the rectangle

1. Create the four vertices of the rectangle with *New Entry -> Basic -> Point*. Two of these points are the extremities of the microstructure, the other two are given such that
   - the rectangle's three sides become parallel to the coordinate axes (so that boundary conditions are easily prescribed)
   - the length of the longer side of the rectangle is long enough compared to the microstructure (we applied a ratio of 5)
2. Connect these vertices with three lines, which forms the three sides of the rectangle: *New Entity -> Build -> Edge*.

3. Create the rectangle by connecting the three line segments constructed in the previous step with the boundary lines of the fourth side, obtained by exploding the boundary grains: *New Entity -> Build -> Wire*.
4. Delete the original "artificial" grain as it will be replaced by the new one.
5. Create the surface enclosed by the rectangle: *New Entity -> Build -> Face*, and select the wire created before. Perform steps 1-5 for the other rectangle (on the other side of the microstructure) as well.
6. In order to create a conforming mesh on the whole domain (i.e. on the microstructure and on the two rectangles), we need to create a compound surface: *New Entity -> Build -> Compound* and select the grains plus the two rectangles.
7. It is not enough to create the mesh, we also need to know which elements belong to which grains. To allow this, we explode the compound surface: select the compound object created in the previous step as the *Main Object* in *New Entity -> Explode*. The *Sub-shape Type* is *Face*, as before.

The geometry is now impeccable, let us start meshing.

6.2 Mesh

Select the *Mesh* module.

1. Create the mesh
   1. Choose *Mesh -> Create Mesh* from the menu. The geometry on which the mesh will be created is the compound surface.
   2. The mesh type in this study is *Triangular* and the algorithm is *NETGEN 1D-2D*. Choose *NETGEN 2D Parameters* as a hypothesis and experiment with the settings to suit your needs. Accept the changes.
   3. Choose *Mesh -> Compute* to generate the mesh with the chosen settings.

   If you want to alter the mesh, change the hypothesis and compute the new mesh.
2. Obtain the sub-meshes for the grains

   The segmented image contains regions that are not part of the recrystallized region, but they belong to the homogeneous region. We want to handle them in the same way as the two artificial grains. We do not need to merge the surfaces, just put them in the same element group. Therefore, we create
   - a common element group for the elements lying in the homogeneous region
   - one element group for each grain in the heterogeneous (recrystallized) region

   using *Mesh -> Create Groups from Geometry* and selecting all the 250 faces of the geometry. To form a single group for the heterogeneous region, merge the corresponding element groups in *Mesh -> Union Groups*. Once done, delete the groups that were used in forming the union.

3. We will explicitly need to prescribe boundary conditions on the left and right sides of the rectangular domain. For this, the nodes on those sides are collected with *Mesh -> Create Group* and set the *Elements Type* to *Node*. Select the nodes on the left edge and give the node set a name. Repeat it for the nodes on the right.
4. Export the mesh Click on *File -> Export -> MED file*. The sub-meshes (element groups, node groups) are also exported.

The mesh is ready for further processing. We have another *guide* that discusses how to handle the MED file from within Python.

CHAPTER

SEVEN

PROCESSING A .MED FILE

After exporting the mesh from Salome to a MED file, we may want to perform certain operations on it. The MEDCoupling tool of Salome provides C++ and Python APIs for this purpose. However, that requires the user to

- have Salome installed as those APIs are available from the Salome kernel
- get to know the API

Moreover, it can happen that some mesh processing functionalities they may want to use does not exist. Since meshes consisting of cells of the same type (e.g. triangles) can be represented as homogeneous and contiguous arrays, converting the mesh from MED to numpy arrays seems a reasonable choice. This is what our *med* module does: it provides a thin wrapper around *MEDCoupling* to extract the mesh and the defined groups (cell and vertex groups) from the MED file and convert them to numpy arrays. This way, the user who deals with numerical modelling can implement their mesh processing algorithms based on numpy arrays, which is fast and straightforward. Furthermore, the person who performs the CAD operations and has Salome installed, can use our *med* module to export the mesh to numpy arrays so that the numerical analyst can directly work on it without having to have Salome installed and without any knowledge on the *MEDCoupling* API.

If you want to know more about the implementation details, read the documentation for the *med module*.

7.1 Using the module

To use our *med* module, access to the *MEDLoader* module from Salome is required. In the following, we assume that Salome has been installed and added to the path, so the command `salome` is available. If you

- want to use the Python REPL:

```
$ salome shell -- python
Python 3.6.5 (default, Dec 16 2019, 16:42:15)
[GCC 7.3.0] on linux
Type "help", "copyright", "credits" or "license" for more information.
```

  Now, you have access to the *MEDCoupling* Python API. E.g.

```
>>> from MEDLoader import MEDFileData
```

- want to use the PyCharm IDE

```
$ salome shell "path_to_PyCharm/bin/pycharm.sh"
```

  This will start PyCharm. In the IDE (PyCharm in this example), set the interpreter to that of Salome's Python. For me, it is located at `BINARIES-UB18.04/Python/bin/python3`, where `UB18.04` refers to the fact that I downloaded a pre-compiled Salome binaries for Ubuntu 18.04.

To learn more about the `salome` command, read the manual.

CHAPTER

EIGHT

ALGORITHMS

The goal of this document is to provide more low-level algorithmic details than what is given in our paper. In fact, the material presented here is complimentary to the paper. The paper concentrates on the intuition behind the methods and shows the high-level structure, also citing the relevant literature.

8.1 From image to geometry

It is recommended to read Section 2.3 of the paper first and then this section.

The algorithm to construct a geometrical representation out of a segmented image is complex. To reduce the complexity, we created composable parts. We start with some notions below. Then the main steps of the algorithm is discussed in the upcoming subsections.

Grains can have different *representations*. When represented as an image (input in our algorithm), it is a set of pixels labelled with the same positive integer. A grain can be given different geometrical representations. It can be the assembly of primitive shapes, usually triangles. One can also describe a grain by its boundary. For example, piecewise linear boundary segments lead to a *polygon*, connecting spline curves lead to a *splinegon*. A grain can also be represented as a *cycle of a graph*.

We make distinction between *topological* and *geometrical* data. Topological data includes connectivity, neighbourhood and membership information. Coordinates of points are examples for geometrical data. Separating these two terms allows us to build abstractions in the code, making it understandable and extensible.

8.1.1 Skeleton of the image

Based on the segmented/labelled image, *skan* builds the skeleton network, as demonstrated on a sample image below. The different pixel colors represent different labels.

As a preprocessing step, we create an additional labelled region that surrounds the original labelled image. The reason is that this way, *skan* will create branches along the boundary of the original image, which will close the boundary grains. It also simplifies the algorithms we will use later because the boundary interfaces can be handled in the same way as the internal ones: every interface separates exactly two grains.

8.1.2 Which branches form a grain?

The question arises: given the branches, how to reconstruct the grains? First, let us try a graph theoretic approach. In the example below, we want to identify the three grains denoted by roman numerals. The network of branches can be represented as a graph, in which the vertices are the end points and the edges correspond to the branches.

Adequately selected cycles in this graph would give the grains. However, as discussed in the paper, determining the grains based on the graph exclusively would be very challenging because of the following characteristics.

- For general microstructures, the graph contains multiple edges (see the example above), which rules out many graph processing methods.
- Finding all the elementary cycles in the graph is too costly for graphs coming from realistic microstructures. Even if we found all the cycles, we would need a criterion to choose which ones correspond to grains. E.g. the cycle $\bar{6} - \bar{2} - \bar{3} - \bar{5}$ does not encompass a single grain but the union of two grains.
- Another technique to find the correct cycles would be the minimum cycle basis. However, this basis is not unique so there is no guarantee that we find the adequate cycles.

The solution is to use both topological and geometrical information. The skeleton is superimposed on the labelled image (from which it was constructed by *skan*) and the labels around a given skeleton node or end point is detected. Staying with the example in the *first subsection*, the scheme is shown below.

In the following, we describe an algorithm to find out which two grains are incident to a branch (remember that *always two grains neighbor a branch*).

Algorithm

The neighbor search around every node of a branch is performed and the two most common labels are chosen. Since in the image representation the grain is a set of pixels having the same label, the selected two labels give the neighboring two grains to a branch.

Neighbor definitions

As described in the paper, certain scenarios necessitate to consider various neighborhood definitions. For those definitions, see the documentation of the `grains.utils.neighborhood` function.

Going back to the first configuration in the beginning of this section, the algorithm gives the following branch-grain connectivities.

$$\begin{aligned}\bar{1} &: [\mathrm{I}]\\ \bar{2} &: [\mathrm{II}]\\ \bar{3} &: [\mathrm{I}, \mathrm{II}]\\ \bar{4} &: [\mathrm{III}, \mathrm{II}]\\ \bar{5} &: [\mathrm{I}, \mathrm{III}]\\ \bar{6} &: [\mathrm{II}, \mathrm{I}]\end{aligned}$$

Inverting this relationship gives the grain-branch connectivities:

$$\begin{aligned}\mathrm{I} &: [\bar{1}, \bar{3}, \bar{5}, \bar{6}]\\ \mathrm{II} &: [\bar{2}, \bar{3}, \bar{6}, \bar{4}]\\ \mathrm{III} &: [\bar{5}, \bar{4}]\end{aligned}$$

The grain-branch connectivities are an intermediate representation (topological-geometrical). It is independent of how we geometrically represent a grain later.

8.1.3 Grains as oriented planar surfaces

The previous part of the reconstruction algorithm determined which branches bound a grain. In order to obtain a surface representation of a grain, the boundary must be oriented and hence the branches must be connected in the appropriate order. The following figure demonstrates for grain II the working of a brute-force algorithm.

The branches are interlaced based on their common junctions. The arrows show which branches follow in order. Note that the default orientation of branches $\bar{3}$ and $\bar{4}$ needs to be swapped.

Finally, we arrive at a fully geometrical description because each grain is now given by a series of points (nodes and end points) along its boundary.

8.1.4 Geometrical representations of grains

Now that we have a list of points, we can build two geometrical representations of a grain. In the *polygon representation*, the list of points are the consecutive vertices of the polygon. Their coordinates are stacked, the first vertex being repeated to "close" the polygon. In the *spline representation*, the list of points on each branch act as a knots of a B-spline. Once the bounding splines have been constructed, the planar spline surface (splinegon) is spanned by those bounding splines.

CHAPTER

NINE

PROGRAM DESIGN

CristalX is not a black-box library such as BLAS, neither is a GUI-based application intended for end-users. It is rather an easy-to-use and extensible set of Python codes that provide the basic functionalities that scientists can extend based on their needs. The following ideas were kept in mind while writing and maintaining *CristalX*.

- Driven by actual needs

Only implement features that are currently used. Adding extra features requires more testing, possibly more dependencies and therefore code bloat, and increases the cognitive load of the user. Instead, the emphasis is on creating a stable minimum core library that can be easily extended according to users' demands. Consequently, application code is separated from the core modules.

- Build on well-established packages

We rely on the scientific Python stack: *NumPy* for array manipulations, *SciPy* for interpolation and some other computations, *Matplotlib* for visualization and *scikit-image* for image processing. This ensures interoperability with other scientific codes and that our software is hopefully bug-free.

- Minimize the dependencies

Rapid prototyping is essential in scientific code development and Python is an excellent choice to satisfy this requirement. At the same time, relying on fast libraries ensures that the computations are reasonably fast. The libraries mentioned in the previous point are easy to install, often already pre-installed in certain Python distributions.

- High-quality documentation

Future contributors will benefit from the rich documentation. Python doctests are extensively used, serving both as test cases and as examples of usage. The docstrings conform to the *numpydoc* style guide.

- We strive for decoupling the modules

Although part of the *grains* package, if the modules are independent, they can be reused in other projects too just by copy-pasting the required functions.

- Do not overuse classes

In the prototyping phase, prefer using free functions to methods. As an idea evolves, you will naturally find data and algorithms that belong together, and can refactor free functions into member functions of a class.

- Do not use deep hierarchies

Initially, stay away from excessive nesting to avoid fragmenting the code base. If the project grows big, you can still refactor the code by introducing deeper hierarchies. Deep nesting causes unnecessary cognitive load and it also makes the code more verbose at the caller's site. Compare

```
import package1.package2.module
```

with

```
import package.module
```

- Gradually refactor code

As more and more features are added to the project, we will often find that similar tasks emerge in different contexts. It is a good time to think about how they can be generalized and to reconsider your model. This way, you will come up with utility functions best put into *utils.py*.

- Start writing code only after careful thinking

It is no point in writing code before you completely understand your problem domain you want to model. It is more efficient to build abstractions in your head or on paper, then to split it into modular chunks, and only after that start coding.

- Write the documentation *before* the code

If you document the function parameters and the return values in advance, as well as construct a doctest, you are enforced to think about the problem deeply and to create a good interface. Moreover, it guarantees that the documentation is not missing (what you would anyway have to write at some point, so why not at the beginning?).

- Give doctest-compatible examples

You hit two birds with the same stone: provide an example for the user and get some confidence that your code works as intended (at least for the particular example). As mentioned in the previous point, write them *before* the actual code implementation. Doctests do not replace careful testing.

- Keep the documentation as part of your code

The problem with wiki pages is that they are version controlled in a different Git repository. It makes it longer to change a hosting service (e.g. moving from GitHub to GitLab), you need to maintain two repositories, cannot change the documentation and the code in the same commit, and you have to rely on the rendering capabilities of the hosting service (e.g. GitHub cannot render math). It is therefore better to keep the documentation as part of your project in a dedicated directory (`docs/` in our case), use a documentation generator (*Sphinx* in our case) and host it online (on *Read the Docs* in our case).

CHAPTER

TEN

CODING CONVENTIONS

CHAPTER

ELEVEN

DOCUMENTATION

Writing documentation is necessary when you contribute to this project, either by writing code or by changing/extending the external documents. In this section, we give tips how you can write them. This is an opinionated topic and it lays down how it is currently done. Feel free to suggest new ideas.

Whenever you write the documentation, first *test it locally* before pushing changes: Read the Docs spends about 1000 seconds to build the documentation.

It took me a long time to experiment with the Sphinx settings that provide the output what you can see in the rendered documentation. Some notes concerning these efforts can be found in the Notes section. Another way to learn about Sphinx documentation is by reading the source of the existing documentation. On each page of the HTML documentation, the header contains a *View page source* hyperlink.

11.1 Code documentation

As shown in the *figure*, codes are written either as Python files or as Jupyter notebooks. With the proper extensions (see the `docs/source/conf.py` file), both of them are automatically included in the documentation by Sphinx. In what follows, we concentrate on documenting Python files.

The docstings are written in RST, following the numpydoc style, using the Napoleon Sphinx extension.

Provide doctests to demonstrate the use of the function you write and to provide minimal testing.

The line length is 100 characters, as defined in the `/.editorconfig` file.

11.2 External documentation

The external documentation is written in reStructuredText (RST) and in Markdown. Sphinx, by default, uses RST, extending it with more capabilities. However, recommonmark can parse Markdown files and automatically convert them to RST at documentation build time. This is a great help as more people are used to the simple Markdown than to the more complex (and more capable) RST. Actually, the current document you read was also written in Markdown. Of course, it is perfectly fine if you write the documentation exclusively in RST.

Currently, the structure of the documentation is written in RST, and most of the external documentation in Markdown.

CHAPTER

TWELVE

DEVELOPMENT

Intro . . .

12.1 General workflow

The development workflow can be followed in the following figure.

1. You write the Python source codes (.py) and the Jupyter notebooks (.ipynb) on your local machine. If you want, you can create the documentation locally using Sphinx.
2. When a logical unit has been finished, you commit the changes with `git push`. This will upload the new version of the modified files to a remote repository (currently GitHub). If you edit files in the remote repository and you want those changes to be present in your local copy, you can use `git pull`. For more details on Git, read the manual.
3. Several commit hooks are attached to the remote repository. When they detect a change, certain actions are activated. One the one hand, the online version of the documentation, hosted on Read the Docs will be updated. On the other hand, static analyzers will reanalyze the new version of the code. Some of them may create a pull request based on their recommendations.

12.2 Profiling

I use Pyinstrument for profiling the code. It comes with the *CristalX* installation.

Otherwise, you can install it with `pip install pyinstrument` or by *conda* after the *conda-forge* channel has been activated.

```
conda install -c conda-forge pyinstrument
```

As Pyinstrument has no dependencies, you can safely install it to your current environment. If you do not want to take a risk, create a new environment. With *conda*, you can do e.g.

```
conda create -n pyinstrument python=3.7 scipy matplotlib
conda activate pyinstrument
conda install -c conda-forge pyinstrument
```

The *profiling* module provides a wrapper around Pyinstrument. Put the code you want to profile in the `profile` context manager, e.g.

```
>>> import random
>>> from grains.profiling import profile
>>> with profile('html') as p:
...     for _ in range(1000000):
...         rand_num = random.uniform(1, 2.2)
```

For more details see the *API reference*.

CHAPTER

THIRTEEN

CONTRIBUTING

CristalX is an open-source project that welcomes contributions of any kind.

13.1 What can you help in?

The major fields in which you can help are the following (in increasing complexity).

13.1.1 Use cases

If you use *CristalX* in your project, let us know. Parts of your code, if they are general enough to be incorporated, could be included in *CristalX*. Make contact with us by *opening an issue*.

13.1.2 Documentation

If the documentation of some functions

- is missing
- is incomprehensible
- does not contain examples
- is not rendered properly

or if the code examples break, *open a pull request*. Similarly, open a pull request if the guides

- contain typos
- are incomprehensible

13.1.3 Code

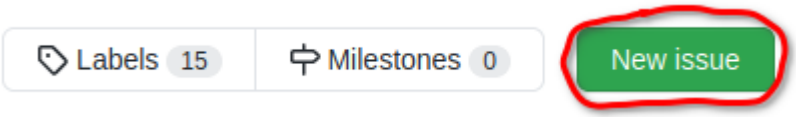
- You can report bugs by *opening an issue*.
- If you want to help but do not know where to start, consider the currently open issues, especially the ones with the help wanted label.
- You can implement new features. First of all, *contact us* if you plan to work on a non-trivial feature. This will save work for you. Use the *fork & PR* workflow.

13.2 How to contribute

First, create a GitHub account. There are two ways to contribute.

13.2.1 Open an issue

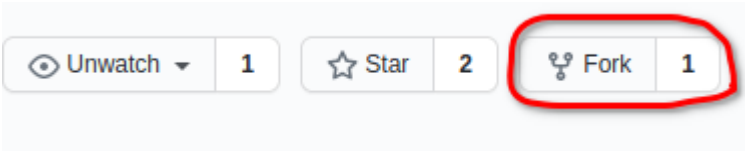
To open a new issue, click on the green button on the *Issues* page.



13.2.2 Fork & pull request

At the moment, there are no code formatting guidelines, the best is to follow the formatting of the existing code.

1. Fork the GitHub repository by clicking on the *Fork* button at the top right corner.



2. Install *CristalX locally* by cloning your fork (`git clone`).
3. Create a new branch.

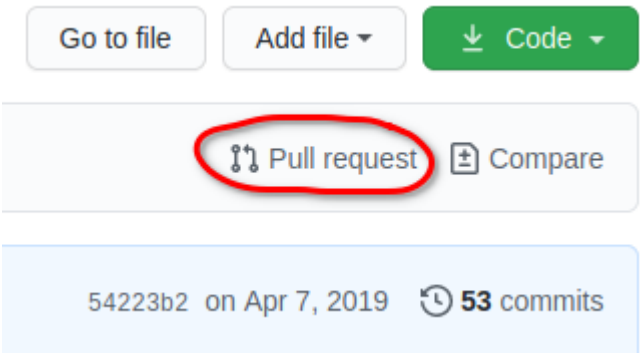
   Do not work on the default (*master*) branch but create a new feature branch, e.g.

```
git checkout -b new_feature
```

4. Make your changes.

   Add or modify files and regularly commit your changes to your local clone with meaningful commit messages (`git commit`). Do not forget to test your code: if you do not provide unit tests, at least write doctests.

5. Push your changes to your remote fork on GitHub (`git push`).
6. Visit your forked repository on GitHub and click on the *Pull request* button. See the GitHub documentation for details.



7. Keep your fork up to date

   While you work on your forked repository, changes may be committed to the original (called *upstream*) repository. To make sure you keep your fork up to date with the upstream repository, follow the instructions in the GitHub documentation.

This was a basic overview, for more details check out the following documents:

- https://gist.github.com/Chaser324/ce0505fbed06b947d962
- https://github.com/susam/gitpr

CHAPTER

FOURTEEN

VERSIONING

The versioning of *CristalX* starts with 1.0.0 and it somewhat follows the rules of Semantic Versioning 2.0.0, with the syntax MAJOR.MINOR.PATCH, where MAJOR introduces significant changes, MINOR comes with smaller changes, and PATCH provides a fixture or a tiny improvement either in the code or in the documentation.

14.1 Why not SemVer?

Semantic Versioning (SemVer) is a widely used versioning scheme, applicable for **public APIs**. Its purpose is to be rigorous on how to indicate when a bug fix, new features or incompatible changes in the public API are introduced. There is an excellent discussion about it here and a detailed guide here. Many criticize it for not being indicative about the rate of important changes. E.g. 1.8.5 –> 1.9.0 may include dozens of relevant improvements, while 1.9.5 –> 2.0.0 may merely be a simple clean-up that changes the public API. However, SemVer was never meant to be used for software version numbers.

CristalX is not a library, but a collection of tools that operate at a high level. Most of its functions are exposed to the user, except the ones marked with a leading underscore or two leading underscores. However, the public API would be a subset of these functions: e.g. the functions of the *utils* module are exposed but they are mostly intended to be used by other modules, not by the user. As *CristalX* is not a library but rather a tool for rapid prototyping, semantic versioning would not make much sense.

14.2 Why not CalVer?

Calendar Versioning (CalVer) is an alternative to SemVer. *CristalX* may not come with regular changes in the future or it will get updates at irregular intervals. We do not want to give the impression that relevant changes are introduced linearly in time. Moreover, the changelog and the time stamp in the git commits clearly show when new releases are published.

14.3 Our versioning

As there is no unconditionally best versioning system, we came up with our own, which seems to fit well for research code like *CristalX*. The starting point is SemVer with some differences. Our versioning is intended for humans. The MAJOR version in increased only for substantially new features. This is, of course, subjective but we want to avoid large MAJOR version numbers as e.g. in Firefox. The guideline to follow is that the novelty of a feature makes the MAJOR version increase, not the number of additions. Here are some examples. Assume that we are at 1.2.3. We fixed a set of related bugs in the code: 1.2.3 –> 1.2.4. Then we implemented several functionalities to speed up the code: 1.2.4 –> 1.3.0. A new module was created and several others were modified that allowed us to carry out groundbreaking research: 1.3.0 –> 2.0.0. An existing algorithm was improved to handle the corner cases: 2.0.0 –> 2.1.0.

Similarly to SemVer, when one of the digits increases, the ones right to it are set to zero (e.g. 1.0.1 –> 1.0.2, 1.0.3 –> 1.1.0, 1.8.6 –> 2.0.0).

We try to keep backward compatibility. Insignificant changes are postponed, and are included as part of a MINOR release. If you often feel the need to introduce changes to the function signatures, rather **add** new functions and give **deprecation notices** than remove or modify existing ones. This does not lead to code bloat in the long run because deprecated syntax is removed from time to time. To mark a function, a method or a class as deprecated, import the `deprecated` function from the *deprecation* package and follow its syntax.

The *master* branch of the Git repository contains the latest developments since the last published release. These unreleased modifications are allowed to contain incompatibilities (changes in the function signatures, etc.) compared to the latest release. This flexibility is essential for rapid prototyping in research codes like *CristalX*. However, these possible incompatibilities must be fixed for the next release, see the previous paragraph.

14.3.1 Connection with the Git workflow

The version numbers are reflected in the tag names. Your normal Git workflow stays the same: commit modifications and push them to the remote repository. When you want to mark a commit yet to be included in a certain version, type

```
git tag -m "Concise message" v<version_number>
```

where `<version_number>` has the form MAJOR.MINOR.PATCH. Note that it is preceded by the `v` letter, conventionally used for tags. As an example:

```
git tag -m "Initial release." v1.0.0
```

Keep the tag message short: the detailed changes since the previous version are collected in the changelog.

The tag is pushed by

```
git push --tags
```

Whenever you publish a tag, and hence update the changelog, also create a release for that tag on GitHub. Copy the changes the new version brings from the changelog to the description of the release. In this regard, we follow the way of JabRef. The zipped size of *CristalX* is quite small, so size constraint will not be a problem on GitHub.

CHAPTER

FIFTEEN

SEGMENTATION

This module contains the Segmentation class, responsible for the image segmentation of grain-based materials (rocks, metals, etc.)

15.1 Classes

Segmentation	Segmentation of grain-based microstructures

15.1.1 grains.segmentation.Segmentation

class grains.segmentation.**Segmentation**(*image_location*, *save_location=None*, *interactive_mode=True*)

Segmentation of grain-based microstructures

original_image
Matrix representing the initial, unprocessed image.

Type ndarray

save_location
Directory where the processed images are saved

Type str

__init__(*image_location*, *save_location=None*, *interactive_mode=True*)
Initialize the class with file paths and with some options

Parameters

- **image_location** (*str*) – Path to the image to be segmented, file extension included.
- **save_location** (*str, optional*) – Path to directory where images will be outputted. If not given, the same directory is used where the input image is loaded from.
- **interactive_mode** (*bool, optional*) – When True, images of each image manipulation step are plotted and details are shown in the console. Default is False.

Returns *None.*

Methods

__init__(image_location[, save_location, ...])	Initialize the class with file paths and with some options
create_skeleton(boundary_image)	Use thinning on the grain boundary image to obtain a single-pixel wide skeleton.
filter_image(window_size[, image_matrix])	Median filtering on an image.
find_grain_boundaries(segmented_image)	Find the grain boundaries.
initial_segmentation(*args)	Perform the quick shift superpixel segmentation on an image.
merge_clusters(segmented_image[, threshold])	Merge tiny superpixel clusters.
save_array(filename, array)	Save an image as a numpy array.
save_image(filename, array[, is_label_image])	Save an image as a numpy array.
watershed_segmentation(skeleton)	Watershed segmentation of a granular microstructure.

class grains.segmentation.**Segmentation**(*image_location*, *save_location=None*, *interactive_mode=True*)

Bases: object

Segmentation of grain-based microstructures

original_image
Matrix representing the initial, unprocessed image.

Type ndarray

save_location
Directory where the processed images are saved

Type str

create_skeleton(*boundary_image*)
Use thinning on the grain boundary image to obtain a single-pixel wide skeleton.

Parameters **boundary_image** (*bool ndarray*) – A binary image containing the objects to be skeletonized.

Returns **skeleton** (*bool ndarray*) – Thinned image.

filter_image(*window_size*, *image_matrix=None*)
Median filtering on an image. The median filter is useful in our case as it preserves the important borders (i.e. the grain boundaries).

Parameters

- **window_size** (*int*) – Size of the sampling window.
- **image_matrix** (*3D ndarray with size 3 in the third dimension, optional*) – Input image to be filtered. If not given, the original image is used.

Returns **filtered_image** (*3D ndarray with size 3 in the third dimension*) – Filtered image, output of the median filter algorithm.

find_grain_boundaries(*segmented_image*)
Find the grain boundaries.

Parameters **segmented_image** (*ndarray*) – Label image, output of a segmentation.

Returns **boundary** (*bool ndarray*) – A bool ndarray, where True represents a boundary pixel.

initial_segmentation (**args*)
Perform the quick shift superpixel segmentation on an image. The quick shift algorithm is invoked with its default parameters.

Parameters ***args** (*3D numpy array with size 3 in the third dimension*) – Input image to be segmented. If not given, the original image is used.

Returns **segment_mask** (*ndarray*) – Label image, output of the quick shift algorithm.

merge_clusters (*segmented_image*, *threshold=5*)
Merge tiny superpixel clusters. Superpixel segmentations result in oversegmented images. Based on graph theoretic tools, similar clusters are merged.

Parameters

- **segmented_image** (*ndarray*) – Label image, output of a segmentation.
- **threshold** (*float, optional*) – Regions connected by edges with smaller weights are combined.

Returns **merged_superpixels** (*ndarray*) – The new labelled array.

save_array (*filename*, *array*)
Save an image as a numpy array. The array is saved in the standard numpy format, into the directory determined by the *save_location* attribute.

Parameters

- **filename** (*str*) – The array is saved under this name, with extension .npy
- **array** (*ndarray*) – An image represented as a numpy array.

save_image (*filename*, *array*, *is_label_image=False*)
Save an image as a numpy array. The array is saved in the standard numpy format, into the directory determined by the *save_location* attribute.

Parameters

- **filename** (*str*) – The array is saved under this name, with extension .npy
- **array** (*ndarray*) – An image represented as a numpy array.
- **is_label_image** (*bool*) – True if the array represents a labeled image.

watershed_segmentation (*skeleton*)
Watershed segmentation of a granular microstructure. Uses the watershed transform to label non-overlapping grains in a cellular microstructure given by the grain boundaries.

Parameters **skeleton** (*bool ndarray*) – A binary image, the skeletonized grain boundaries.

Returns **segmented** (*ndarray*) – Label image, output of the watershed segmentation.

CHAPTER

SIXTEEN

GALA

A trimmed version of the Gala project (https://github.com/janelia-flyem/gala) with some additions (new function, added documentation for the existing ones). Gala is licensed by the Janelia Farm License: http://janelia-flyem.github.io/janelia_farm_license.html

16.1 Functions

imextendedmin(image, h[, connectivity])	Extended-minima transform.
hminima(a, thresh)	Suppress all minima that are shallower than thresh.
imhmin(a, thresh)	Suppress all minima that are shallower than thresh.
morphological_reconstruction(marker, mask[, ...])	Perform morphological reconstruction of the marker into the mask.
regional_minima(a[, connectivity])	Find the regional minima in an ndarray.
complement(a)	

16.1.1 grains.gala_light.imextendedmin

grains.gala_light.**imextendedmin**(*image*, *h*, *connectivity=1*)

Extended-minima transform. The extended minima transform is the regional minima of the h-minima transform. The implementation follows the MATLAB function under the same name.

Parameters

- **image** (*ndarray*) – The input array on which to perform imextendedmin.
- **h** (*float*) – Any local minima shallower than this will be flattened.
- **connectivity** (*int, optional*) – Determines which elements are considered as neighbors of the central element. Elements up to a squared distance of *connectivity* from the center are considered neighbors. If connectivity=1, no diagonal elements are neighbors.

Returns *bool ndarray* – True at places of the extended minima.

16.1.2 grains.gala_light.hminima

grains.gala_light.**hminima**(*a*, *thresh*)

Suppress all minima that are shallower than thresh.

Parameters

- **a** (*array*) – The input array on which to perform hminima.
- **thresh** (*float*) – Any local minima shallower than this will be flattened.

Returns **out** (*array*) – A copy of the input array with shallow minima suppressed.

16.1.3 grains.gala_light.imhmin

grains.gala_light.**imhmin**(*a*, *thresh*)

Suppress all minima that are shallower than thresh.

Parameters

- **a** (*array*) – The input array on which to perform hminima.
- **thresh** (*float*) – Any local minima shallower than this will be flattened.

Returns **out** (*array*) – A copy of the input array with shallow minima suppressed.

16.1.4 grains.gala_light.morphological_reconstruction

grains.gala_light.**morphological_reconstruction**(*marker*, *mask*, *connectivity=1*)

Perform morphological reconstruction of the marker into the mask.

See the Matlab image processing toolbox documentation for details: http://www.mathworks.com/help/toolbox/images/f18-16264.html

16.1.5 grains.gala_light.regional_minima

grains.gala_light.**regional_minima**(*a*, *connectivity=1*)
Find the regional minima in an ndarray. As written in the MATLAB documentation of the imregionalmin function: "Regional minima are connected components of pixels with a constant intensity value, surrounded by pixels with a higher value."

16.1.6 grains.gala_light.complement

grains.gala_light.**complement**(*a*)

grains.gala_light.**complement**(*a*)

grains.gala_light.**hminima**(*a*, *thresh*)
Suppress all minima that are shallower than thresh.

Parameters

- **a** (*array*) – The input array on which to perform hminima.
- **thresh** (*float*) – Any local minima shallower than this will be flattened.

Returns **out** (*array*) – A copy of the input array with shallow minima suppressed.

grains.gala_light.**imextendedmin**(*image*, *h*, *connectivity=1*)
Extended-minima transform. The extended minima transform is the regional minima of the h-minima transform. The implementation follows the MATLAB function under the same name.

Parameters

- **image** (*ndarray*) – The input array on which to perform imextendedmin.
- **h** (*float*) – Any local minima shallower than this will be flattened.
- **connectivity** (*int, optional*) – Determines which elements are considered as neighbors of the central element. Elements up to a squared distance of *connectivity* from the center are considered neighbors. If connectivity=1, no diagonal elements are neighbors.

Returns *bool ndarray* – True at places of the extended minima.

grains.gala_light.**imhmin**(*a*, *thresh*)
Suppress all minima that are shallower than thresh.

Parameters

- **a** (*array*) – The input array on which to perform hminima.
- **thresh** (*float*) – Any local minima shallower than this will be flattened.

Returns **out** (*array*) – A copy of the input array with shallow minima suppressed.

grains.gala_light.**morphological_reconstruction**(*marker*, *mask*, *connectivity=1*)
Perform morphological reconstruction of the marker into the mask.

See the Matlab image processing toolbox documentation for details: http://www.mathworks.com/help/toolbox/images/f18-16264.html

grains.gala_light.**regional_minima**(*a*, *connectivity=1*)
Find the regional minima in an ndarray. As written in the MATLAB documentation of the imregionalmin function: "Regional minima are connected components of pixels with a constant intensity value, surrounded by pixels with a higher value."

CHAPTER

SEVENTEEN

ANALYSIS

This module contains the Analysis class, responsible for the analysis of segmented grain-based microstructures.

All the examples assume that the modules *numpy* and *matplotlib.pyplot* were imported as *np* and *plt*, respectively.

17.1 Classes

Analysis	Analysis of grain assemblies.

17.1.1 grains.analysis.Analysis

class grains.analysis.**Analysis**(*label_image*, *interactive_mode=False*)

Analysis of grain assemblies.

original_image

Matrix representing the initial, unprocessed image.

Type ndarray

save_location

Directory where the processed images are saved

Type str

__init__(*label_image*, *interactive_mode=False*)

Initialize the class with file paths and with some options

Parameters

- **label_image** (*ndarray*) – Segmented image.
- **interactive_mode** (*bool, optional*) – When True, images of each image manipulation step are plotted and details are shown in the console. Default is False.

Returns *None.*

Methods

__init__(label_image[, interactive_mode])	Initialize the class with file paths and with some options
compute_properties()	Determines relevant properties of the grains.
set_scale([pixel_per_unit])	Defines a scale for performing computations in that unit.
show_grains([grain_property])	Display the grains, optionally with a property superposed.
show_properties([gui])	Displays previously computed properties of the grains

17.2 Functions

feret_diameter(prop)	Determines the maximum Feret diameter.
plot_prop(prop[, pixel_per_unit, show_axis])	Plots relevant region properties into a single figure.
plot_grain_characteristic(characteristic, ...)	Plots the distribution of a given grain characteristic.
show_label_image(label_image[, alpha])	Displays a labeled image.
label_image_skeleton(label_image)	Skeleton of a labeled image.
thicken_skeleton(skeleton, thickness)	Thickens a skeleton by morphological dilation.
label_image_apply_mask(label_image, mask, value)	Changes parts of a labeled image to a given value.

17.2.1 grains.analysis.feret_diameter

grains.analysis.**feret_diameter**(*prop*)

Determines the maximum Feret diameter.

Parameters **prop** (*RegionProperties*) – Describes a labeled region.

Returns **max_feret_diameter** (*float*) – Maximum Feret diameter of the region.

See also:

skimage.measure.regionprops() Measure properties of labeled image regions

Examples

```
>>> import numpy as np
>>> from skimage.measure import regionprops
>>> image = np.ones((2,2), dtype=np.int8)
>>> prop = regionprops(image)[0]
>>> feret_diameter(prop)
2.23606797749979
```

17.2.2 grains.analysis.plot_prop

grains.analysis.**plot_prop**(*prop*, *pixel_per_unit=1*, *show_axis=True*)

Plots relevant region properties into a single figure. Four subfigures are created, giving the region's

- image, its area and its center
- filled image, its area
- bounding box, its area
- convex image, its area

Parameters

- **prop** (*RegionProperties*) – Describes a labeled region.
- **pixel_per_unit** (*float or int, optional*) – Number of pixels contained in a certain unit. The default is 1, in which case all measurements are performed in pixel units.

Returns **fig** (*matplotlib.figure.Figure*) – The figure object is returned in case further manipulations are necessary.

17.2.3 grains.analysis.plot_grain_characteristic

grains.analysis.**plot_grain_characteristic**(*characteristic*, *centers*, *interpolation='linear'*, *grid_size=(100, 100)*, ***kwargs*)

Plots the distribution of a given grain characteristic.

One way to gain insight into a grain assembly is to plot the distribution of a certain grain property in the domain the grains occupy. In this function, for each grain, and arbitrary (scalar) quantity is associated to the center of the grain. In case of *n* grains, *n* data points span the interpolant and the given characteristic is interpolated on a grid of the AABB of the grain centers.

Parameters

- **characteristic** (*ndarray*) – Characteristic property, the distribution of which is sought. A 1D numpy array.
- **centers** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a grain, and the two columns giving the Cartesian coordinates of the grain center.
- **interpolation** (*{'nearest', 'linear', 'cubic'}, optional*) – Type of the interpolation for creating the distribution. The default is *'linear'*.
- **grid_size** (*tuple of int, optional*) – 2-tuple, the size of the grid on which the data is interpolated. The default is (100, 100).

Other Parameters

- **center_marker** (*str, optional*) – Marker indicating the center of the grains. The default is *'P'*. For a list of supported markers, see the documentation. If you do not want the centers to be shown, choose *'none'*.
- **show_axis** (*bool, optional*) – If True, the axes are displayed. The default is False.

Returns *None*

See also:

`scipy.interpolate.griddata()`

Notes

This function knows nothing about how the center of a grain is determined and what characteristic features a grain has. It only performs interpolation and visualization, hence decoupling the plotting from the actual representation of grains and their characteristics. For instance, a grain can be represented as a spline surface, as a polygon, as an assembly of primitives (often triangles), as pixels, just to mention some typical scenarios. Calculating the center of a grain depends on the grain representation at hand. Similarly, one can imagine various grain characteristics, such as area, diameter, Young modulus.

Examples

Assume that the grain centers are sampled from a uniformly random distribution on the unit square.

```
>>> n_data = 100
>>> points = np.random.random((n_data, 2))
```

The quantity we want to plot has a parabolic distribution with respect to the position of the grain centers.

```
>>> func = lambda x, y: 1 - (x-0.5)**2 - (y-0.5)**2
>>> plot_grain_characteristic(func(points[:, 0], points[:, 1]), points, center_
↪marker='*')
>>> plt.show()
```

17.2.4 grains.analysis.show_label_image

grains.analysis.**show_label_image**(*label_image*, *alpha=1*)

Displays a labeled image.

A random color is associated with each labeled region. If boundary pixels are present in the image, they are plotted in black.

Parameters

- **label_image** (*ndarray*) – Labeled input image, represented as a 2D numpy array of non-negative integers. The label 0 is assumed to denote a boundary pixel.
- **alpha** (*float, optional*) – Opacity of colorized labels. Must be within [0, 1].

Returns *None*

17.2.5 grains.analysis.label_image_skeleton

grains.analysis.**label_image_skeleton**(*label_image*)

Skeleton of a labeled image.

The skeleton of a labeled image is a single-pixel wide network that separates the labeled regions.

Parameters **label_image** (*ndarray*) – Labeled input image, represented as a 2D numpy array of positive integers.

Returns *ndarray* – A 2D bool numpy array having the same size as `label_image`, where True represents the skeleton pixels.

See also:

thicken_skeleton()

17.2.6 grains.analysis.thicken_skeleton

grains.analysis.**thicken_skeleton**(*skeleton*, *thickness*)
Thickens a skeleton by morphological dilation.

Parameters

- **skeleton** (*ndarray*) – Skeleton of a binary image, represented as a bool 2D numpy array.
- **thickness** (*int*) – Thickness of the resulting boundaries.

Returns *ndarray* – A 2D bool numpy array, where True represents the thickened skeleton.

See also:

label_image_skeleton()

17.2.7 grains.analysis.label_image_apply_mask

grains.analysis.**label_image_apply_mask**(*label_image*, *mask*, *value*)
Changes parts of a labeled image to a given value.

Convenience function, equivalent to `label_image[mask] = value` but the original array `label_image` is *not* overwritten.

Parameters

- **label_image** (*ndarray*) – Labeled input image, represented as a 2D numpy array of positive integers.
- **mask** (*ndarray*) – Boolean array of the same size as `label_image`, marking the pixels that will be replaced by `value`.
- **value** (*int*) – The masked pixels are replaced by this value.

Returns *ndarray* – Copy of the input image, its selected pixels being replaced by the given value.

class grains.analysis.**Analysis**(*label_image*, *interactive_mode=False*)
Bases: object

Analysis of grain assemblies.

original_image
Matrix representing the initial, unprocessed image.

Type ndarray

save_location
Directory where the processed images are saved

Type str

compute_properties()
Determines relevant properties of the grains. The area of each grain is determined in the units previously given in the *set_scale* method.

Parameters

- **window_size** (*int*) – Size of the sampling window.
- **image_matrix** (*3D ndarray with size 3 in the third dimension, optional*) – Input image to be filtered. If not given, the original image is used.

Returns **filtered_image** (*3D ndarray with size 3 in the third dimension*) – Filtered image, output of the median filter algorithm.

set_scale (*pixel_per_unit=1*)

Defines a scale for performing computations in that unit. Image measures (area, diameter, etc.) are performed on a matrix corresponding to a label image. Therefore, the result of all the computations are obtained in pixel units. It is often of interest to access the results in physical units (mm, cm, inch, etc.). Manually converting pixels, pixel squares, etc. to pyhsical units, physical unit sqaures, etc. are tedious and error prone. Once the conversion between a pixel and a physical unit is given, all the subsequent calculations are performed in the desired physical unit.

Parameters **pixel_per_unit** (*float or int or scalar ndarray, optional*) – Number of pixels contained in a certain unit. The default is 1, in which case all measurements are performed in pixel units.

Returns *None.*

show_grains (*grain_property=None*)

Display the grains, optionally with a property superposed.

Parameters

grain_property (***{None, 'area', 'centroid', 'coordinate',}*** **– 'equivalent_diameter', 'feret_diameter', 'label'}** optional

If not None, the selected property is shown on the grain as text.

Returns *None.*

show_properties (*gui=False*)

Displays previously computed properties of the grains

Parameters **gui** (*bool, optional*) – If true, the grain properties are shown in a GUI. If false, they are printed to stdout. The default is False. The GUI requires the *dfgui* modul, which can be obtained from https://github.com/bluenote10/PandasDataFrameGUI

Returns *None.*

grains.analysis.**feret_diameter** (*prop*)

Determines the maximum Feret diameter.

Parameters **prop** (*RegionProperties*) – Describes a labeled region.

Returns **max_feret_diameter** (*float*) – Maximum Feret diameter of the region.

See also:

skimage.measure.regionprops() Measure properties of labeled image regions

Examples

```
>>> import numpy as np
>>> from skimage.measure import regionprops
>>> image = np.ones((2,2), dtype=np.int8)
>>> prop = regionprops(image)[0]
>>> feret_diameter(prop)
2.23606797749979
```

grains.analysis.**label_image_apply_mask** (*label_image*, *mask*, *value*)

Changes parts of a labeled image to a given value.

Convenience function, equivalent to `label_image[mask] = value` but the original array `label_image` is *not* overwritten.

Parameters

- **label_image** (*ndarray*) – Labeled input image, represented as a 2D numpy array of positive integers.
- **mask** (*ndarray*) – Boolean array of the same size as `label_image`, marking the pixels that will be replaced by `value`.
- **value** (*int*) – The masked pixels are replaced by this value.

Returns *ndarray* – Copy of the input image, its selected pixels being replaced by the given value.

`grains.analysis.`**`label_image_skeleton`**(*label_image*)

Skeleton of a labeled image.

The skeleton of a labeled image is a single-pixel wide network that separates the labeled regions.

Parameters **label_image** (*ndarray*) – Labeled input image, represented as a 2D numpy array of positive integers.

Returns *ndarray* – A 2D bool numpy array having the same size as `label_image`, where True represents the skeleton pixels.

See also:

`thicken_skeleton()`

`grains.analysis.`**`plot_grain_characteristic`**(*characteristic*, *centers*, *interpolation='linear'*, *grid_size=(100, 100)*, ***kwargs*)

Plots the distribution of a given grain characteristic.

One way to gain insight into a grain assembly is to plot the distribution of a certain grain property in the domain the grains occupy. In this function, for each grain, and arbitrary (scalar) quantity is associated to the center of the grain. In case of *n* grains, *n* data points span the interpolant and the given characteristic is interpolated on a grid of the AABB of the grain centers.

Parameters

- **characteristic** (*ndarray*) – Characteristic property, the distribution of which is sought. A 1D numpy array.
- **centers** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a grain, and the two columns giving the Cartesian coordinates of the grain center.
- **interpolation** (*{'nearest', 'linear', 'cubic'}, optional*) – Type of the interpolation for creating the distribution. The default is *'linear'*.
- **grid_size** (*tuple of int, optional*) – 2-tuple, the size of the grid on which the data is interpolated. The default is (100, 100).

Other Parameters

- **center_marker** (*str, optional*) – Marker indicating the center of the grains. The default is *'P'*. For a list of supported markers, see the documentation. If you do not want the centers to be shown, choose *'none'*.
- **show_axis** (*bool, optional*) – If True, the axes are displayed. The default is False.

Returns *None*

See also:

`scipy.interpolate.griddata()`

Notes

This function knows nothing about how the center of a grain is determined and what characteristic features a grain has. It only performs interpolation and visualization, hence decoupling the plotting from the actual representation of grains and their characteristics. For instance, a grain can be represented as a spline surface, as a polygon, as an assembly of primitives (often triangles), as pixels, just to mention some typical scenarios. Calculating the center of a grain depends on the grain representation at hand. Similarly, one can imagine various grain characteristics, such as area, diameter, Young modulus.

Examples

Assume that the grain centers are sampled from a uniformly random distribution on the unit square.

```
>>> n_data = 100
>>> points = np.random.random((n_data, 2))
```

The quantity we want to plot has a parabolic distribution with respect to the position of the grain centers.

```
>>> func = lambda x, y: 1 - (x-0.5)**2 - (y-0.5)**2
>>> plot_grain_characteristic(func(points[:, 0], points[:, 1]), points, center_
↪marker='*')
>>> plt.show()
```

grains.analysis.**plot_prop**(*prop*, *pixel_per_unit=1*, *show_axis=True*)

Plots relevant region properties into a single figure. Four subfigures are created, giving the region's

- image, its area and its center
- filled image, its area
- bounding box, its area
- convex image, its area

Parameters

- **prop** (*RegionProperties*) – Describes a labeled region.
- **pixel_per_unit** (*float or int, optional*) – Number of pixels contained in a certain unit. The default is 1, in which case all measurements are performed in pixel units.

Returns **fig** (*matplotlib.figure.Figure*) – The figure object is returned in case further manipulations are necessary.

grains.analysis.**show_label_image**(*label_image*, *alpha=1*)

Displays a labeled image.

A random color is associated with each labeled region. If boundary pixels are present in the image, they are plotted in black.

Parameters

- **label_image** (*ndarray*) – Labeled input image, represented as a 2D numpy array of non-negative integers. The label 0 is assumed to denote a boundary pixel.
- **alpha** (*float, optional*) – Opacity of colorized labels. Must be within [0, 1].

Returns *None*

grains.analysis.**thicken_skeleton**(*skeleton*, *thickness*)

Thickens a skeleton by morphological dilation.

Parameters

- **skeleton** (*ndarray*) – Skeleton of a binary image, represented as a bool 2D numpy array.
- **thickness** (*int*) – Thickness of the resulting boundaries.

Returns *ndarray* – A 2D bool numpy array, where True represents the thickened skeleton.

See also:

label_image_skeleton()

grains.analysis.**truecolor2label**(*color_image*)

Truecolor image into labeled image.

It is often the case that you need to deal with a labeled image that was saved as a truecolor image (e.g. RGB). A labeled region is then the set of pixels with the same colors.

Parameters **color_image** (*ndarray*) – 3D array, the first two dimensions corresponding to the image pixels, the third one for the channels (e.g. RGB, HSV, CMYK, etc.).

Returns *ndarray* – Labeled image, represented as a 2D numpy array of non-negative integers.

CHAPTER

EIGHTEEN

MESHING

18.1 Classes

SkeletonGeometry	
QuadSkeletonGeometry	
TriSkeletonGeometry	
FixedDict	https://stackoverflow.com/a/14816446/4892892
OOF2	

18.1.1 grains.meshing.SkeletonGeometry

class grains.meshing.**SkeletonGeometry**(*leftright_periodicity*, *topbottom_periodicity*)

abstract **__init__**(*leftright_periodicity*, *topbottom_periodicity*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(leftright_periodicity, ...)	Initialize self.

18.1.2 grains.meshing.QuadSkeletonGeometry

class grains.meshing.**QuadSkeletonGeometry**(*leftright_periodicity=False*, *topbottom_periodicity=False*)

__init__(*leftright_periodicity=False*, *topbottom_periodicity=False*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__([leftright_periodicity, ...])	Initialize self.

18.1.3 grains.meshing.TriSkeletonGeometry

class grains.meshing.**TriSkeletonGeometry**(*leftright_periodicity=False*, *topbottom_periodicity=False*, *arrangement='conservative'*)

__init__(*leftright_periodicity=False*, *topbottom_periodicity=False*, *arrangement='conservative'*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__([leftright_periodicity, ...])	Initialize self.

18.1.4 grains.meshing.FixedDict

class grains.meshing.**FixedDict**(*dictionary*)
https://stackoverflow.com/a/14816446/4892892

__init__(*dictionary*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(dictionary)	Initialize self.

18.1.5 grains.meshing.OOF2

class grains.meshing.**OOF2**

__init__()
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__	Initialize self.
create_material(name) **Parameters** **name** (*TYPE*) – DESCRIPTION.	
create_microstructure([name])	Creates a microstructure from an image.

Continued on next page

Table 6 – continued from previous page

create_skeleton(nelem_x, nelem_y, geometry)	
load_pixelgroups(microstructure_file)	**Parameters** **microstructure_file** (*str*) – DESCRIPTION.
materials2groups(materials[, groups])	**Parameters** • **materials** (*list of str*) – DESCRIPTION.
pixel2group()	
read_image(label_image)	
save_microstructure([name])	
save_pixelgroups([name])	**Parameters** **name** (*str*) – DESCRIPTION.
show()	**returns** *None*.
write_script([name])	

Attributes

script

class grains.meshing.**FixedDict**(*dictionary*)

Bases: object

https://stackoverflow.com/a/14816446/4892892

class grains.meshing.**OOF2**

Bases: object

create_material(*name*)

Parameters **name** (*TYPE*) – DESCRIPTION.

Raises **Exception** – DESCRIPTION.

Returns *None*.

create_microstructure(*name=None*)

Creates a microstructure from an image.

Parameters **name** (*str, optional*) – Path to the image on which the microstucture is created, file extension included. If not given, the microstructure is given the same name as the input image.

Raises **Exception** – DESCRIPTION.

Returns *None*.

create_skeleton(*nelem_x*, *nelem_y*, *geometry*, *name=None*)

load_pixelgroups(*microstructure_file*)

Parameters **microstructure_file** (*str*) – DESCRIPTION.

Returns *None.*

materials2groups(*materials*, *groups=None*)

Parameters

- **materials** (*list of str*) – DESCRIPTION.
- **groups** (*list of int, optional*) – DESCRIPTION. The default is None.

Returns *None.*

pixel2group()

read_image(*label_image*)

save_microstructure(*name=None*)

save_pixelgroups(*name=None*)

Parameters **name** (*str*) – DESCRIPTION.

Returns *None.*

script = []

show()

Returns *None.*

write_script(*name=None*)

class grains.meshing.**QuadSkeletonGeometry**(*leftright_periodicity=False*, *topbottom_periodicity=False*)

Bases: *grains.meshing.SkeletonGeometry*

class grains.meshing.**SkeletonGeometry**(*leftright_periodicity*, *topbottom_periodicity*)

Bases: abc.ABC

class grains.meshing.**TriSkeletonGeometry**(*leftright_periodicity=False*, *topbottom_periodicity=False*, *arrangement='conservative'*)

Bases: *grains.meshing.SkeletonGeometry*

grains.meshing.**nt**

alias of grains.meshing.modules

CHAPTER

NINETEEN

CAD

CHAPTER

TWENTY

MED

Extracting and processing meshes from .med files. The functions were tested on the MEDCoupling API, version 9.4.0.

Todo: Support renumbering (https://docs.salome-platform.org/latest/dev/MEDCoupling/user/html/data_optimization.html).

Getting help:

- This module relies on the Python interface of MEDCoupling. Click here for the latest documentation.
- User's manual for the Python interface
- To know more about the MED file format, which is a specialization of HDF5, see the documentation. For a discussion on the relation between the MED format and the APIS, see this page and that one.
- The definitions, such as *group*, used in this module are from the development guide.
- A (mostly English) tutorial for the Python interface to MEDCoupling is also useful. Particularly interesting are the mesh manipulation examples
- Main page of the documentation

20.1 Functions

read_mesh	Reads a mesh file in .med format.
get_nodes	Obtains the nodes and the node groups of a mesh.
get_elements	Obtains the elements for each group of a mesh.

20.1.1 grains.med.read_mesh

grains.med.**read_mesh**(*filename*)

Reads a mesh file in .med format. Only one mesh, the first one, is supported. However, that mesh can contain groups.

Parameters **filename** (*str*) – Path to the mesh file.

Returns *MEDFileUMesh* – Represents an unstructured mesh. For details, see the manual on https://docs.salome-platform.org/latest/dev/MEDCoupling/developer/classMEDCoupling_1_1MEDFileUMesh.html

20.1.2 grains.med.get_nodes

grains.med.**get_nodes**(*mesh*)

Obtains the nodes and the node groups of a mesh.

Parameters **mesh** (*MEDFileUMesh*) – Unstructured mesh.

Returns

- **nodes** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a node, and the two columns giving the Cartesian coordinates of the nodes.
- **node_groups** (*dict*) – The keys in the dictionary are the node group names, while the values are list of integers, giving the nodes that belong to the particular group.

See also:

get_elements(), getGroupArr

20.1.3 grains.med.get_elements

grains.med.**get_elements**(*mesh*, *numbering='global'*)

Obtains the elements for each group of a mesh.

Elements of the same dimension as the mesh are collected (e.g. faces for a 2D mesh).

Todo: put those elements that do not belong to any group into an automatically created group

Todo: support ordering *elements* in alphabetical order

Todo: implement the *'global'* strategy

Parameters

- **mesh** (*MEDFileUMesh*) – Unstructured mesh.
- **numbering** (*{'global'}, optional*) –

  Determines how to allocate element numbers in the mesh. 'global': numbers the elements without taking into account which group they belong to. Use this strategy if you are not sure whether an element belongs to more than one group. 'group': numbers the elements group-wise. This is much faster than the *'global'* strategy, but use this option if you are sure that the groups of the mesh do not contain common elements.

  The default is 'global'.

Returns

- **elements** (*ndarray*) – Element-node connectivities in a 2D numpy array, in which each row corresponds to an element and the columns are the nodes of the elements. It is assumed that all the elements have the same number of nodes.
- **element_groups** (*dict*) – The keys in the dictionary are the element group names, while the values are list of integers, giving the elements that belong to the particular group.

Warning: Currently, elements that do not fit into any groups are discarded.

See also:

get_nodes(), change_node_numbering()

Notes

The element-node connectivities are read from the mesh. If you want to change the ordering of the nodes, use the change_node_numbering() function.

Both this and the *get_nodes()* function relies on getGroupsOnSpecifiedLev to obtain the groups based on a parameter, called *meshDimRelToMaxExt*. This parameter designates the relative dimension of the mesh entities whose IDs are required. If it is 1, it denotes the nodes. If 0, entities of the same dimension as the mesh are meant (e.g. group of volumes for a 3D mesh, or group of faces for a 2D mesh). When -1, entities of spatial dimension immediately below that of the mesh are collected (e.g. group of faces for a 3D mesh, or group of edges for a 2D mesh). For -2, entities of two dimensions below that of the mesh are fetched (e.g. group of edges for a 3D mesh).

grains.med.**get_elements**(*mesh*, *numbering='global'*)

Obtains the elements for each group of a mesh.

Elements of the same dimension as the mesh are collected (e.g. faces for a 2D mesh).

Todo: put those elements that do not belong to any group into an automatically created group

Todo: support ordering *elements* in alphabetical order

Todo: implement the *'global'* strategy

Parameters

- **mesh** (*MEDFileUMesh*) – Unstructured mesh.
- **numbering** (*{'global'}, optional*) –

  Determines how to allocate element numbers in the mesh. 'global': numbers the elements without taking into account which group they belong to. Use this strategy if you are not sure whether an element belongs to more than one group. 'group': numbers the elements group-wise. This is much faster than the *'global'* strategy, but use this option if you are sure that the groups of the mesh do not contain common elements.

  The default is 'global'.

Returns

- **elements** (*ndarray*) – Element-node connectivities in a 2D numpy array, in which each row corresponds to an element and the columns are the nodes of the elements. It is assumed that all the elements have the same number of nodes.
- **element_groups** (*dict*) – The keys in the dictionary are the element group names, while the values are list of integers, giving the elements that belong to the particular group.

Warning: Currently, elements that do not fit into any groups are discarded.

See also:

get_nodes(), change_node_numbering()

Notes

The element-node connectivities are read from the mesh. If you want to change the ordering of the nodes, use the change_node_numbering() function.

Both this and the *get_nodes()* function relies on getGroupsOnSpecifiedLev to obtain the groups based on a parameter, called *meshDimRelToMaxExt*. This parameter designates the relative dimension of the mesh entities whose IDs are required. If it is 1, it denotes the nodes. If 0, entities of the same dimension as the mesh are meant (e.g. group of volumes for a 3D mesh, or group of faces for a 2D mesh). When -1, entities of spatial dimension immediately below that of the mesh are collected (e.g. group of faces for a 3D mesh, or group of edges for a 2D mesh). For -2, entities of two dimensions below that of the mesh are fetched (e.g. group of edges for a 3D mesh).

grains.med.**get_nodes**(*mesh*)

Obtains the nodes and the node groups of a mesh.

Parameters **mesh** (*MEDFileUMesh*) – Unstructured mesh.

Returns

- **nodes** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a node, and the two columns giving the Cartesian coordinates of the nodes.
- **node_groups** (*dict*) – The keys in the dictionary are the node group names, while the values are list of integers, giving the nodes that belong to the particular group.

See also:

get_elements(), getGroupArr

grains.med.**read_mesh**(*filename*)

Reads a mesh file in .med format. Only one mesh, the first one, is supported. However, that mesh can contain groups.

Parameters **filename** (*str*) – Path to the mesh file.

Returns *MEDFileUMesh* – Represents an unstructured mesh. For details, see the manual on https://docs.salome-platform.org/latest/dev/MEDCoupling/developer/classMEDCoupling_1_1MEDFileUMesh.html

CHAPTER

TWENTYONE

SALOME

The documentation generated from this file is available on https://cristalx.readthedocs.io/en/latest/api.html#module-grains.salome.

The aim of this *module* is to manage geometry and mesh operations on two-dimensional microstructures that tessellate a domain. This has the important consequence that the domain is assumed to consist of non-overlapping shapes that cover it. After generating a *conforming* mesh, each element belongs to a single group and no element exists outside the group. More precisely, elements that do not belong to any group are not taken into account by the `Mesh` class. They can still be accessed by the functions of Salome, but the use of such lower-level abstractions is against the philosophy of encapsulation this module provides.

The non-goals of this module include everything not related to the tessellation nature of 2D microstructures. The emphasis is on readability and not on speed.

This file can be used either as a module or as a script.

21.1 Using as a module

Developers, implementing new features, will use *salome.py* as a Python module. Although this module is part of the `grains` package in the CristalX project, it does not rely on the other modules of `grains`. This ensures that it can be used standalone and *run as a script* in the Salome environment. It only uses language constructs available in Python 3.6, and external packages shipped with Salome 9.4.0 onwards. To enable debugging, code completion and other useful development methods, consult with the documentation on ... Most classes contain a protected variable that holds the underlying Salome object. Unless you debug, it is not necessary to directly deal with Salome objects programmatically.

21.2 Using as a script

When *salome.py* is run as a script, the contents in the `if __name__ == "__main__":` block is executed. Edit it to suit your needs. Similarly to the case when *used as a module*, the script can only be run from Salome's own Python interpreter: either from the shell or from the GUI. To run it from the shell (including the GUI's built-in Python command prompt), type

```
exec(open("<path_to_CristalX>/grains/salome.py", "rb").read())
```

You can also execute the script from the GUI by clicking on *File* → *Load Script*...

21.3 Classes

Geometry	Represents the geometrical entities of a two-dimensional tessellated domain.
Face	Closed part of a plane.
Edge	A shape corresponding to a curve, and bounded by a vertex at each extremity.
Interface	An edge between two faces.
Mesh	Performs mesh manipulations on a tessellated geometry.
FaceMesh	Mesh on a face, part of the whole mesh.
InterfaceMesh	Mesh on an interface, part of the whole mesh.
CohesiveZone	Constructs zero-thickness elements along the interfaces.
GUI	Using GUI-related functionalities in Salome.

21.3.1 grains.salome.Geometry

class grains.salome.**Geometry**(*name='microstructure'*)

Represents the geometrical entities of a two-dimensional tessellated domain.

A *Geometry* object knows about the faces that tessellate the domain, and about the edges and interfaces that separate the faces.

Parameters **name** (*str, optional*) – Name of the geometry.

See also:

Face, *Edge*, *Interface*

__init__(*name='microstructure'*)

Initialize self. See help(type(self)) for accurate signature.

Methods

__init__([name])	Initialize self.
create_interfaces()	Constructs unique interfaces that separate the faces.
extract_edges()	Decomposes each face into edges.
extract_faces()	Decomposes the geometry into faces.
load(step_file)	Loads the geometry from a STEP file.

21.3.2 grains.salome.Face

class grains.salome.**Face**(*face*, *name*)

Closed part of a plane.

A *Face* knows about the *Edge* objects that bound it.

Parameters

- **face** (*GEOM_Object of shape type 'FACE'*) – The main Salome object wrapped by this class.
- **name** (*str*) – Name of the face.

See also:

GEOM_Object, Shape type

__init__ (*face*, *name*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(face, name)	Initialize self.

21.3.3 grains.salome.Edge

class grains.salome.**Edge**(*edge*, *name*)
A shape corresponding to a curve, and bounded by a vertex at each extremity.

An *Edge* knows about the *Face* it is part of, and the faces neighboring it.

Parameters

- **edge** (*GEOM_Object of shape type 'EDGE'*) – The main Salome object wrapped by this class.
- **name** (*str*) – Name of the edge.

See also:

GEOM_Object, Shape type

__init__ (*edge*, *name*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(edge, name)	Initialize self.
length()	Length of the edge.

21.3.4 grains.salome.Interface

class grains.salome.**Interface**(*edge*, *name*, *neighboring_faces*)
An edge between two faces.

Similar to an *Edge*, but two neighboring *Face* objects share a common *Interface*. An *Interface* knows about the two faces that it separates.

Parameters

- **edge** (*GEOM_Object of shape type 'EDGE'*) – The main Salome object wrapped by this class.
- **name** (*str*) – Name of the interface.
- **neighboring_faces** (*list of Face*) – The two neighboring faces.

See also:

Edge, *Face*

__init__ (*edge*, *name*, *neighboring_faces*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(edge, name, neighboring_faces)	Initialize self.
length()	Length of the interface.

21.3.5 grains.salome.Mesh

class grains.salome.**Mesh** (*geometry*, *name='Mesh'*)
Performs mesh manipulations on a tessellated geometry.

Parameters

- **geometry** (*Geometry*) – Geometry object on which the mesh exists.
- **name** (*str, optional*) – Name of the mesh.

See also:

Geometry, *FaceMesh*, *InterfaceMesh*

__init__ (*geometry*, *name='Mesh'*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(geometry[, name])	Initialize self.
element_edge_normal(element, edge)	Outward-pointing unit normal to an element edge.
generate()	Generates a mesh on the geometry.
generate_element_nodes(elements)	Nodes of selected elements, returned one at a time.
incident_elements(edge[, element_type])	Searches for elements incident to an edge.
incident_face_mesh(interface_mesh)	Face meshes incident to an interface mesh.
obtain_face_meshes()	Retrieves the elements of the mesh on each face.
obtain_interface_meshes()	Obtains the 1D interfacial mesh for each interface.
one_ring(node[, definition])	Elements around a node.
point_in_element(element, point)	Checks whether a point is in an element.

21.3.6 grains.salome.FaceMesh

class grains.salome.**FaceMesh** (*face_mesh*, *name*, *on_face*)
Mesh on a face, part of the whole mesh.

Parameters

- **face_mesh** (*smeshBuilder.Mesh.GroupOnGeom*) – The main Salome object wrapped by this class.
- **name** (*str*) – Name of the face mesh.
- **on_face** (*Face*) – Geometrical face on which this mesh exists.

__init__ (*face_mesh*, *name*, *on_face*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(face_mesh, name, on_face)	Initialize self.
elements()	Retrieves the elements of the face mesh.
nodes()	Retrieves the nodes of the face mesh.

21.3.7 grains.salome.InterfaceMesh

class grains.salome.**InterfaceMesh** (*interface_mesh*, *name*, *on_interface*)
Mesh on an interface, part of the whole mesh.

Parameters

- **interface_mesh** (*smeshBuilder.Mesh.GroupOnGeom*) – The main Salome object wrapped by this class.
- **name** (*str*) – Name of the interface mesh.
- **on_interface** (*Interface*) – Interface on which this mesh exists.

__init__ (*interface_mesh*, *name*, *on_interface*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(interface_mesh, name, on_interface)	Initialize self.
elements()	Retrieves the elements of the interface mesh.
elements_by_nodes(nodes)	Connecting elements to given nodes.
endpoint_nodes()	Nodes at the extremities of the interface mesh.
nodes()	Retrieves the nodes of the interface mesh.

21.3.8 grains.salome.CohesiveZone

class grains.salome.**CohesiveZone** (*mesh*)
Constructs zero-thickness elements along the interfaces.

Parameters **mesh** (*Mesh*) – Mesh into which the cohesive elements will be inserted.

__init__ (*mesh*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(mesh)	Initialize self.
create_cohesive_elements()	Creates zero-thickness quadrilateral elements along the interfaces.
decouple_faces()	Decouples the face meshes along the interfaces.

21.3.9 grains.salome.GUI

class grains.salome.**GUI**

Using GUI-related functionalities in Salome.

Notes

A part of Salome's GUI is exposed to Python. To get an idea of what is available, see https://docs.salome-platform.org/latest/gui/GUI/text_user_interface.html

__init__()

Initialize self. See help(type(self)) for accurate signature.

Methods

__init__	Initialize self.
assert_salome_desktop()	Checks if Salome's GUI is available, and raises an exception if it is not.
has_desktop()	Indicates if the Salome GUI is running.
show(obj[, show_only])	Shows objects in Salome's GUI.
update_object_browser()	Refreshes Salome's object browser.
view([view])	Sets the viewpoint.

Attributes

component_map

class grains.salome.**CohesiveZone**(*mesh*)

Bases: object

Constructs zero-thickness elements along the interfaces.

Parameters **mesh** (*Mesh*) – Mesh into which the cohesive elements will be inserted.

_affected_elements(*interface_mesh*)

Face elements whose nodes must be renumbered when duplicating an interface mesh.

Parameters **interface_mesh** (*InterfaceMesh*) – The original interface mesh that will be duplicated.

Returns **elements** (*set*) – Elements of the mesh that require node renumbering.

See also:

_enrich_interfaces()

_correct_junction_nodes()
Post-processing to handle inconsistent interface nodes at the junctions.

The interface-wise creation of new edge elements in *_affected_elements()* may result in edge element nodes that do not connect the opposite face element nodes on the two sides of the interface. This function checks the edge element nodes at the junctions and renumbers them so that they hold the same label as the face element nodes they connect to.

Returns *None.*

See also:

decouple_faces(), *_affected_elements()*, smeshBuilder.Mesh.FindCoincidentNodesOnPart(), smeshBuilder.Mesh.ChangeElemNodes()

_enrich_interfaces()
Inserts new interface elements and nodes into the mesh.

Although Salome has built-in functionality for duplicating nodes and creating elements, even accessible from the GUI with *Modification -> Transformation -> Duplicate Nodes and/or Elements*, it does not work with multiple intersecting interfaces or for closed interfaces. The reason is that the first step of the two-step procedure Salome performs fails in such situations. Therefore, this method uses a modified algorithm for the first step, and then calls the second step. These steps are the following:

1. Find the elements (called affected elements) in the mesh whose node numbers need to be changed due to the topological changes in the mesh caused by the introduction of new nodes.

2. The affected elements are fed to an existing function in Salome, which returns the 1D elements it creates from the duplicated nodes. The new interface mesh is stored in the *CohesiveZone* object.

Returns *None.*

See also:

decouple_faces(), *_affected_elements()*, smeshBuilder.Mesh.DoubleNodeElemGroups(), smeshBuilder.Mesh.MakeGroupByIds()

_generate_cohesive_element(*bottom_element*, *top_element*)
Creates a zero-thickness quadrilateral element.

Parameters

- **bottom_element** (*int*) – Edge element that will form the bottom edge of the cohesive element.
- **top_element** (*int*) – Edge element that will form the top edge of the cohesive element. It is assumed that the top element geometrically overlaps with the bottom element.

Returns *list of int* – The four nodes of the cohesive element, numbered counter-clockwise. The node ordering adheres to the node numbering in Abaqus.

See also:

Mesh.incident_elements(), *Mesh.element_edge_normal()*, smeshBuilder.Mesh.GetElemNodes(), smeshBuilder.Mesh.GetNodeXYZ()

create_cohesive_elements()
Creates zero-thickness quadrilateral elements along the interfaces.

It is necessary that the mesh has already been decoupled along the interfaces by the *decouple_faces()* method. That method introduced duplicated nodes and edge elements along the interfaces. The purpose of this method is to tie each interface (edge) element to its corresponding duplicate in order to form a

four-noded zero-thickness element, referred to as cohesive element. The bottom edge of the new cohesive element corresponds to the original edge element, while its top edge is formed by the duplicated interface edge element.

Returns **cohesive_elements** (*list*) – List of nodes that form the cohesive elements. The node numbering follows the node ordering of Salome, which is the same as the node ordering in Abaqus.

See also:

decouple_faces(), *_generate_cohesive_element()*, smeshBuilder.Mesh.AddFace()

decouple_faces()

Decouples the face meshes along the interfaces.

The algorithm consists of two main steps. First, new interface meshes are created that overlap with the existing ones and contain independent nodes and interface elements. In the same step, the incident face mesh nodes are updated to reflect the topological changes. However, in this method, extra nodes are introduced at the junctions, leading to a kinematic inconsistency. Therefore, the extraneous interface mesh nodes are renumbered in the second step of the algorithm.

Returns *None.*

See also:

create_cohesive_elements()

class grains.salome.**Edge**(*edge*, *name*)

Bases: object

A shape corresponding to a curve, and bounded by a vertex at each extremity.

An *Edge* knows about the *Face* it is part of, and the faces neighboring it.

Parameters

- **edge** (*GEOM_Object of shape type 'EDGE'*) – The main Salome object wrapped by this class.
- **name** (*str*) – Name of the edge.

See also:

GEOM_Object, Shape type

length()

Length of the edge.

Returns *float* – Length of the edge.

See also:

geomBuilder.BasicProperties

class grains.salome.**Face**(*face*, *name*)

Bases: object

Closed part of a plane.

A *Face* knows about the *Edge* objects that bound it.

Parameters

- **face** (*GEOM_Object of shape type 'FACE'*) – The main Salome object wrapped by this class.

- **name** (*str*) – Name of the face.

See also:

GEOM_Object, Shape type

class grains.salome.**FaceMesh**(*face_mesh*, *name*, *on_face*)
Bases: object

Mesh on a face, part of the whole mesh.

Parameters

- **face_mesh** (*smeshBuilder.Mesh.GroupOnGeom*) – The main Salome object wrapped by this class.
- **name** (*str*) – Name of the face mesh.
- **on_face** (*Face*) – Geometrical face on which this mesh exists.

elements()
Retrieves the elements of the face mesh.

Returns *list of int* – Elements belonging to the face mesh.

See also:

SMESH.SMESH_IDSource.GetIDs()

nodes()
Retrieves the nodes of the face mesh.

Returns *list of int* – Nodes belonging to the face mesh.

See also:

SMESH.SMESH_GroupBase.GetNodeIDs()

class grains.salome.**GUI**
Bases: object

Using GUI-related functionalities in Salome.

Notes

A part of Salome's GUI is exposed to Python. To get an idea of what is available, see https://docs.salome-platform.org/latest/gui/GUI/text_user_interface.html

exception SalomeNoDesktop
Bases: Exception

Raised when Salome is run without desktop, but a desktop functionality is invoked.

classmethod _get_component(*obj*)
Determines the component of an object.

This function maps a class of this module to the Salome module the class uses. For instance, class *Face* is mapped to 'GEOM'.

Parameters **obj** – Any object for which the component name is looked for.

Returns *str or None* – The name of the component the object belongs to. If an object of an unsupported class is given, None is returned. For the list of supported classes, see the component_map member of *GUI* class.

See also:

show()

static assert_salome_desktop()
Checks if Salome's GUI is available, and raises an exception if it is not.

This function acts as a helper function when relying on Salome's GUI.

Raises ***SalomeNoDesktop*** – If Salome's GUI is not available.

component_map = {<class 'grains.salome.Geometry'>: 'GEOM', <class 'grains.salome.Face':

static has_desktop()
Indicates if the Salome GUI is running.

Returns *bool* – True if Salome's GUI is available, False otherwise.

classmethod show(*obj*, *show_only=False*)
Shows objects in Salome's GUI.

Todo: Support list of objects.

Parameters

- **obj** (*iterable*) – The object(s) to be shown in Salome. Objects of the following classes are supported: Geometry, Face, Edge, Interface, Mesh, FaceMesh, InterfaceMesh.
- **show_only** (*bool, optional*) – If True, the other objects are hidden. The default value is False.

Returns *None*

Raises

- ***SalomeNoDesktop*** – If Salome's GUI is not available.
- **TypeError** – If `obj` is not an object that can be displayed.
- **ValueError** – If the given object does not exist in the Salome study.

Examples

For example, you can display an interface mesh and a face mesh by calling

```
GUI.show([interface_mesh, face_mesh])
```

where `interface_mesh` and `face_mesh` are *InterfaceMesh* and *FaceMesh* objects respectively. This way of using the *show* method provides great flexibility as different types of objects can be handled at the same time.

static update_object_browser()
Refreshes Salome's object browser.

Only makes sense if executed with the GUI enabled.

Returns *None*

See also:

has_desktop()

classmethod view(*view='top'*)
Sets the viewpoint.

Parameters **view** (*{'front', 'back', 'top', 'bottom', 'left', 'right'}, optional*) – Position from which the scene is viewed. The default is 'top'.

Returns *None*

class grains.salome.**Geometry**(*name='microstructure'*)
Bases: object

Represents the geometrical entities of a two-dimensional tessellated domain.

A *Geometry* object knows about the faces that tessellate the domain, and about the edges and interfaces that separate the faces.

Parameters **name** (*str, optional*) – Name of the geometry.

See also:

Face, *Edge*, *Interface*

_find_overlapping_edges()
Finds edges that are on top of each other.

Overlapping edges have the same length. Although its converse is not true in general, we will assume so. This part of the algorithm (i.e. deciding the overlapping edges) can later be refined.

Returns **overlapping_edges** (*list*) – Each member of the list contains a list of (supposedly) two Edge objects.

See also:

create_interfaces(), *Edge.length()*

static _has_smaller_ID(*edges*)
Selects the edge with a smaller ID.

When generating mesh with the NETGEN plugin of Salome, if several edges overlap, only the edge with the smallest ID holds a mesh. The purpose of this function is to find the edge with the smaller ID out of two overlapping edges.

Parameters **edges** (*list of Edge*) – List of two Edge objects.

Returns *Edge* – Either the first or the second element of the input list, depending on which of them has a smaller ID.

See also:

create_interfaces()

Notes

For a detailed discussion on this highly important issue, see the corresponding forum thread.

create_interfaces()
Constructs unique interfaces that separate the faces.

Based on the edges (obtained by exploding the mesh), interfaces are created. Interfaces are unique separators of two neighboring faces. In other words,

- if the edge is a boundary edge, no interface is created,
- two neighboring faces have two overlapping edges, of which one is defined to be an interface.

It is assumed that the edges and faces of the geometry have already been obtained.

Returns *None.*

See also:

extract_faces(), *extract_edges()*

extract_edges()
Decomposes each face into edges.

This method must be called after the *extract_faces()* method, otherwise it has no effect.

Returns *None.*

See also:

extract_faces()

extract_faces()
Decomposes the geometry into faces.

Returns *None.*

See also:

extract_edges()

load(*step_file*)
Loads the geometry from a STEP file.

Parameters **step_file** (*str*) – The STEP file containing the geometry.

Returns *None.*

class grains.salome.**Interface**(*edge*, *name*, *neighboring_faces*)
Bases: object

An edge between two faces.

Similar to an *Edge*, but two neighboring *Face* objects share a common *Interface*. An *Interface* knows about the two faces that it separates.

Parameters

- **edge** (*GEOM_Object of shape type 'EDGE'*) – The main Salome object wrapped by this class.
- **name** (*str*) – Name of the interface.
- **neighboring_faces** (*list of Face*) – The two neighboring faces.

See also:

Edge, *Face*

length()
Length of the interface.

Returns *float* – Length of the interface.

See also:

geomBuilder.BasicProperties

class grains.salome.**InterfaceMesh**(*interface_mesh*, *name*, *on_interface*)
Bases: object

Mesh on an interface, part of the whole mesh.

Parameters

- **interface_mesh** (*smeshBuilder.Mesh.GroupOnGeom*) – The main Salome object wrapped by this class.
- **name** (*str*) – Name of the interface mesh.
- **on_interface** (*Interface*) – Interface on which this mesh exists.

elements()
Retrieves the elements of the interface mesh.

Returns *list of int* – Elements belonging to the interface mesh.

See also:

SMESH.SMESH_IDSource.GetIDs()

elements_by_nodes(*nodes*)
Connecting elements to given nodes.

Parameters **nodes** (*list of int*) – Nodes for which we want to find the connecting elements.

Returns *list of int* – Elements that are incident to the given nodes.

See also:

smeshBuilder.Mesh.GetElementsByNodes()

endpoint_nodes()
Nodes at the extremities of the interface mesh.

Returns **ep_nodes** (*list of int*) – Nodes of the end points of the interface on which the interface mesh is defined. If the interface is open, it has two end points. When closed, the two end points coincide and instead of the two coinciding nodes, a single node is returned.

nodes()
Retrieves the nodes of the interface mesh.

Returns *list of int* – Nodes belonging to the interface mesh.

See also:

SMESH.SMESH_GroupBase.GetNodeIDs()

class grains.salome.**Mesh**(*geometry*, *name='Mesh'*)
Bases: object

Performs mesh manipulations on a tessellated geometry.

Parameters

- **geometry** (*Geometry*) – Geometry object on which the mesh exists.
- **name** (*str, optional*) – Name of the mesh.

See also:

Geometry, *FaceMesh*, *InterfaceMesh*

class ElementType
Bases: enum.Enum

Subset of the element types recognized by Salome.

This enumeration is for convenience. Only those elements of Salome are considered that are relevant for the *Mesh* class.

See also:

SMESH.ElementType

ALL

EDGE

FACE

NODE

element_edge_normal(*element*, *edge*)
Outward-pointing unit normal to an element edge.

The edge is assumed to be planar.

Parameters

- **element** (*int*) – ID of the element.
- **edge** (*list of int*) – Edge of the element for which the normal is to be found. The edge is given by its two nodes.

Returns **normal** (*tuple of float*) – Outward-pointing unit normal.

See also:

point_in_element()

generate()
Generates a mesh on the geometry.

Todo: Do not hardcode values and explain the need for consistent orientation.

generate_element_nodes(*elements*)
Nodes of selected elements, returned one at a time.

Parameters **elements** (*iterable*) – Element IDs.

Yields *list of int* – The first entry of the list is the element ID, the remaining entries are the node IDs of the element.

incident_elements(*edge*, *element_type=None*)
Searches for elements incident to an edge.

Parameters

- **edge** (*list of int*) – An edge of an element, given by its two nodes.
- **element_type** (*Mesh.ElementType, optional*) – Perform the search for the given element type only.

Returns *list of int* – Element IDs that are incident to the given edge.

See also:

smeshBuilder.Mesh.GetNodeInverseElements()

incident_face_mesh(*interface_mesh*)
Face meshes incident to an interface mesh.

Todo: Use this method in _affected_elements as well.

Parameters **interface_mesh** (*InterfaceMesh*) – Interface mesh for which the connecting face meshes are sought.

Returns **face_mesh** (*list of FaceMesh*) – Face meshes incident to an interface mesh.

Raises **Exception** – If no face mesh is incident to the interface mesh.

obtain_face_meshes()
Retrieves the elements of the mesh on each face.

Returns *None.*

obtain_interface_meshes()
Obtains the 1D interfacial mesh for each interface.

Returns *None.*

one_ring(*node*, *definition='connecting'*)
Elements around a node.

Parameters

- **node** (*int*) – Node ID for which the one-ring is searched.
- **definition** (*{'connecting', 'surrounding'}, optional*) – What you mean by neighboring elements. See the notes below.

Returns *list* – List of integers (element IDs).

Notes

One should make a distinction between elements *connecting* to a node and elements *surrounding* a node. For a mesh with no overlapping nodes, the two definitions give the same elements. However, if multiple nodes are located at the same geometrical point, it can happen that the incident elements are not connected to the same node.

point_in_element(*element*, *point*)
Checks whether a point is in an element.

This method is implemented for 2D meshes only.

Parameters

- **element** (*int*) – Element of the mesh.
- **point** (*tuple of float*) – Point coordinates (x,y).

Returns *bool* – True if the given element contains the given point.

Raises

- **Exception** – If the mesh is not two-dimensional.
- **ValueError** – If the element does not exist in the mesh.

Notes

This method calls an efficient *matplotlib* function to determine whether a point is in a polygon. For alternative implementations, see this discussion.

See also:

`matplotlib.path.Path.contains_point()`

CHAPTER

TWENTYTWO

GEOMETRY

This module implements computational geometry algorithms, needed for other modules.

All the examples assume that the modules *numpy* and *matplotlib.pyplot* were imported as *np* and *plt*, respectively.

22.1 Classes

Mesh	Data structure for a general mesh.
TriMesh	Unstructured triangular mesh.
Polygon	Represents a polygon.

22.1.1 grains.geometry.Mesh

class grains.geometry.**Mesh**(*vertices*, *cells*)

Data structure for a general mesh.

This class by no means wants to provide intricate functionalities and does not strive to be efficient at all. Its purpose is to give some useful features the project relies on. The two main entities in the mesh are the *vertices* and the *cells*. They are expected to be passed by the user, so reading from various mesh files is not implemented. This keeps the class simple, requires few package dependencies and keeps the class focused as there are powerful tools to convert among mesh formats (see e.g. meshio).

Parameters

- **vertices** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a vertex, and the two columns giving the Cartesian coordinates of the vertex.
- **cells** (*ndarray*) – Cell-vertex connectivities in a 2D numpy array, in which each row corresponds to a cell and the columns are the vertices of the cells. It is assumed that all the cells have the same number of vertices.

See also:

change_vertex_numbering

Notes

Although not necessary, it is highly recommended that the local vertex numbering in the cells are the same, either clockwise or counter-clockwise. Some methods, such as *get_boundary()* even requires it. If you are not sure whether the cells you provide have a consistent numbering, it is better to renumber them by calling the *change_vertex_numbering()* method.

__init__(*vertices*, *cells*)

Todo: Error checking

Methods

__init__(vertices, cells)	
associate_field(vertex_values[, name])	Associates a scalar, vector or tensor field to the nodes.
create_cell_set(name, cells)	Forms a group from a set of cells.
create_vertex_set(name, vertices)	Forms a group from a set of vertices.
get_boundary()	Extracts the boundary of the mesh.
get_edges()	Constructs edge-cell connectivities of the mesh.

22.1.2 grains.geometry.TriMesh

class grains.geometry.**TriMesh**(*vertices*, *cells*)

Unstructured triangular mesh.

Vertices and cells are both stored as numpy arrays. This makes the simple mesh manipulations easy and provides interoperability with the whole scientific Python stack.

Parameters

- **vertices** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a vertex, and the two columns giving the Cartesian coordinates of the vertex.
- **cells** (*ndarray*) – Cell-vertex connectivities in a 2D numpy array, in which each row corresponds to a cell and the columns are the vertices of the cells. It is assumed that all the cells have the same number of vertices.

__init__(*vertices*, *cells*)

Error checking

Methods

__init__(vertices, cells)	
associate_field(vertex_values[, name])	Associates a scalar, vector or tensor field to the nodes.
cell_area(cell)	Computes the area of a cell.
cell_set_area(cell_set)	Computes the area of a cell set.
cell_set_to_mesh(cell_set)	Creates a mesh from a cell set.
change_vertex_numbering(orientation[, inplace])	Changes cell vertex numbering.
create_cell_set(name, cells)	Forms a group from a set of cells.
create_vertex_set(name, vertices)	Forms a group from a set of vertices.
get_boundary()	Extracts the boundary of the mesh.
get_edges()	Constructs edge-cell connectivities of the mesh.
plot(*args, **kwargs)	Plots the mesh.
plot_field(component, *args[, show_mesh])	Plots a field on the mesh.
rotate(angle[, point, inplace])	Rotates a 2D mesh about a given point by a given angle.
sample_mesh(sample[, param])	Provides sample meshes.
scale(factor[, inplace])	Scales the geometry by modifying the coordinates of the vertices.
write_inp(filename)	Writes the mesh to an Abaqus .inp file.

Attributes

plot_options

22.1.3 grains.geometry.Polygon

class grains.geometry.**Polygon**(*vertices*)

Represents a polygon.

This class works as expected as long as the given polygon is *simple*, i.e. it is not self-intersecting and does not contain holes.

A simple class that has *numpy* and *matplotlib* (for the visualization) as the only dependencies. It does not want to provide extensive functionalities (for those, check out Shapely). The polygon is represented by its vertices, given in a consecutive order.

Parameters **vertices** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a vertex, and the two columns giving the Cartesian coordinates of the vertex.

Raises

- **Exception** – If all the vertices of the polygon lie along the same line. If the polygon is not given in R^2.
- **ValueError** – If the polygon does not have at least 3 vertices.

Examples

Try to give a "polygon", in which all vertices are collinear

```
>>> poly = Polygon(np.array([[0, 0], [1, 1], [2, 2]]))
Traceback (most recent call last):
...
Exception: All vertices are collinear. Not a valid polygon.
```

Now we give a valid polygon:

```
>>> pentagon = Polygon(np.array([[2, 1], [0, 0], [0.5, 3], [-1, 4], [3, 5]]))
```

Use Python's *print* function to display basic information about a polygon:

```
>>> print(pentagon)
A non-convex polygon with 5 vertices, oriented clockwise.
```

__init__(*vertices*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(vertices)	Initialize self.
area()	Signed area of the polygon.
centroid()	Centroid of the polygon.
diameter([definition])	Diameter of the polygon.
is_convex()	Decides whether the polygon is convex.
orientation()	Orientation of the polygon.
plot(*args, **kwargs)	Plots the polygon.

Attributes

plot_options

22.2 Functions

is_collinear(points[, tol])	Decides whether a set of points is collinear.
squared_distance(x, y)	Squared Euclidean distance between two points.
distance_matrix(points)	A symmetric square matrix, containing the pairwise squared Euclidean distances among points.
_polygon_area(x, y)	Computes the signed area of a non-self-intersecting, possibly concave, polygon.

22.2.1 grains.geometry.is_collinear

grains.geometry.**is_collinear**(*points*, *tol=None*)

Decides whether a set of points is collinear.

Works in any dimensions.

Parameters

- **points** (*ndarray*) – 2D numpy array with N columns, each row corresponding to a point, and the N columns giving the Cartesian coordinates of the point.
- **tol** (*float, optional*) – Tolerance value passed to numpy's *matrix_rank* function. This tolerance gives the threshold below which SVD values are considered zero.

Returns *bool* – True for collinear points.

See also:

`numpy.linalg.matrix_rank()`

Notes

The algorithm for three points is from Tim Davis.

Examples

Two points are always collinear

```
>>> is_collinear(np.array([[1, 0], [1, 5]]))
True
```

Three points in 3D which are supposed to be collinear (returns false due to numerical error)

```
>>> is_collinear(np.array([[0, 0, 0], [1, 1, 1], [5, 5, 5]]), tol=0)
False
```

The previous example with looser tolerance

```
>>> is_collinear(np.array([[0, 0, 0], [1, 1, 1], [5, 5, 5]]), tol=1e-14)
True
```

22.2.2 grains.geometry.squared_distance

grains.geometry.**squared_distance**(*x*, *y*)

Squared Euclidean distance between two points.

For points $x(x_1, ..., x_n)$ and $y(y_1, ...y_n)$ the following metric is computed

$$\sum_{i=1}^{n}(x_i - y_i)^2$$

Parameters **x, y** (*ndarray*) – 1D numpy array, containing the coordinates of the two points.

Returns *float* – Squared Euclidean distance.

See also:

distance_matrix()

Examples

```
>>> squared_distance(np.array([0, 0, 0]), np.array([1, 1, 1]))
3.0
```

22.2.3 grains.geometry.distance_matrix

grains.geometry.**distance_matrix**(*points*)

A symmetric square matrix, containing the pairwise squared Euclidean distances among points.

Parameters **points** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a point, and the two columns giving the Cartesian coordinates of the points.

Returns **dm** (*ndarray*) – Distance matrix.

See also:

squared_distance()

Examples

```
>>> points = np.array([[1, 1], [3, 0], [-1, -1]])
>>> distance_matrix(points)
array([[ 0.,  5.,  8.],
       [ 5.,  0., 17.],
       [ 8., 17.,  0.]])
```

22.2.4 grains.geometry._polygon_area

grains.geometry.**_polygon_area**(*x*, *y*)

Computes the signed area of a non-self-intersecting, possibly concave, polygon.

Directly taken from http://rosettacode.org/wiki/Shoelace_formula_for_polygonal_area#Python

Parameters **x, y** (*list*) – Coordinates of the consecutive vertices of the polygon.

Returns *float* – Area of the polygon.

Warning: If numpy vectors are passed as inputs, the resulting area is incorrect! WHY?

Notes

The code is not optimized for speed and for numerical stability. Intended to be used to compute the area of finite element cells, in which case the numerical stability is not an issue (unless the cell is degenerate). As this function is called possibly as many times as the number of cells in the mesh, no input checking is performed.

Examples

```
>>> _polygon_area([0, 1, 1], [0, 0, 1])
0.5
```

class grains.geometry.**Mesh**(*vertices*, *cells*)
Bases: abc.ABC

Data structure for a general mesh.

This class by no means wants to provide intricate functionalities and does not strive to be efficient at all. Its purpose is to give some useful features the project relies on. The two main entities in the mesh are the *vertices* and the *cells*. They are expected to be passed by the user, so reading from various mesh files is not implemented. This keeps the class simple, requires few package dependencies and keeps the class focused as there are powerful tools to convert among mesh formats (see e.g. meshio).

Parameters

- **vertices** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a vertex, and the two columns giving the Cartesian coordinates of the vertex.
- **cells** (*ndarray*) – Cell-vertex connectivities in a 2D numpy array, in which each row corresponds to a cell and the columns are the vertices of the cells. It is assumed that all the cells have the same number of vertices.

See also:

change_vertex_numbering

Notes

Although not necessary, it is highly recommended that the local vertex numbering in the cells are the same, either clockwise or counter-clockwise. Some methods, such as *get_boundary()* even requires it. If you are not sure whether the cells you provide have a consistent numbering, it is better to renumber them by calling the *change_vertex_numbering()* method.

static _ismatrix(*array*)
Decides whether the input is a matrix.

Parameters **array** (*ndarray*) – Numpy array to be checked.

Returns *bool* – True if the input is a 2D array. Otherwise, False.

See also:

_isvector()

static _isvector(*array*)
Decides whether the input is a vector.

Parameters **array** (*ndarray*) – Numpy array to be checked.

Returns *bool* – True if the input is a 1D array or if it is a column or row vector. Otherwise, False.

See also:

_ismatrix()

associate_field(*vertex_values*, *name='field'*)
Associates a scalar, vector or tensor field to the nodes.

Only one field can be present at a time. If you want to use a new field, call this method again with the new field values, which will replace the previous ones.

Parameters

- **vertex_values** (*ndarray*) – Field values at the nodes.
- **name** (*str, optional*) – Name of the field. If not given, it will be 'field'.

Returns *None*

create_cell_set (*name*, *cells*)
Forms a group from a set of cells.

Parameters

- **name** (*str*) – Name of the cell set.
- **cells** (*list*) – List of cells to be added to the set.

Returns *None*

create_vertex_set (*name*, *vertices*)
Forms a group from a set of vertices.

Parameters

- **name** (*str*) – Name of the vertex set.
- **vertices** (*list*) – List of vertices to be added to the set.

get_boundary ()
Extracts the boundary of the mesh.

It is expected that all the cells have the same orientation, i.e. the cell vertices are consistently numbered (either clockwise or counter-clockwise). See the constructor for details.

Returns

- **boundary_vertices** (*ndarray*) – Ordered 1D ndarray of vertices, the boundary vertices of the mesh.
- **boundary_edges** (*dict*) – The keys of the returned dictionary are 2-tuples, representing the two vertices of the boundary edges, while the values are the list of cells containing a particular boundary edge. The dictionary is ordered: the consecutive keys represent the consecutive boundary edges. Although a boundary edge is part of a single cell, that cell is given in a list so as to maintain the same format as the one used in the *get_edges()* method.

Notes

The reason why consistent cell vertex numbering is demanded is because in that case the boundary edges are oriented in such a way that the second vertex of a boundary edge is the first vertex of the boundary edge it connects to.

Examples

Let us consider the same example mesh as the one described in the *get_edges()* method.

```
>>> mesh = TriMesh(np.array([[0, 0], [1, 0], [2, 0], [0, 2], [0, 1], [1, 1]]),
...                np.array([[0, 1, 5], [4, 5, 3], [5, 4, 0], [2, 5, 1]]))
```

We extract the boundary of that mesh using

```
>>> bnd_vertices, bnd_edges = mesh.get_boundary()
>>> bnd_vertices
array([0, 1, 2, 5, 3, 4])
>>> bnd_edges
{(0, 1): [0], (1, 2): [3], (2, 5): [3], (5, 3): [1], (3, 4): [1], (4, 0): [2]}
```

get_edges()

Constructs edge-cell connectivities of the mesh.

The cells of the mesh do not necessarily have to have a consistent vertex numbering.

Returns **edges** (*dict*) – The keys of the returned dictionary are 2-tuples, representing the two vertices of the edges, while the values are the list of cells containing a particular edge.

Notes

We traverse through the cells of the mesh, and within each cell the edges. The edges are stored as new entries in a dictionary if they are not already stored. Checking if a key exists in a dictionary is performed in O(1). The number of edges in a cell is independent of the mesh density. Therefore, the time complexity of the algorithm is O(N), where N is the number of cells in the mesh.

See also:

get_boundary()

Examples

We show an example for a triangular mesh (as the *Mesh* class is abstract).

```
>>> mesh = TriMesh(np.array([[0, 0], [1, 0], [2, 0], [0, 2], [0, 1], [1, 1]]),
...                np.array([[0, 1, 5], [4, 5, 3], [5, 4, 0], [2, 5, 1]]))
>>> edges = mesh.get_edges()
>>> edges
{(0, 1): [0], (1, 5): [0, 3], (5, 0): [0, 2], (4, 5): [1, 2], (5, 3): [1],
(3, 4): [1], (4, 0): [2], (2, 5): [3], (1, 2): [3]}
>>> mesh.plot(cell_labels=True, vertex_labels=True)
>>> plt.show()
```

class grains.geometry.**Polygon**(*vertices*)

Bases: object

Represents a polygon.

This class works as expected as long as the given polygon is *simple*, i.e. it is not self-intersecting and does not contain holes.

A simple class that has *numpy* and *matplotlib* (for the visualization) as the only dependencies. It does not want to provide extensive functionalities (for those, check out Shapely). The polygon is represented by its vertices, given in a consecutive order.

Parameters **vertices** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a vertex, and the two columns giving the Cartesian coordinates of the vertex.

Raises

- **Exception** – If all the vertices of the polygon lie along the same line. If the polygon is not given in R^2.
- **ValueError** – If the polygon does not have at least 3 vertices.

Examples

Try to give a "polygon", in which all vertices are collinear

```
>>> poly = Polygon(np.array([[0, 0], [1, 1], [2, 2]]))
Traceback (most recent call last):
...
Exception: All vertices are collinear. Not a valid polygon.
```

Now we give a valid polygon:

```
>>> pentagon = Polygon(np.array([[2, 1], [0, 0], [0.5, 3], [-1, 4], [3, 5]]))
```

Use Python's *print* function to display basic information about a polygon:

```
>>> print(pentagon)
A non-convex polygon with 5 vertices, oriented clockwise.
```

area()
Signed area of the polygon.

The signed area is computed by the shoelace formula[1]

$$A = \frac{1}{2}\sum_{i=1}^{N}(x_i y_{i+1} - x_{i+1} y_i)$$

Returns *float* – Signed area.

References

Examples

```
>>> poly = Polygon(np.array([[0, 0], [1, 0], [1, 1], [-1, 1]]))
>>> poly.area()
1.5
>>> poly = Polygon(np.array([[-1, 1], [1, 1], [1, 0], [0, 0]]))
>>> poly.area()
-1.5
```

centroid()
Centroid of the polygon.

[1] http://paulbourke.net/geometry/polygonmesh/centroid.pdf

The centroid is computed according to the following formula[2]

$$C_x = \frac{1}{6A}\sum_{i=1}^{N}(x_i + x_{i+1})(x_i y_{i+1} - x_{i+1} y_i)$$

$$C_y = \frac{1}{6A}\sum_{i=1}^{N}(y_i + y_{i+1})(x_i y_{i+1} - x_{i+1} y_i)$$

where A is the signed area determined by the `area()` method and x_i, y_i are the vertex coordinates with $x_{N+1} = x_1$ and $y_{N+1} = y_1$.

Returns *tuple* – 2-tuple, the coordinates of the centroid.

References

Examples

```
>>> poly = Polygon(np.array([[0, 0], [0, 1], [1, 1], [1, 0]]))
>>> poly.centroid()
(0.5, 0.5)
>>> poly = Polygon(np.array([[2, 1], [0, 0], [0.5, 3], [-1, 4], [3, 5]]))
>>> poly.centroid()
(1.254..., 2.807...)
```

diameter (*definition='set'*)

Diameter of the polygon.

Multiple definitions are supported for the diameter:

- *Diameter of a set*. The polygon is considered as a set A of points comprised

of the polygon vertices. Let (X, d) be a metric space. The diameter of the set is defined as

$$\operatorname{diam}(A) = \sup\{d(x, y) \mid x, y \in A\}. \tag{22.1}$$

Here, the Euclidean metric is used.

- *Equivalent diameter*. Diameter of the circle of the same area as that of the polygon.

Parameters **definition** (*{'set', 'equivalent'}, optional*) – The default is 'set'.

Returns *float* – Diameter of the polygon, based on the chosen definition.

Notes

When `definition` is 'set', computing the diameter by (22.1) is equivalent to determining the distance of the furthest points in the convex hull of A. Therefore, the diameter will always be the distance between two points on the convex hull of A. Then for each vertex of the hull finding which other hull vertex is farthest away from it, the *rotating caliper* algorithm can be used. Our brute-force method is simpler as it needs neither the convex hull nor the rotating caliper algorithm: all the pairwise distances among the polygon vertices are computed and the largest one is chosen. Pair of points a maximum distance apart. Since the polygons in our applications do not have that many vertices, this simplistic approach is a viable alternative.

[2] http://paulbourke.net/geometry/polygonmesh/centroid.pdf

Examples

```
>>> poly = Polygon(np.array([[2, 5], [0, 1], [4, 3], [4, 5]]))
>>> poly.diameter('set')
5.6568542...
>>> poly.diameter('equivalent')
3.1915382...
>>> poly = Polygon(np.array([[2, 1], [3, -4], [-1, -1], [-4, -2], [-3, 0]]))
>>> poly.diameter('set')
7.2801098...
>>> poly.diameter('equivalent')
4.2967398...
```

is_convex()
Decides whether the polygon is convex.

Returns *bool* – True if the polygon is convex. False otherwise.

Notes

The algorithm works by checking if all pairs of consecutive edges in the polygon are either all clockwise or all counter-clockwise oriented. This method is valid only for simple polygons. The implementation follows this code, extended for the case when two consecutive edges are collinear. If the polygon was not simple, a more complicated algorithm would be needed, see e.g. here.

Examples

A triangle is always convex:

```
>>> poly = Polygon(np.array([[1, 1], [0, 1], [0, 0]]))
>>> poly.is_convex()
True
```

Let us define a concave deltoid:

```
>>> poly = Polygon(np.array([[-1, -1], [0, 1], [1, -1], [0, 5]]))
>>> poly.is_convex()
False
```

Give a polygon that has two collinear edges:

```
>>> poly = Polygon(np.array([[0.5, 0], [1, 0], [1, 1], [0, 1], [0, 0]]))
>>> poly.is_convex()
True
```

orientation()
Orientation of the polygon.

Returns *str* – ‘cw’ if the polygon has clockwise orientation, ‘ccw’ if counter-clockwise.

plot(**args*, ***kwargs*)
Plots the polygon.

Parameters **ax** (*matplotlib.axes.Axes, optional*) – The *Axes* instance the polygon resides in. The default is None, in which case a new *Axes* within a new figure is created.

Other Parameters

- **show_axes** (*bool, optional*) – If True, the coordinate system is shown. The default is True.
- **vertex_labels** (*bool, optional*) – If True, vertex labels are shown. The default is False.
- **args, kwargs** (*optional*) – Additional arguments and keyword arguments to be specified. Those arguments are the ones supported by `matplotlib.axes.Axes.plot()`.

Returns *None*

Examples

Consider the pentagon used in the example of the constructor. Plot it in black with red diamond symbols representing its vertices. Moreover, display the vertex numbers and do not show the coordinate system.

```
>>> pentagon = Polygon(np.array([[2, 1], [0, 0], [0.5, 3], [-1, 4], [3, 5]]))
>>> pentagon.plot('k-d', vertex_labels=True, markerfacecolor='r', show_
↪axes=False)
>>> plt.show()
```

plot_options = {'ax': None, 'show_axes': True, 'vertex_labels': False}

class grains.geometry.**TriMesh**(*vertices*, *cells*)

Bases: *grains.geometry.Mesh*

Unstructured triangular mesh.

Vertices and cells are both stored as numpy arrays. This makes the simple mesh manipulations easy and provides interoperability with the whole scientific Python stack.

Parameters

- **vertices** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a vertex, and the two columns giving the Cartesian coordinates of the vertex.
- **cells** (*ndarray*) – Cell-vertex connectivities in a 2D numpy array, in which each row corresponds to a cell and the columns are the vertices of the cells. It is assumed that all the cells have the same number of vertices.

cell_area(*cell*)

Computes the area of a cell.

Parameters **cell** (*int*) – Cell label.

Returns **area** (*float*) – Area of the cell.

See also:

cell_set_area()

cell_set_area(*cell_set*)

Computes the area of a cell set.

Parameters **cell_set** (*str*) – Name of the cell set.

Returns **area** (*float*) – Area of the cell set.

See also:

cell_area()

cell_set_to_mesh(*cell_set*)

Creates a mesh from a cell set.

The cell orientation is preserved. I.e. if the cells had a consistent orientation (clockwise or counter-clockwise), the cells of the new mesh inherit this property.

Parameters **cell_set** (*str*) – Name of the cell set being used to construct the new mesh. The cell set must be present in the `cell_sets` member variable of the current mesh object.

Returns *TriMesh* – A new *TriMesh* object, based on the selected cell set of the original mesh.

Notes

The implementation is based on https://stackoverflow.com/a/13572640/4892892.

Examples

```
>>> mesh = TriMesh(np.array([[0, 0], [1, 0], [0, 1], [1, 1]]),
...                np.array([[0, 1, 2], [1, 3, 2]]))
>>> mesh.create_cell_set('set', [1])
>>> new_mesh = mesh.cell_set_to_mesh('set')
>>> new_mesh.cells  # note that the vertices have been relabelled
array([[0, 2, 1]])
>>> new_mesh.vertices
array([[1, 0],
       [0, 1],
       [1, 1]])
>>> new_mesh.plot(cell_labels=True, vertex_labels=True)
>>> plt.show()
```

change_vertex_numbering(*orientation*, *inplace=False*)

Changes cell vertex numbering.

Parameters

- **orientation** (*{'ccw', 'cw'}*) – Vertex numbering within a cell, either *'ccw'* (counter-clockwise, default) or *'cw'* (clock-wise).
- **inplace** (*bool, optional*) – If True, the vertex ordering is updated in the mesh object. The default is False.

Returns **reordered_cells** (*ndarray*) – Same format as the `cells` member variable, with the requested vertex ordering.

Notes

Supposed to be used with planar P1 or Q1 finite s.

Examples

```
>>> mesh = TriMesh(np.array([[1, 1], [3, 5], [7,3]]), np.array([0, 1, 2]))
>>> mesh.change_vertex_numbering('ccw')
array([[2, 1, 0]])
```

plot(**args*, ***kwargs*)

Plots the mesh.

Parameters **ax** (*matplotlib.axes.Axes, optional*) – The *Axes* instance the mesh resides in. The default is None, in which case a new *Axes* within a new figure is created.

Other Parameters

- **cell_sets, vertex_sets** (*bool, optional*) – If True, the cell/vertex sets (if exist) are highlighted in random colors. The default is True.
- **cell_legends, vertex_legends** (*bool, optional*) – If True, cell/vertex set legends are shown. The default is False. For many sets, it is recommended to leave these options as False, otherwise the plotting becomes very slow.
- **cell_labels, vertex_labels** (*bool, optional*) – If True, cell/vertex labels are shown. The default is False. Recommended to be left False in case of many cells/vertices. Cell labels are positioned in the centroids of the cells.
- **args, kwargs** (*optional*) – Additional arguments and keyword arguments to be specified. Those arguments are the ones supported by `matplotlib.axes.Axes.plot()`.

Returns *None*

Notes

If you do not want to plot the cells, only the vertices, pass the `'.'` option, e.g.:

```
mesh.plot('k.')
```

to plot the vertices in black. Here, `mesh` is a *TriMesh* object.

Examples

A sample mesh is constructed by creating uniformly randomly distributed points on the rectangular domain [-1, 1] x [1, 2]. These points will constitute the vertices of the mesh, while its cells are the Delaunay triangles on the vertices.

```
>>> from grains.geometry import TriMesh
>>> msh = TriMesh(*TriMesh.sample_mesh(1))
```

The cells are drawn in greeen, in 3 points of line width, and the vertices of the mesh are shown in blue.

```
>>> msh.plot('go-', linewidth=3, markerfacecolor='b', vertex_labels=True)
>>> plt.show()
```

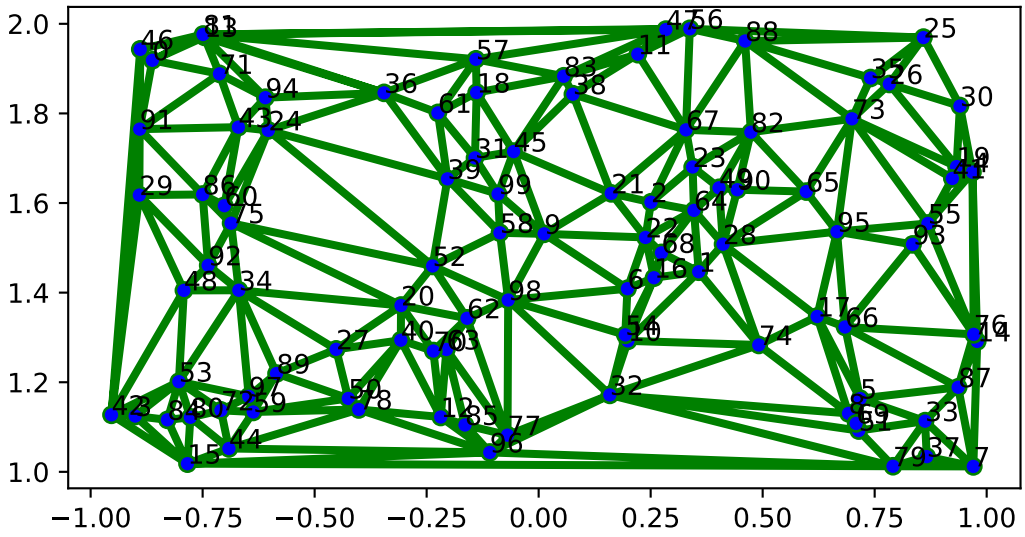
Notes

The plotting is done by calling `triplot()`, which internally makes a deep copy of the triangles. This increases the memory usage in case of many elements.

plot_field(*component*, **args*, *show_mesh=True*, ***kwargs*)

Plots a field on the mesh.

The aim of this method is to support basic post-processing for finite element visualization. Only the basic contour plot type is available. For vector or tensor fields, the components to be plotted must be chosen. For faster and more comprehensive plotting capabilities, turn to well-established scientific visualization software, such as ParaView or Mayavi. Another limitation of the *`plot_field()`* method is that field values are assumed to be associated to the vertices of the mesh, which restricts us to $P1$ Lagrange elements.


2.0
1.8
1.6
1.4
1.2
1.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

Parameters

- **component** (*int*) – Positive integer, the selected component of the field to be plotted. Components are indexed from 0.
- **show_mesh** (*bool, optional*) – If True, the underlying mesh is shown. The default is True.
- **ax** (*matplotlib.axes.Axes, optional*) – The *Axes* instance the plot resides in. The default is None, in which case a new *Axes* within a new figure is created.

Other Parameters **See them described in the :meth:`plot` method.**

Returns *None*

See also:

plot()

Examples

The following example considers the same type of mesh as in the example shown for *plot()*.

```
>>> msh = TriMesh(*TriMesh.sample_mesh(1))
```

We pretend that the field is an analytical function, evaluated at the vertices.

```
>>> field = lambda x, y: 1 - (x + y**2) * np.sign(x)
>>> field = field(msh.vertices[:, 0], msh.vertices[:, 1])
```

We associate this field to the mesh and plot it with and without the mesh

```
>>> msh.associate_field(field, 'analytical field')
>>> _, (ax1, ax2) = plt.subplots(1, 2)
>>> msh.plot_field(0, 'bo-', ax=ax1, linewidth=1, markerfacecolor='k')
>>> msh.plot_field(0, ax=ax2, show_mesh=False)
>>> plt.show()
```

plot_options = {'ax': None, 'cell_labels': False, 'cell_legends': False, 'cell_sets': '

rotate (*angle*, *point=(0, 0)*, *inplace=False*)

Rotates a 2D mesh about a given point by a given angle.

Parameters

- **angle** (*float*) – Angle of rotation, in radians.
- **point** (*list or tuple, optional*) – Coordinates of the point about which the mesh is rotated. If not given, it is the origin.
- **inplace** (*bool, optional*) – If True, the vertex positions are updated in the mesh object. The default is False.

Returns **rotated_vertices** (*ndarray*) – Same format as the `vertices` member variable, with the requested rotation.

Notes

Rotating a point P given by its coordinates in the global coordinate system as $P(x, y)$ around a point $A(x, y)$ by an angle α is done as follows.

1. The coordinates of P in the local coordinate system, the origin of which is A, is expressed as

$$P(x', y') = P(x, y) - A(x, y).$$

2. The rotation is performed in the local coordinate system as $P'(x', y') = RP(x', y')$, where R is the rotation matrix:

$$R = \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix}.$$

3. The rotated point P' is expressed in the original (global) coordinate system:

$$P'(x, y) = P'(x', y') + A(x, y).$$

static sample_mesh(*sample*, *param=100*)
Provides sample meshes.

Parameters

- **sample** (*int*) – Integer, giving the sample mesh to be considered. Possibilities:
- **param** – Parameters to the sample meshes. Possibilities:

Returns

- **nodes** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a vertex, and the two columns giving the Cartesian coordinates of the vertices.
- **cells** (*ndarray*) – Cell-vertex connectivity in a 2D numpy array, in which each row corresponds to a cell and the columns are the vertices of the cells. It is assumed that all the cells have the same number of vertices.

scale(*factor*, *inplace=False*)
Scales the geometry by modifying the coordinates of the vertices.

Parameters

- **factor** (*float*) – Each vertex coordinate is multiplied by this non-negative number.
- **inplace** (*bool, optional*) – If True, the vertex positions are updated in the mesh object. The default is False.

Returns *None.*

write_inp(*filename*)
Writes the mesh to an Abaqus .inp file.

Parameters **filename** (*str*) – Path to the mesh file.

Returns *None*

grains.geometry.**_polygon_area**(*x*, *y*)
Computes the signed area of a non-self-intersecting, possibly concave, polygon.

Directly taken from http://rosettacode.org/wiki/Shoelace_formula_for_polygonal_area#Python

Parameters **x, y** (*list*) – Coordinates of the consecutive vertices of the polygon.

Returns *float* – Area of the polygon.

Warning: If numpy vectors are passed as inputs, the resulting area is incorrect! WHY?

Notes

The code is not optimized for speed and for numerical stability. Intended to be used to compute the area of finite element cells, in which case the numerical stability is not an issue (unless the cell is degenerate). As this function is called possibly as many times as the number of cells in the mesh, no input checking is performed.

Examples

```
>>> _polygon_area([0, 1, 1], [0, 0, 1])
0.5
```

grains.geometry.**distance_matrix**(*points*)

A symmetric square matrix, containing the pairwise squared Euclidean distances among points.

Parameters **points** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a point, and the two columns giving the Cartesian coordinates of the points.

Returns **dm** (*ndarray*) – Distance matrix.

See also:

squared_distance()

Examples

```
>>> points = np.array([[1, 1], [3, 0], [-1, -1]])
>>> distance_matrix(points)
array([[ 0.,  5.,  8.],
       [ 5.,  0., 17.],
       [ 8., 17.,  0.]])
```

grains.geometry.**is_collinear**(*points*, *tol=None*)

Decides whether a set of points is collinear.

Works in any dimensions.

Parameters

- **points** (*ndarray*) – 2D numpy array with N columns, each row corresponding to a point, and the N columns giving the Cartesian coordinates of the point.
- **tol** (*float, optional*) – Tolerance value passed to numpy's *matrix_rank* function. This tolerance gives the threshold below which SVD values are considered zero.

Returns *bool* – True for collinear points.

See also:

numpy.linalg.matrix_rank()

Notes

The algorithm for three points is from Tim Davis.

Examples

Two points are always collinear

```
>>> is_collinear(np.array([[1, 0], [1, 5]]))
True
```

Three points in 3D which are supposed to be collinear (returns false due to numerical error)

```
>>> is_collinear(np.array([[0, 0, 0], [1, 1, 1], [5, 5, 5]]), tol=0)
False
```

The previous example with looser tolerance

```
>>> is_collinear(np.array([[0, 0, 0], [1, 1, 1], [5, 5, 5]]), tol=1e-14)
True
```

grains.geometry.**squared_distance**(*x*, *y*)

Squared Euclidean distance between two points.

For points $x(x_1, ..., x_n)$ and $y(y_1, ...y_n)$ the following metric is computed

$$\sum_{i=1}^{n}(x_i - y_i)^2$$

Parameters **x, y** (*ndarray*) – 1D numpy array, containing the coordinates of the two points.

Returns *float* – Squared Euclidean distance.

See also:

distance_matrix()

Examples

```
>>> squared_distance(np.array([0, 0, 0]), np.array([1, 1, 1]))
3.0
```

CHAPTER

TWENTYTHREE

ABAQUS

Warning: This module will substantially be rewritten. See this issue.

This module allows to create and manipulate Abaqus input files through the Abaqus keywords, thereby providing automation. Note that it is not intended to be a complete API to Abaqus. If you want fine control over the whole Abaqus ecosystem, consult with the Abaqus Scripting Reference Guide (*ASRG*). However, *ASRG* needs Abaqus to be installed, moreover, you must use the Python interpreter embedded into Abaqus. That version of Python is very old even in the latest versions of Abaqus. Furthermore, if you need to use custom Python packages for your work, chances are high that they will not work with the embedded interpreter, and may even crash the installation. To use this module, no Abaqus installation is needed. In fact, only functions from the Python standard library are used.

The documentation of Abaqus version 2017 is hosted on the following website: https://abaqus-docs.mit.edu/2017/English/SIMACAEEXCRefMap/simaexc-c-docproc.htm. Throughout the documentation of this module (*grains.abaqus*), we will make references to that website. If the links cease to exist, please let me know by opening an issue. Alternatively, once you have registered, you can browse the documentation on the official website.

23.1 Classes

Geometry	Geometrical operations on the mesh.
Material	Adds, removes, modifies materials.
Procedure	Handling analysis steps during the simulation.

23.1.1 grains.abaqus.Geometry

class grains.abaqus.**Geometry**

Geometrical operations on the mesh.

__init__()

Initialize self. See help(type(self)) for accurate signature.

Methods

__init__()	Initialize self.
read(inp_file)	Reads material data from an Abaqus .inp file.
scale(factor)	Scales the geometry by modifying the coordinates of the nodes.
write([output_file])	Writes material data to an Abaqus .inp file.

23.1.2 grains.abaqus.Material

class grains.abaqus.**Material**(*from_Abaqus=False*)

Adds, removes, modifies materials. Requirements: be able to - create an empty .inp file, containing only the materials - add materials to an existing .inp file

TODO: only document public attributes! .. attribute:: materials

materials, their behaviors and their parameters are stored here. Intended for internal representation. To view them, use the *show* method, to write them to an input file, use the *write* method.

type dict

read(*inp_file*)

Reads material data from an Abaqus .inp file.

write(*output_file=None*)

Writes material data to an Abaqus .inp file.

remove(*inp_file*, *output_file=None*)

Removes material definitions from an Abaqus .inp file.

create(*inp_file*)

Creates empty Abaqus .inp file.

show()

Shows material data as it appears in the Abaqus .inp file.

Notes

The aim of this class is to programmatically add, remove, modify materials in a format understandable by Abaqus. This class does not target editing materials through a GUI (that can be done in Abaqus CAE).

__init__(*from_Abaqus=False*)

Parameters **from_Abaqus** (*bool, optional*) – True if the input file was generated by Abaqus. The default is False. Abaqus generates input files with a consistent format. This allows certain optimizations: the input file may not need to be completely traversed to extract the materials. Third-party programs sometimes generate .inp files, which are valid but do not follow the Abaqus pattern. In this case, it cannot be predicted where the material definition ends in the file – the whole file needs to be traversed.

Returns *None.*

Methods

__init__([from_Abaqus])	**Parameters from_Abaqus** (*bool, optional*) – True if the input file was generated by Abaqus. The default is False.

add_linearelastic(material, E, nu)	Adds linear elastic behavior to a given material.
add_material(material)	Defines a new material by its name.
add_plastic(material, sigma_y, epsilon_p)	Adds metal plasticity behavior to a given material.
add_sections(inp_file[, output_file])	Adds section definitions to an Abaqus .inp file.
create(inp_file)	Creates empty Abaqus .inp file.
read(inp_file)	Reads material data from an Abaqus .inp file.
remove(inp_file[, output_file])	Removes material definitions from an Abaqus .inp file.
show()	Shows material data as it appears in the Abaqus .inp file.
write([output_file])	Writes material data to an Abaqus .inp file.

23.1.3 grains.abaqus.Procedure

class grains.abaqus.**Procedure**(*from_Abaqus=False*)

Handling analysis steps during the simulation.

TODO: only document public attributes!

steps

analysis steps, each step collecting the necessary information. Intended for internal representation. To view them, use the *show()* method, to write them to an input file, use the *write()* method.

Type dict

__init__(*from_Abaqus=False*)

Parameters from_Abaqus (*bool, optional*) – True if the input file was generated by Abaqus. The default is False. Abaqus generates input files with a consistent format. This allows certain optimizations: the input file may not need to be completely traversed to extract the materials. Third-party programs sometimes generate .inp files, which are valid but do not follow the Abaqus pattern. In this case, it cannot be predicted where the material definition ends in the file – the whole file needs to be traversed.

Returns *None.*

Methods

__init__([from_Abaqus])	**Parameters from_Abaqus** (*bool, optional*) – True if the input file was generated by Abaqus. The default is False.

Continued on next page

Table 4 – continued from previous page

add_analysis(step[, time_period, ...])	Adds an analysis type to a given step.
add_boundary_condition(name, step, nodes, ...)	Adds boundary condition to a given step.
create_step(name[, nlgeom, max_increments])	Defines a new step.
read(inp_file)	Reads procedure data from an Abaqus .inp file.
show()	Shows the text for the *step* module, as it appears in the Abaqus .inp file.
write([output_file])	Writes step definition data to an Abaqus .inp file.

23.2 Functions

extract(keyword)	Obtains Abaqus keyword and its parameters.
validate_file(file, caller)	Input or output file validation.

23.2.1 grains.abaqus.extract

grains.abaqus.**extract**(*keyword*)

Obtains Abaqus keyword and its parameters.

Parameters **keyword** (*str*) –

Some examples: '*Elastic, type=ORTHOTROPIC' '*Damage Initiation, criterion=HASHIN' '*Nset, nset=Set-1, generate'

Returns **separated** (*list*) – DESCRIPTION.

23.2.2 grains.abaqus.validate_file

grains.abaqus.**validate_file**(*file*, *caller*)

Input or output file validation.

Parameters

- **file** (*str*) – Existing Abaqus .inp file or a new .inp file to be created.
- **caller** (*{'read', 'write', 'create'}*) – Method name that called this function.

Returns *None.*

class grains.abaqus.**Geometry**

Bases: object

Geometrical operations on the mesh.

_Geometry__format()

Formats the material data in the Abaqus .inp format. The internal representation of the material data in converted to a string understood by Abaqus.

abaqus_format [list] List of strings, each element of the list corresponding to a line (with

line ending) in the Abaqus .inp file. In case of no

material, an empty list is returned.

The output is a list so that further concatenation operations are easy. If you want a string, merge the elements of the list:

output = ''.join(output)

This is what the *show* method does.

read(*inp_file*)

Reads material data from an Abaqus .inp file.

Parameters **inp_file** (*str*) – Abaqus input (.inp) file to be created.

Returns *None.*

Notes

- This method is designed to read material data. Although the logic could be used to process other properties (parts, assemblies, etc.) in an input file, they are not yet implemented in this class.
- This method assumes that the input file is valid. If it is, the material data can be extacted. If not, the behavior is undefined: the program can crash or return garbage. This is by design: the single responsibility principle dictates that the validity of the input file must be provided by other methods. If the input file was generated from within Abaqus CAE, it is guaranteed to be valid. The *write* method of this class also ensures that the resulting input file is valid. This design choice also makes the program logic simpler. For valid syntax in the input file, check the Input Syntax Rules section in the Abaqus user's guide.
- To read material data from an input file, one has to identify the structure of .inp files in Abaqus. Abaqus is driven by keywords and corresponding data. For a list of accepted keywords, consult the Abaqus Keywords Reference Guide. There are three types of input lines in Abaqus:
  - keyword line: begins with a star, followed by the name of the keyword. Parameters, if any, are separated by commas and are given as parameter-value pairs. Keywords and parameters are not case sensitive. Example:

    *ELASTIC, TYPE=ISOTROPIC, DEPENDENCIES=1

    Some keywords can only be defined once another keyword has already been defined. E.g. the keyword ELASTIC must come after MATERIAL in a valid .inp file.
  - data line: immediately follows a keyword line. All data items must be separated by commas. Example:

    -12.345, 0.01, 5.2E-2, -1.2345E1
  - **comment line: starts with ** and is ignored by Abaqus. Example:** ** This is a comment line
- Internally, the materials are stored in a dictionary. It holds the material data read from the file. The keys in this dictionary are the names of the materials, and the values are dictionaries themselves. Each such dictionary stores a behavior for the given material. E.g. an elastoplastic material is governed by an elastic and a plastic behavior. The parameters for each behavior are stored in a list.

scale(*factor*)

Scales the geometry by modifying the coordinates of the nodes.

Parameters **factor** (*float*) – Each nodal coordinate is multiplied by this non-negative number.

Returns *None.*

Notes

The modification happens in-place.

write(*output_file=None*)
Writes material data to an Abaqus .inp file.

Parameters **output_file** (*str, optional*) – Output file name to write the modifications into. If not given, the original file name is appended with '_mod'.

Returns *None.*

Notes

- If the output file name is the same as the input file, the original .inp file will be overwritten. This is strongly not recommended.
- The whole content of the original input file is read to memory. It might be a problem for very large .inp files. In that case, a possible implementation could be the following:
  1. Remove old material data
  2. Append new material data to the proper position in the file

  Appending is automatically done at the end of the file. Moving the material description to the end of the file is not possible in general because defining materials cannot be done from any module, i.e. the *MATERIAL keyword cannot follow an arbitrary keyword. In this case, Abaqus throws an AbaqusException with the following message:

  It can be suboption for the following keyword(s)/level(s): model

class grains.abaqus.**Material**(*from_Abaqus=False*)
Bases: object

Adds, removes, modifies materials. Requirements: be able to - create an empty .inp file, containing only the materials - add materials to an existing .inp file

TODO: only document public attributes! .. attribute:: materials

materials, their behaviors and their parameters are stored here. Intended for internal representation. To view them, use the *show* method, to write them to an input file, use the *write* method.

type dict

read(*inp_file*)
Reads material data from an Abaqus .inp file.

write(*output_file=None*)
Writes material data to an Abaqus .inp file.

remove(*inp_file*, *output_file=None*)
Removes material definitions from an Abaqus .inp file.

create(*inp_file*)
Creates empty Abaqus .inp file.

show()
Shows material data as it appears in the Abaqus .inp file.

Notes

The aim of this class is to programmatically add, remove, modify materials in a format understandable by Abaqus. This class does not target editing materials through a GUI (that can be done in Abaqus CAE).

_Material__format()

Formats the material data in the Abaqus .inp format. The internal representation of the material data in converted to a string understood by Abaqus.

abaqus_format [list] List of strings, each element of the list corresponding to a line (with

line ending) in the Abaqus .inp file. In case of no

material, an empty list is returned.

The output is a list so that further concatenation operations are easy. If you want a string, merge the elements of the list:

output = ''.join(output)

This is what the *show* method does.

static _Material__isnumeric(*x*)

Decides if the input is a scalar number.

Parameters **x** (*any type*) – Input to be tested.

Returns *bool* – True if the given object is a scalar number.

add_linearelastic(*material*, *E*, *nu*)

Adds linear elastic behavior to a given material.

Parameters

- **material** (*str*) – Name of the material the behavior belongs to.
- **E** (*int, float*) – Young's modulus.
- **nu** (*int, float*) – Poisson's ratio.

Returns *None.*

add_material(*material*)

Defines a new material by its name.

Parameters **material** (*str*) – Name of the material to be added. A material can have multiple behaviors (e.g. elastoplastic).

Returns *None.*

add_plastic(*material*, *sigma_y*, *epsilon_p*)

Adds metal plasticity behavior to a given material.

Parameters

- **material** (*str*) – Name of the material the behavior belongs to.
- **sigma_y** (*int, float*) – Yield stress.
- **epsilon_p** (*int, float*) – Plastic strain.

Returns *None.*

static add_sections(*inp_file*, *output_file=None*)

Adds section definitions to an Abaqus .inp file.

Defines properties for elements by associating materials to them. The element set containing the elements for which the material behavior is being defined is assumed to have the same name as that of the material. E.g. if materials with names *mat-1* and *mat-2* exist, element sets with names *mat-1* and *mat-2* must also exist. If such element sets do not exist, Abaqus will throw a warning and the section assignment will not be successful.

Parameters

- **inp_file** (*str*) – Abaqus .inp file from which the materials should be removed.
- **output_file** (*str, optional*) – Output file name to write the modifications into. If not given, the original file name is appended with '_mod'.

Returns *None.*

Notes

If fine control is required for associating custom material names to custom element set names, that can be done from the Abaqus GUI. The purpose of this method is automation for large number of element sets, each associated to a (possibly distinct) material. In that case, custom element set names are not reasonable any more, and having the same names for the element sets and for the materials is completely meaningful.

create(*inp_file*)

Creates empty Abaqus .inp file.

Parameters **inp_file** (*str*) – Abaqus input file to be created. If an extension is not given, the default .inp is used.

Returns *None.*

read(*inp_file*)

Reads material data from an Abaqus .inp file.

Parameters **inp_file** (*str*) – Abaqus input (.inp) file to be created.

Returns *None.*

Notes

- This method is designed to read material data. Although the logic could be used to process other properties (parts, assemblies, etc.) in an input file, they are not yet implemented in this class.
- This method assumes that the input file is valid. If it is, the material data can be extacted. If not, the behavior is undefined: the program can crash or return garbage. This is by design: the single responsibility principle dictates that the validity of the input file must be provided by other methods. If the input file was generated from within Abaqus CAE, it is guaranteed to be valid. The *write* method of this class also ensures that the resulting input file is valid. This design choice also makes the program logic simpler. For valid syntax in the input file, check the Input Syntax Rules section in the Abaqus user's guide.
- To read material data from an input file, one has to identify the structure of .inp files in Abaqus. Abaqus is driven by keywords and corresponding data. For a list of accepted keywords, consult the Abaqus Keywords Reference Guide. There are three types of input lines in Abaqus:
  - keyword line: begins with a star, followed by the name of the keyword. Parameters, if any, are separated by commas and are given as parameter-value pairs. Keywords and parameters are not case sensitive. Example:

    *ELASTIC, TYPE=ISOTROPIC, DEPENDENCIES=1

Some keywords can only be defined once another keyword has already been defined. E.g. the keyword ELASTIC must come after MATERIAL in a valid .inp file.

- data line: immediately follows a keyword line. All data items must be separated by commas. Example:

  -12.345, 0.01, 5.2E-2, -1.2345E1

- **comment line: starts with ** and is ignored by Abaqus. Example:** ** This is a comment line

- Internally, the materials are stored in a dictionary. It holds the material data read from the file. The keys in this dictionary are the names of the materials, and the values are dictionaries themselves. Each such dictionary stores a behavior for the given material. E.g. an elastoplastic material is governed by an elastic and a plastic behavior. The parameters for each behavior are stored in a list.

static remove(*inp_file*, *output_file=None*)
Removes material definitions from an Abaqus .inp file.

Parameters

- **inp_file** (*str*) – Abaqus .inp file from which the materials should be removed.
- **output_file** (*str, optional*) – Output file name to write the modifications into. If not given, the original file name is appended with '_mod'.

Returns *None.*

show()
Shows material data as it appears in the Abaqus .inp file.

Returns *None.*

write(*output_file=None*)
Writes material data to an Abaqus .inp file.

Parameters **output_file** (*str, optional*) – Output file name to write the modifications into. If not given, the original file name is appended with '_mod'.

Returns *None.*

Notes

- If the output file name is the same as the input file, the original .inp file will be overwritten. This is strongly not recommended.
- The whole content of the original input file is read to memory. It might be a problem for very large .inp files. In that case, a possible implementation could be the following:
  1. Remove old material data
  2. Append new material data to the proper position in the file

  Appending is automatically done at the end of the file. Moving the material description to the end of the file is not possible in general because defining materials cannot be done from any module, i.e. the *MATERIAL keyword cannot follow an arbitrary keyword. In this case, Abaqus throws an AbaqusException with the following message:

  It can be suboption for the following keyword(s)/level(s): model

class grains.abaqus.**Procedure**(*from_Abaqus=False*)
Bases: object

Handling analysis steps during the simulation.

TODO: only document public attributes!

steps
analysis steps, each step collecting the necessary information. Intended for internal representation. To view them, use the *show()* method, to write them to an input file, use the *write()* method.

Type dict

_Procedure__format()

Formats the data in the Abaqus .inp format. The internal representation of the steps data in converted to a string understood by Abaqus.

abaqus_format [list] List of strings, each element of the list corresponding to a line (with

line ending)

in the Abaqus .inp file. In case of no data, an empty list is returned.

The output is a list so that further concatenation operations are easy. If you want a string, merge the elements of the list: `output = ''.join(output)` This is what the *show()* method does.

add_analysis(*step*, *time_period=1.0*, *initial_increment=None*, *min_increment=0*, *max_increment=None*)
Adds an analysis type to a given step.

Note: Currently only static stress/displacement analysis is supported, indicated by the STATIC Abaqus keyword. No optional parameters are supported.

Todo: Check user inputs. Define exceptions (*ValueError* class) with the error messages Abaqus CAE throws.

Parameters

- **step** (*str*) – Name of the step the analysis type belongs to.
- **initial_increment** (*float, optional*) – Initial time increment. This value will be modified as required if the automatic time stepping scheme is used. If this entry is zero or is not specified, a default value that is equal to the total time period of the step is assumed.
- **time_period** (*float, optional*) – Time period of the step. The default is 1.0.
- **min_increment** (*float, optional*) – Only used for automatic time incrementation. If ABAQUS/Standard finds it needs a smaller time increment than this value, the analysis is terminated. If this entry is zero, a default value of the smaller of the suggested initial time increment or 1e–5 times the total time period is assumed.
- **max_increment** (*float, optional*) – Maximum time increment allowed. Only used for automatic time incrementation. If this value is not specified, no upper limit is imposed, i.e. `max_increment = time_period`.

Returns *None*

Examples

```
>>> proc = Procedure()
>>> proc.create_step('Step-1', max_increments=1000)
>>> proc.add_analysis('Step-1', initial_increment=0.001, min_increment=1e-8)
```

add_boundary_condition(*name*, *step*, *nodes*, *first_dof*, *last_dof=None*, *magnitude=0.0*)

Adds boundary condition to a given step.

Boundary conditions can be prescribed on node sets, using the Abaqus keyword BOUNDARY. Optional parameters are not supported.

Multiple boundary conditions can be given on the same node set. It is the responsibility of the user to ensure that the constraints are compatible.

Note: Currently, boundary conditions can only be defined in a user-defined step, and not in the initial step.

Parameters

- **name** (*str*) – Name of the boundary condition to be added. Boundary condition names must be unique.
- **step** (*str*) – Name of the step the boundary condition belongs to.
- **nodes** (*str or int*) – If a string, the label of the node set, if a positive integer, the label of a single node on which the boundary condition is prescribed.
- **first_dof** (*int*) – First degree of freedom constrained.
- **last_dof** (*int, optional*) – Last degree of freedom constrained. Not necessary to be given if only one degree of freedom is being constrained.
- **magnitude** (*float*) – Magnitude of the variable. If this magnitude is a rotation, it must be given in radians. The default value is 1.0.

Returns *None*

Examples

Let us consider a two-dimensional structure, fixed on a part of its boundary (called *'left'*), and displaced on another part (called *'right'*). First, we create an analysis step (named *'Step-1'*).

```
>>> proc = Procedure()
>>> proc.create_step('Step-1', max_increments=1000)
```

Now, we prescribe the zero displacements.

```
>>> proc.add_boundary_condition('fixed', 'Step-1', 'left', first_dof=1, last_
↪dof=2)
```

Since we did not specify the magnitude of the displacement components, they are zero by default. The other boundary condition prescribes different values for the horizontal and vertical components. Hence, they are given separately.

```
>>> proc.add_boundary_condition('pulled_right', 'Step-1', 'right', first_
↪dof=1, magnitude=2)
>>> proc.add_boundary_condition('fixed_right', 'Step-1', 'right', first_dof=2,
↪ magnitude=0)
```

Note that we can also prescribe boundary conditions at a particular node, e.g.

```
>>> proc.add_boundary_condition('at_node', 'Step-1', 1, first_dof=2,␣
↪magnitude=-1.2)
```

where we set the vertical displacement component to -1.2 at node 1.

create_step(*name*, *nlgeom=False*, *max_increments=100*)

Defines a new step.

A *step* is the fundamental part of the simulation workflow in Abaqus. Among the available options, only the *NLGEOM* and *INC* options are supported currently.

Todo: Check in the *write()* method whether every step contains an analysis, as this is required by Abaqus.

Parameters

- **name** (*str*) – Name of the analysis step to be added. Step names must be unique.
- **nlgeom** (*bool, optional*) – Omit this parameter or set to False to perform a geometrically linear analysis during the current step. Set it to True to indicate that geometric nonlinearity should be accounted for during the step. Once the `nlgeom` option has been switched on, it will be active during all subsequent steps in the analysis. The default is False.
- **max_increments** (*int*) – The analysis will stop if the maximum number of increments is exceeded before the complete solution for the step has been obtained. The default is 100.

Returns *None*

read(*inp_file*)

Reads procedure data from an Abaqus .inp file.

Parameters **inp_file** (*str*) – Abaqus input (.inp) file to be created.

Returns *None.*

Notes

- This method is designed to read material data. Although the logic could be used to process other properties (parts, assemblies, etc.) in an input file, they are not yet implemented in this class.
- This method assumes that the input file is valid. If it is, the material data can be extacted. If not, the behavior is undefined: the program can crash or return garbage. This is by design: the single responsibility principle dictates that the validity of the input file must be provided by other methods. If the input file was generated from within Abaqus CAE, it is guaranteed to be valid. The *write* method of this class also ensures that the resulting input file is valid. This design choice also makes the program logic simpler. For valid syntax in the input file, check the Input Syntax Rules section in the Abaqus user's guide.

- To read material data from an input file, one has to identify the structure of .inp files in Abaqus. Abaqus is driven by keywords and corresponding data. For a list of accepted keywords, consult the Abaqus Keywords Reference Guide. There are three types of input lines in Abaqus:
  - keyword line: begins with a star, followed by the name of the keyword. Parameters, if any, are separated by commas and are given as parameter-value pairs. Keywords and parameters are not case sensitive. Example:

    *ELASTIC, TYPE=ISOTROPIC, DEPENDENCIES=1

    Some keywords can only be defined once another keyword has already been defined. E.g. the keyword ELASTIC must come after MATERIAL in a valid .inp file.
  - data line: immediately follows a keyword line. All data items must be separated by commas. Example:

    -12.345, 0.01, 5.2E-2, -1.2345E1
  - **comment line: starts with ** and is ignored by Abaqus. Example:** ** This is a comment line
- Internally, the materials are stored in a dictionary. It holds the material data read from the file. The keys in this dictionary are the names of the materials, and the values are dictionaries themselves. Each such dictionary stores a behavior for the given material. E.g. an elastoplastic material is governed by an elastic and a plastic behavior. The parameters for each behavior are stored in a list.

show()
Shows the text for the *step* module, as it appears in the Abaqus .inp file.

Returns *None.*

write(*output_file=None*)
Writes step definition data to an Abaqus .inp file.

Parameters **output_file** (*str, optional*) – Output file name to write the modifications into. If not given, the original file name is appended with '_mod'.

Returns *None.*

Notes

- If the output file name is the same as the input file, the original .inp file will be overwritten. This is strongly not recommended.
- The whole content of the original input file is read to memory. It might be a problem for very large .inp files. In that case, a possible implementation could be the following:
  1. Remove old material data
  2. Append new material data to the proper position in the file

  Appending is automatically done at the end of the file. Moving the material description to the end of the file is not possible in general because defining materials cannot be done from any module, i.e. the *MATERIAL keyword cannot follow an arbitrary keyword. In this case, Abaqus throws an AbaqusException with the following message:

  It can be suboption for the following keyword(s)/level(s): model

grains.abaqus.**extract**(*keyword*)
Obtains Abaqus keyword and its parameters.

Parameters **keyword** (*str*) –

Some examples: '*Elastic, type=ORTHOTROPIC' '*Damage Initiation, criterion=HASHIN' '*Nset, nset=Set-1, generate'

Returns **separated** (*list*) – DESCRIPTION.

grains.abaqus.**validate_file** (*file*, *caller*)

Input or output file validation.

Parameters

- **file** (*str*) – Existing Abaqus .inp file or a new .inp file to be created.
- **caller** (*{'read', 'write', 'create'}*) – Method name that called this function.

Returns *None.*

CHAPTER

TWENTYFOUR

DIC

This module is used to process field values obtained by digital image correlation (DIC). Plotting, comparison with numerical solutions, etc. are implemented.

24.1 Classes

DIC	Performs operations on digital image correlation data.

24.1.1 grains.dic.DIC

class grains.dic.**DIC**(*u*, *v*)

Performs operations on digital image correlation data.

Parameters **u, v** (*ndarray*) – The two components of the displacement field, discretized on a rectangular grid.

Raises **ValueError** – If the displacement components are not discretized on the same grid or if the grid size is not at least 3-by-3. This latter requirement is not a problem in practice (which camera is not capable of shooting photos in 9 pixels resolution?), while it allows the evaluation of the numerical derivatives with second order accuracy on the boundaries too.

Notes

Throughout the class methods, the following terms are used. When not precised, *image* refers to the DIC data plotted as an image. We can perceive the image as a *pixel grid*, in which the vertices are the centres of the pixels. An image coordinate system (X, Y) can be defined on this grid such that the vertices have integer coordinates, the origin A is at the top left hand corner, and the Y-axis points towards the right, while the X-axis points to the bottom. When the experimental result is compared with a numerical solution (assumed to be available at the *nodes* of a *mesh*), one needs to map values defined on the DIC grid onto the nodes of the mesh, and vice versa. The mesh exists on the physical domain, for which a physical coordinate system (x, y) is attached to. Hence, there is a need to express (X, Y) in terms of (x, y). Let $A(a_x, a_y)$ be the origin of the (X, Y) coordinate system given in terms of the x, y coordinates, and $s[\mathrm{pixel}/\mathrm{mm}]$ is the scale for the DIC image. The coordinate transformation is then given by

The DIC grid in the physical coordinate system (x, y) is called *physical grid*.

It should be noted that the special alignment of (x, y) with respect to (X, Y) is not a major constraint. In practical applications (when a Cartesian coordinate system is used), the orientation of (x, y) in this way is a convention.

__init__ (*u*, *v*)
Initialize self. See help(type(self)) for accurate signature.

Methods

__init__(u, v)	Initialize self.
equivalent_strain(strain_tensor, strain_measure)	Computes a scalar quantity from the strain tensor.
plot_displacement(component[, ax])	Plots a component of the displacement field.
plot_physicalgrid([ax])	Plots the DIC grid in the physical coordinate system.
plot_pixelgrid([ax])	Plots the DIC grid in the image coordinate system.
plot_strain(component[, minval, maxval, ...])	Plots a component of the infinitesimal strain tensor.
plot_superimposedmesh(mesh, *args, **kwargs)	Plots the DIC grid with a mesh superimposed on it.
project_onto_grid(nodes, nodal_values[, method])	Project a numerically computed field onto the DIC grid.
project_onto_mesh(nodes[, method])	Project the experimental displacement field onto a mesh.
set_transformation(origin, ...)	Sets the transformation rule between the pixel and the physical coordinate systems.
strain(strain_measure)	Computes the strain tensor from the displacement vector.

24.2 Functions

plot_strain(strain[, minval, maxval, ...])	Plots a scalar strain field.

24.2.1 grains.dic.plot_strain

grains.dic.**plot_strain** (*strain*, *minval=None*, *maxval=None*, *colorbar=True*, *label=''*)
Plots a scalar strain field.

Parameters

- **strain** (*ndarray*) – Scalar strain field sampled on an m-by-n grid, given as a 2D numpy array.
- **minval, maxval** (*float, optional*) – Set the color scaling for the image by fixing the values that map to the colormap color limits. If `minval` is not provided, the limit is determined from the minimum value of the data. Similarly for `maxval`.
- **colorbar** (*bool, optional*) – If True, a horizontal colorbar is placed below the strain map. The default is True.
- **label** (*str, optional*) – Label describing the strain field. LaTeX code is also accepted, e.g. *r'$varepsilon_{yy}$'*. If not given, no text is displayed.

Returns *None*

See also:

DIC.strain()

Deprecated since version 1.1.0: This will be removed in 1.3.0. This function will be a static method of the DIC class. See also the deprecation warning of *DIC.plot_strain()*.

class grains.dic.**DIC**(*u*, *v*)

Bases: object

Performs operations on digital image correlation data.

Parameters **u, v** (*ndarray*) – The two components of the displacement field, discretized on a rectangular grid.

Raises **ValueError** – If the displacement components are not discretized on the same grid or if the grid size is not at least 3-by-3. This latter requirement is not a problem in practice (which camera is not capable of shooting photos in 9 pixels resolution?), while it allows the evaluation of the numerical derivatives with second order accuracy on the boundaries too.

Notes

Throughout the class methods, the following terms are used. When not precised, *image* refers to the DIC data plotted as an image. We can perceive the image as a *pixel grid*, in which the vertices are the centres of the pixels. An image coordinate system (X, Y) can be defined on this grid such that the vertices have integer coordinates, the origin A is at the top left hand corner, and the Y-axis points towards the right, while the X-axis points to the bottom. When the experimental result is compared with a numerical solution (assumed to be available at the *nodes* of a *mesh*), one needs to map values defined on the DIC grid onto the nodes of the mesh, and vice versa. The mesh exists on the physical domain, for which a physical coordinate system (x, y) is attached to. Hence, there is a need to express (X, Y) in terms of (x, y). Let $A(a_x, a_y)$ be the origin of the (X, Y) coordinate system given in terms of the x, y coordinates, and $s[\mathrm{pixel}/\mathrm{mm}]$ is the scale for the DIC image. The coordinate transformation is then given by

The DIC grid in the physical coordinate system (x, y) is called *physical grid*.

It should be noted that the special alignment of (x, y) with respect to (X, Y) is not a major constraint. In practical applications (when a Cartesian coordinate system is used), the orientation of (x, y) in this way is a convention.

static equivalent_strain(*strain_tensor*, *strain_measure*)

Computes a scalar quantity from the strain tensor.

Parameters

- **strain_tensor** (*ndarray*) – Components of the strain tensor $\boldsymbol{\varepsilon}$ as an $m \times n \times 3$ array. The first two dimensions correspond to the grid points they are determined at, the third dimension gives the components of the tensor in the following order: $\varepsilon_{11}, \varepsilon_{12}, \varepsilon_{22}$.
- **strain_measure** (*{'von Mises'}*) – One of the following strain measures.
  - 'von Mises'

$$\varepsilon_M := \sqrt{\frac{2}{3}\boldsymbol{\varepsilon}^{\mathrm{dev}} : \boldsymbol{\varepsilon}^{\mathrm{dev}}} = \sqrt{\frac{2}{3}\left(\boldsymbol{\varepsilon} : \boldsymbol{\varepsilon} - \frac{1}{3}(\mathrm{tr}\boldsymbol{\varepsilon})^2\right)}$$

where $\boldsymbol{\varepsilon}^{\mathrm{dev}}$ is the deviatoric part of the strain tensor. This can further be simplified (see the notes below) to

$$\varepsilon_M = \frac{2}{3}\sqrt{\varepsilon_{11}^2 + \varepsilon_{22}^2 + 3\varepsilon_{12}^2 - \varepsilon_{11}\varepsilon_{22}}$$

Returns *ndarray* – Equivalent strain at the grid points, given as an $m \times n$ numpy array.

See also:

strain()

Notes

Under plane stress conditions, ε_{33} is not zero, but it is computed as

$$\varepsilon_{33} = -\frac{\nu}{E}(\sigma_{11} + \sigma_{22})$$

Since the stresses are not known from the DIC, one must settle with plane strain conditions where $\varepsilon_{33} = 0$. This is what we follow in the *DIC* class. We remark that in stereo-DIC multiple cameras are used, which allows the measurement of ε_{33}.

plot_displacement(*component*, *ax=None*)

Plots a component of the displacement field.

Parameters

- **component** (*{1, 2}*) – Component to be plotted, where 1 corresponds to the first, 2 corresponds to the second component of the displacement field.
- **ax** (*matplotlib.axes.Axes, optional*) – The *Axes* instance the grid resides in. The default is None, in which case a new *Axes* within a new figure is created.

Returns *None*

See also:

plot_strain()

plot_physicalgrid(*ax=None*)

Plots the DIC grid in the physical coordinate system.

This method is only available once the relation between the image coordinate system and the physical coordinate system has been set up by the *set_transformation()* method.

Parameters **ax** (*matplotlib.axes.Axes, optional*) – The *Axes* instance the grid resides in. The default is None, in which case a new *Axes* within a new figure is created.

Returns **ax** (*matplotlib.axes.Axes*)

See also:

plot_pixelgrid()

Notes

See in the *plot_pixelgrid()* method.

plot_pixelgrid(*ax=None*)
Plots the DIC grid in the image coordinate system.

Parameters **ax** (*matplotlib.axes.Axes, optional*) – The *Axes* instance the grid resides in. The default is None, in which case a new *Axes* within a new figure is created.

Returns **ax** (*matplotlib.axes.Axes*)

See also:

plot_physicalgrid()

Notes

For a DIC image with $m \times n$ number of pixels, the number of grid lines is $(m+1)+(n+1)$. Plotting all these lines would not only slow down the program, it would also make the grid practically indistinguishable from a filled rectangle. Therefore, for high resolution images, only grid lines around the boundary of the image are plotted. The target resolution above which this strategy is used can be given in the class constructor.

plot_strain(*component*, *minval=None*, *maxval=None*, *colorbar=True*)
Plots a component of the infinitesimal strain tensor.

The partial derivatives of the displacement field are computed with numerical differentiation.

Parameters

- **component** (*tuple, {(1,1), (1,2), (2,1), (2,2)}*) – Component to be plotted, where
  - (1,1) denotes ε_{11}
  - (1,2) and (2,1) denote $\varepsilon_{12} = \varepsilon_{21}$
  - (2,2) denotes ε_{22}

  for the infinitesimal strain tensor

$$\varepsilon = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} \\ \varepsilon_{21} & \varepsilon_{22} \end{pmatrix}$$

- **minval, maxval** (*float, optional*) – Set the color scaling for the image by fixing the values that map to the colormap color limits. If `minval` is not provided, the limit is determined from the minimum value of the data. Similarly for `maxval`.
- **colorbar** (*bool, optional*) – If True, a horizontal colorbar is placed below the strain map. The default is True.

Returns *None*

See also:

plot_displacement(), `numpy.gradient()`

Deprecated since version 1.1.0: This will be removed in 1.3.0. This method will be modified to perform the plotting only. The computation of the various strain measures will be done in the *strain()* method. The function that replaces this function will keep the same name and is currently implemented outside this class.

plot_superimposedmesh(*mesh*, **args*, ***kwargs*)
Plots the DIC grid with a mesh superimposed on it.

Since the finite element mesh represents a physical domain, the DIC grid is plotted in the physical coordinate system, which is determined by the *set_transformation()* method.

Note: Maybe no need to couple this module with the *geometry* module just for the sake of this function. It is probably easier to simply pass the nodes and the elements, and call *triplot*.

Parameters

- **mesh** (*Mesh*) – A subclass of *grains.geometry.Mesh* to be plotted along with the physical DIC grid.
- **args** (*optional*) – The same as for matplotlib.axes.Axes.plot(). The settings given here influence the mesh plotting.
- **kwargs** (*optional*) – The same as for matplotlib.axes.Axes.plot(). The settings given here influence the mesh plotting.

Returns **ax** (*matplotlib.axes.Axes*) – The Axes object on which the plot is drawn.

See also:

grains.geometry.TriMesh.plot()

Examples

Let us create a grid and a random mesh (the same as in the *Examples* section of the *project_onto_mesh()*).

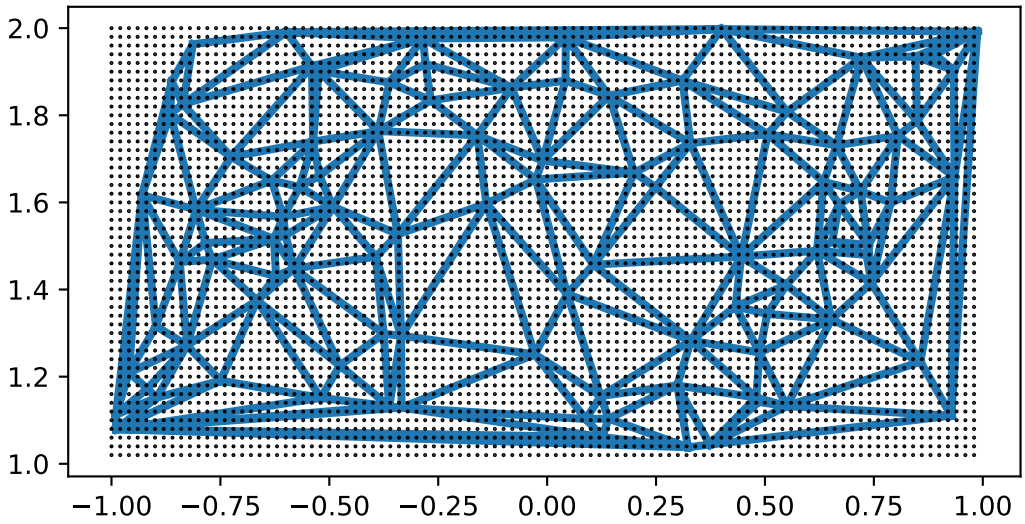
```
>>> from grains.dic import DIC
>>> from grains.geometry import TriMesh
>>> x_grid, y_grid = np.mgrid[-1:1:100j, 1:2:50j]
>>> exact_solution = lambda x, y: 1 - (x + y**2) * np.sign(x)
>>> grid = DIC(np.random.rand(*np.shape(x_grid.T)), np.random.rand(*np.
↪shape(x_grid.T)))
>>> grid.set_transformation((-1, 2), 50)
>>> n_nodes = 100  # modify this to see how good the interpolated solution is
>>> msh = TriMesh(*TriMesh.sample_mesh(1, n_nodes))
>>> grid.plot_superimposedmesh(msh, linewidth=3, markerfacecolor='b')
>>> plt.show()
```

project_onto_grid(*nodes*, *nodal_values*, *method='linear'*)
Project a numerically computed field onto the DIC grid.

Todo: Use the example code of this method to create the plotting method of this class. When done, rewrite the example with the methods.

Parameters

- **nodes** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a node of the mesh, and the two columns giving the Cartesian coordinates of the nodes.


2.0
1.8
1.6
1.4
1.2
1.0
−1.00
−0.75
−0.50
−0.25
0.00
0.25
0.50
0.75
1.00

- **nodal_values** (*ndarray*) – 1D numpy array (vector), the numerically computed field at the nodes of the mesh.
- **method** (*{'nearest', 'linear', 'cubic'}, optional*) – Type of the interpolation. The default is linear.

Returns *ndarray* – 2D numpy array, the projected field values at the physical DIC grid points.

See also:

project_onto_mesh(), scipy.interpolate.griddata()

Examples

The DIC grid and the nodal finite element values (interpolated in-between, which is an errenous way to visualize discontinuous functions) can be seen in the upper left and lower left figures, respectively.

```
>>> from grains.dic import DIC
>>> from grains.geometry import TriMesh
>>> x_grid, y_grid = np.mgrid[-1:1:100j, 1:2:50j]
>>> exact_solution = lambda x, y: 1 - (x + y**2) * np.sign(x)
>>> grid = DIC(exact_solution(x_grid, y_grid).T, exact_solution(x_grid,y_
↪grid).T)
>>> grid.set_transformation((-1, 2), 50)
```

The finite element solution is obtained at the nodes (upper right figure) of the mesh. Here, we assumed that the nodes are sampled from a uniformly random distribution on $[-1, 1] \times [1, 2]$.

```
>>> n_nodes = 100  # modify this to see how good the interpolated solution is
```

For the sake of this example, we also assume that the nodal values are "exact", i.e. they admit the function values at the nodes. In reality, of course, this will not be the case, but this allows us to investigate the effect moving from the FE mesh to the DIC grid.

```
>>> mesh = TriMesh(*TriMesh.sample_mesh(1, n_nodes))
>>> fe_values = exact_solution(mesh.vertices[:, 0], mesh.vertices[:, 1])
>>> mesh.associate_field(fe_values)
>>> interpolated = grid.project_onto_grid(mesh.vertices, fe_values, method=
↪'linear')
```

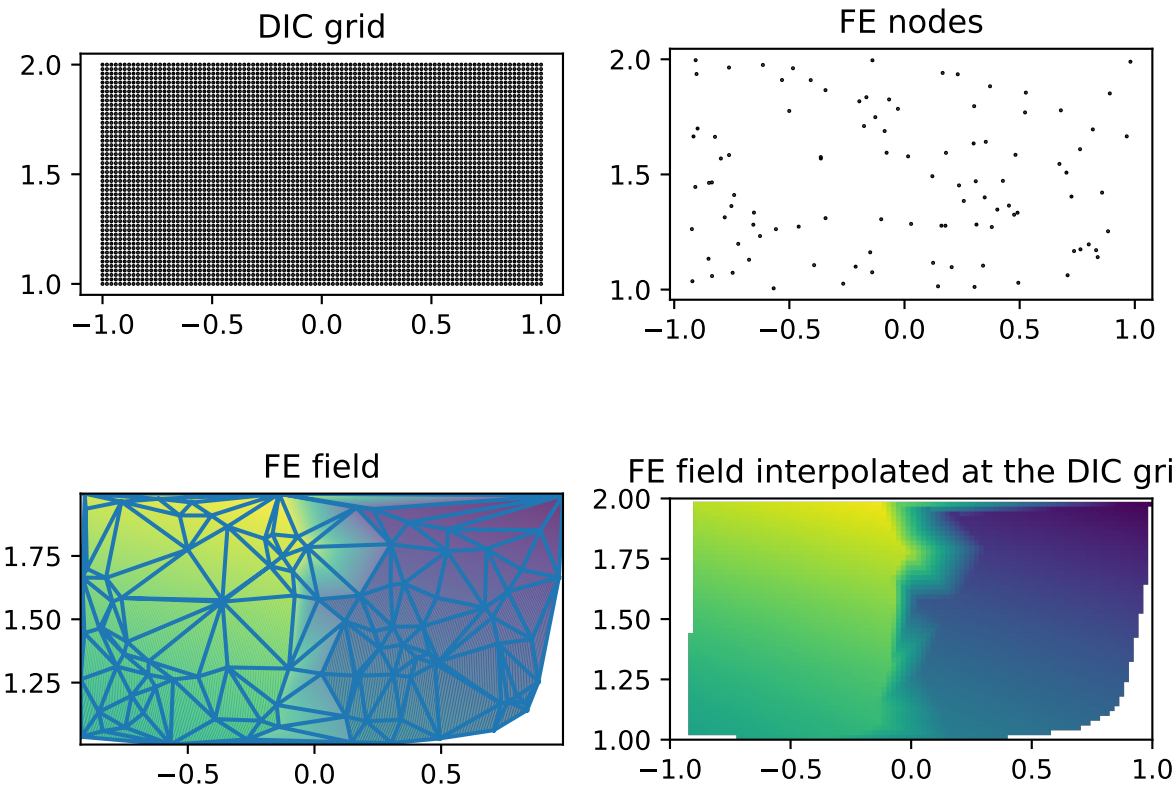
The FE field available at the nodes are interpolated at the DIC grid points, as shown in the lower right figure. Note that no extrapolation is performed, so values are not computed at the grid points lying outside the convex hull of the finite element nodes.

```
>>> ax = []
>>> ax.append(plt.subplot(221))
>>> plt.plot(x_grid, y_grid, 'k.', ms=1)
>>> plt.title('DIC grid')
>>> ax.append(plt.subplot(222))
>>> plt.plot(mesh.vertices[:, 0], mesh.vertices[:, 1], 'k.', ms=1)
>>> plt.title('FE nodes')
>>> ax.append(plt.subplot(223))
>>> mesh.plot_field(0, ax=ax[-1])
>>> plt.title('FE field')
>>> ax.append(plt.subplot(224))
>>> plt.imshow(interpolated, extent=(-1, 1, 1, 2), origin='lower', vmin=-4,␣
↪vmax = 5)
```

(continues on next page)

(continued from previous page)

```
>>> plt.title('FE field interpolated at the DIC grid')
>>> plt.tight_layout()
>>> for a in ax:
...     a.set_aspect('equal', 'box')
>>> plt.show()
```



You are invited to modify this example to simulate a finer mesh by increasing `n_nodes`. Also try different interpolation techniques.

project_onto_mesh (*nodes*, *method='linear'*)

Project the experimental displacement field onto a mesh.

Parameters **nodes** (*ndarray*) – 2D numpy array with 2 columns, each row corresponding to a node of the mesh, and the two columns giving the Cartesian coordinates of the nodes.

Returns

- **u_nodes, v_nodes** (*ndarray*) – 1D numpy arrays (vectors), the components of the projected displacement field at the given `nodes`.
- **method** (*{'nearest', 'linear', 'cubic'}, optional*) – Type of the interpolation. The default is linear.

See also:

project_onto_grid()

Examples

Suppose we have measured field data, obtained by DIC. The experimental field values are obtained as an image. The pixel centers of this image form a grid, each grid point having an associated scalar value, the value of the measured field. In this example, we pretend that the measured field is given as a function. The DIC grid and the measured field values can be seen in the upper left and lower left figures, respectively.

```
>>> from grains.dic import DIC
>>> from grains.geometry import TriMesh
>>> x_grid, y_grid = np.mgrid[-1:1:100j, 1:2:50j]
>>> exact_solution = lambda x, y: 1 - (x + y**2) * np.sign(x)
>>> grid = DIC(exact_solution(x_grid, y_grid).T, exact_solution(x_grid,y_
↪grid).T)
```

The finite element solution is obtained at the nodes (upper right figure) of the mesh. Here, we assumed that the nodes are sampled from a uniformly random distribution on $[-1, 1] \times [1, 2]$.

```
>>> n_nodes = 100  # modify this to see how good the interpolated solution is
>>> mesh = TriMesh(*TriMesh.sample_mesh(1, n_nodes))
```

For the sake of this example, we also assume that the nodal values are "exact", i.e. they are the function values at the nodes. In reality, of course, this will not be the case, but this allows us to investigate the effect moving from the FE mesh to the DIC grid.

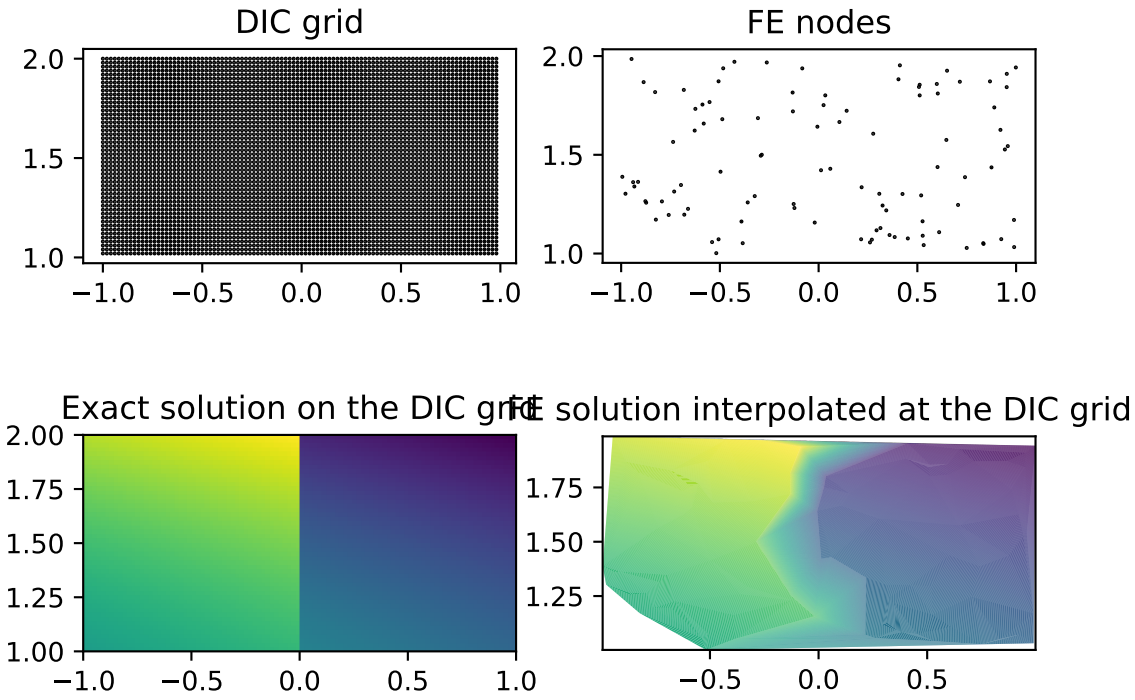
```
>>> grid.set_transformation((-1, 2), 50)
>>> fe_values = exact_solution(mesh.vertices[:, 0], mesh.vertices[:, 1])
>>> interpolated = grid.project_onto_mesh(mesh.vertices, 'nearest')
```

The FE solution available at the nodes are interpolated at the DIC grid points, as shown in the lower right figure. Interpolation with continuous functions cannot resolve well the discontinuity present in the "exact solution", i.e. in the measurement data. A discontinuous manufactured solution was intentionally prepared to illustrate this.

```
>>> ax = []
>>> ax.append(plt.subplot(221))
>>> grid.plot_physicalgrid(ax[0])
>>> plt.title('DIC grid')
>>> ax.append(plt.subplot(222))
>>> mesh.plot('k.', ax=ax[1], markersize=1)
>>> plt.title('FE nodes')
>>> ax.append(plt.subplot(223))
>>> plt.imshow(exact_solution(x_grid, y_grid).T, extent=(-1, 1, 1, 2),␣
↪origin='lower',
...            vmin=-4, vmax = 5)
>>> plt.title('Exact solution on the DIC grid')
>>> ax.append(plt.subplot(224))
>>> interpolated[0][np.isnan(interpolated[0])] = 0
>>> mesh.associate_field(interpolated[0])
>>> mesh.plot_field(0, show_mesh=False, ax=ax[3])
>>> plt.title('FE solution interpolated at the DIC grid')
>>> plt.show()
```

You are invited to modify this example to simulate a finer mesh by increasing `n_nodes`. Also try different interpolation techniques.

set_transformation(*origin*, *pixels_per_physicalunit*)
Sets the transformation rule between the pixel and the physical coordinate systems.


DIC grid
FE nodes
Exact solution on the DIC grid
FE solution interpolated at the DIC grid
2.0
1.5
1.0
−1.0
−0.5
0.0
0.5
1.0
2.00
1.75
1.50
1.25
1.00

To determine the position and the size of the DIC image in the physical space, a transformation rule needs to be given, as described in the *Notes* section of the `DIC` class.

Parameters

- **origin** (*tuple*) – 2-tuple of float, the coordinates of the origin of the DIC grid (upper left corner) in the physical coordinate system.
- **pixels_per_physicalunit** (*float*)

Returns *None*

strain (*strain_measure*)

Computes the strain tensor from the displacement vector.

The symmetric strain tensor $\boldsymbol{\varepsilon}$ with components

$$\boldsymbol{\varepsilon} = \begin{pmatrix} \varepsilon_{11} & \varepsilon_{12} \\ \varepsilon_{21} & \varepsilon_{22} \end{pmatrix}$$

is computed for the given strain measure. The partial derivatives of the displacement field (u, v), available on an $m \times n$ grid, are computed with numerical differentiation with second order accuracy.

Parameters **strain_measure** (*{'infinitesimal', 'Green-Lagrange'}*) – One of the following strain measures.

- 'infinitesimal'

$$\begin{aligned} \varepsilon_{11} &= \frac{\partial u}{\partial x} \\ \varepsilon_{12} &= \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\right) \\ \varepsilon_{22} &= \frac{\partial v}{\partial y} \end{aligned}$$

- 'Green-Lagrange'

$$\begin{aligned} \varepsilon_{11} &= \frac{1}{2}\left(2\frac{\partial u}{\partial x} + \left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial v}{\partial x}\right)^2\right) \\ \varepsilon_{12} &= \frac{1}{2}\left(\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} + \frac{\partial u}{\partial x}\frac{\partial u}{\partial y} + \frac{\partial v}{\partial x}\frac{\partial v}{\partial y}\right) \\ \varepsilon_{22} &= \frac{1}{2}\left(2\frac{\partial v}{\partial y} + \left(\frac{\partial u}{\partial y}\right)^2 + \left(\frac{\partial v}{\partial y}\right)^2\right) \end{aligned}$$

Returns **strain_tensor** (*ndarray*) – Components of the strain tensor as an $m \times n \times 3$ array. The first two dimensions correspond to the grid points they are determined at, the third dimension gives the components of the tensor in the following order: $\varepsilon_{11}, \varepsilon_{12}, \varepsilon_{22}$.

See also:

`equivalent_strain()`, `plot_strain()`, `numpy.gradient()`

Notes

The derivatives of the displacement field are computed in the the physical coordinate system.

Examples

Consider a rectangular body with a linear displacement function in horizontal direction and no displacement vertically. The deformation of the body is such that only the horizontal strain is nonzero.

```
>>> u = np.array([[0, 1e-3, 2e-3, 3e-3], [0, 1e-3, 2e-3, 3e-3], [0, 1e-3, 2e-
↪3, 3e-3]])
>>> v = np.zeros((3,4))
>>> d = DIC(u, v)
>>> E = d.strain('infinitesimal')
>>> E[:, :, 0]
array([[0.001, 0.001, 0.001, 0.001],
       [0.001, 0.001, 0.001, 0.001],
       [0.001, 0.001, 0.001, 0.001]])
>>> np.allclose(E[:, :, 2], 0)
True
>>> np.allclose(E[:, :, 1], 0)
True
```

The Green-Lagrange strain tensor is slightly different. Comparing with the infinitesimal strain tensor shows how good the assumption of small deformations is.

```
>>> E_gl = d.strain('Green-Lagrange')
>>> E_gl[:, :, 0] - E[:, :, 0]
array([[5.e-07, 5.e-07, 5.e-07, 5.e-07],
       [5.e-07, 5.e-07, 5.e-07, 5.e-07],
       [5.e-07, 5.e-07, 5.e-07, 5.e-07]])
```

The other two strain components remain zero.

```
>>> np.allclose(E_gl[:, :, 1:2], 0)
True
```

grains.dic.**plot_strain**(*strain*, *minval=None*, *maxval=None*, *colorbar=True*, *label=''*)

Plots a scalar strain field.

Parameters

- **strain** (*ndarray*) – Scalar strain field sampled on an m-by-n grid, given as a 2D numpy array.
- **minval, maxval** (*float, optional*) – Set the color scaling for the image by fixing the values that map to the colormap color limits. If `minval` is not provided, the limit is determined from the minimum value of the data. Similarly for `maxval`.
- **colorbar** (*bool, optional*) – If True, a horizontal colorbar is placed below the strain map. The default is True.
- **label** (*str, optional*) – Label describing the strain field. LaTeX code is also accepted, e.g. *r'$varepsilon_{yy}$'*. If not given, no text is displayed.

Returns *None*

See also:

DIC.strain()

Deprecated since version 1.1.0: This will be removed in 1.3.0. This function will be a static method of the DIC class. See also the deprecation warning of *DIC.plot_strain()*.

CHAPTER

TWENTYFIVE

SIMULATION

25.1 Functions

data_Pierre	Yield stresses and average grain diameters from Pierre's thesis.
hallpetch_constants	Determines the two Hall-Petch constants.
hallpetch	Computes the yield stress from the Hall-Petch relation.
hallpetch_plot	Plots the Hall-Petch formula for given grain sizes and yield stresses.
change_domain	Extends or crops the domain an image fills.
nature_of_deformation	Characterizes the intergranular/intragranular deformations.

25.1.1 grains.simulation.data_Pierre

grains.simulation.**data_Pierre**()

Yield stresses and average grain diameters from Pierre's thesis.

Returns

- **sigma_y** (*list of floats*) – Yield stresses.
- **d** (*list of floats*) – Diameters of the grains.

25.1.2 grains.simulation.hallpetch_constants

grains.simulation.**hallpetch_constants**(*sigma_y*, *d*)

Determines the two Hall-Petch constants. Given available measurements for the grains sizes and the yield stresses, the two constants in the Hall-Petch formula are computed.

Parameters

- **sigma_y** (*list of floats*) – Yield stresses.
- **d** (*list of floats*) – Diameters of the grains.

Returns

- **sigma_0** (*float*) – Starting stress for dislocation movement (material constant).
- **k** (*float*) – Strengthening coefficient (material constant).

Notes

If two data points are given in the inputs (corresponding to two measurements), the output parameters have unique values:

k = (sigma_y[0] - sigma_y[1]) / (1/sqrt(d[0]) - 1/sqrt(d[1])) sigma_0 = sigma_y[0] - k/sqrt(d[0])

If there are more than two measurements, the resulting linear system is overdetermined. In both cases, the outputs are determined using least squares fitting.

25.1.3 grains.simulation.hallpetch

grains.simulation.**hallpetch**(*sigma_0*, *k*, *d*)

Computes the yield stress from the Hall-Petch relation.

Parameters

- **sigma_0** (*float*) – Starting stress for dislocation movement (material constant).
- **k** (*float*) – Strengthening coefficient (material constant).
- **d** (*float or list of floats*) – Diameter of the grain.

Returns **sigma_y** (*float or list of floats*) – Yield stress.

25.1.4 grains.simulation.hallpetch_plot

grains.simulation.**hallpetch_plot**(*sigma_y*, *d*, *units=('MPa'*, *'mm')*)

Plots the Hall-Petch formula for given grain sizes and yield stresses.

Parameters

- **sigma_y** (*ndarray*) – Yield stresses.
- **d** (*ndarray*) – Grain diameters.
- **units** (*2-tuple of str, optional*) – Units for the yield stress and the grain diameters. The default is ("MPa","mm").

Returns **fig** (*matplotlib.figure.Figure*) – The figure object is returned in case further manipulations are necessary.

25.1.5 grains.simulation.change_domain

grains.simulation.**change_domain**(*image*, *left*, *right*, *bottom*, *top*, *padding_value=nan*)

Extends or crops the domain an image fills.

The original image is extended, cropped or left unchanged in the left, right, bottom and top directions by padding the corresponding 2D or 3D array with a given value or removing existing elements. Non-integer image length is avoided by rounding up. This choice prevents ending up with an empty image during cropping or no added pixel during extension.

Parameters

- **image** (*ndarray*) – 2D or 3D numpy array representing the original image.
- **left, right** (*float*) – When positive, the domain is extended, when negative, the domain is cropped by the given value relative to the image width.

- **bottom, top** (*float*) – When positive, the domain is extended, when negative, the domain is cropped by the given value relative to the image height.
- **padding_value** (*float, optional*) – Value for the added pixels. The default is numpy.nan.

Returns **changed_image** (*ndarray*) – 2D or 3D numpy array representing the modified domain.

Examples

Crop an image at the top, extended it at the bottom and on the left, and leave it unchanged on the right. Note the rounding for non-integer pixels.

```
>>> import numpy as np
>>> image = np.array([[0.1, 0.2, 0.3], [0.4, 0.5, 0.6], [0.7, 0.8, 0.9]])
>>> modified = change_domain(image, 0.5, 0, 1/3, -1/3, 0)
>>> image  # no in-place modification, the original image is not overwritten
array([[0.1, 0.2, 0.3],
       [0.4, 0.5, 0.6],
       [0.7, 0.8, 0.9]])
>>> modified
array([[0. , 0. , 0.4, 0.5, 0.6],
       [0. , 0. , 0.7, 0.8, 0.9],
       [0. , 0. , 0. , 0. , 0. ]])
```

25.1.6 grains.simulation.nature_of_deformation

`grains.simulation.`**`nature_of_deformation`**(*microstructure*, *strain_field*, *interface_width=3*, *visualize=True*)

Characterizes the intergranular/intragranular deformations.

To decide whether the strain localization is intergranular (happens along grain boundaries, also called interfaces) or intragranular in a given microstructure, the strain field is projected on the microstructure. Here, by strain field we mean a scalar field, often called *equivalent strain* that is derived from a strain tensor.

It is irrelevant for this function whether the strain field is obtained from a numerical simulation or from a (post-processed) full-field measurement. All what matters is that the strain field be available on a grid of the same size as the microstructure.

The strain field is assumed to be localized on an interface if its neighborhood, with band width defined by the user, contains higher strain values than what is outside the band (i.e. the grain interiors). A too large band width identifies small grains to have boundary only, without any interior. This means that even if the strain field in reality localizes inside such small grains, the localization is classified as intergranular. However, even for extreme deformations, one should not expect that the strain localizes on an interface with a single-point width. Moreover, using a too small band width is susceptible to the exact position of the interfaces, which are extracted from the grain microstructure. A judicial balance needs to be achieved in practice.

Parameters

- **microstructure** (*ndarray*) – Labelled image corresponding to the segmented grains in a grain microstructure.
- **strain_field** (*ndarray*) – Discrete scalar field of the same size as the `microstructure`.
- **interface_width** (*int, optional*) – Thickness of the band around the interfaces.
- **visualize** (*bool, optional*) – If True, three plots are created. Two of them show the deformation field within the bands and outside the bands. They are linked together, so when

you pan or zoom on one, the other plot will follow. The third plot contains two histograms on top of each other, giving the frequency of the strain values within the bands and outside the bands.

Returns

- **boundary_strain** (*ndarray*) – Copy of `strain_field`, but values outside the band are set to NaN.
- **bulk_strain** (*ndarray*) – Copy of `strain_field`, but values within the band are set to NaN.
- **bands** (*ndarray*) – Boolean array of the same size as `strain_field`, with True values corresponding to the band.

See also:

grains.dic.DIC.strain() Computes a strain tensor from the displacement field.

grains.dic.DIC.equivalent_strain() Extracts a scalar quantity from a strain tensor.

matplotlib.pyplot.hist() Plots a histogram.

Notes

1. From the modelling viewpoint, it is important to know whether the strain localizes to the grain boundaries or it is dominant within the grains as well. In the former case, simplifications in the models save computational time in the simulations.
2. In dynamics, the evolution of the strain field is relevant. E.g. an initially intergranular deformation can turn into diffuse localization that occurs within the grains as well. In that case, a strain field must be obtained at each time step, and this function can be called for each such instance.

Examples

The following figure was created by this function with `visualize` set to *True* and `band_width` chosen to be 3.

`grains.simulation.`**`change_domain`**(*image*, *left*, *right*, *bottom*, *top*, *padding_value=nan*)

Extends or crops the domain an image fills.

The original image is extended, cropped or left unchanged in the left, right, bottom and top directions by padding the corresponding 2D or 3D array with a given value or removing existing elements. Non-integer image length is avoided by rounding up. This choice prevents ending up with an empty image during cropping or no added pixel during extension.

Parameters

- **image** (*ndarray*) – 2D or 3D numpy array representing the original image.
- **left, right** (*float*) – When positive, the domain is extended, when negative, the domain is cropped by the given value relative to the image width.
- **bottom, top** (*float*) – When positive, the domain is extended, when negative, the domain is cropped by the given value relative to the image height.
- **padding_value** (*float, optional*) – Value for the added pixels. The default is numpy.nan.

Returns **changed_image** (*ndarray*) – 2D or 3D numpy array representing the modified domain.

Examples

Crop an image at the top, extended it at the bottom and on the left, and leave it unchanged on the right. Note the rounding for non-integer pixels.

```
>>> import numpy as np
>>> image = np.array([[0.1, 0.2, 0.3], [0.4, 0.5, 0.6], [0.7, 0.8, 0.9]])
>>> modified = change_domain(image, 0.5, 0, 1/3, -1/3, 0)
>>> image  # no in-place modification, the original image is not overwritten
array([[0.1, 0.2, 0.3],
       [0.4, 0.5, 0.6],
       [0.7, 0.8, 0.9]])
>>> modified
array([[0. , 0. , 0.4, 0.5, 0.6],
       [0. , 0. , 0.7, 0.8, 0.9],
       [0. , 0. , 0. , 0. , 0. ]])
```

grains.simulation.**data_Pierre**()
Yield stresses and average grain diameters from Pierre's thesis.

Returns

- **sigma_y** (*list of floats*) – Yield stresses.
- **d** (*list of floats*) – Diameters of the grains.

grains.simulation.**hallpetch**(*sigma_0*, *k*, *d*)
Computes the yield stress from the Hall-Petch relation.

Parameters

- **sigma_0** (*float*) – Starting stress for dislocation movement (material constant).
- **k** (*float*) – Strengthening coefficient (material constant).
- **d** (*float or list of floats*) – Diameter of the grain.

Returns **sigma_y** (*float or list of floats*) – Yield stress.

grains.simulation.**hallpetch_constants**(*sigma_y*, *d*)
Determines the two Hall-Petch constants. Given available measurements for the grains sizes and the yield stresses, the two constants in the Hall-Petch formula are computed.

Parameters

- **sigma_y** (*list of floats*) – Yield stresses.
- **d** (*list of floats*) – Diameters of the grains.

Returns

- **sigma_0** (*float*) – Starting stress for dislocation movement (material constant).
- **k** (*float*) – Strengthening coefficient (material constant).

Notes

If two data points are given in the inputs (corresponding to two measurements), the output parameters have unique values:

k = (sigma_y[0] - sigma_y[1]) / (1/sqrt(d[0]) - 1/sqrt(d[1])) sigma_0 = sigma_y[0] - k/sqrt(d[0])

If there are more than two measurements, the resulting linear system is overdetermined. In both cases, the outputs are determined using least squares fitting.

grains.simulation.**hallpetch_plot**(*sigma_y*, *d*, *units=('MPa'*, *'mm')*)

Plots the Hall-Petch formula for given grain sizes and yield stresses.

Parameters

- **sigma_y** (*ndarray*) – Yield stresses.
- **d** (*ndarray*) – Grain diameters.
- **units** (*2-tuple of str, optional*) – Units for the yield stress and the grain diameters. The default is ("MPa","mm").

Returns **fig** (*matplotlib.figure.Figure*) – The figure object is returned in case further manipulations are necessary.

grains.simulation.**nature_of_deformation**(*microstructure*, *strain_field*, *interface_width=3*, *visualize=True*)

Characterizes the intergranular/intragranular deformations.

To decide whether the strain localization is intergranular (happens along grain boundaries, also called interfaces) or intragranular in a given microstructure, the strain field is projected on the microstructure. Here, by strain field we mean a scalar field, often called *equivalent strain* that is derived from a strain tensor.

It is irrelevant for this function whether the strain field is obtained from a numerical simulation or from a (post-processed) full-field measurement. All what matters is that the strain field be available on a grid of the same size as the microstructure.

The strain field is assumed to be localized on an interface if its neighborhood, with band width defined by the user, contains higher strain values than what is outside the band (i.e. the grain interiors). A too large band width identifies small grains to have boundary only, without any interior. This means that even if the strain field in reality localizes inside such small grains, the localization is classified as intergranular. However, even for extreme deformations, one should not expect that the strain localizes on an interface with a single-point width. Moreover, using a too small band width is susceptible to the exact position of the interfaces, which are extracted from the grain microstructure. A judicial balance needs to be achieved in practice.

Parameters

- **microstructure** (*ndarray*) – Labelled image corresponding to the segmented grains in a grain microstructure.
- **strain_field** (*ndarray*) – Discrete scalar field of the same size as the `microstructure`.
- **interface_width** (*int, optional*) – Thickness of the band around the interfaces.
- **visualize** (*bool, optional*) – If True, three plots are created. Two of them show the deformation field within the bands and outside the bands. They are linked together, so when you pan or zoom on one, the other plot will follow. The third plot contains two histograms on top of each other, giving the frequency of the strain values within the bands and outside the bands.

Returns

- **boundary_strain** (*ndarray*) – Copy of `strain_field`, but values outside the band are set to NaN.

- **bulk_strain** (*ndarray*) – Copy of `strain_field`, but values within the band are set to NaN.
- **bands** (*ndarray*) – Boolean array of the same size as `strain_field`, with True values corresponding to the band.

See also:

grains.dic.DIC.strain() Computes a strain tensor from the displacement field.

grains.dic.DIC.equivalent_strain() Extracts a scalar quantity from a strain tensor.

matplotlib.pyplot.hist() Plots a histogram.

Notes

1. From the modelling viewpoint, it is important to know whether the strain localizes to the grain boundaries or it is dominant within the grains as well. In the former case, simplifications in the models save computational time in the simulations.
2. In dynamics, the evolution of the strain field is relevant. E.g. an initially intergranular deformation can turn into diffuse localization that occurs within the grains as well. In that case, a strain field must be obtained at each time step, and this function can be called for each such instance.

Examples

The following figure was created by this function with `visualize` set to *True* and `band_width` chosen to be 3.

CHAPTER

TWENTYSIX

UTILITIES

This module provides *general* utility functions used by the **grains** package. The specific helper functions reside in the proper module. For example, a function that works on a general list goes here, but a computational geometry algorithm goes to the **geometry** module. The functions in the **utils** module can be interesting for other projects too, partly because of their general scope, and partly because of the few dependencies.

26.1 Functions

duplicates	Set of duplicate elements in a sequence.
toggle	Return True for False values and False for True values in a list.
index_list	Index a list by another list.
flatten_list	Merge a list of lists to a single list.
argsorted	Return the indices that would sort a list or a tuple.
map_inplace	Apply a function to each member of an iterable in-place.
non_unique	Finds indices of non-unique elements in a 1D or 2D ndarray.
parse_kwargs	Compares keyword arguments with defaults.
compress	Creates a zip archive from a single file.
decompress	Decompresses the contents of a zip archive into the current directory.
decompress_inmemory	Decompresses the contents of a zip archive into a dictionary.
neighborhood	Neighboring points to a grid point.

26.1.1 grains.utils.duplicates

grains.utils.**duplicates**(*sequence*)

Set of duplicate elements in a sequence.

Parameters **sequence** (*sequence types (list, tuple, string, etc.)*) – Sequence possibly containing repeating elements.

Returns *set* – Set of unique values.

Notes

Copied from https://stackoverflow.com/a/9836685/4892892

Examples

Note that the order of the elements in the resulting set does not matter.

```
>>> a = [1, 2, 3, 2, 1, 5, 6, 5, 5, 5]  # list
>>> duplicates(a)
{1, 2, 5}
>>> a = (1, 1, 0, -1, -1, 0)  # tuple
>>> duplicates(a)
{0, 1, -1}
>>> a = 'abbcdkc'  # string
>>> duplicates(a)
{'c', 'b'}
```

26.1.2 grains.utils.toggle

grains.utils.**toggle**(*lst*)

Return True for False values and False for True values in a list.

Parameters **lst** (*list*) – An arbitrary list, possibly containing other lists.

Returns *list* – Element-wise logical not operator applied on the input list.

Notes

Solution taken from https://stackoverflow.com/a/51122372/4892892.

Examples

```
>>> toggle([True, False])
[False, True]
>>> toggle(['h', 0, 2.3, -2, 5, []])
[False, True, False, False, False, True]
```

26.1.3 grains.utils.index_list

grains.utils.**index_list**(*lst*, *indices*)

Index a list by another list.

Parameters

- **lst** (*list*) – List to be indexed.
- **indices** (*list*) – Indices of the original list that will form the new list.

Returns *list* – Members of *lst*, selected by *indices*.

Examples

```
>>> index_list(['c', ['nested', 'list'], 13], [1, 2])
[['nested', 'list'], 13]
```

26.1.4 grains.utils.flatten_list

grains.utils.**flatten_list**(*nested_list*)

Merge a list of lists to a single list.

Parameters **nested_list** (*list*) – List containing other lists.

Returns *list* – Flattened list.

Notes

- Only a single level (i.e. list of lists) is handled, see the second example.
- Several methods, such as list comprehension, monoid and loops, are proposed in https://stackoverflow.com/questions/952914/how-to-make-a-flat-list-out-of-list-of-lists. Here, the list comprehension approach is used.

Examples

```
>>> nested_list = [['some'], ['items']]
>>> flatten_list(nested_list)
['some', 'items']
>>> multiply_nested_list = [[['item'], 'within', 'item']]
>>> flatten_list(multiply_nested_list)
[['item'], 'within', 'item']
```

26.1.5 grains.utils.argsorted

grains.utils.**argsorted**(*sequence*, *reverse=False*)

Return the indices that would sort a list or a tuple.

Implementation is taken from https://stackoverflow.com/a/6979121/4892892.

Parameters

- **sequence** (*list, tuple*) – Input sequence in which the sorted indices to be found.
- **reverse** (*bool*) – If set to True, then the elements are sorted as if each comparison was reversed.

Returns *list* – List of indices that would sort the input list/tuple.

See also:

`sorted()`, `numpy.argsort()`

Examples

```
>>> argsorted([2, 1.1, 1.1])
[1, 2, 0]
>>> argsorted([2, 1.1, 1.1], reverse=True)
[0, 1, 2]
>>> argsorted(())
[]
```

26.1.6 grains.utils.map_inplace

grains.utils.**map_inplace**(*function*, *__iterable*)

Apply a function to each member of an iterable in-place.

Parameters

- **function** (*function object*) – Function to be applied to the entries of the iterable.
- **__iterable** (*iterable*) – Iterable.

Notes

Comprehensions or functional tools work on iterators, thereby not modifying the original container (https://stackoverflow.com/a/4148523/4892892). For in-place modification, the conventional for loop approach is used (https://stackoverflow.com/a/4148525/4892892).

Examples

```
>>> lst = ['2', 2]; func = lambda x: x*2
>>> map_inplace(func, lst); lst
['22', 4]
>>> lifespan = {'cat': 15, 'dog': 12}; die_early = lambda x: x/2
>>> map_inplace(die_early, lifespan); lifespan
{'cat': 7.5, 'dog': 6.0}
```

26.1.7 grains.utils.non_unique

grains.utils.**non_unique**(*array*, *axis=None*)

Finds indices of non-unique elements in a 1D or 2D ndarray.

Parameters

- **array** (*ndarray*) – Array in which the non-unique elements are searched.
- **axis** (*{None, 0, 1}, optional*) – The axis to operate on. If None, *array* will be flattened. If an integer, the subarrays indexed by the given axis will be flattened and treated as the elements of a 1-D array with the dimension of the given axis. Object arrays or structured arrays that contain objects are not supported if the *axis* kwarg is used. The default is None.

Returns

- **nonunique_values** (*list*) – Unique (individual, row or column) entries.

- **nonunique_indices** (*list*) – Each element of the list corresponds to non-unique elements, whose indices are given in a 1D numpy array.

Examples

In a 1D array, the repeated values and their indices are found by

```
>>> val, idx = non_unique(np.array([1, -1, 0, -1, 2, 5, 0, -1]))
>>> val
[-1, 0]
>>> idx
[array([1, 3, 7]), array([2, 6])]
```

In the matrix below, we can see that rows 0 and 2 are identical, as well as rows 1 and 4.

```
>>> val, idx = non_unique(np.array([[1, 3], [2, 4], [1, 3], [-1, 0], [2, 4]]),␣
↪axis=0)
>>> val
[array([1, 3]), array([2, 4])]
>>> idx
[array([0, 2]), array([1, 4])]
```

By transposing the matrix above, the same holds for the columns.

```
>>> val, idx = non_unique(np.array([[1, 2, 1, -1, 2], [3, 4, 3, 0, 4]]), axis=1)
>>> val
[array([1, 3]), array([2, 4])]
>>> idx
[array([0, 2]), array([1, 4])]
```

If the dimensions along which to find the duplicates are not given, the input is flattened and the indexing happens in C-order (row-wise).

```
>>> val, idx = non_unique(np.array([[1, 2, 1, -1, 2], [3, 4, 3, 0, 4]]))
>>> val
[1, 2, 3, 4]
>>> idx
[array([0, 2]), array([1, 4]), array([5, 7]), array([6, 9])]
```

26.1.8 grains.utils.parse_kwargs

grains.utils.**parse_kwargs**(*kwargs*, *defaults*)

Compares keyword arguments with defaults.

Allows processing keyword arguments supplied to a function by the user by comparing them with an admissible set of options defined by the developer. There are three cases:

1. The keyword given by the user is present in the set the developer provides. Then the value belonging to the keyword overrides the default value.

2. The keyword given by the user is *not* present in the set the developer provides. In this case, the unrecognized keyword, along with its value, is saved separately.

3. The keyword existing in the set the developer provides is not given by the user. Then the default value is used.

Parameters

- **kwargs** (*dict*) – Keyword arguments (parameter-value pairs) passed to a function.
- **defaults** (*dict*) – Default parameter-value pairs.

Returns

- **parsed** (*dict*) – Dictionary with the same keys as `defaults`, the parsed parameter-value pairs.
- **unknown** (*dict*) – Dictionary containing the parameter-value pairs not present in `defaults`.

Notes

The default values, given in the input dictionary `defaults`, are never overwritten.

Examples

```
>>> default_options = {'opt1': 1, 'opt2': 'string', 'opt3': [-1, 0]}
>>> user_options = {'opt3': [2, 3, -1], 'opt2': 'string',  'opt4': -2.14}
>>> parsed_options, unknown_options = parse_kwargs(user_options, default_options)
>>> parsed_options
{'opt1': 1, 'opt2': 'string', 'opt3': [2, 3, -1]}
>>> unknown_options
{'opt4': -2.14}
```

26.1.9 grains.utils.compress

`grains.utils.`**`compress`**(*filename*, *level=9*)

Creates a zip archive from a single file.

Parameters

- **filename** (*str*) – Name of the file to be compressed.
- **level** (*int, optional*) – Level of compression. Integers 0 through 9 are accepted. The default is 9.

Returns *None.*

See also:

`zipfile.ZipFile`

26.1.10 grains.utils.decompress

`grains.utils.`**`decompress`**(*filename*, *path=None*)

Decompresses the contents of a zip archive into the current directory.

Parameters

- **filename** (*str*) – Name of the zip archive.
- **path** (*str, optional*) – Directory to extract to. The default is the directory the function is called from.

See also:

`zipfile.ZipFile`

26.1.11 grains.utils.decompress_inmemory

`grains.utils.`**`decompress_inmemory`**(*filename*)

Decompresses the contents of a zip archive into a dictionary.

Parameters **filename** (*str*) – Name of the zip archive.

Returns **data** (*dict*) – The keys of the dictionary are the compressed file names (without extension), the corresponding values are their contents.

See also:

`zipfile.ZipFile`

26.1.12 grains.utils.neighborhood

`grains.utils.`**`neighborhood`**(*center*, *radius*, *norm*, *method='ball'*, *bounds=None*)

Neighboring points to a grid point.

Given a point in a subspace of $\mathbb{Z}^n$, the neighboring points are determined based on the specified rules.

Todo: Currently, the neighbors are deterministically but not systematically ordered. Apart from testing purposes, this does not seem to be a big issue. Still, a logical ordering is desirable. E.g. ordering in increasing coordinate values, first in the first dimension and lastly in the last dimension.

Parameters

- **center** (*tuple of int*) – Point x_0 around which the neighborhood is searched. It must be an n-tuple of integers, where n is the spatial dimension.
- **radius** (*int, positive*) – Radius of the ball or sphere in which the neighbors are searched. If the radius is 1, the immediate neighbors are returned.
- **norm** (*{1, inf}*) – Type of the vector norm $\|x - x_0\|$, where x is a point whose distance is searched from the center x_0.

Type	Name	Definition
1	1-norm	$\|x\|_1 = \sum_{i=1}^{n} \|x_i\|$
numpy.inf	maximum norm	$\|x\|_\infty = \max\{\|x_1\|, \ldots, \|x_n\|\}$

  where inf means numpy's np.inf object.
- **method** (*{'ball', 'sphere'}, optional*) – Specifies the criterion of how to decide whether a point x is in the neighborhood of x_0. The default is 'ball'.

  For 'ball':

$$\|x - x_0\| \leq r$$

  For 'sphere':

$$\|x - x_0\| = r$$

where r is the radius passed as the `radius` parameter and the type of the norm is taken based on the `norm` input parameter.

- **bounds** (*list of tuple, optional*) – Restricts the neighbors within a box. The dimensions of the n-dimensional box are given as a list of 2-tuples: [(x_1_min, x_1_max), ... , (x_n_min, x_n_max)]. The default value is an unbounded box in all dimensions. Use np.inf to indicate unbounded values.

Returns **neighbors** (*tuple of ndarray*) – Tuple of length n, each entry being a 1D numpy array: the integer indices of the points that are in the neighborhood of `center`.

Notes

1. The von Neumann neighborhood with range r is a special case when `radius=r`, `norm=1` and `method='ball'`.

2. The Moore neighborhood with range r is a special case when `radius=r`, `norm=np.inf` and `method='ball'`.

Examples

Find the Moore neighborhood with range 2 the point (1) on the half-line [0, inf).

```
>>> neighborhood((1,), 2, np.inf, bounds=[(0, np.inf)])
(array([0, 1, 2, 3]),)
```

Find the von Neumann neighborhood with range 2 around the point (2, 2), restricted on the domain [0, 4] x [0, 3].

```
>>> neighborhood((2, 2), 2, 1, bounds=[(0, 4), (0, 3)])
(array([2, 1, 2, 3, 0, 1, 2, 3, 4, 1, 2, 3]), array([0, 1, 1, 1, 2, 2, 2, 2, 2, 3,
↪ 3, 3]))
```

Find the Moore neighborhood with range 1 around the point (0, -4) such that the neighbors lie on the half-plane [0, 2] x (-inf, -4].

```
>>> neighborhood((0, -4), 1, np.inf, bounds=[(0, 2), (-np.inf, -4)])
(array([0, 1, 0, 1]), array([-5, -5, -4, -4]))
```

Find the sphere of radius 2, measured in the 1-norm, around the point (-1, 0, 3), within the half-space {(x,y,z) in Z^3 | y>=0}.

```
>>> neighborhood((-1, 0, 3), 2, 1, 'sphere', [(-np.inf, np.inf), (0, np.inf), (-
↪np.inf, np.inf)])
(array([-3, -2, -2, -1, -1,  0,  0,  1, -2, -1, -1,  0, -1]),
 array([0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 2]),
 array([3, 2, 4, 1, 5, 2, 4, 3, 3, 2, 4, 3, 3]))
```

`grains.utils.`**`argsorted`**(*sequence*, *reverse=False*)

Return the indices that would sort a list or a tuple.

Implementation is taken from https://stackoverflow.com/a/6979121/4892892.

Parameters

- **sequence** (*list, tuple*) – Input sequence in which the sorted indices to be found.

- **reverse** (*bool*) – If set to True, then the elements are sorted as if each comparison was reversed.

Returns *list* – List of indices that would sort the input list/tuple.

See also:

`sorted()`, `numpy.argsort()`

Examples

```
>>> argsorted([2, 1.1, 1.1])
[1, 2, 0]
>>> argsorted([2, 1.1, 1.1], reverse=True)
[0, 1, 2]
>>> argsorted(())
[]
```

`grains.utils.`**`compress`**(*filename*, *level=9*)

Creates a zip archive from a single file.

Parameters

- **filename** (*str*) – Name of the file to be compressed.
- **level** (*int, optional*) – Level of compression. Integers 0 through 9 are accepted. The default is 9.

Returns *None.*

See also:

`zipfile.ZipFile`

`grains.utils.`**`decompress`**(*filename*, *path=None*)

Decompresses the contents of a zip archive into the current directory.

Parameters

- **filename** (*str*) – Name of the zip archive.
- **path** (*str, optional*) – Directory to extract to. The default is the directory the function is called from.

See also:

`zipfile.ZipFile`

`grains.utils.`**`decompress_inmemory`**(*filename*)

Decompresses the contents of a zip archive into a dictionary.

Parameters **filename** (*str*) – Name of the zip archive.

Returns **data** (*dict*) – The keys of the dictionary are the compressed file names (without extension), the corresponding values are their contents.

See also:

`zipfile.ZipFile`

`grains.utils.`**`duplicates`**(*sequence*)

Set of duplicate elements in a sequence.

Parameters **sequence** (*sequence types (list, tuple, string, etc.)*) – Sequence possibly containing repeating elements.

Returns *set* – Set of unique values.

Notes

Copied from https://stackoverflow.com/a/9836685/4892892

Examples

Note that the order of the elements in the resulting set does not matter.

```
>>> a = [1, 2, 3, 2, 1, 5, 6, 5, 5, 5]  # list
>>> duplicates(a)
{1, 2, 5}
>>> a = (1, 1, 0, -1, -1, 0)  # tuple
>>> duplicates(a)
{0, 1, -1}
>>> a = 'abbcdkc'  # string
>>> duplicates(a)
{'c', 'b'}
```

grains.utils.**flatten_list**(*nested_list*)

Merge a list of lists to a single list.

Parameters **nested_list** (*list*) – List containing other lists.

Returns *list* – Flattened list.

Notes

- Only a single level (i.e. list of lists) is handled, see the second example.
- Several methods, such as list comprehension, monoid and loops, are proposed in https://stackoverflow.com/questions/952914/how-to-make-a-flat-list-out-of-list-of-lists. Here, the list comprehension approach is used.

Examples

```
>>> nested_list = [['some'], ['items']]
>>> flatten_list(nested_list)
['some', 'items']
>>> multiply_nested_list = [[['item'], 'within', 'item']]
>>> flatten_list(multiply_nested_list)
[['item'], 'within', 'item']
```

grains.utils.**index_list**(*lst*, *indices*)

Index a list by another list.

Parameters

- **lst** (*list*) – List to be indexed.
- **indices** (*list*) – Indices of the original list that will form the new list.

Returns *list* – Members of *lst*, selected by *indices*.

Examples

```
>>> index_list(['c', ['nested', 'list'], 13], [1, 2])
[['nested', 'list'], 13]
```

grains.utils.**map_inplace**(*function*, *__iterable*)

Apply a function to each member of an iterable in-place.

Parameters

- **function** (*function object*) – Function to be applied to the entries of the iterable.
- **__iterable** (*iterable*) – Iterable.

Notes

Comprehensions or functional tools work on iterators, thereby not modifying the original container (https://stackoverflow.com/a/4148523/4892892). For in-place modification, the conventional for loop approach is used (https://stackoverflow.com/a/4148525/4892892).

Examples

```
>>> lst = ['2', 2]; func = lambda x: x*2
>>> map_inplace(func, lst); lst
['22', 4]
>>> lifespan = {'cat': 15, 'dog': 12}; die_early = lambda x: x/2
>>> map_inplace(die_early, lifespan); lifespan
{'cat': 7.5, 'dog': 6.0}
```

grains.utils.**neighborhood**(*center*, *radius*, *norm*, *method='ball'*, *bounds=None*)

Neighboring points to a grid point.

Given a point in a subspace of $\mathbb{Z}^n$, the neighboring points are determined based on the specified rules.

Todo: Currently, the neighbors are deterministically but not systematically ordered. Apart from testing purposes, this does not seem to be a big issue. Still, a logical ordering is desirable. E.g. ordering in increasing coordinate values, first in the first dimension and lastly in the last dimension.

Parameters

- **center** (*tuple of int*) – Point x_0 around which the neighborhood is searched. It must be an n-tuple of integers, where n is the spatial dimension.
- **radius** (*int, positive*) – Radius of the ball or sphere in which the neighbors are searched. If the radius is 1, the immediate neighbors are returned.
- **norm** (*{1, inf}*) – Type of the vector norm $\|x - x_0\|$, where x is a point whose distance is searched from the center x_0.

Type	Name	Definition
1	1-norm	$\|x\|_1 = \sum_{i=1}^{n} \|x_i\|$
numpy.inf	maximum norm	$\|x\|_\infty = \max\{\|x_1\|, \ldots, \|x_n\|\}$

where inf means numpy's np.inf object.

- **method** (*{'ball', 'sphere'}, optional*) – Specifies the criterion of how to decide whether a point x is in the neighborhood of x_0. The default is 'ball'.

  For 'ball':

  $$\|x - x_0\| \leq r$$

  For 'sphere':

  $$\|x - x_0\| = r$$

  where r is the radius passed as the `radius` parameter and the type of the norm is taken based on the `norm` input parameter.

- **bounds** (*list of tuple, optional*) – Restricts the neighbors within a box. The dimensions of the n-dimensional box are given as a list of 2-tuples: [(x_1_min, x_1_max), ... , (x_n_min, x_n_max)]. The default value is an unbounded box in all dimensions. Use np.inf to indicate unbounded values.

Returns **neighbors** (*tuple of ndarray*) – Tuple of length n, each entry being a 1D numpy array: the integer indices of the points that are in the neighborhood of `center`.

Notes

1. The von Neumann neighborhood with range r is a special case when `radius=r`, `norm=1` and `method='ball'`.

2. The Moore neighborhood with range r is a special case when `radius=r`, `norm=np.inf` and `method='ball'`.

Examples

Find the Moore neighborhood with range 2 the point (1) on the half-line [0, inf).

```
>>> neighborhood((1,), 2, np.inf, bounds=[(0, np.inf)])
(array([0, 1, 2, 3]),)
```

Find the von Neumann neighborhood with range 2 around the point (2, 2), restricted on the domain [0, 4] x [0, 3].

```
>>> neighborhood((2, 2), 2, 1, bounds=[(0, 4), (0, 3)])
(array([2, 1, 2, 3, 0, 1, 2, 3, 4, 1, 2, 3]), array([0, 1, 1, 1, 2, 2, 2, 2, 2, 3,
↪ 3, 3]))
```

Find the Moore neighborhood with range 1 around the point (0, -4) such that the neighbors lie on the half-plane [0, 2] x (-inf, -4].

```
>>> neighborhood((0, -4), 1, np.inf, bounds=[(0, 2), (-np.inf, -4)])
(array([0, 1, 0, 1]), array([-5, -5, -4, -4]))
```

Find the sphere of radius 2, measured in the 1-norm, around the point (-1, 0, 3), within the half-space {(x,y,z) in Z^3 | y>=0}.

```
>>> neighborhood((-1, 0, 3), 2, 1, 'sphere', [(-np.inf, np.inf), (0, np.inf), (-
↪np.inf, np.inf)])
(array([-3, -2, -2, -1, -1,  0,  0,  1, -2, -1, -1,  0, -1]),
 array([0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 2]),
 array([3, 2, 4, 1, 5, 2, 4, 3, 3, 2, 4, 3, 3]))
```

grains.utils.**non_unique**(*array*, *axis=None*)

Finds indices of non-unique elements in a 1D or 2D ndarray.

Parameters

- **array** (*ndarray*) – Array in which the non-unique elements are searched.
- **axis** (*{None, 0, 1}, optional*) – The axis to operate on. If None, *array* will be flattened. If an integer, the subarrays indexed by the given axis will be flattened and treated as the elements of a 1-D array with the dimension of the given axis. Object arrays or structured arrays that contain objects are not supported if the *axis* kwarg is used. The default is None.

Returns

- **nonunique_values** (*list*) – Unique (individual, row or column) entries.
- **nonunique_indices** (*list*) – Each element of the list corresponds to non-unique elements, whose indices are given in a 1D numpy array.

Examples

In a 1D array, the repeated values and their indices are found by

```
>>> val, idx = non_unique(np.array([1, -1, 0, -1, 2, 5, 0, -1]))
>>> val
[-1, 0]
>>> idx
[array([1, 3, 7]), array([2, 6])]
```

In the matrix below, we can see that rows 0 and 2 are identical, as well as rows 1 and 4.

```
>>> val, idx = non_unique(np.array([[1, 3], [2, 4], [1, 3], [-1, 0], [2, 4]]),␣
↪axis=0)
>>> val
[array([1, 3]), array([2, 4])]
>>> idx
[array([0, 2]), array([1, 4])]
```

By transposing the matrix above, the same holds for the columns.

```
>>> val, idx = non_unique(np.array([[1, 2, 1, -1, 2], [3, 4, 3, 0, 4]]), axis=1)
>>> val
[array([1, 3]), array([2, 4])]
>>> idx
[array([0, 2]), array([1, 4])]
```

If the dimensions along which to find the duplicates are not given, the input is flattened and the indexing happens in C-order (row-wise).

```
>>> val, idx = non_unique(np.array([[1, 2, 1, -1, 2], [3, 4, 3, 0, 4]]))
>>> val
[1, 2, 3, 4]
>>> idx
[array([0, 2]), array([1, 4]), array([5, 7]), array([6, 9])]
```

grains.utils.**parse_kwargs**(*kwargs*, *defaults*)

Compares keyword arguments with defaults.

Allows processing keyword arguments supplied to a function by the user by comparing them with an admissible set of options defined by the developer. There are three cases:

1. The keyword given by the user is present in the set the developer provides. Then the value belonging to the keyword overrides the default value.

2. The keyword given by the user is *not* present in the set the developer provides. In this case, the unrecognized keyword, along with its value, is saved separately.

3. The keyword existing in the set the developer provides is not given by the user. Then the default value is used.

Parameters

- **kwargs** (*dict*) – Keyword arguments (parameter-value pairs) passed to a function.
- **defaults** (*dict*) – Default parameter-value pairs.

Returns

- **parsed** (*dict*) – Dictionary with the same keys as `defaults`, the parsed parameter-value pairs.
- **unknown** (*dict*) – Dictionary containing the parameter-value pairs not present in `defaults`.

Notes

The default values, given in the input dictionary `defaults`, are never overwritten.

Examples

```
>>> default_options = {'opt1': 1, 'opt2': 'string', 'opt3': [-1, 0]}
>>> user_options = {'opt3': [2, 3, -1], 'opt2': 'string',  'opt4': -2.14}
>>> parsed_options, unknown_options = parse_kwargs(user_options, default_options)
>>> parsed_options
{'opt1': 1, 'opt2': 'string', 'opt3': [2, 3, -1]}
>>> unknown_options
{'opt4': -2.14}
```

grains.utils.**toggle**(*lst*)

Return True for False values and False for True values in a list.

Parameters **lst** (*list*) – An arbitrary list, possibly containing other lists.

Returns *list* – Element-wise logical not operator applied on the input list.

Notes

Solution taken from https://stackoverflow.com/a/51122372/4892892.

Examples

```
>>> toggle([True, False])
[False, True]
>>> toggle(['h', 0, 2.3, -2, 5, []])
[False, True, False, False, False, True]
```

CHAPTER

TWENTYSEVEN

PROFILING

This module implements profiling facilities so that user code can be tested for speed.

27.1 Functions

profile([output_format, output_filename, ...])	Profiles a block of code with Pyinstrument.

27.1.1 grains.profiling.profile

grains.profiling.**profile**(*output_format='html'*, *output_filename=None*, *html_open=False*)

Profiles a block of code with Pyinstrument.

Intended to be used in a *with* statement.

Parameters

- **output_format** (*{'html', 'text'}, optional*) – Shows the result either as text or in an HTML file. If `output_format = 'html'`, the file is saved according to the `output_filename` parameter. The default is 'html'.
- **output_filename** (*str, optional*) – Only taken into account if `output_format = 'html'`. If not given (default), the html output is saved to the same directory the caller resides. The name of the html file is the same as that of the caller.
- **html_open** (*bool, optional*) – Only taken into account if `output_format = 'html'`. If True, the generated HTML file is opened in the default browser. The default is False.

Notes

In the implementation, we move two levels up in the stack frame, one for exiting the context manager and one for exiting this generator. This assumes that *profile()* was called as a context manager. As a good practice, provide the `output_filename` input argument.

Examples

Measure the time needed to generate 1 million uniformly distributed random numbers.

```
>>> import random
>>> with profile('html') as p:
...     for _ in range(1000000):
...         rand_num = random.uniform(1, 2.2)
```

grains.profiling.**profile**(*output_format='html'*, *output_filename=None*, *html_open=False*)

Profiles a block of code with Pyinstrument.

Intended to be used in a *with* statement.

Parameters

- **output_format** (*{'html', 'text'}, optional*) – Shows the result either as text or in an HTML file. If `output_format = 'html'`, the file is saved according to the `output_filename` parameter. The default is 'html'.
- **output_filename** (*str, optional*) – Only taken into account if `output_format = 'html'`. If not given (default), the html output is saved to the same directory the caller resides. The name of the html file is the same as that of the caller.
- **html_open** (*bool, optional*) – Only taken into account if `output_format = 'html'`. If True, the generated HTML file is opened in the default browser. The default is False.

Notes

In the implementation, we move two levels up in the stack frame, one for exiting the context manager and one for exiting this generator. This assumes that *`profile()`* was called as a context manager. As a good practice, provide the `output_filename` input argument.

Examples

Measure the time needed to generate 1 million uniformly distributed random numbers.

```
>>> import random
>>> with profile('html') as p:
...     for _ in range(1000000):
...         rand_num = random.uniform(1, 2.2)
```

CHAPTER

TWENTYEIGHT

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28.1 Index

CHAPTER

TWENTYNINE

CHANGELOG

All notable changes to this project will be documented in this file. The format is based on Keep a Changelog, and this project **does not** adhere to Semantic Versioning. We refer to GitHub issues by their numbers. If there is no issue associated to the change, the commit hashes implementing the change are linked.

29.1 Unreleased

29.2 1.1.0 - 2021-03-04

29.2.1 Added

- Grains embedded into other grains are now identified in the splinegon creation algorithm. 4cef7ec, 6c4ad0a
- Computation of the infinitesimal and Green-Lagrange strain tensors for DIC displacement field. 7eaa0b5, 9e5466e
- Computation of the equivalent von Mises strain. 2b9b0be
- Characterization of the strain localization (intergranular/intragranular) in the microstructure. a74f954, 13576f7
- The README file shows how to cite our paper. #30
- Added a new segmented microstructure (6b539ba) and the corresponding DIC measurements (3c845e7).

29.2.2 Deprecated

- The content of `dic.DIC.plot_strain` will be replaced with that of `dic.plot_strain` in version 1.3.0. The latter function will be removed. b8633c2

29.3 1.0.1 - 2020-11-19

29.3.1 Added

- Document on describing the versioning scheme we will follow. e74474c
- Added a changelog to the project. b48821b, f6ca9c1

29.3.2 Removed

- The documentation no longer shows the recent git commits. 1fd3a50

29.4 1.0.0 - 2020-11-16

This is the initial release of *CristalX*.

CHAPTER

THIRTY

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