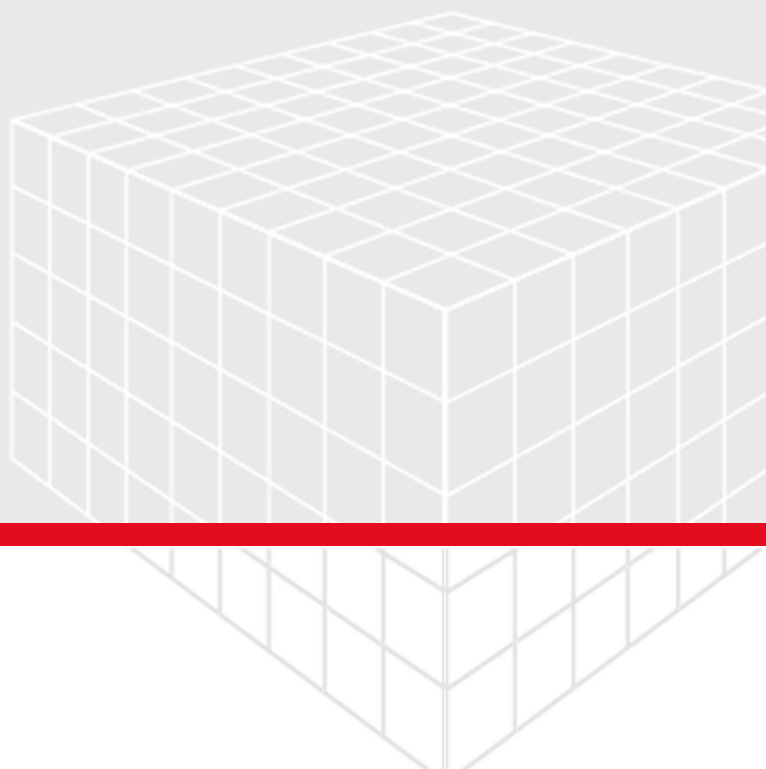


# GrainFind

## User Guide

**GEODICT Release 2026**

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**GEO**DICT

<https://doi.org/10.30423/userguide.geodict>

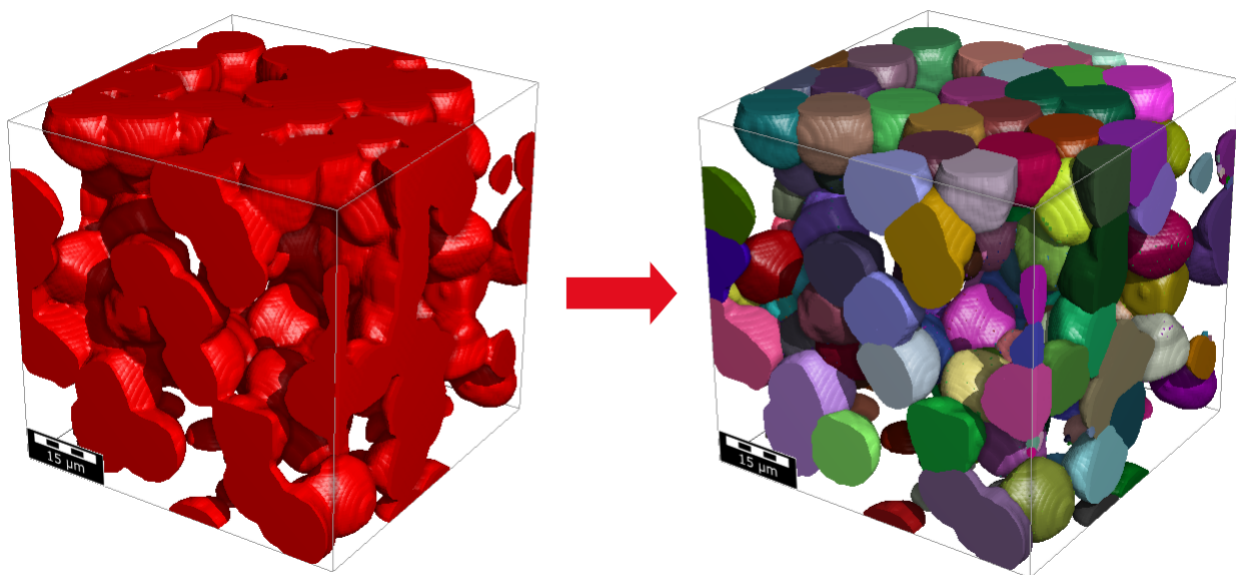
# GrainFind

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# 1 GrainFind

Use the **GrainFind** module to identify individual grains in structures where the grain boundaries are unknown. For each identified grain, the module computes an individual best-fit shape and its orientation in the structure. This makes it possible to perform simulations on the structure that were previously impossible, such as simulations of mechanical properties that depend on grain orientation. Additionally, the structural information can be used with the GrainGeo module to generate similar structures, or digital twins, of the original structure.

Potential applications include identifying grains in battery electrodes in electrochemistry and using information about individual grains to foster a thorough understanding of rock structure in Digital Rock Physics. GrainFind can also characterize particles in particle filtration applications.



Additional to the grain identification, it is also possible to **Identify Binder (AI)** using machine learning technologies. Please note that for this feature a special license is required.

Moreover, the grain size distribution can be estimated through the **Estimate Grain Diameters** command.



## New in GeoDict 2026

- New output option [Save Grain-Network Model as \\*.gad](#)<sup>[28]</sup> in Identify Grains.

## Learn to use GrainFind

- [Identify Grains](#)<sup>[5]</sup>  
Identify individual grains and their geometrical properties.
- [Identify Binder \(AI\)](#)<sup>[66]</sup>  
Separate binder from grains and get a binder distribution over the Z-layers.

### Learn to use GrainFind

- [Estimate Grain Diameters](#)<sup>77</sup>  
Determine grain diameters and separate the grains into different classes.
- [References](#)<sup>92</sup>  
Publications cited in this chapter.



#### Join the conversation

Visit the Community on [GeoDict Forum](#) to be inspired and get answers to top questions.

Find illustrative application examples on the [website](#).

Our tutorials and seminar videos give you a first hands-on experience. They are collected in the [Learning Center](#).

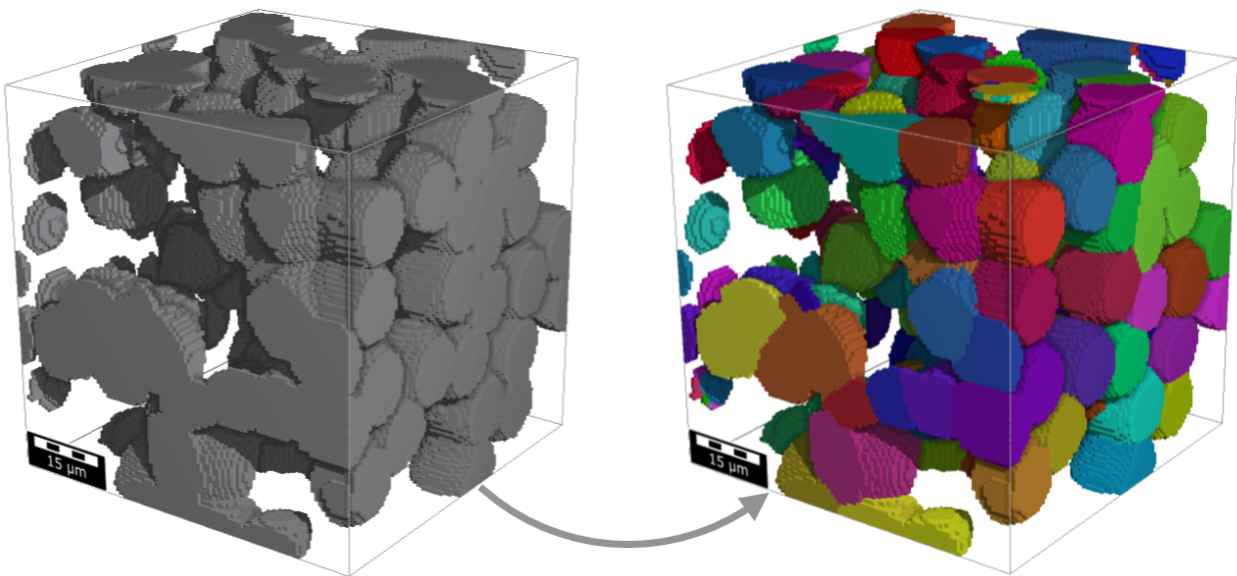
Send your [Support Request](#) to our technical Support.



## 1.1 Identify Grains

With **Identify Grains**, individual grains are identified and analyzed in a given structure. The method introduces a segmentation of the grains, based on a distance transformation, which identifies the number of grains, as well as the grain volume, sphericity, and the orientation of the grains. Based on the statistical properties of the identified grains, a [digital twin of the structure can be created with GrainGeo](#)<sup>[62]</sup>. Find more details about the theory behind **Identify Grains** in the [Theoretical Background](#)<sup>[5]</sup> section.

To successfully identify grains, the parameters for the command must be chosen carefully. The built-in default values cannot be set to deliver the best possible results for all applications. Best practice is to carry out a parameter study for the solver parameters at the beginning of the analysis.



The Identify Grains command:

- [Theoretical Background](#)<sup>[5]</sup>  
Learn more about the theory behind the grain identification.
- [Options](#)<sup>[13]</sup>  
Set the parameters for the identification.
- [Results](#)<sup>[31]</sup>  
View the computed results.
- [Connecting GrainFind analysis results with GrainGeo](#)<sup>[62]</sup>  
Learn how you can use Identify Grains results to generate digital twins.

### 1.1.1 Theoretical Background

The grain identification process in GrainFind is mainly based on the [Watershed Algorithm](#)<sup>[7]</sup> (WA, [https://en.wikipedia.org/wiki/Watershed\\_\(image\\_processing\)](https://en.wikipedia.org/wiki/Watershed_(image_processing))) that is widely used for the segmentation of image data. The challenge of identifying individual grains in a connected

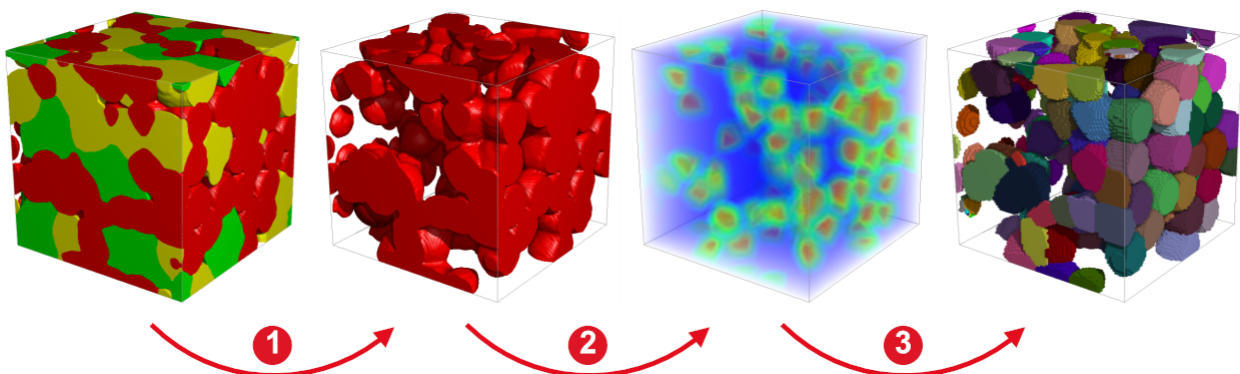
structure can be performed through a segmentation of the structure. The algorithm for the grain identification consists of the following steps:

1. Converting the image into a distance map using the Euclidean Distance Transform (EDT).
2. Identifying local maxima in the distance map and converting them to grain seeds as starting point for the WA.
3. Identifying individual grains by a grain-border determination through the WA.
4. Post-processing of the identified grains.
  - a. Handling of grain fragments
  - b. Handling of boundary grains

Only the parameterization of the watershed transform algorithm (choosing a [minimum grain diameter](#)<sup>[15]</sup>) and the post-processing ([reconnection of grain fragments](#)<sup>[19]</sup>, [boundary grain handling](#)<sup>[22]</sup>, etc.) require user input. The complexity of the algorithm – such as the EDT - is hidden “under the hood”.

The main steps to run the watershed algorithm for grain identification are:

1. Select the material to be analyzed
2. On the chosen material, the EDT is carried out as a preparation for the watershed transform
3. The watershed transform is conducted based on the EDT.



In many cases, the result of the watershed transform is enough to identify the grains. Otherwise, further steps are required.

### Understand the Theory behind Identify Grains

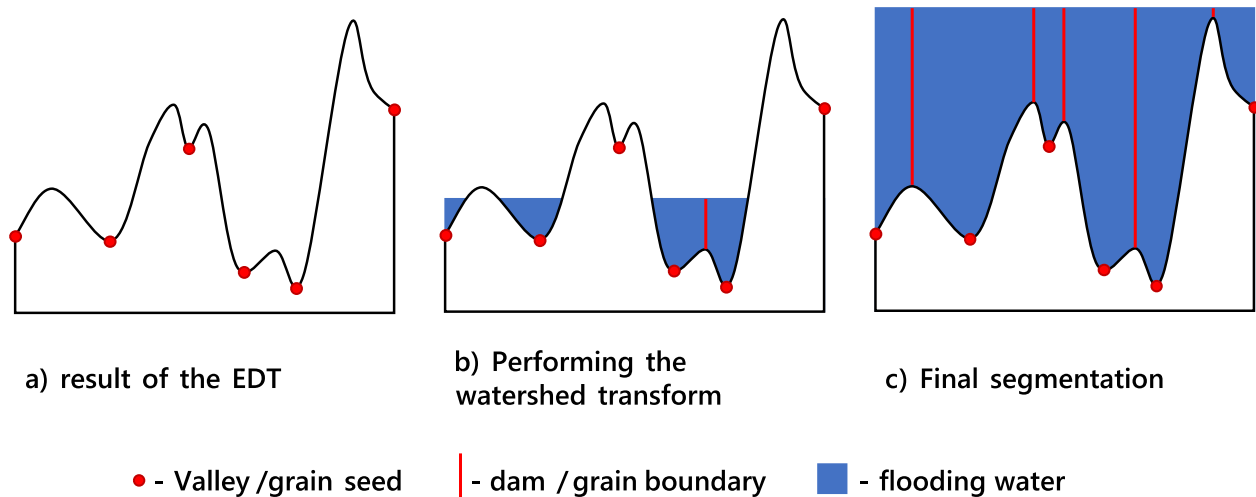
- [Watershed Algorithm](#)<sup>[7]</sup>  
Learn about the concept of the Watershed Algorithm.
- [Sphericity parameters](#)<sup>[7]</sup>  
Learn how the Sheppard and the Krumbein sphericities are computed.
- [Results of Identify Grains](#)<sup>[8]</sup>  
Get an overview of the computed scalar values.

## Watershed Algorithm

The watershed algorithm (WA) is a segmentation algorithm commonly used in image processing. The WA is based on the Euclidean Distance Transform (EDT). Grain seeds are placed in the local maxima of the EDT, and in those seeds, grains start to “grow”. In the growing process, grain boundaries are formed as soon as grains touch.

The concept behind the watershed algorithm transform can be understood more easily in a 2D example. In this representation, the EDT can be regarded as a topographical relief where high values represent valleys and low values represent peaks. This topography is continuously “flooded with water”, starting from the deepest valleys. As soon as the water from neighboring valley begins to mix, a dam is created (corresponding to the grain boundary). The result is a topography with water-filled valleys and dams that separate them. The identified valleys represent the grains and the dams that separate them denote the grain boundaries.

In the figure below, the progression of the watershed algorithm is illustrated. On the left side, the topographical relief corresponding to the EDT is shown where the grain seeds (valley bottom) are marked in red. This topography is successively flooded with water, and dams are formed between adjacent valleys.



Known information about the grain space, i.e., the minimal grain diameter, can be used to adjust the results of the Watershed Algorithm.

## Sphericity parameters

While there are many definitions of sphericity, the two sphericity indices given in the GrainFind output are those defined by [Sheppard \(2006\)](#)<sup>[92]</sup> (optional) and [Krumbein \(1941\)](#)<sup>[92]</sup>.

### Sheppard Sphericity

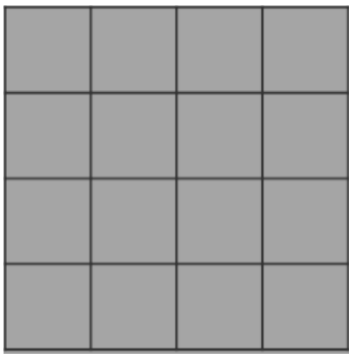
Based on Sheppard, the sphericity  $P_s$  of a grain is defined as the ratio of the inner radius  $R_i$  of a grain to its equivalent radius  $R_e$ .

$$P_S = \frac{R_i}{R_e}$$

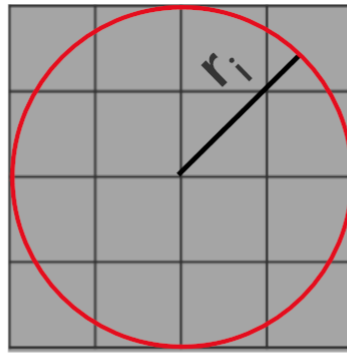
(1) Sheppard Sphericity

The *equivalent radius*  $R_e$  is the radius of a sphere with the same volume as the grain. The *inner radius*  $R_i$  is the radius of the largest sphere which fits into the grain. The inner radius can be computed based on the Euclidean Distance Transform (EDT).

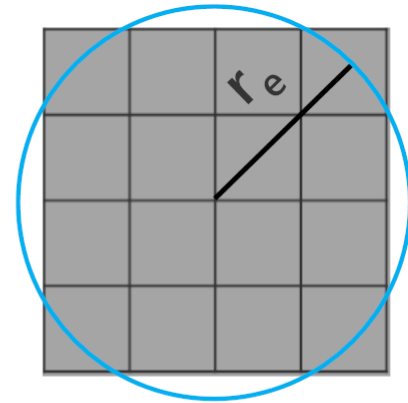
Sphericity values range between 0 and 1. The more the grain resembles a sphere, the higher is its sphericity value. A value of 1 marks a perfect spherical grain. In the example below, the sphericity of the square shaped grain is  $2/2.26 = 0.88$ .



Grain geometry



Inner radius  
 $r_i = 2$  voxel



Equivalent radius  
 $r_e = 2.26$  voxel

## Krumbein Sphericity

To calculate sphericity based on Krumbein, three principal axes ( $a$ ,  $b$ ,  $c$ ) of the grains fit-shape are determined. The Krumbein sphericity  $P_K$  is then calculated using the length of these axes as

$$P_K = \sqrt[3]{\frac{bc}{a^2}}$$

(2) Krumbein Sphericity

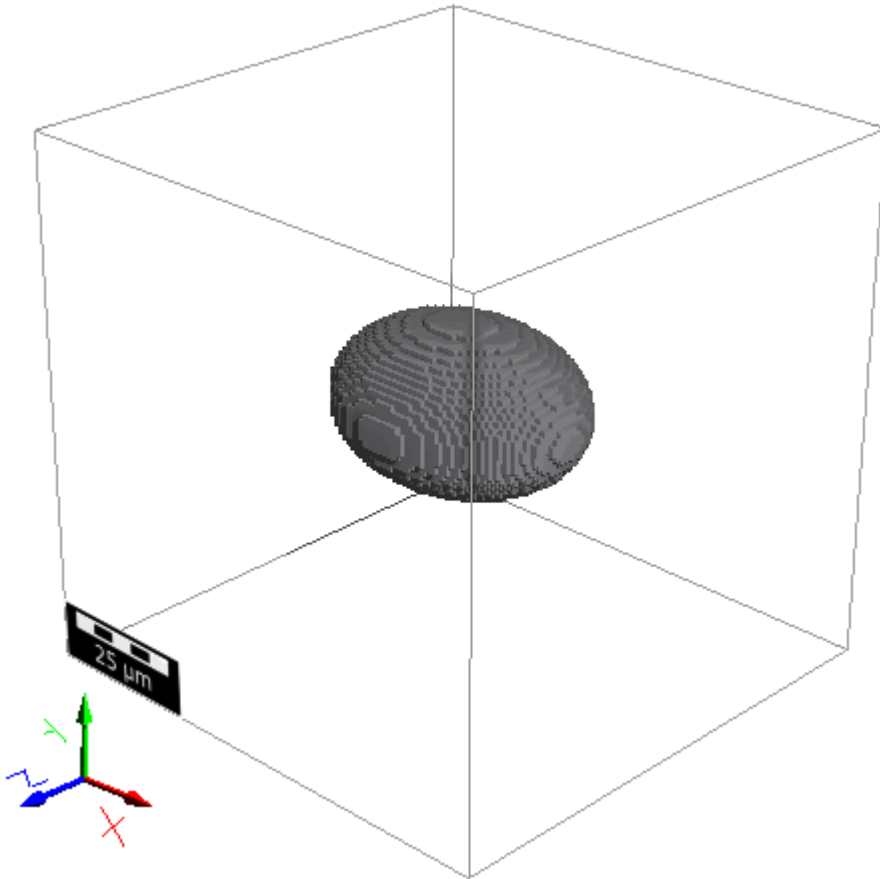
where  $a$  is length of the longest axis, while  $b$  and  $c$  are the lengths of the two shorter axes.

Analogously to the Sheppard sphericity, the values for the Krumbein sphericity range between 0 and 1, with 1 characterizing perfectly spherical grains.

## Results of Identify Grains

The parameters of the [Grain-Fit Shapes](#)<sup>[23]</sup> are used to compute further scalar values of the grains. We show the parameters graphically with the help of a simple structure, that contains

one ellipsoidal grain with dimensions 50  $\mu\text{m}$  x 30  $\mu\text{m}$  x 40  $\mu\text{m}$  in the center of an empty domain with voxel length 1  $\mu\text{m}$ .



The three Grain-Fit Shapes are all described by three values. For the **Ellipsoids** three diameters are needed, for the **Short Ellipsoidal Fibers** two diameters and the length of the fiber are required, and the **Box** is described by the three side lengths.

In the following, we set

- $a$  to be the length of the longest of the three values,
- $b$  to be the length of the medium value,
- $c$  to be the length of the shortest value.

## Computed Scalar Values

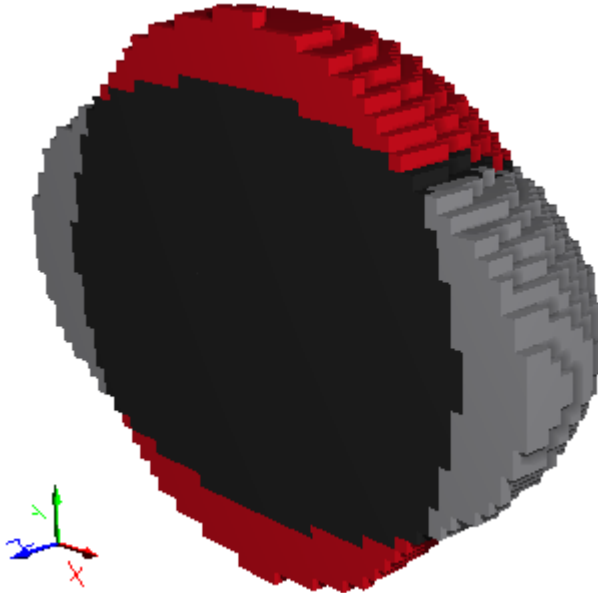
- **Volume:** The volume of the grain is simply determined by the number of voxels the grain contains. To get a volume in metrical units, it is multiplied by the cubed voxel length:

$$V = \#(\text{pore voxels}) * (\text{voxel length})^3$$

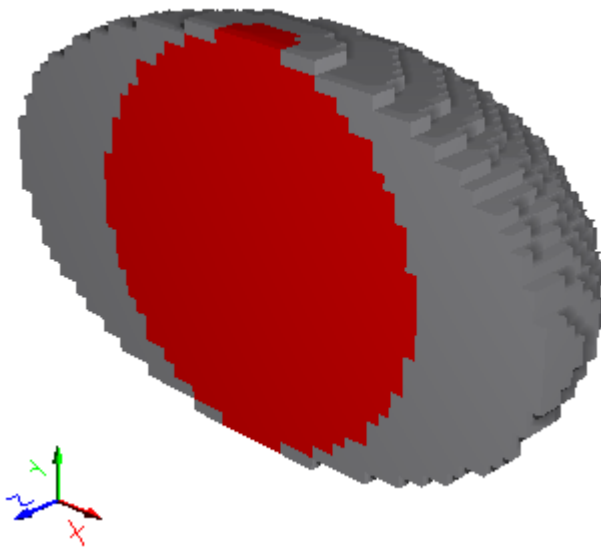
(3) Volume

In the example, the grain consists of 31384 voxels, so that the grain volume is  $31384 \mu\text{m}^3$ .

- **Equivalent Diameter:** The equivalent diameter is the diameter of the sphere which has the same volume as the grain. Below, the volume equivalent sphere for the example (which has a diameter of  $39 \mu\text{m}$ ) is shown in red and was added to the initial ellipsoid using the Add command of LayerGeo. The black part represents the overlap.



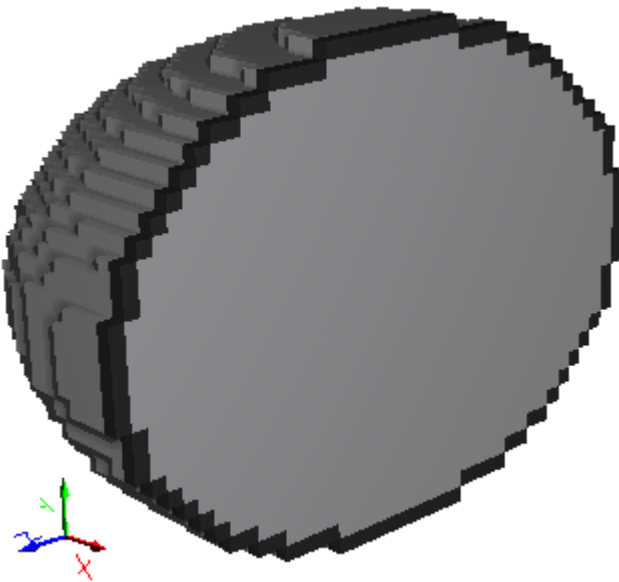
- **Inner Diameter:** The inner diameter is the diameter of the largest sphere that can be inscribed into the grain. Below, the inscribed sphere for the example, which has a diameter of  $30 \mu\text{m}$ , is shown in red and was added to the ellipsoid structure with LayerGeo.



**Important!** Note that the Inner Diameter is only calculated if the option **Save Inscribed-Sphere Diameters and Sheppard Sphericities** was checked in the [Output](#)

[Options](#) of the grain-identification options.

- **Shortest Fit Diameter:** This is the shortest diameter ( $c$ ) of the shape fitted into the grain. For the example, the shortest diameter is 30  $\mu\text{m}$ .
- **Intermediate Fit Diameter:** This is the intermediate diameter ( $b$ ) of the shape fitted into the grain. For the example, the intermediate diameter is 40  $\mu\text{m}$ .
- **Longest Fit Diameter:** This is the longest diameter ( $a$ ) of the shape fitted into the grain. For the example, the longest diameter is 50  $\mu\text{m}$ .
- **Perimeter:** The computed perimeter is the shortest perimeter around the shape fitted into the grain. As an ellipsoid is defined by three diameters, the perimeter is computed as the perimeter of the ellipse formed from the two smallest of those three diameters. For the example structure the perimeter would be the length of the black line, which is 110  $\mu\text{m}$ .



- **Krumbein Sphericity:** The Krumbein Sphericity is a measure for the sphericity of the grain, based on the three principal axes ( $a$ ,  $b$ ,  $c$ ) of the fitted shape. If the Krumbein Sphericity is close to 1, the shape is nearly a sphere. In the example above, the Krumbein Sphericity is 0.78, which means that the diameters differ much.

$$P_K = \sqrt[3]{\frac{bc}{a^2}}$$

(4) Krumbein  
Sphericity

- **Sheppard Sphericity:** The Sheppard Sphericity is defined as the diameter of the inscribed sphere divided by the diameter of the volume-equivalent sphere. For the example, the Sheppard Sphericity of the grain is 0.76.



**Important!** Note that the Sheppard Sphericity is only calculated if the option **Save Inscribed-Sphere Diameters and Sheppard Sphericities** was checked in the [Output Options](#) of the grain-identification options.

- **Aspect Ratio:** The shape fitted into the grain is defined by three diameters. The aspect ratio is computed as

$$\text{aspect ratio} = \frac{c}{a} \quad (5) \text{ Aspect Ratio}$$

where the shortest diameter  $c$  is divided by the largest diameter  $a$ , which is 0.6 for the example.

- **Surface Area:** The surface of the grains is estimated by an algorithm based on MatDict's **Estimate Surface Area** command (see also J. Ohser, F. Mücklich). The Area (or Surface) Probability is defined by computing the surface area of each segmented grain (using the same algorithm as in MatDict's Estimate Surface Area command) and then weighting the grains by that value. The computed surface area does also include the surface between different grains, not only the area between pore and solid material. For the example, the surface is 4985  $\mu\text{m}^2$ .
- **Surface-to-Volume Ratio:** The estimated surface area of the grain is divided by the volume of the grain. For the example a value of 0.159 is obtained.
- **Surface Smoothness:** This is the surface of the fitted shape divided by the estimated surface of the grain. Usually, the estimated grain surface is larger than the surface of the fitted shape. Hence, the surface smoothness is usually below 1. Only if the shape of the grain is very similar to the fitted shape, then the surface estimation might be a little smaller than the surface of the fitted shape. The latter is the case in the example, where the surface smoothness is 1.002.
- **Cut-Surface Ratio:** The Cut-Surface Ratio measures how much of the grain surface is part of the domain boundary. The interface of the grain with the domain boundary is the **Cut Surface**, which is then divided by the remaining surface of the grain. Thus, it is a measure for the quality of boundary grains. For example, a Cut-Surface Ratio of 1 means that the interface of the grain with the domain boundary is as large as the remaining surface of the grain. In the example, the grain has no boundary contacts and thus the cut surface area and the cut-surface ratio are both 0.



**Important!** Note that the domain boundaries, that were set to be periodic, do not contribute to the interface of the grain with the domain boundary. Particularly, if all domain boundaries are set to be periodic, the cut-surface ratio will always be zero. Also, if [Remove Grain Fragments at Domain Boundary](#) was activated, then the cut surface ratio is zero, too, because there will be no grains left that have an interface with the domain boundaries.

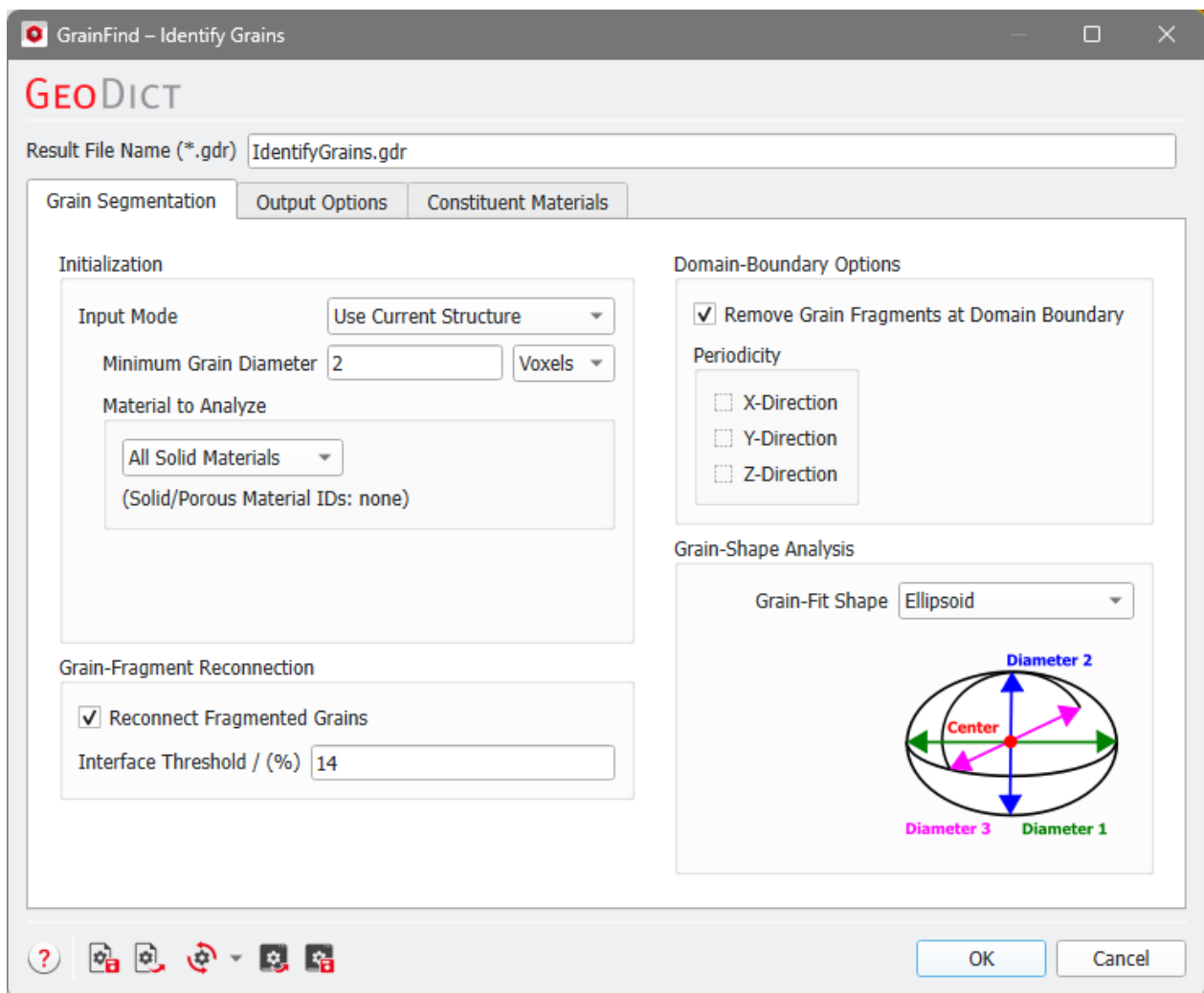


- **Mass:** If a density is assigned to the [analyzed material](#), each grain has a mass which can be calculated from its volume.
- **Moment of Inertia:** It depends on the mass distribution of the grains and is only computed if a density is assigned.
- **Coordination Number:** This is the number of contacts of a grain to other grains. In the example the coordination number is 0 as only one grain exists.

## 1.1.2 Options

The **Identify Grains** dialog opens when clicking the **Edit...** button and includes the **Grain Segmentation** tab, the **Output Options** tab, and the **Constituent Materials** tab.

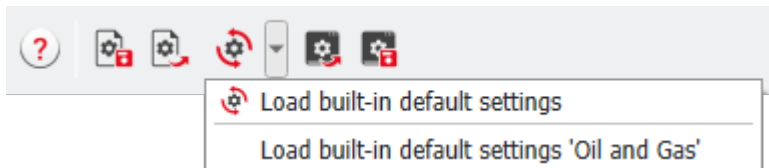
At the top of the dialog, enter the **Result File Name**. The result file is saved in the chosen project folder (**File** → **Choose Project Folder** in the menu bar).



The built-in default icon comes with a selection of different presets. Clicking on the little arrow shows several additional preset options.

The usual built-in default settings will load the settings according to the current GeoDict edition. You can change the current GeoDict edition from the **Settings menu** as described in

the Graphical User Interface chapter.



In **GrainFind - Identify Grains** find edition-specific presets for the **Standard Edition** and the **Oil and Gas Edition**.

In the Oil and Gas edition, the [Interface Threshold](#)<sup>[19]</sup> is increased from 14% to 80%, because the grains in rocks tend to share large interfaces. With a larger interface threshold, they are not merged.

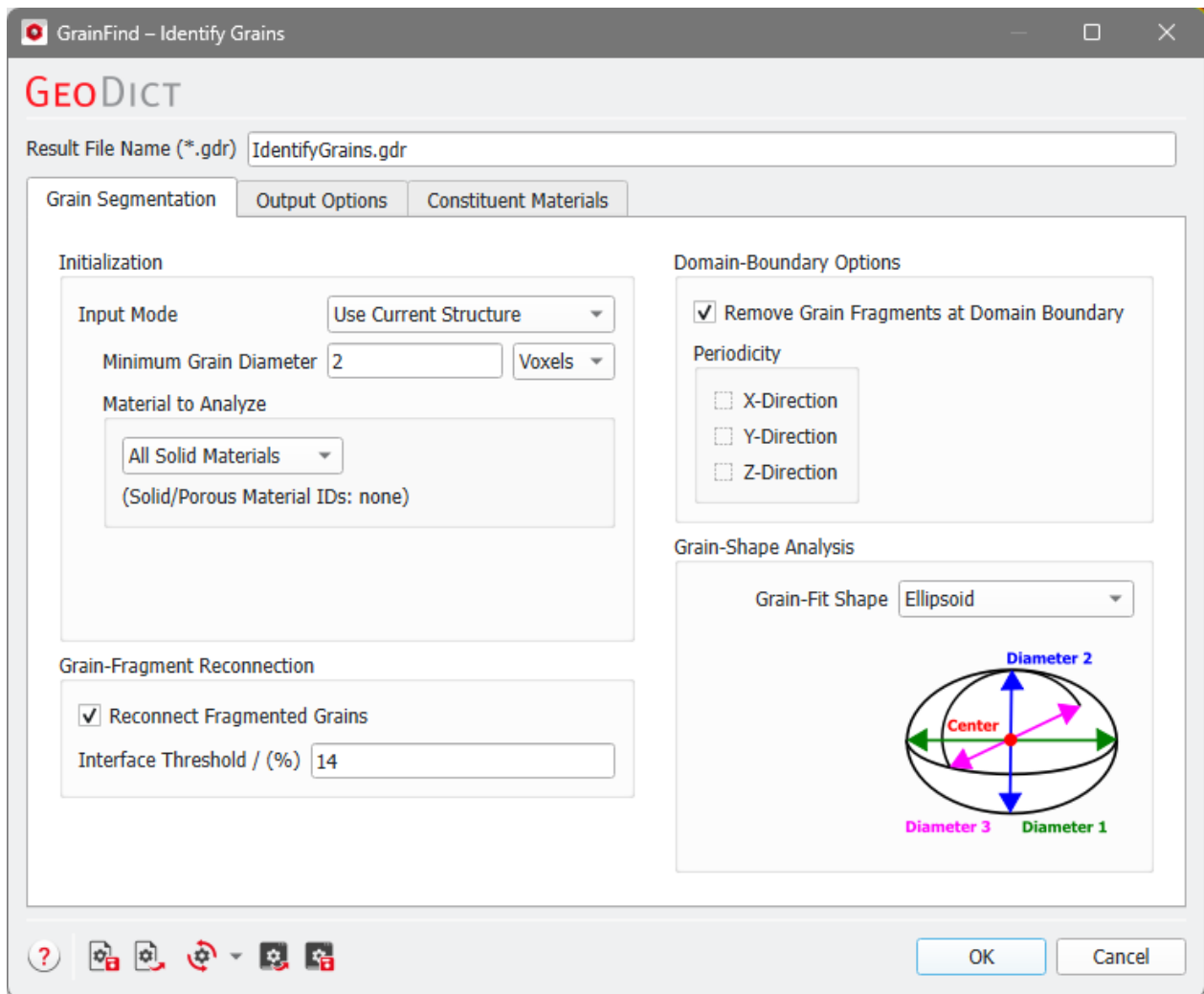
In the [Output Options](#)<sup>[28]</sup> tab, additional files are saved: **Save Grain-Size Distribution (Volume-Equivalent Diameter) as \*.gsd** and **Save Inscribed-Sphere Diameters and Sheppard Sphericities**.

Identify Grains Options:

- [Grain Segmentation](#)<sup>[14]</sup>  
Set the parameters for the identification.
- [Output Options](#)<sup>[28]</sup>  
Select which additional files should be saved.
- [Constituent Materials](#)<sup>[30]</sup>  
Enter the density of the materials in the structure.

## Grain Segmentation

The parameters under the **Grain Segmentation** tab are grouped into four panels: **Initialization**, **Grain-Fragment Reconnection**, **Domain-Boundary Options**, and **Grain-Shape Analysis**.

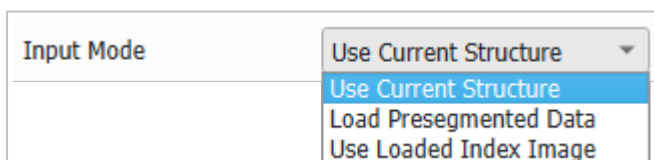


The Grain Segmentation tab:

- [Initialization](#)<sup>15</sup>  
Select the Input for the analysis.
- [Grain-Fragment Reconnection](#)<sup>19</sup>  
Select whether grain fragments should be merged before analyzing them.
- [Domain-Boundary Options](#)<sup>22</sup>  
Choose if grains touching the boundary should be removed before the analysis.
- [Grain Shape Analysis](#)<sup>23</sup>  
Select which shape should be fitted to the grains.

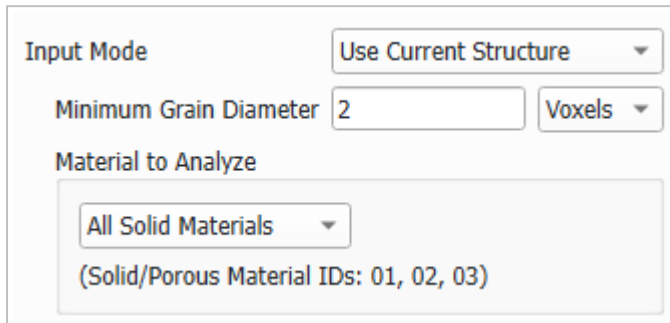
## Initialization

From the pull-down menu, select what should be the basis for the analysis.



## Use Current Structure

Select **Use Current Structure** to use the structure currently in memory. Below, enter the **Minimum Grain Diameter**, which defines the minimum size an individual grain must have for the analysis. The unit of **Minimum Grain Diameter** can be selected as **Voxels** or **m**.



The screenshot shows a software interface with the following elements:

- Input Mode:** A dropdown menu set to "Use Current Structure".
- Minimum Grain Diameter:** A text input field containing the value "2".
- Unit:** A dropdown menu set to "Voxels".
- Material to Analyze:** A dropdown menu set to "All Solid Materials".
- Material IDs:** A text label below the dropdown showing "(Solid/Porous Material IDs: 01, 02, 03)".

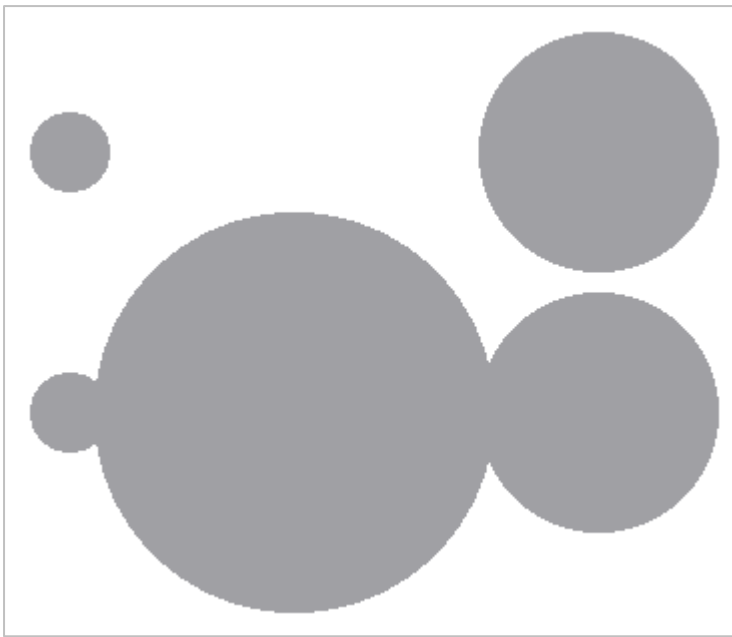


**Note!** The initialization of the grain segmentation (the watershed algorithm) might be time consuming for large structures. Thus, the options **Load Presegmented Data** or **Use Loaded Index Image** are useful when performing parameter studies with GrainFind – Identify Grains, where the initialization is kept unchanged while other parameters are varied.

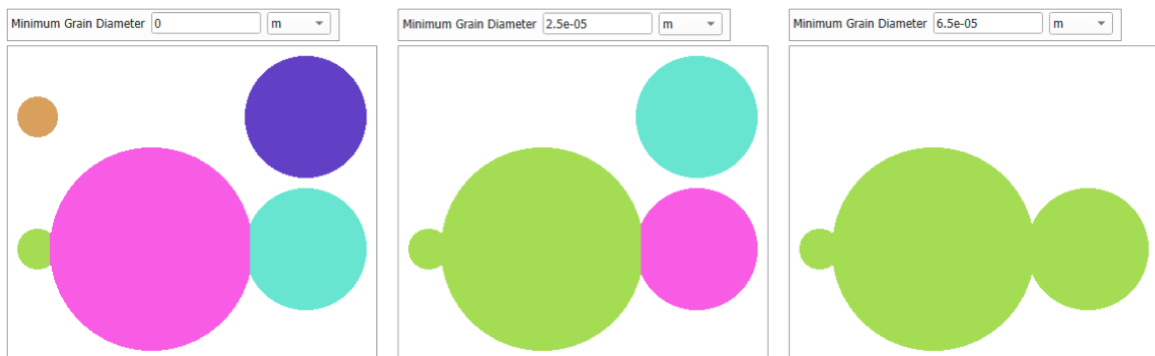
### ✓ Minimum Grain Diameter

This parameter determines which grains to keep and which grains to neglect or combine with others. If smaller grains exist which are connected to larger grains, the grains are combined and count as one grain. Single grains with a diameter smaller than the **Minimum Grain Diameter** are neglected.

In the next figure, the effect of the choice for **Minimum Grain Diameter** in the initialization step (of the watershed algorithm) is illustrated using the visualization of \*.g32 files. The original structure contains spherical grains with diameters 100  $\mu\text{m}$ , 60  $\mu\text{m}$ , and 20  $\mu\text{m}$ , and some grains touch so they share an interface.

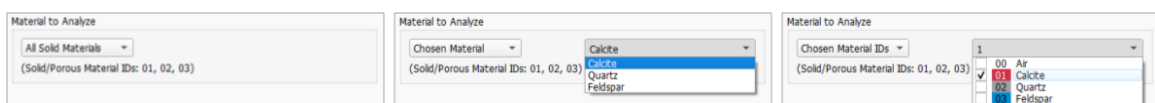


With **Minimum Grain Diameter** set to zero, all five grains are identified as single grains. When setting the **Minimum Grain Diameter** to 25  $\mu\text{m}$ , the single 20  $\mu\text{m}$  grain is neglected, while the 20  $\mu\text{m}$  grain connected to the larger grain is merged and so only three grains are identified. Analogously, for a choice of 65  $\mu\text{m}$ , only one single merged grain is detected while the smaller grains are neglected.



## ✓ Material To Analyze

Under **Material to Analyze**, define the part of the structure to be considered in the analysis. Either the complete structure can be analyzed (**All Solid Materials**), an individual material can be selected (**Chosen Material**) or a choice of Material IDs can be made (**Chosen Material IDs**). If the selection includes multiple Material IDs they are combined and analyzed as one single material.



The specific materials can be selected in the [Constituent Materials](#) tab. The material info is used to compute the grain mass and the moment of inertia and is contained in the Map tab of the Result Viewer.

## Load Presegmented Data

If you want to import already segmented data from an index-image file (\*.g32 or \*.leS) select **Load Presegmented Data**. In this case **Browse** for the file you want to load below.

|                                  |                          |           |
|----------------------------------|--------------------------|-----------|
| Input Mode                       | Load Presegmented Data ▼ |           |
| Grain-Index Image (*.g32; *.leS) | Grains.g32               | Browse... |
| Pore Material                    | Air...                   |           |
| Grain Material                   | Calcite (Solid)...       |           |



**Know how!** For **Load Presegmented Data**, the difference between the \*.g32 and \*.leS formats is that \*.g32 is a binary format, which produces comparatively smaller files but is not human readable, and \*.leS is an ASCII-format which is human readable, but produces larger files. Furthermore, loading a \*.g32 file into GeoDict is much faster than loading a \*.leS file. Therefore, we recommend to use the \*.g32 option.

For the presegmented data you have to define the **Grain Material** and the surrounding **Pore Material** by clicking on the corresponding buttons and choosing the material. For this Input Mode the Constituent Materials tab is not available and thus grayed-out.

## Use Loaded Index Image

Alternatively, you can use the currently loaded \*.g32 file by selecting **Use Loaded Index Image**. Then, the name of the \*.g32 file will be displayed below or it is shown that no Index Image is loaded.

|                           |                          |  |
|---------------------------|--------------------------|--|
| Input Mode                | Use Loaded Index Image ▼ |  |
| Grain-Index Image (*.g32) | Grains.g32               |  |
| Pore Material             | Air...                   |  |
| Grain Material            | Calcite (Solid)...       |  |

|                           |                          |  |
|---------------------------|--------------------------|--|
| Input Mode                | Use Loaded Index Image ▼ |  |
| Grain-Index Image (*.g32) | <No Index Image Loaded>  |  |
| Pore Material             | Air...                   |  |
| Grain Material            | Calcite (Solid)...       |  |

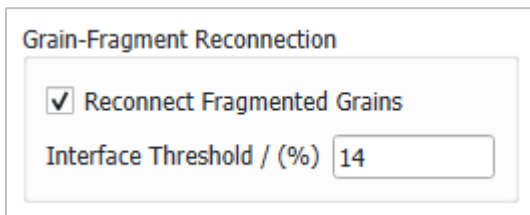


**Know how!** Check **Use Loaded Index Image** if the presegmented data is already loaded into GeoDict. In that case, it can be used directly and it is not necessary to load it again.

When choosing the loaded index image as input you have to define the **Grain Material** and the surrounding **Pore Material** by clicking on the corresponding buttons. For this Input Mode the Constituent Materials tab is not available and thus grayed-out.

## Grain-Fragment Reconnection

In some cases (e.g., for complex grain shapes), the watershed algorithm in step 1 tends to over-segment the grains. This means, that sometimes grains are identified as multiple grains (**Fragmented Grains**) when, in fact, they may be a single grain with a complex shape. Activate the checkbox **Reconnect Fragmented Grains** to merge connected grains depending on the value chosen for **Interface Threshold**.



Grain-Fragment Reconnection

☒ Reconnect Fragmented Grains

Interface Threshold / (%) 14

The probability that two grain fragments belong to the same grain is measured with the interface ratio. This interface ratio compares the interface area of two touching grain fragments with the surface area of the grain fragment with the smaller surface.

$$\text{interface ratio} = \frac{\text{interface of touching fragments}}{\min(\text{surface of object 1, surface of object 2})} \quad \text{(6) Interface Ratio}$$

For the computation of the interface ratio, the grain surfaces and interfaces need to be computed. The surface area estimation is based on Estimate Surface Area from MatDict (see also [J. Ohser, F. Mücklich](#)<sup>[92]</sup>).

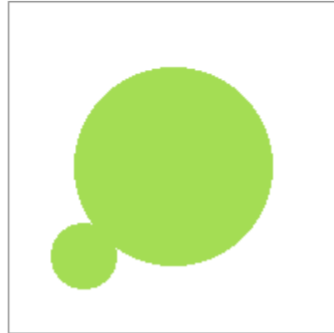
If the *interface ratio* is larger than the percentage chosen for the **Interface Threshold**, the two grain fragments are merged and only one grain is reported as identified.

For example, if the **Interface Threshold** is set to the default **14**, the shared interface of two grains must be larger than 14% of the total surface of the smaller grain for the two grains to be merged. The next example shows two structures in which a big grain and a small grain touch with different interface surface between them. Depending on the surface of the interface, the value of **Interface Threshold** at which the two grains stop being reconnected and are detected as two (instead of only one) is very different.

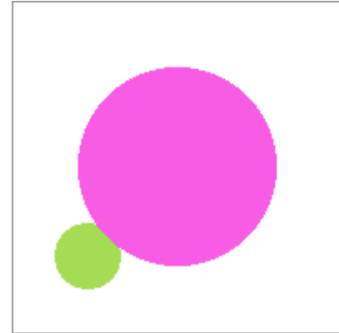
When the two grains share a small interface, a low value of **Interface Threshold** (7) is enough to separate the two grains. When the two grains instead share a large interface, a higher value of **Interface Threshold** (15) is needed to separate the two grains. The default value of **Interface Threshold** (14) would be appropriate to separate the two grains sharing a small interface, but not the grains sharing a large interface.

### Small Interface

Interface Threshold / (%)

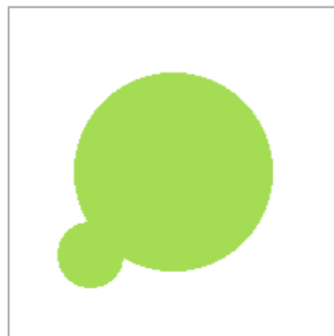
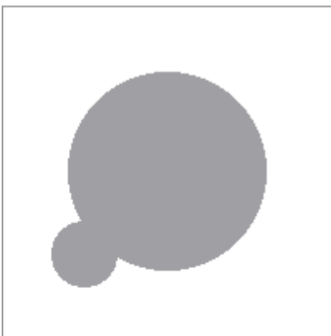


Interface Threshold / (%)

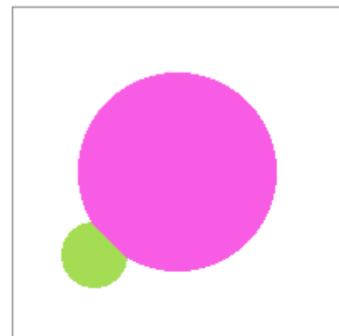


### Large Interface

Interface Threshold / (%)



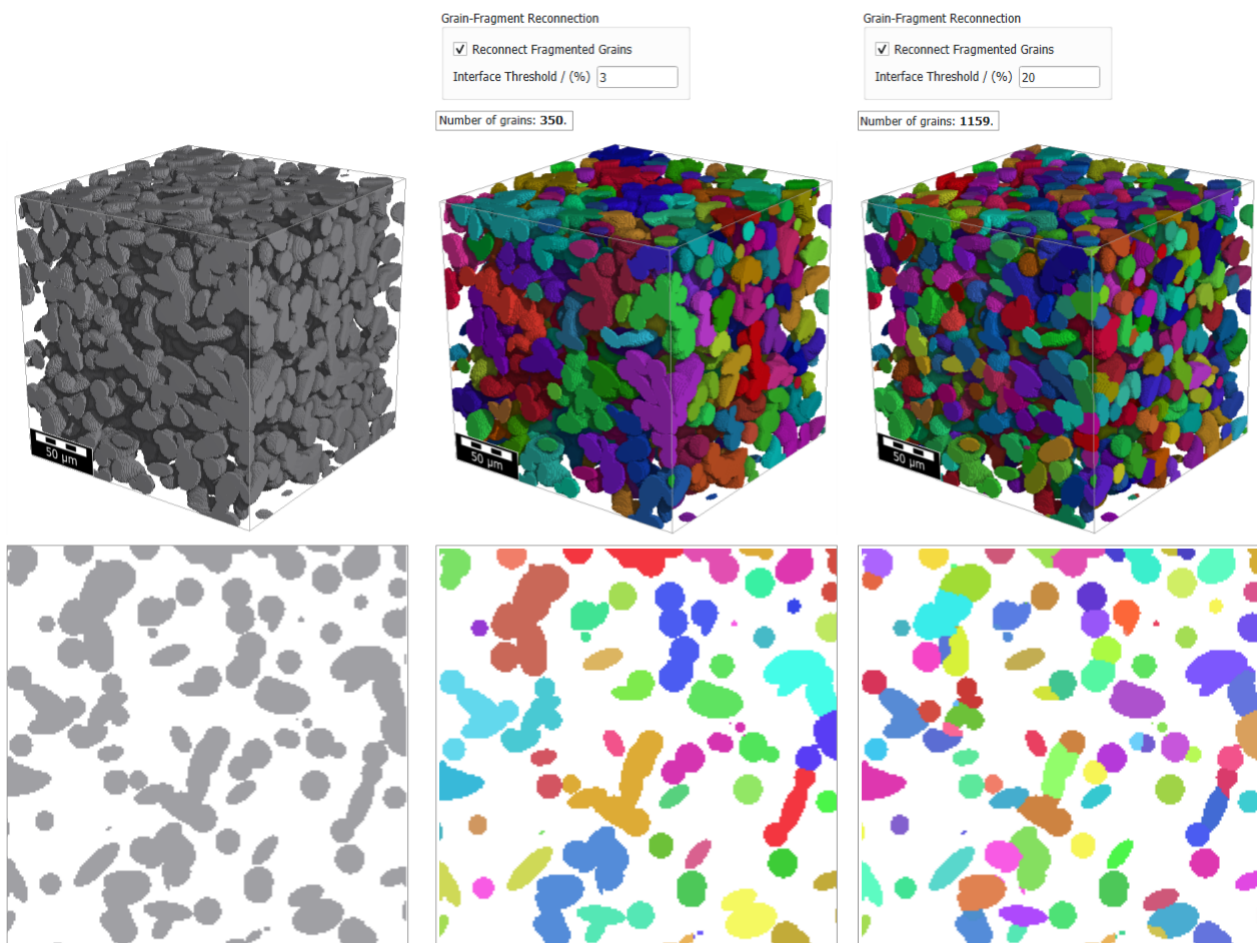
Interface Threshold / (%)



The value for the **Interface Threshold** must be chosen carefully depending on the size of grains in the structure. With a low threshold, more grains are merged (and less grains are identified).

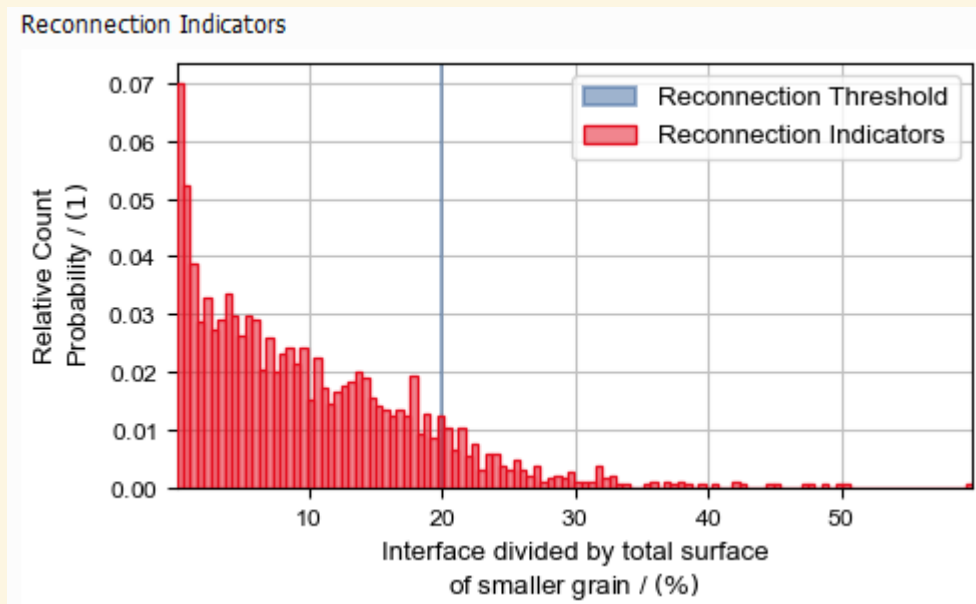
In the figures below (using the visualization of \*.g32 files), observe the effect of different choices for the **Interface Threshold**. For this example, the **Minimal Grain Diameter** is always 2  $\mu\text{m}$ . With a very low Interface Threshold value of 3%, several large and complex grains are identified in the structure that may not correspond to single grains. With a value of 20%, the grains may be over-segmented with many small grains being detected.





**Know how!** Use the **Reconnection Indicators** histogram under the **Results** → **Plots** subtab in the Result Viewer to find an appropriate **Interface Threshold** for the structure. As described above, the ratio of the interface area between two grains and the total surface of the smaller grain is computed. This ratio of all grain interfaces and the selected **Interface Threshold** are plotted in the **Reconnection Indicator** histogram.

The following ratio histogram belongs to the example structure and the interface threshold of 20% is marked in blue. Observe that many grain interfaces have a ratio smaller than 20%, thus only few grains are merged together.

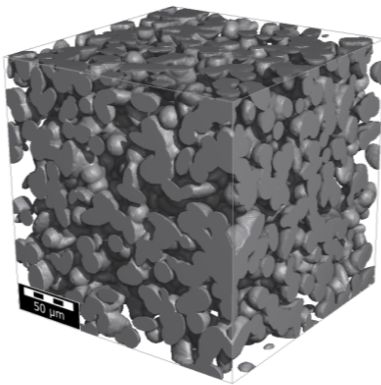


## Domain-Boundary Options

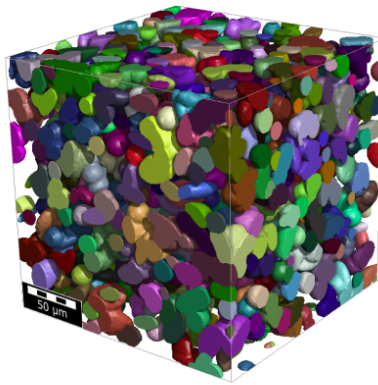
In the **Domain-Boundary Options** panel, the handling of boundary grains is defined.

The screenshot shows the "Domain-Boundary Options" panel. It includes a checked checkbox labeled "Remove Grain Fragments at Domain Boundary". Below this is a section titled "Periodicity" containing three unchecked checkboxes: "X-Direction", "Y-Direction", and "Z-Direction".

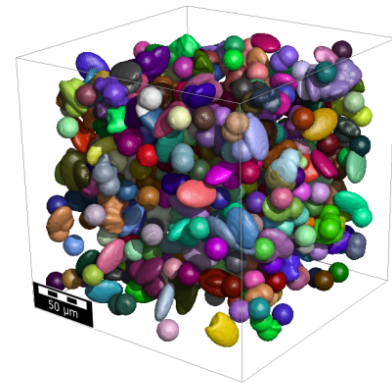
When **Remove Grain Fragments at Domain Boundary** is checked, all grains touching the domain boundary, after the initialization and the grain-fragment reconnection are done, are removed. This might improve the results, since boundary grains which do not lie entirely within the domain might lead to incorrect grain shape estimates. The visualizations below are loaded from the Result Viewer of the \*.gdr result file (under the [Grain Visualization tab](#)<sup>58</sup>).



Grain space to analyze



Grain space after Grain Reconnection



Grain space after grain fragment removal at domain boundaries

When **Remove Grain Fragments at Domain Boundary** is unchecked, the **Periodicity** options become available. By checking the X-, Y-, or Z-Direction checkboxes, the grain space is treated as periodic in the chosen direction(s) before the grain segmentation. Otherwise, when **Periodicity** is not chosen in a direction, the structure is assumed to end at the domain boundary.

**Domain-Boundary Options**

☐ Remove Grain Fragments at Domain Boundary

**Periodicity**

☒ X-Direction  
☒ Y-Direction  
☒ Z-Direction



**Important!** Periodicity should only be chosen for real periodic structures, otherwise it might lead to strange results (with grains which are treated as connected but are distant from each other in reality).

## Grain Shape Analysis

After the grain identification step (defined by the parameters under **Initialization**, **Grain-Fragment Reconnection**, and **Domain-Boundary Options**), the shape of the grains is analyzed. This analysis is done by fitting one selected object type into the identified grains. Choose the **Grain-Fit Shape** that fits best to the grain shapes appearing in your structure.

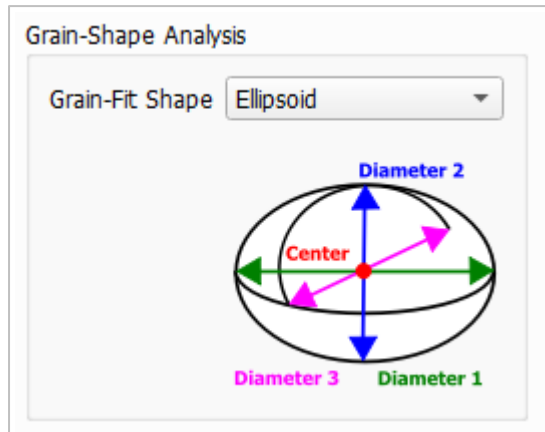
**Grain-Shape Analysis**

Grain-Fit Shape

Ellipsoid  
**Ellipsoid**  
 Short Elliptical Fiber  
 Box

✓ Fit Shape Ellipsoid

An ellipsoid can be fitted to the identified grains.



To define such an ellipsoid, a center point and three diameters are needed.

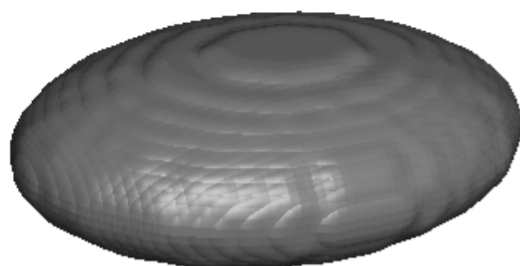
In the following, we set

- $a$  to be the length of the longest of the three diameters,
- $b$  to be the length of the medium diameter,
- $c$  to be the length of the shortest diameter.

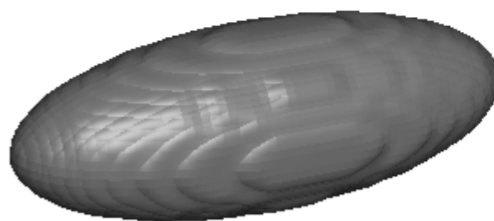
A pair of diameters is similar if its size ratio (the smaller diameter is divided by the larger diameter) is larger than 0.875. Two diameters differ, if their ratio is smaller than 0.875.

Four shapes for the ellipsoids can be fitted into the grain:

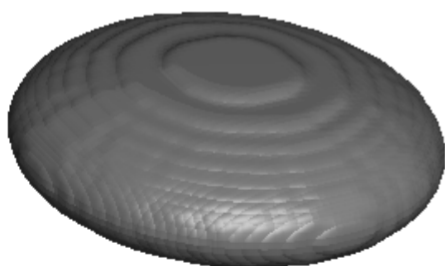
- An ellipsoid is formed as a **Flat Bar**, if all three diameters  $a$ ,  $b$ , and  $c$  differ much from each other.
- A **Prolate Spheroid** has one bigger diameter,  $a$ , and the two smaller diameters,  $b$  and  $c$ , are similar to each other. Its shape is similar to a cigar.
- The two bigger diameters ( $a$  and  $b$ ) of an **Oblate Spheroid** are similar. Thus, it can be compared to a disk.
- For a **Sphere** all three diameters  $a$ ,  $b$ , and  $c$  are similar.



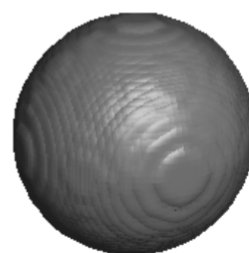
Flat Bar



Prolate Spheroid



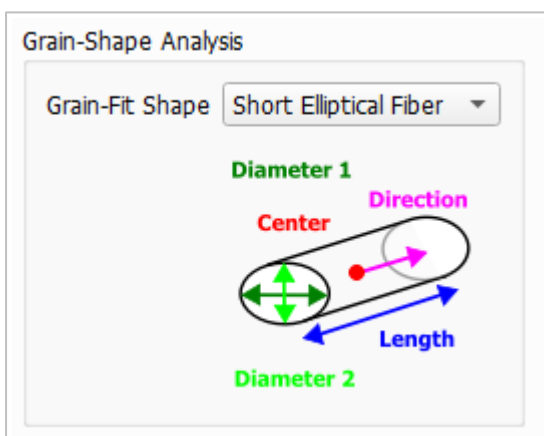
Oblate Spheroid



Sphere

### ✓ Fit Shape Short Elliptical Fiber

Select to fit a short elliptical fiber into the grains.



To define such a **Short Elliptical Fiber**, a center point, two diameters and a length are needed.

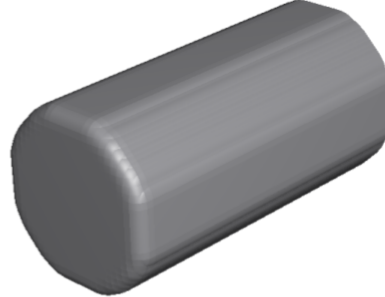
Four shapes for the short elliptical fibers can be fitted into the grain:

- A fiber is **Elliptical**, if the two diameters are different.
- It is **Circular**, if the two diameters are the same.

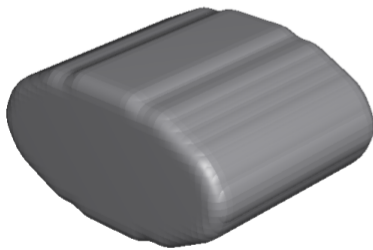
- An **Elliptical Stub** has at least one diameter larger than the length and the diameters are different.
- The **Circular Stub** is the same as above, but with equal diameters.



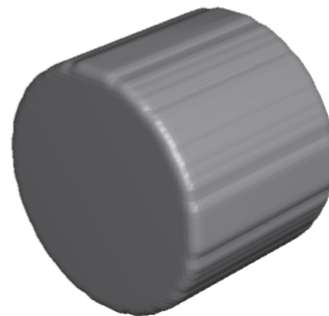
Elliptical



Circular



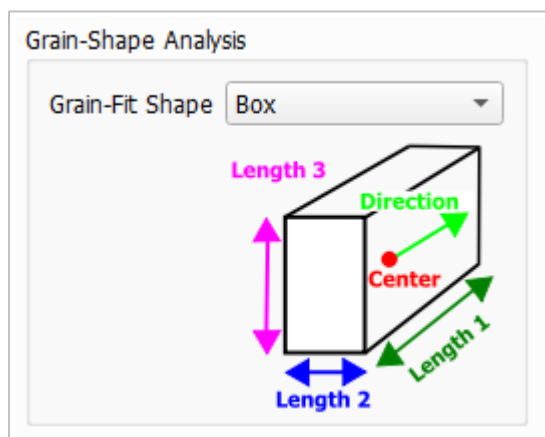
Elliptical Stub



Circular Stub

### ✓ Fit Shape Box

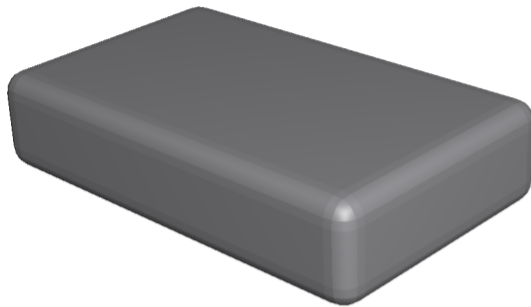
With the last option, a box is fitted into the grains.



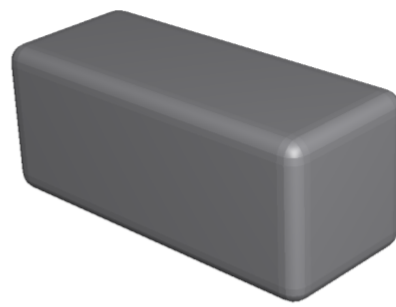
To define such a **Box**, a center point and three lengths are needed.

Four shapes of a box can be fitted into the grain:

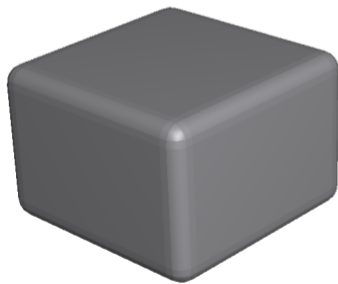
- If the all three lengths differ a box is called **Flat Bar**.
- For a **Rectangular Bar** the two shorter lengths are equal.
- For a **Rectangular Disk** the two larger lengths are equal.
- If all three lengths are equal the box is a **Cube**.



**Flat Bar**



**Rectangular Bar**



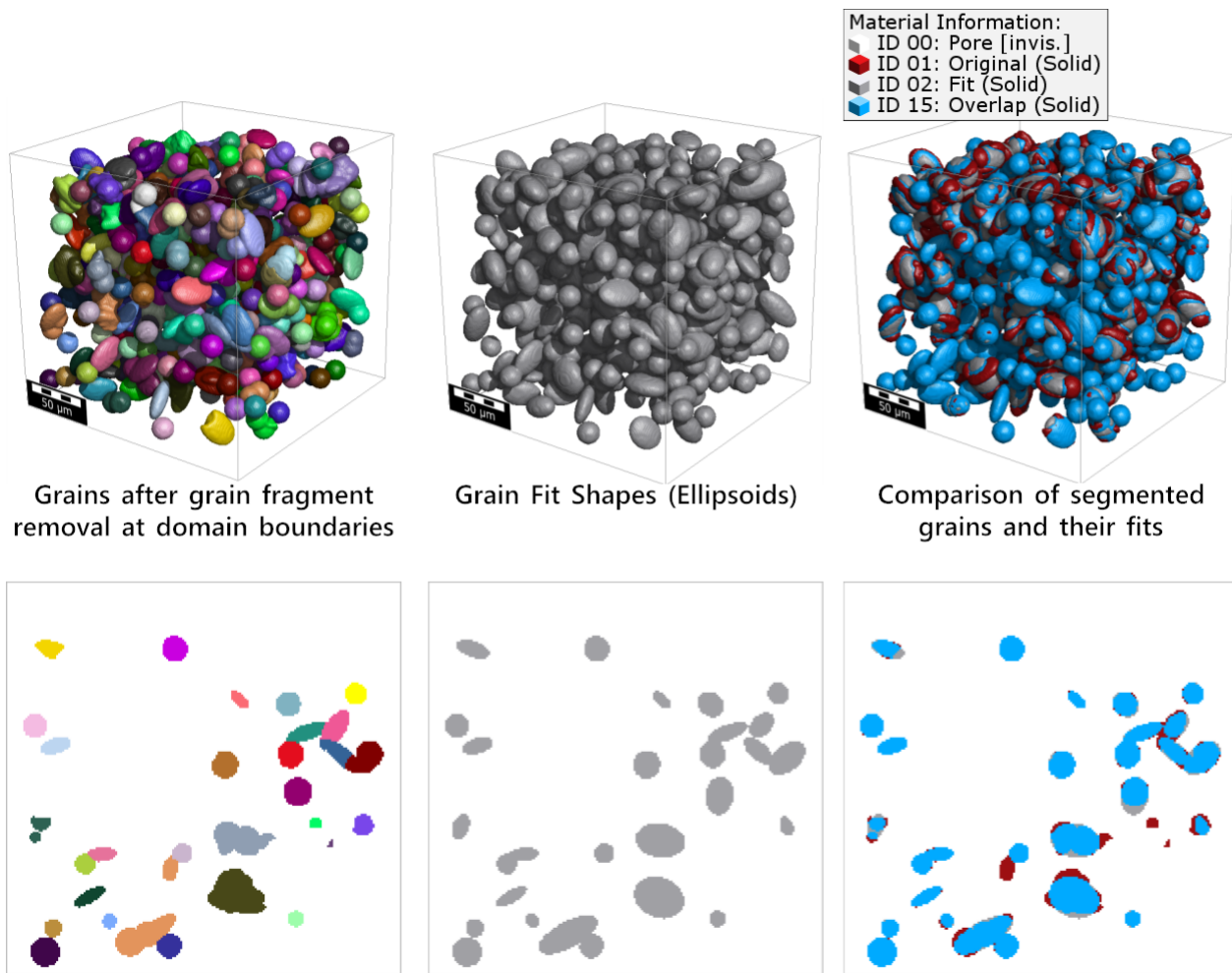
**Rectangular Disk**



**Cube**

The following figure shows the results of **Grain-Shape Analysis** on a grain structure. These visualizations are loaded from the Result Viewer of the \*.gdr result file (under the [Grain Visualization tab](#)<sup>57</sup>).

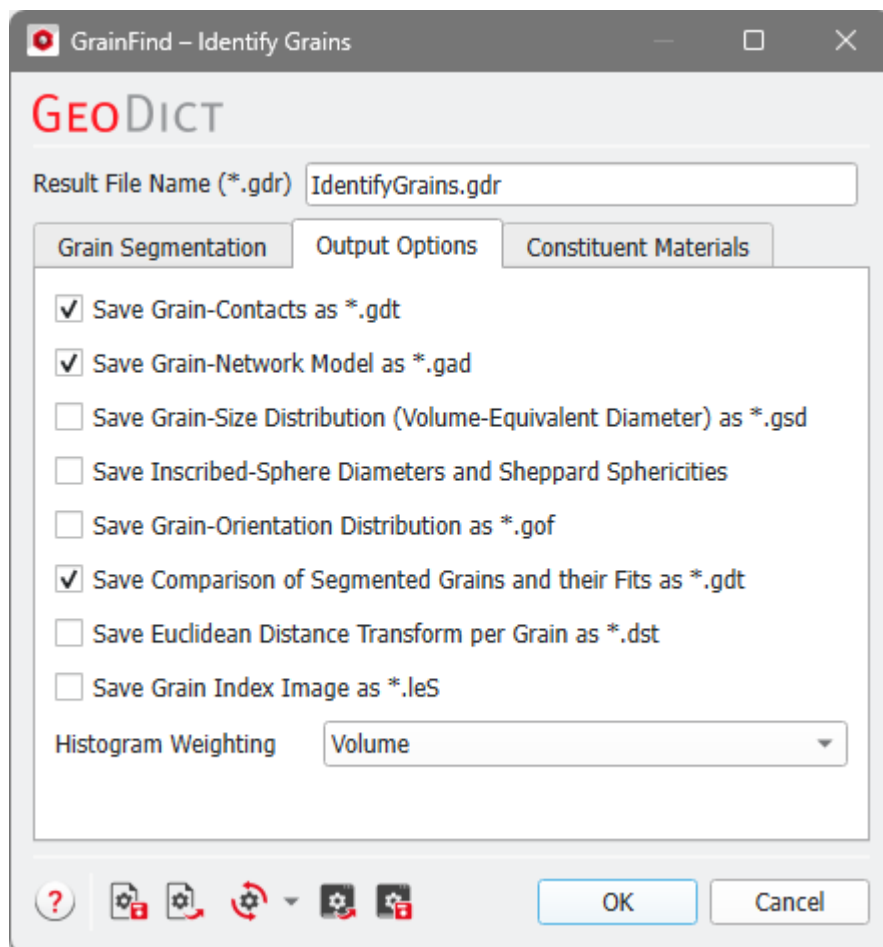
On the **left**, the structure is shown after grains are identified, and the grain fragments are removed at the domain boundary. The **middle** image shows the shapes of ellipsoids fitted to the grains. The **right** image shows a comparison between the identified grains (red) and the ellipsoid shapes fitted to them (gray). The matching voxels are shown in blue. This visualization provides a validation of the fitting to the ellipsoid shapes. A fitting is considered very good when a high percentage of overlap is observed, meaning the fitted shapes accurately cover the grainss.



## Output Options

Under the **Output Options** tab, choose which additional results should be computed and saved. Load the files for visualization in the Result Viewer under the [Grain Visualization](#) <sup>50</sup> tab. Some of these options need an additional computing effort and are unchecked by default. Shown below is the default selection of the output options for the Standard Edition.





**Note!** The following files are always saved as Output, independent of the selection in this tab:

- A Grain Index Image as \*.g32 file
- The Grain Fit Shapes as \*.gad file
- Intermediate Result of Watershed Transformation as \*.gdt file

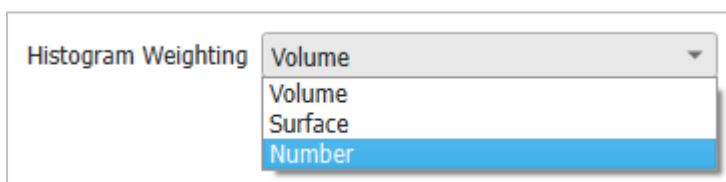
- Check **Save Grain-Contacts as \*.gdt** to save a structure file, where the grains have Material ID 01 and the contact areas have Material ID 02.
- The option **Save Grain-Network Model as \*.gad** is selected by default and creates a file containing analytic objects to represent the network. The grains are represented by spheres (Material ID 01) and the connections between them are modeled by cylinders (Material ID 02).
- Check **Save Grain-Size Distribution (Volume-Equivalent Diameter) as \*.gsd** to save the computed grain size distribution as a volume field. This information can be used, e.g., for visualization of the volume field of the Volume-Equivalent Diameter or for further analysis with Python.



**Know how!** You can modify the fields of the volume file after the computation in the [post-processing widget](#)<sup>[34]</sup> in the Result Viewer.

- When **Save Inscribed-Sphere Diameters and Sheppard Sphericities** is checked, the diameter of the inscribed sphere for every grain is calculated as volume field and saved. The Sheppard sphericity is computed according to [1](#)<sup>[8]</sup>. Both options need additional computing effort and are unchecked by default.
- Check **Save Grain-Orientation Distribution as \*.gof** to save the orientation of the pores in a volume field and use the orientation information in simulations or for later analysis. For example, when predicting mechanical properties with ElastoDict, anisotropic material properties can be assigned depending on the grain orientation.
- By default selected is to **Save Comparison of Segmented Grains and their Fits as \*.gdt**, which is useful to evaluate the quality of the [Grain-Fit Shapes](#)<sup>[23]</sup> (Ellipsoids, Short Elliptical Fibers, or Boxes). A good accordance of the grain fit shapes and the identified grains is important as a basis for generating good digital twins with **GrainGeo Create – Load GrainFind Result**<sup>[62]</sup>.
- After checking **Save Euclidean Distance Transform per Grain as \*.dst**, the EDT for every grain is calculated individually and the result is saved in one single file (\*.dst format). This option needs additional computing effort and is unchecked by default.
- The resulting grain index image is saved by default in the binary \*.g32 format. With the last option, **Save Grain Index Image as \*.leS**, it can be additionally saved as an ASCII file. This format takes more space and needs longer to write and load into GeoDict, but it is human-readable and can easily be imported into other software.

Choosing **Histogram Weighting** as **Volume**, **Surface**, or **Number** changes the values on the Y-axis of the resulting histogram plots. Then, either the grain volume probability, the grain surface area probability, or the grain count probability is shown. The histogram weighting can also be changed in the [Histogram Plot Options](#)<sup>[48]</sup> in the Result Viewer after the analysis has been run.

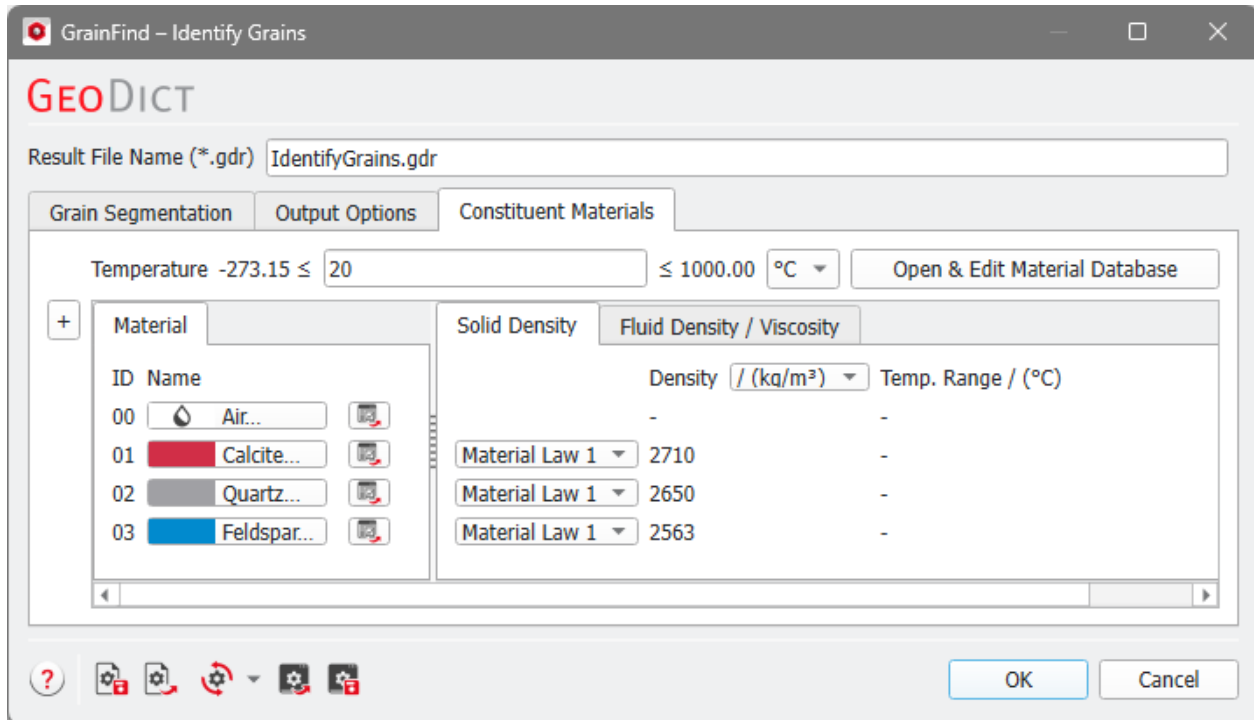


## Constituent Materials

This tab is only available if **Use Current Structure** is chosen as [Input Mode](#)<sup>[15]</sup> in the **Grain Segmentation** tab.

Under the **Constituent Materials** tab, the temperature can be edited if the density of a material is temperature dependent. Additionally, the density of every fluid and solid material in the structure must be specified in this tab. The density can be given in kg/m<sup>3</sup> or g/cm<sup>3</sup>. For materials from the GeoDict Material Database, the density value is entered automatically. If a

material is set to **Manual**, the Material Law changes to **Manual Law** and more laws can be added or deleted by clicking the "+" or "-" button on the right of the corresponding row. You can enter the density for manual materials directly in this tab.



### 1.1.3 Results

After the **Identify Grains** calculation is finished, the resulting files are saved in the project folder and a Result Viewer with the GeoDict result file opens automatically. The created GeoDict result file (\*.gdr) contains six tabs. The computational results are shown under the **Results** tab, and can be loaded for visualization via the **Grain Visualization** tab. The other four tabs (**Input Map**, **Log Map**, **Post Map**, and **Metadata**) display additional information about the computation.

Find more details on the general functionalities in the Result Viewer user guide.

The **Results** tab is the central point for the analysis of the identified grains. It is grouped in three subtabs: **Report**, **Plots**, and **Map**. The **Report** tab shows statistics about the identified grains and the **Plots** tab contains plot options for the analysis of the results. The **Map** tab contains all resulting data from the **Identify Grains** run. This data is the basis for the tables in the **Report** tab and for the plots in the **Plots** tab. On the left, the **Post-Processing Widget** allows you to fine-tune many graphs of the **Plots** tab. Collapse the **Post-Processing Widget** by pulling it to the left.

# GrainFind: Identify Grains

Domain Size: 100 x 100 x 100
Voxel Length: 698.302 nm
Load Structure

Input Map
Log Map
Post Map
Results
Grain Visualization
Create Videos
Metadata

### Scatter Plot

Vertical Axis (y-Axis)
Krumbein Sphericities

Horizontal Axis (x-Axis)
Equivalent Diameters

### Threshold by Scalar Value

Scalar Value
Volume

Number of Bins
10

Thresholding Method
k-Means

Number of Grain Types
2

### Histogram Plot

Histogram Weighting
Number

Histogram Plot Type
Relative

Volume
Number of Bins / (1) 10

Diameter
Number of Bins / (1) 10

Perimeter
Number of Bins / (1) 10

Sphericity and Aspect Ratio
Number of Bins / (1) 10

Surface and Contact
Number of Bins / (1) 10

Surface-to-Volume Ratio
Number of Bins / (1) 10

Surface Smoothness
Number of Bins / (1) 10

Mass
Number of Bins / (1) 10

Moment of Inertia
Number of Bins / (1) 10

GSD Field Choices
Equivalent Diameter, Inner Diameter

Apply

☒ Back-up result file

Plot Options

Report
Plots
Map

## GrainFind

### Main results

- Number of grains: **48**.
- Number of grain contacts: **63** (total grain contact area: 2737.01  $\mu\text{m}^2$ ).
- The index image "**Grains.g32**" and the human-readable index image "Grains.le5" contain the identified grains with their grain tags. These tags are integers ranging from 1 to 48.
- All mean values, all standard deviations, all D10 values, all D50 values, all D90 values, and all histogram values are calculated by **weighting** with the **grain number**. The weighting can be changed in the post-processing widget.

### Grain volume percentage statistics

| Step                            | Grain volume percentage |
|---------------------------------|-------------------------|
| Initial Grain Structure         | 36.6217 %               |
| Watershed with minimal diameter | 36.6217 %               |
| Grain reconnection              | 36.6217 %               |
| Boundary Grain removal          | 16.0704 %               |

### Grain volume statistics

|        | Minimum                 | Maximum                 | Mean value              | Standard deviation      |
|--------|-------------------------|-------------------------|-------------------------|-------------------------|
| Volume | 1.02153 $\mu\text{m}^3$ | 3473.89 $\mu\text{m}^3$ | 1140.03 $\mu\text{m}^3$ | 384.367 $\mu\text{m}^3$ |

### Grain sphericity statistics

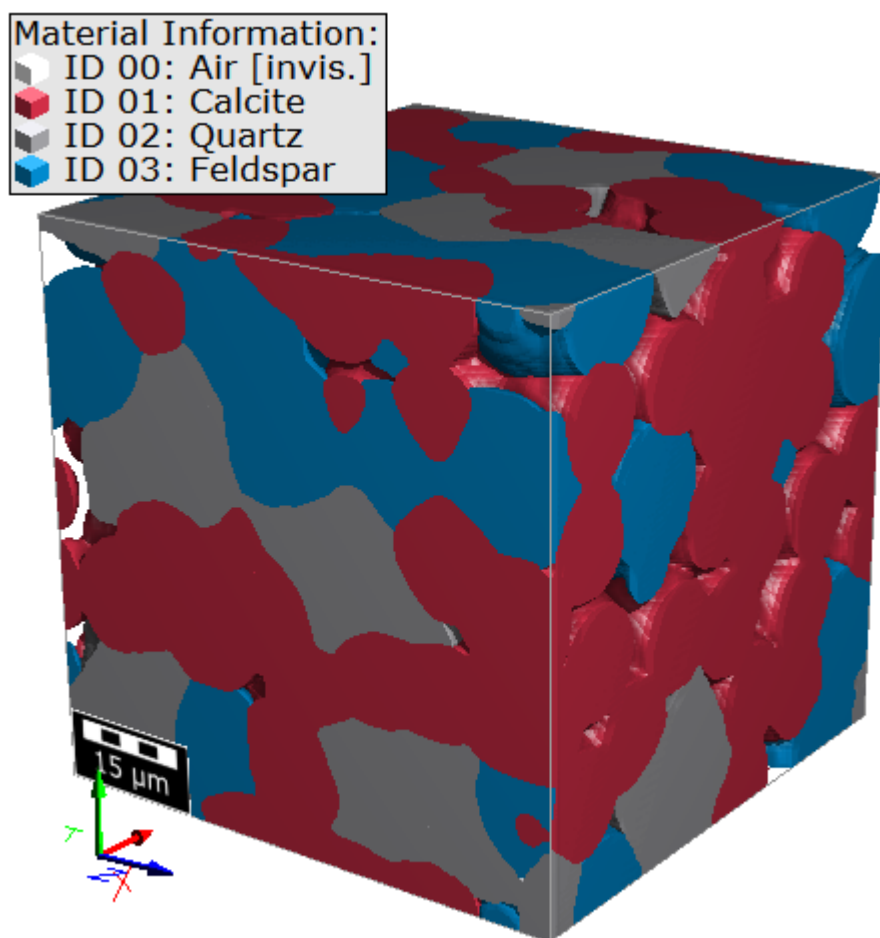
| Sphericities                       | Minimum  | Maximum  | Mean value | Standard deviation |
|------------------------------------|----------|----------|------------|--------------------|
| Krumbein $(b \cdot c / a^2)^{1/3}$ | 0.8016   | 0.984386 | 0.907762   | 0.0374353          |
| Sheppard $r_i/r_e$                 | 0.635032 | 1        | 0.798974   | 0.0456458          |

$r_i$ : inner radius (radius of inscribed sphere)  
 $r_e$ : equivalent radius (radius of volume-equivalent sphere)  
 $a, b, c$ : longest, medium, and shortest diameter of the ellipsoid that have been fitted to the identified grain.

### Grain diameter statistics

|                                      | Minimum               | Maximum               | Mean value           | Standard deviation    | D 10                  | D 50                  | D 90                  |
|--------------------------------------|-----------------------|-----------------------|----------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| Diameter of volume-equivalent sphere | 1.24954 $\mu\text{m}$ | 18.7905 $\mu\text{m}$ | 12.736 $\mu\text{m}$ | 1.90287 $\mu\text{m}$ | 11.5388 $\mu\text{m}$ | 12.5287 $\mu\text{m}$ | 13.5187 $\mu\text{m}$ |

The presented Identify Grains results are computed on this structure with sintered grains, generated with GrainGeo - Sinter. Only Material ID 01 (red) was analyzed.



## Post-Processing Widget

### Scatter Plot

In the **Scatter Plot** panel, you can choose two scalar values to be plotted against each other. By default, the Krumbein Sphericity is plotted against the Equivalent Diameters.

Find out more about the **Scatter Plot** in the [Plots](#)<sup>[38]</sup> topic.

### Threshold by Scalar Value

In the **Threshold by Scalar Value** panel you can choose a scalar value and a thresholding method to classify the grains into a selected number of types.

Find out more about the **Threshold by scalar value** plot in the [Plots](#)<sup>[39]</sup> topic.

### Histogram Plot

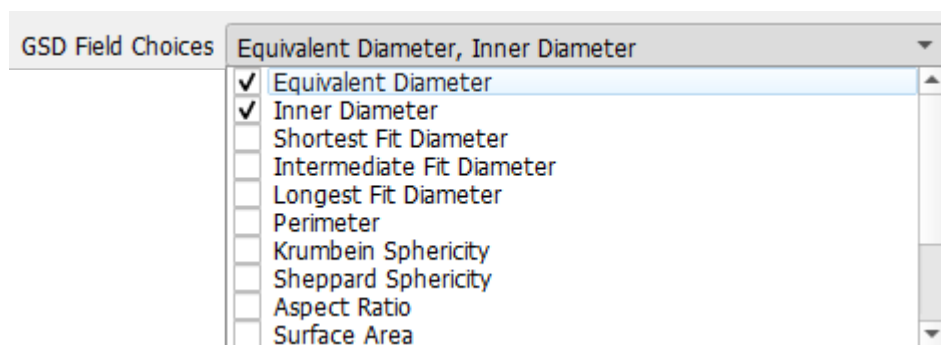
Define the options for the histograms in the Plot tab in the **Histogram Plot** panel. The **Weighting** and **Plot Type** are equal for all histograms, while the bin number can be set individually.

Find more about the Histogram Plot Options in the [Plots](#)<sup>48</sup> topic.

## GSD Field Choices

From the drop-down menu choose the [scalar grain properties](#)<sup>9</sup> that you want to visualize. For every chosen grain property, a volume field is created containing the 3D distribution of this property. These volume fields are saved together in a \*.gsd file (**GeoDict size distribution**). Load this file in the **Grain Visualization** tab under [Load Grain-Size Distribution](#)<sup>52</sup>.

In the example below, where **Equivalent Diameter** and **Inner Diameter** were chosen, the \*.gsd file will contain two volume fields: one with the size distribution of the diameters of volume-equivalent spheres, and one with the inner diameter.



### Identify Grains Results:

- [Report](#)<sup>34</sup>  
See the computed results.
- [Plots](#)<sup>38</sup>  
View result plots.
- [Grain Visualization](#)<sup>50</sup>  
Load results for a graphical visualization.
- [Create Videos](#)<sup>60</sup>  
Use a predefined macro to create a video.

## Report

The **Report** tab shows the **Main results** at the top, and below, in several tables, more detailed statistics. For an explanation of the different computed properties see [Results of Identify Grains](#)<sup>8</sup>.

### ✓ Main results

In the **Main results** section, the number of identified grains and the number and total area of grain contacts is given. For the \*.g32 file (and for the \*.leS file if **Save Grain Index Image as \*.leS** was checked in the [Output Options](#)<sup>[28]</sup> tab) the range of the index numbers is stated. Below, for the mentioned statistical values, the weighting property is given. This is the same as entered for **Histogram Weighting** in the [Output Options](#)<sup>[28]</sup> tab, but you can also change it later in the Post-Processing Widget under the [Histogram Plot Options](#)<sup>[48]</sup>.

#### Main results

- Number of grains: **48**.
- Number of grain contacts: **63** (total grain contact area: 2737.01  $\mu\text{m}^2$ ).
- The index image "**Grains.g32**" and the human-readable index image "Grains.leS" contain the identified grains with their grain tags. These tags are integers ranging from 1 to 48.
- All mean values, all standard deviations, all D10 values, all D50 values, all D90 values, and all histogram values are calculated by **weighting** with the **grain number**. The weighting can be changed in the post-processing widget.

### ✓ Grain volume percentage statistics

In this table the grain volume during the different steps of the identification is displayed. The grain volume percentage after the Watershed transformation is only shown if Current Structure was chosen as Input Mode in the [Identify Grains](#)<sup>[15]</sup> dialog. Then, only grains larger than the minimal grain diameter count for the statistics. The volume percentage after [Grain-Fragment Reconnection](#)<sup>[19]</sup> and [Boundary Grain removal](#)<sup>[22]</sup> are only shown if the corresponding options were selected in the options dialog.

#### Grain volume percentage statistics

| Step                            | Grain volume percentage |
|---------------------------------|-------------------------|
| Initial Grain Structure         | 36.6217 %               |
| Watershed with minimal diameter | 36.6217 %               |
| Grain reconnection              | 36.6217 %               |
| Boundary Grain removal          | 16.0704 %               |

### ✓ Grain volume statistics

For the identified grains, the minimum, maximum, and mean volume and the standard deviation are shown. The mean value and standard deviation are weighted with the chosen **Histogram Weighting** (changeable in the [Post-Processing Widget](#))<sup>[48]</sup>.

**Grain volume statistics**

|        | Minimum                 | Maximum                 | Mean value              | Standard deviation      |
|--------|-------------------------|-------------------------|-------------------------|-------------------------|
| Volume | 1.02153 $\mu\text{m}^3$ | 3473.89 $\mu\text{m}^3$ | 1140.03 $\mu\text{m}^3$ | 384.367 $\mu\text{m}^3$ |

✓ **Grain sphericity statistics**

The statistics for the Krumbein sphericity and the Sheppard sphericity (only if **Save Inscribed-Sphere Diameters and Sheppard Sphericities** was checked in the [Output Options](#) <sup>28</sup> tab) are shown. The mean value and standard deviation are weighted with the chosen **Histogram Weighting** (changeable in the [Post-Processing Widget](#)) <sup>48</sup>.

**Grain sphericity statistics**

| Sphericities                       | Minimum  | Maximum  | Mean value | Standard deviation |
|------------------------------------|----------|----------|------------|--------------------|
| Krumbein $(b \cdot c / a^2)^{1/3}$ | 0.8016   | 0.984386 | 0.907762   | 0.0374353          |
| Sheppard $r_i/r_e$                 | 0.635032 | 1        | 0.798974   | 0.0456458          |

$r_i$ : inner radius (radius of inscribed sphere)

$r_e$ : equivalent radius (radius of volume-equivalent sphere)

$a, b, c$ : longest, medium, and shortest diameter of the ellipsoid that have been fitted to the identified grain.

✓ **Grain diameter statistics**

For different grain diameters the minimum, maximum, and mean value and the standard deviation are shown. The mean value and standard deviation are weighted with the chosen **Histogram Weighting** (changeable in the [Post-Processing Widget](#)) <sup>48</sup>. Additionally, the characteristic diameters D10, D50, D90 are shown. These are the diameters such that 10%, 50%, or 90% of all grains have smaller diameter than the corresponding value. The **Diameter of inscribed sphere** is only computed if **Save Inscribed-Sphere Diameters and Sheppard Sphericities** was checked in the [Output Options](#) <sup>28</sup> tab.

**Grain diameter statistics**

|                                      | Minimum               | Maximum               | Mean value            | Standard deviation    | D 10                  | D 50                  | D 90                  |
|--------------------------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|-----------------------|
| Diameter of volume-equivalent sphere | 1.24954 $\mu\text{m}$ | 18.7905 $\mu\text{m}$ | 12.736 $\mu\text{m}$  | 1.90287 $\mu\text{m}$ | 11.5388 $\mu\text{m}$ | 12.5287 $\mu\text{m}$ | 13.5187 $\mu\text{m}$ |
| Diameter of inscribed sphere         | 1.3966 $\mu\text{m}$  | 11.9326 $\mu\text{m}$ | 10.1102 $\mu\text{m}$ | 1.36103 $\mu\text{m}$ | 9.26589 $\mu\text{m}$ | 10.2338 $\mu\text{m}$ | 11.2017 $\mu\text{m}$ |
| Shortest Diameters                   | 1.02048 $\mu\text{m}$ | 13.3372 $\mu\text{m}$ | 11.559 $\mu\text{m}$  | 1.6116 $\mu\text{m}$  | 10.1519 $\mu\text{m}$ | 12.2154 $\mu\text{m}$ | 13.3323 $\mu\text{m}$ |
| Intermediate Diameters               | 1.22647 $\mu\text{m}$ | 21.928 $\mu\text{m}$  | 12.7731 $\mu\text{m}$ | 2.18487 $\mu\text{m}$ | 11.5482 $\mu\text{m}$ | 12.5852 $\mu\text{m}$ | 13.7249 $\mu\text{m}$ |
| Longest Diameters                    | 1.55881 $\mu\text{m}$ | 22.6858 $\mu\text{m}$ | 14.0317 $\mu\text{m}$ | 2.26718 $\mu\text{m}$ | 12.3007 $\mu\text{m}$ | 14.4699 $\mu\text{m}$ | 15.6471 $\mu\text{m}$ |

✓ **Coordination number statistics**



For the coordination number (number of contacts a grain has to other grains) the minimum, maximum, and mean value and the standard deviation are shown. The mean value and standard deviation are weighted with the chosen **Histogram Weighting** (changeable in the [Post-Processing Widget](#))<sup>48</sup>.

| Coordination number statistics |         |         |            |                    |
|--------------------------------|---------|---------|------------|--------------------|
|                                | Minimum | Maximum | Mean value | Standard deviation |
| Coordination number            | 0       | 7       | 2.625      | 1.56292            |

## ✓ Grain Orientation

At the bottom, the orientation tensor of all grains is shown.

| Grain Orientation |               |               |
|-------------------|---------------|---------------|
| Direction tensor: |               |               |
| <b>0.3631</b>     | 0.0425        | -0.0209       |
| -                 | <b>0.3576</b> | 0.0029        |
| -                 | -             | <b>0.2793</b> |

In detail, let

$$\mathbf{d}_k = \begin{pmatrix} x_k \\ y_k \\ z_k \end{pmatrix}$$

be the unit vector describing the direction of the k-th object and **n** the number of objects. Then the orientation tensor **T** is the sum over the dyadic products of the **d<sub>k</sub>** from all **n** objects, divided by **n**:

$$\mathbf{T} = \frac{1}{n} \left( \sum_{k=1}^n \mathbf{d}_k \mathbf{d}_k^T \right) = \frac{1}{n} \sum_{k=1}^n \begin{pmatrix} x_k x_k & x_k y_k & x_k z_k \\ y_k x_k & y_k y_k & y_k z_k \\ z_k x_k & z_k y_k & z_k z_k \end{pmatrix} = \begin{pmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{pmatrix} \quad \text{(7) Orientation Tensor}$$

The diagonal elements define the orientation strength for the corresponding directions and sum up to 1. Thus, if for example **t<sub>11</sub>=1** (and **t<sub>22</sub>=t<sub>33</sub>=0**), all objects are oriented in the X-direction. For **t<sub>11</sub>=0** all objects are oriented normally to the X-direction and same values for all diagonal elements (**t<sub>11</sub>=t<sub>22</sub>=t<sub>33</sub>= 1/3**) result in a uniform distribution for the object orientation.

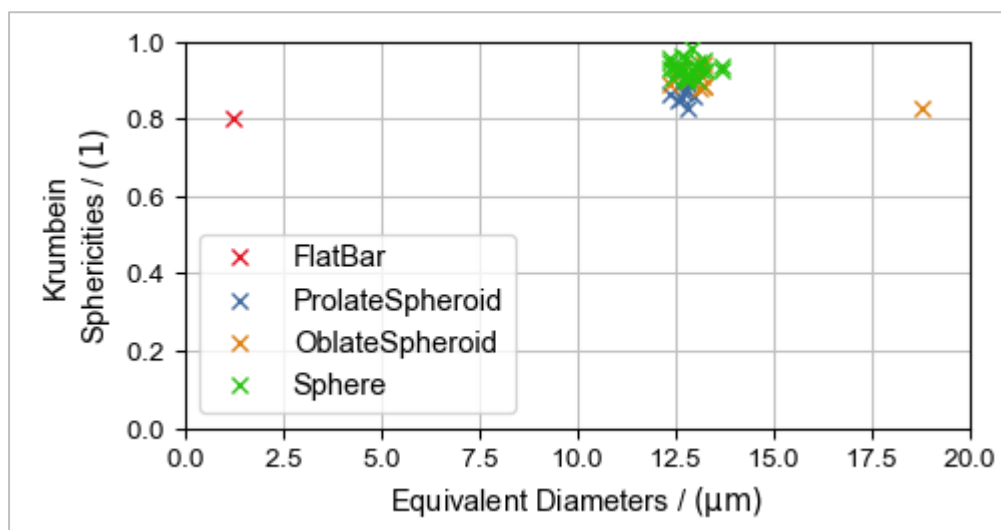
## Plots

The **Plots** tab offers several plots to show the relationship between grain parameters: **Scatter Plot**, **Threshold by scalar value** histogram, **Volume** histogram, **Diameters** histogram, **Perimeter** histogram, **Sphericities** histogram, **Aspect ratio** histogram, **Surfaces And Contacts** histogram, **Mass** histogram, **Moment of Inertia** histogram, **Coordination Number** histogram, the **Orientation** polar plot, and the **Reconnection Indicators** histogram.

Change the plot options in the post-processing widget at the left side of the **Plots** tab. After changes are made, click **Apply...** to use the new values. The changes are also applied to the tables under the [Report](#)<sup>34</sup> subtab.

### ▼ Scatter Plot

In the **Scatter Plot** panel, you can choose two scalar values to be plotted against each other. By default, the Krumbein Sphericity is plotted against the Equivalent Diameters.



You can change the scalar values in the post-processing widget. The different scalar values are explained in [Results of Identify Grains](#)<sup>9</sup>.

Scatter Plot

Vertical Axis (y-Axis) Krumbein Sphericities

Horizontal Axis (x-Axis) Equivalent Diameters

Indices

- Equivalent Diameters
- Inner Diameters
- Shortest Fit Diameters
- Intermediate Fit Diameters
- Longest Fit Diameters
- Perimeter
- Krumbein Sphericities
- Sheppard Sphericities
- Aspect Ratio

The Scatter Plot distinguishes between the four shapes of each object type (Ellipsoids, Short Elliptical Fibers, and Boxes) that are fitted into the grains (see also [Grain Shape Analysis](#)<sup>[23]</sup> for more information).

In the example above, observe in the **Scatter Plot** that all identified grains in the structure are nearly spherical (Krumbein Sphericities close to 1). Nearly all grains have an equivalent diameter around 12.5  $\mu\text{m}$ , except of two outliers.

## ✓ Threshold by scalar value

You can classify the grains in the structure into different types based on a chosen scalar value. Define the parameters in the Post-Processing Widget and control the performance in the **Threshold by scalar value** plot.

The screenshot shows a widget titled "Threshold by Scalar Value" with four input fields:

- Scalar Value:** A dropdown menu with "Volume" selected.
- Number of Bins:** A text input field containing the value "10".
- Thresholding Method:** A dropdown menu with "k-Means" selected.
- Number of Grain Types:** A text input field containing the value "2".

First, select the **Scalar Value** from the drop-down list to determine a threshold for. The default scalar value is **Volume**. All scalar values are described under [Results of Identify Grains](#)<sup>[9]</sup>.

The **Number of Bins** defines how many bins the histogram **Threshold by scalar value** has. With more bins, a more precise threshold value can be found.

To determine the threshold value, three **Thresholding Methods** are available:

The screenshot shows a dropdown menu for "Thresholding Method" with the following options:

- k-Means (highlighted)
- Otsu
- Manual

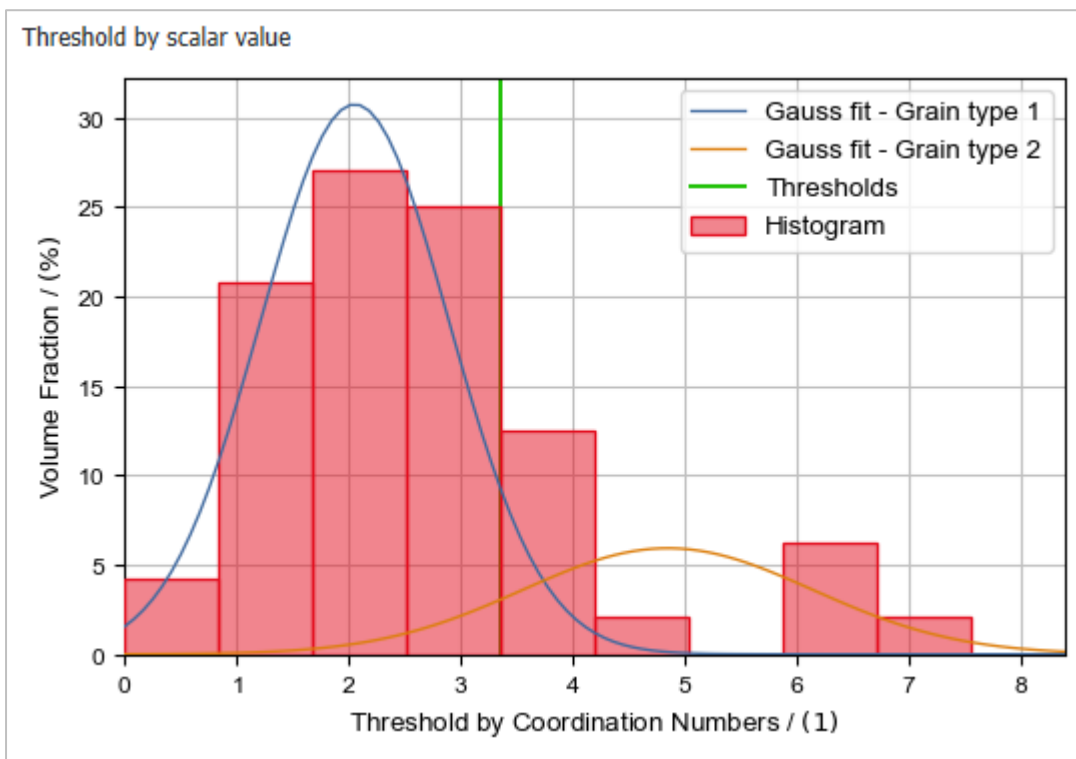
- **k-Means:** uses the k-Means algorithm to find thresholds for the chosen **Number of Grain Types**.
- **Otsu:** uses the Otsu algorithm to find thresholds for the chosen **Number of Grain Types**.
- **Manual:** define your own thresholds by writing a comma-separated list of thresholds into **Threshold(s)**. You implicitly define the number of grain types by the number of thresholds you enter, e.g, if you enter two threshold values this will result in three grain types.

Thresholding Method
Manual

Threshold(s) / (m<sup>3</sup>)

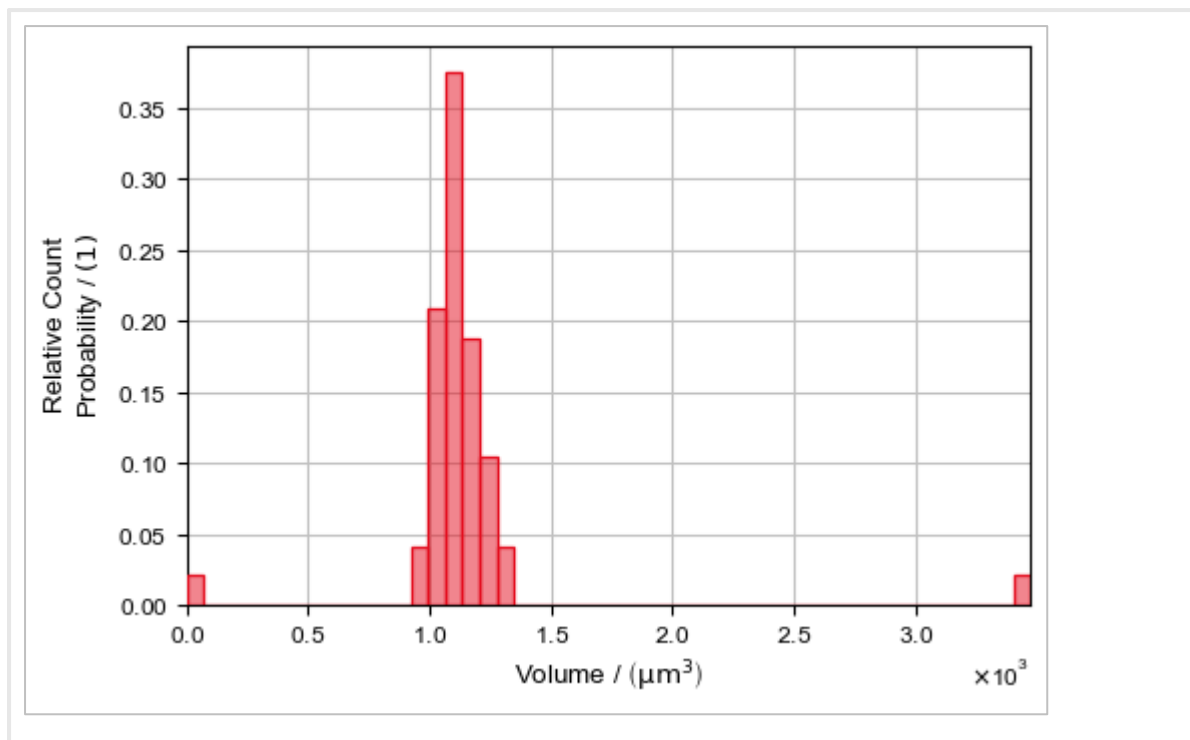
After the settings are applied, the **Threshold by scalar value** plot visualizes the effects. The histogram of the chosen **Scalar Value** is plotted with the entered **Number of Bins**. The computed or entered **Thresholds** are marked as well as the Gauss fit of the grain types. Additionally, a structure containing the different grain types will be created, that can be loaded into GeoDict from the [Grain Visualization tab](#)<sup>55</sup>.

In the example, the grains are separated by their **Coordination Number** into grains with only few contacts to other grains (low coordination number) and many contacts to other grains (higher coordination number).



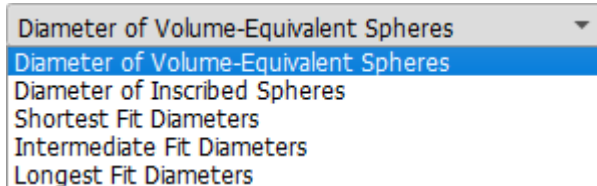
### ✓ Volume histogram

In this tab, the **Volume** of the identified grains is plotted. The [Histogram Plot Options](#)<sup>48</sup> are explained below.



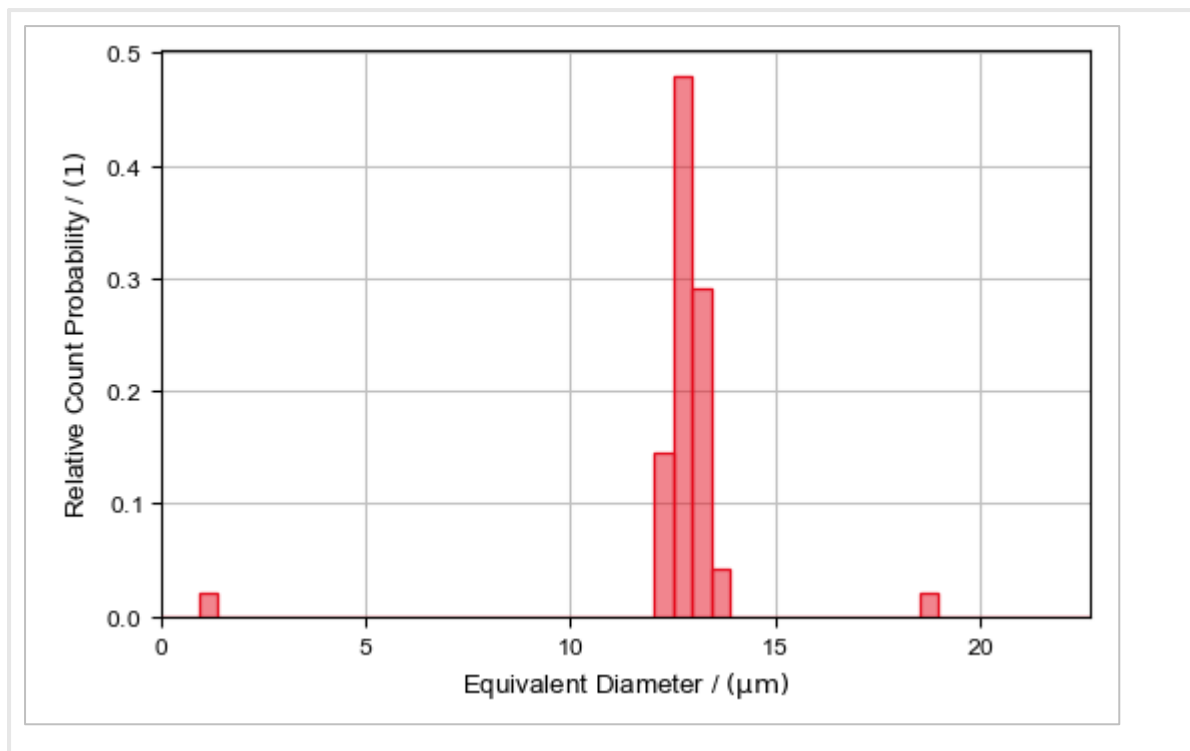
## ✓ Diameters histogram

In the **Diameters** panel you can switch between different plots.



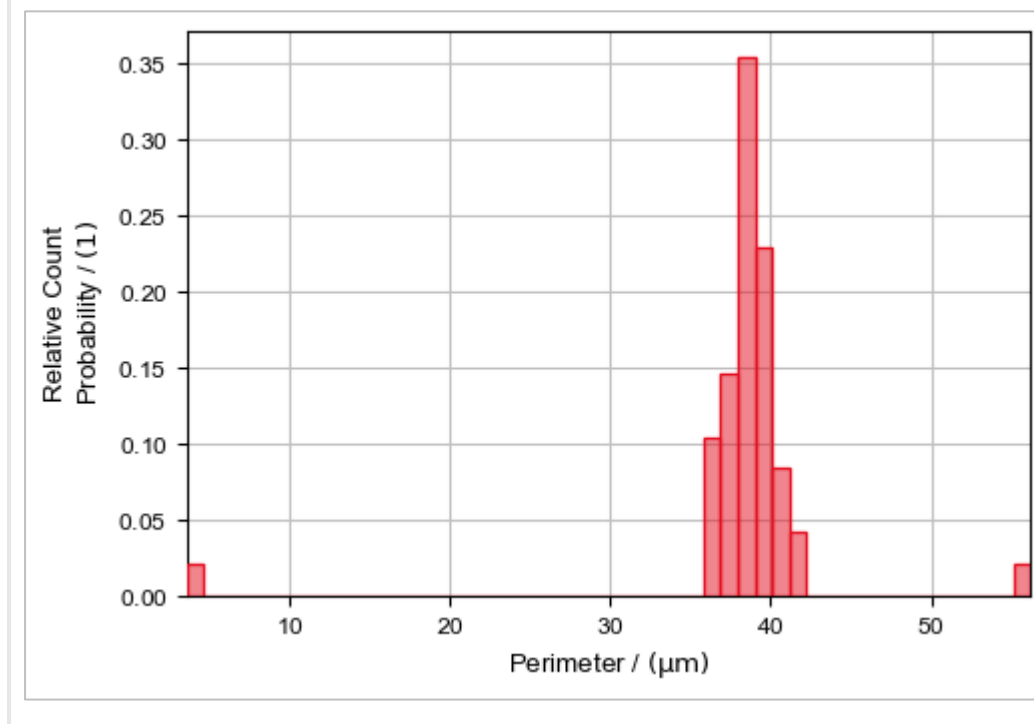
The Diameter of Inscribed Spheres histogram is only available if **Save Inscribed-Sphere Diameters and Sheppard Sphericities** was checked in the [Output Options](#)<sup>[28]</sup> tab.

The [Histogram Plot Options](#)<sup>[48]</sup> are explained below.



## ✓ Perimeter histogram

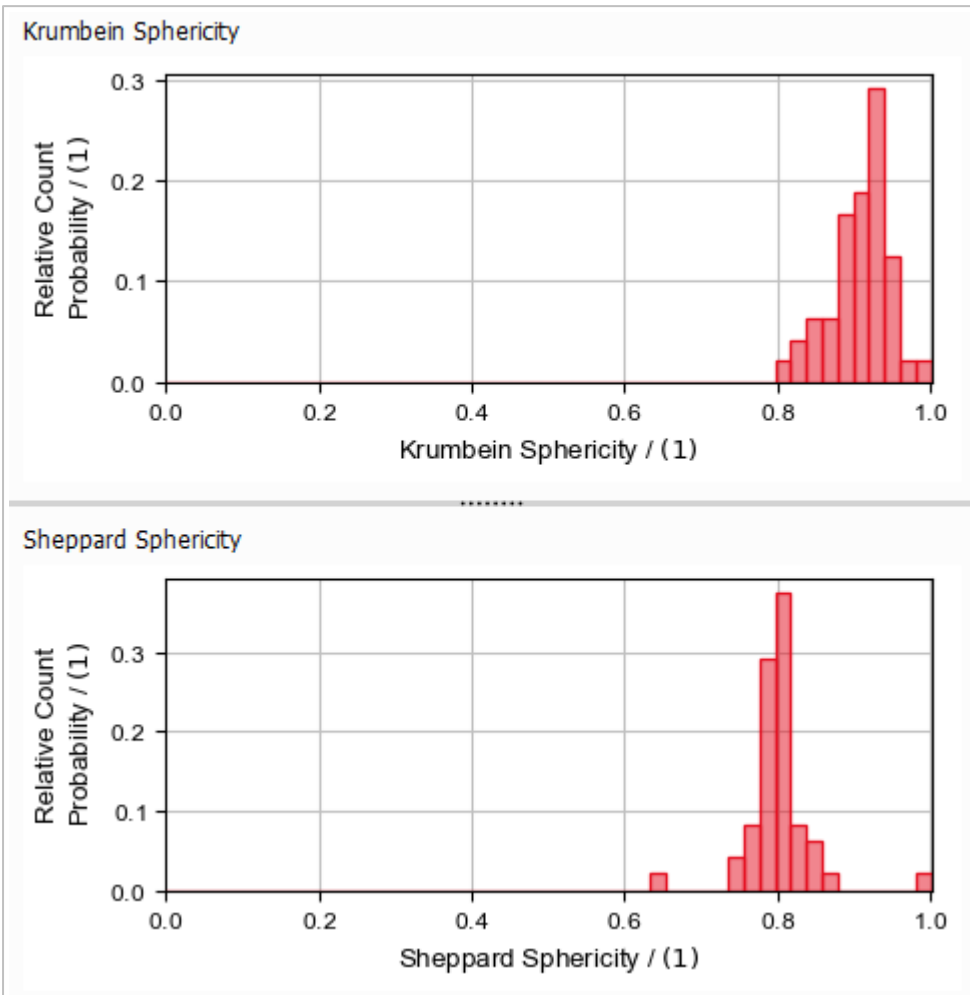
In this tab, the **Perimeter** of the identified grains is plotted. The [Histogram Plot Options](#)<sup>48</sup> are explained below.



## ✓ Sphericities histogram

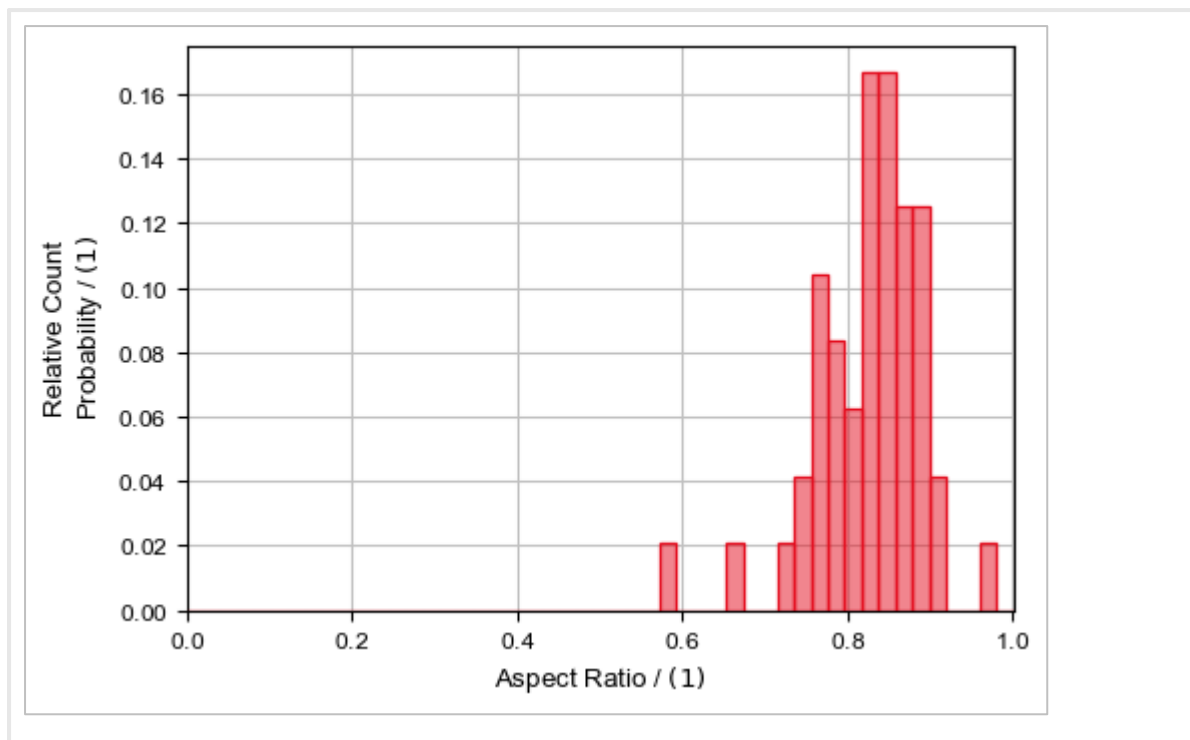
The Krumbein Sphericity and the Sheppard Sphericity (only if **Save Inscribed-Sphere Diameters and Sheppard Sphericities** was checked in the [Output Options](#)<sup>28</sup> tab) are shown in this tab.

The [Histogram Plot Options](#)<sup>48</sup> are explained below.



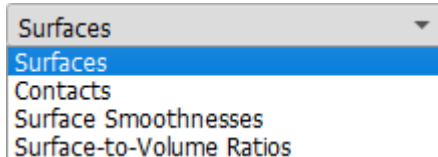
### ✓ Aspect ratio histogram

In this tab, the **Aspect Ratio** of the identified grains is plotted. The [Histogram Plot Options](#)<sup>48</sup> are explained below.



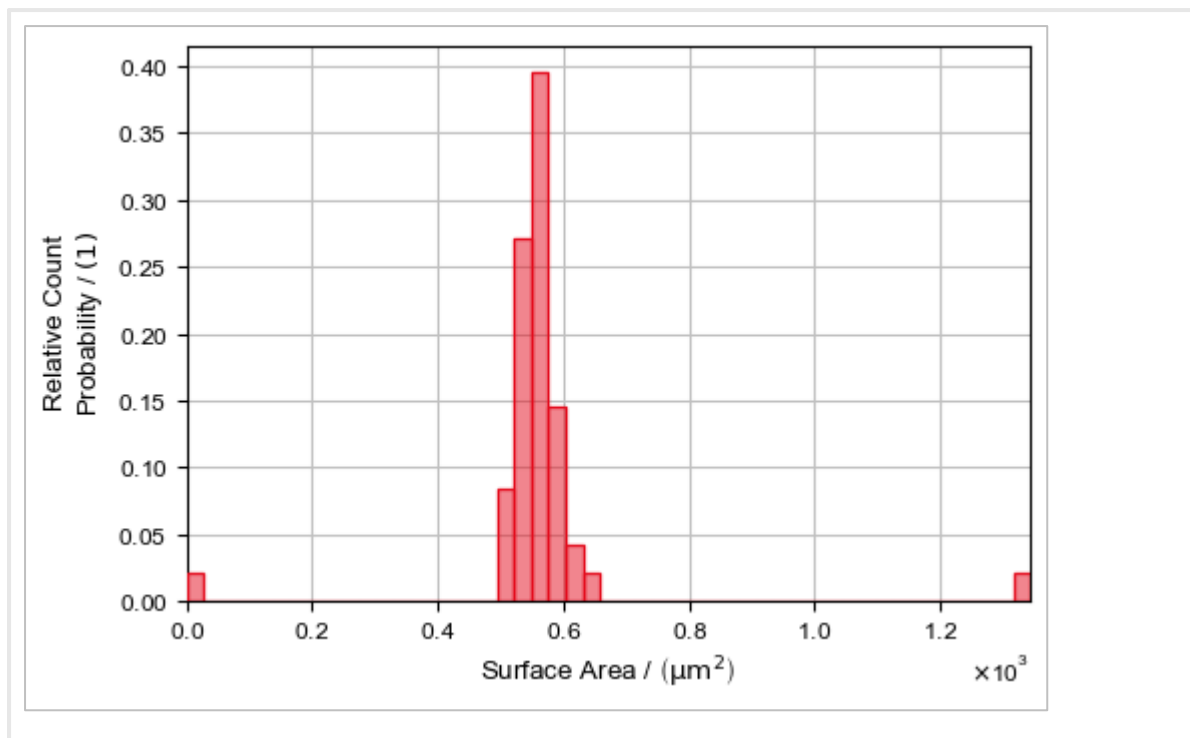
## ✓ Surfaces And Contacts histogram

In the **Surfaces and Contacts** panel you can switch between different plots.



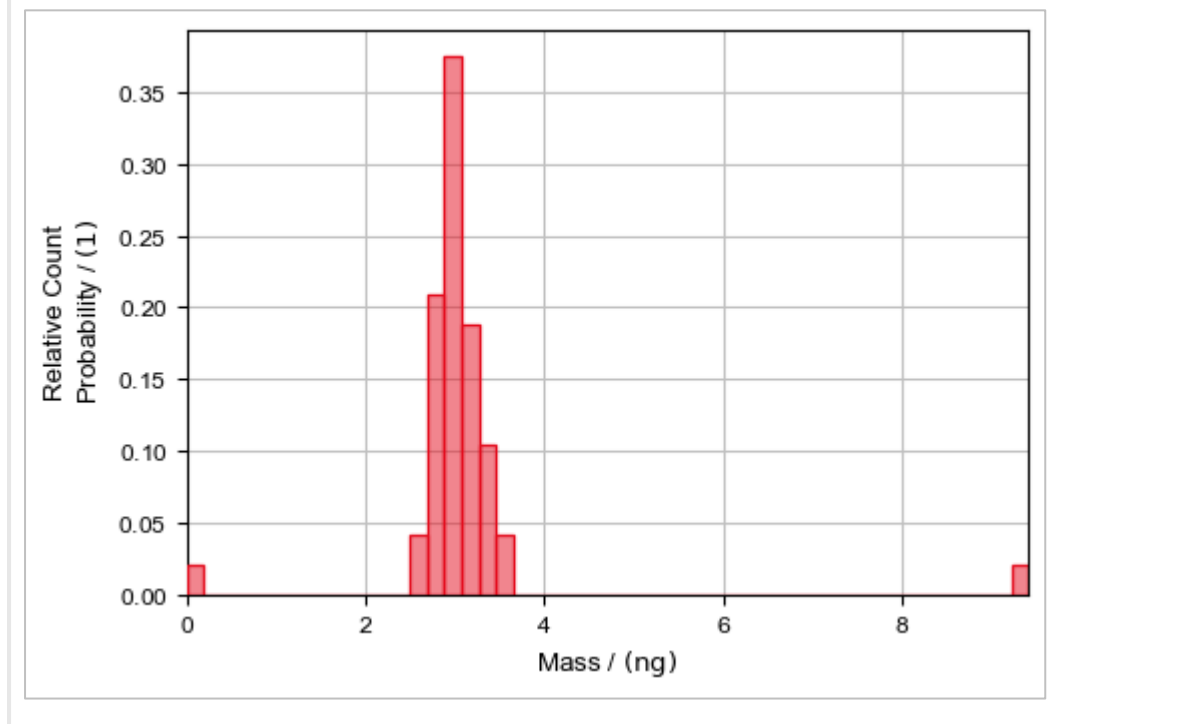
The [Histogram Plot Options](#)<sup>48</sup> are explained below.





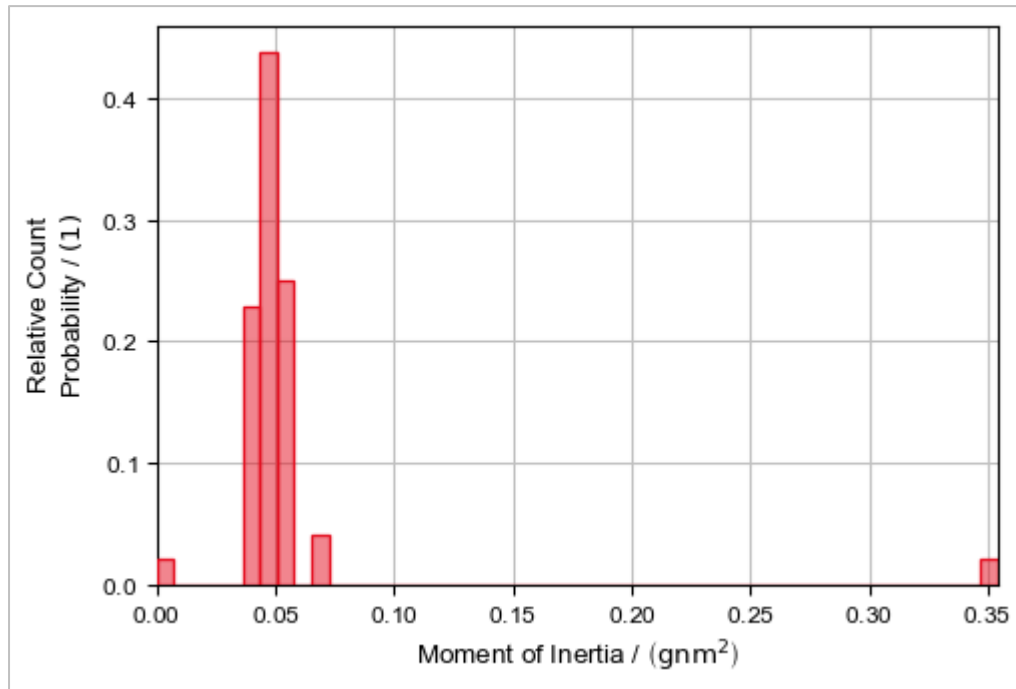
### ✓ Mass histogram

In this tab, the **Mass** histogram of the identified grains is plotted. The [Histogram Plot Options](#)<sup>48</sup> are explained below.



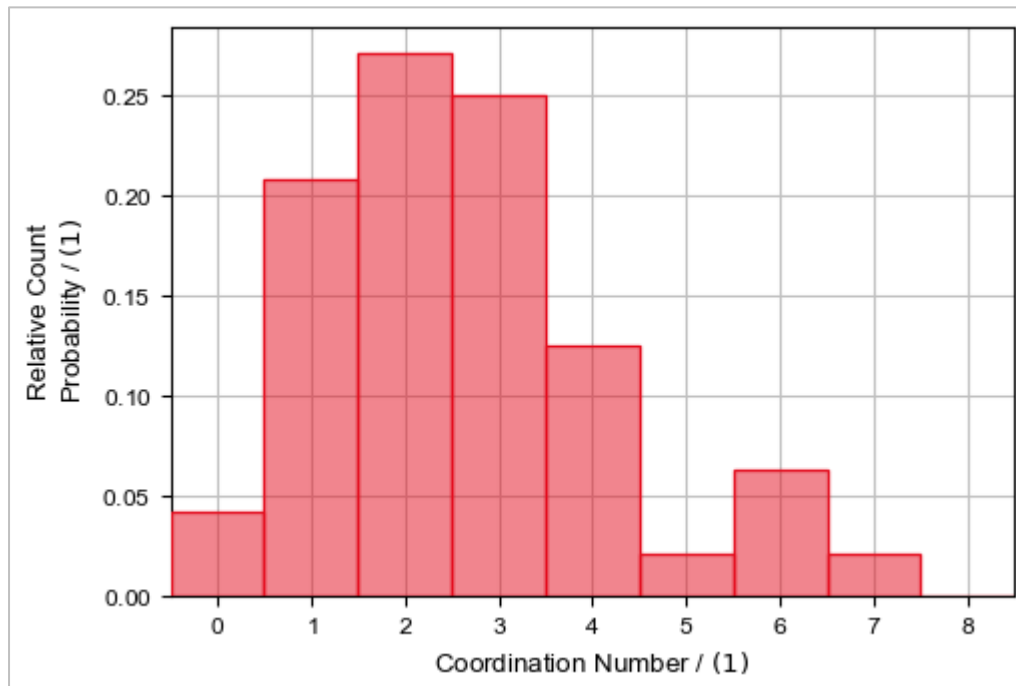
### ✓ Moment of Inertia histogram

In this tab, the **Moment of Inertia** histogram of the identified grains is plotted. The [Histogram Plot Options](#)<sup>48</sup> are explained below.



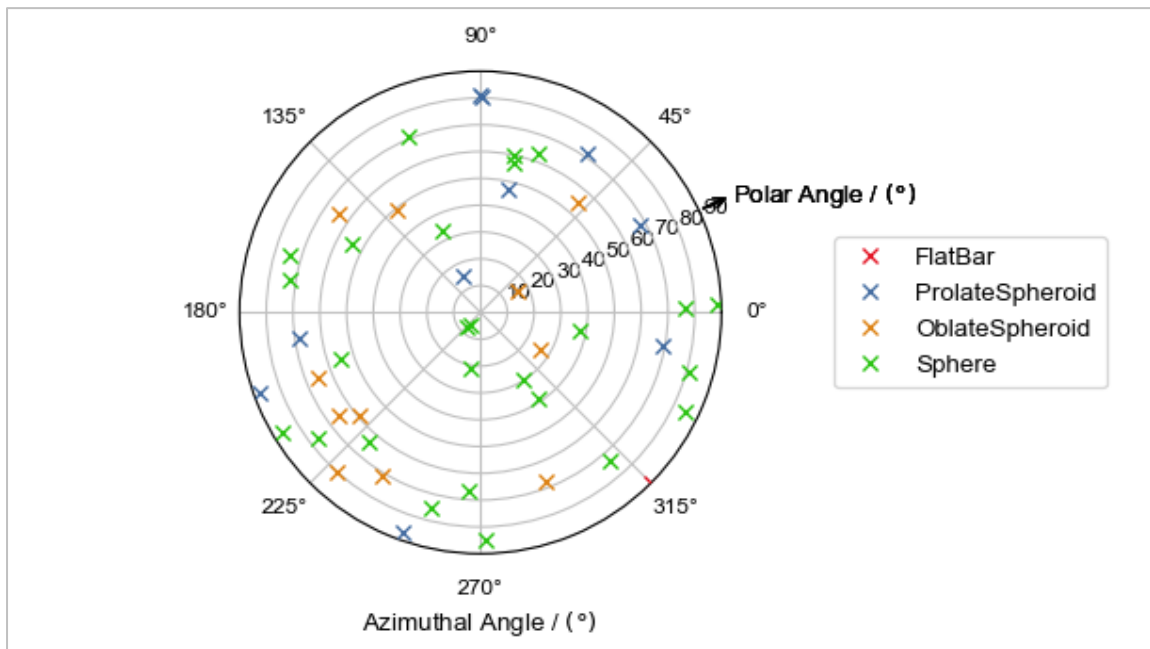
## ✓ Coordination Number histogram

In this tab, the **Coordination Number** (number of contacts a grain has to other grains) of the identified grains is plotted. The [Histogram Plot Options](#)<sup>48</sup> are explained below.



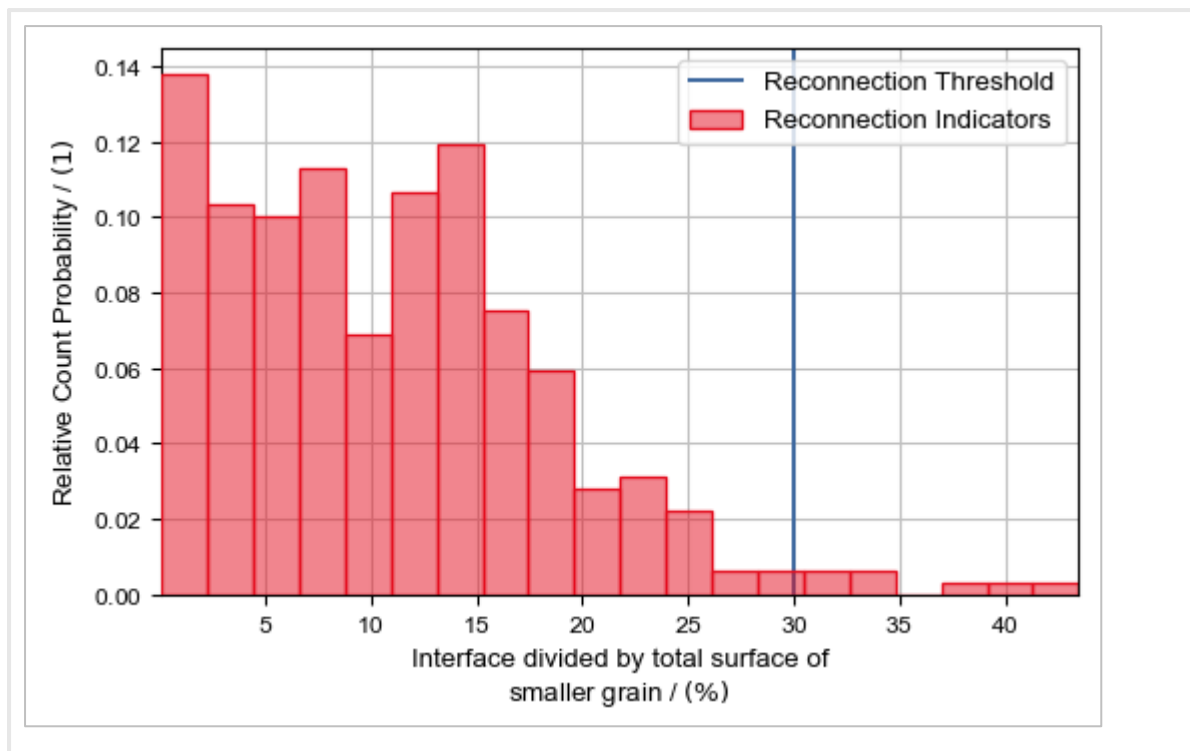
## ✓ Orientation polar plot

In this tab, the orientation of the fitted grain shapes is plotted as polar plot. This plot distinguishes between the four shapes of each object type (Ellipsoids, Short Elliptical Fibers, and Boxes) that are fitted into the grains (see also [Grain Shape Analysis](#)<sup>[23]</sup> for more information).



## ✓ Reconnection Indicators

Use the **Reconnection Indicators** histogram to find an appropriate **Reconnection Threshold** if you want to use [Grain-Fragment Reconnection](#)<sup>[19]</sup> (find more information in this topic).



## ✓ Histogram Plot Options

You can modify the histogram plots with the **Histogram Plot** options in the post-processing widget.

Histogram Plot

Histogram Weighting
Number

Histogram Plot Type
Relative

Volume
Number of Bins / (1) 49

Diameter
Number of Bins / (1) 49

Perimeter
Number of Bins / (1) 49

Sphericity and Aspect Ratio
Number of Bins / (1) 49

Surface and Contact
Number of Bins / (1) 49

Surface-to-Volume Ratio
Number of Bins / (1) 49

Surface Smoothness
Number of Bins / (1) 49

Mass
Number of Bins / (1) 10

Moment of Inertia
Number of Bins / (1) 10

The values on the Y-axes of the histograms in all plots can show **Count Probability**

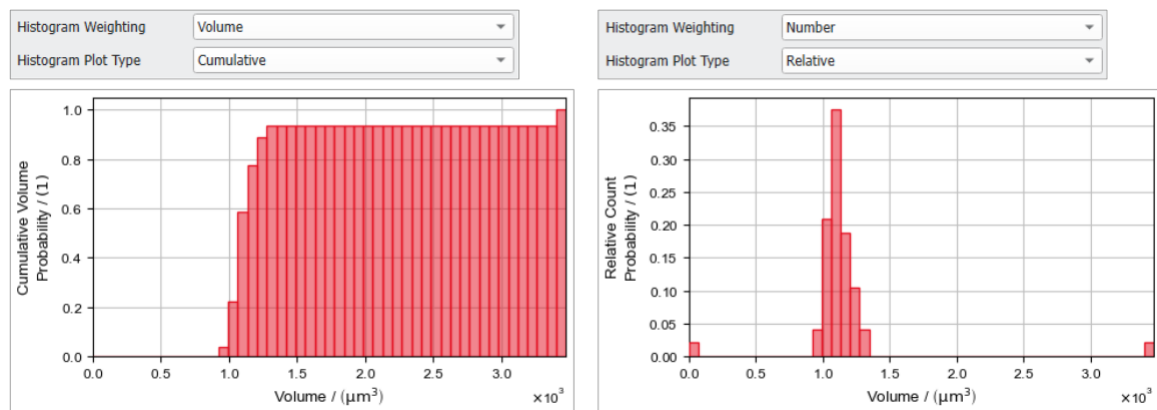
(weighting by **Number**), **Area Probability** (weighting by **Surface**), or **Volume Probability** (weighting by **Volume**), depending on the **Histogram Weighting** you choose. For the Area Probability (weighting by Surface) the surface area of each segmented grain is computed using the same algorithm as in Estimate Surface Area (MatDict) command and then weighting the grains by that value. The computed surface area does also include the surface between different grains, not only the area between grain and pore material.

|                     |         |
|---------------------|---------|
| Histogram Weighting | Volume  |
|                     | Volume  |
|                     | Surface |
|                     | Number  |

Set the **Histogram Plot Type** to **Relative** to compare the individual proportions, or to **Cumulative** to show the accumulation over the data range.

|                     |            |
|---------------------|------------|
| Histogram Plot Type | Relative   |
|                     | Relative   |
|                     | Cumulative |

The example on the left-hand side shows, that the smallest grains make up around 20% of the total grain volume. Compared to the weighting with numbers, around 10% of the grains belong to the smallest grains in the structure.



You can customize the bin size for different histogram plots individually. In general, you can choose between:

- **Number of Bins:** choose how many bins the histogram should have.
- **Bin Size in Units:** choose the bin size for the histogram using the value in the displayed unit (e.g.,  $\mu\text{m}$ ,  $\mu\text{m}^3$ , etc.).
- **Bin Size in Voxels:** choose the bin size for the histogram using the value measure in voxel lengths.

As the different histogram plots show different results, only those choices are available which make sense for the corresponding plot.

|                             |                      |            |         |
|-----------------------------|----------------------|------------|---------|
| Volume                      | Number of Bins ▾     | / (1)      | 49      |
| Diameter                    | Bin Size in Units ▾  | / (nm)     | 2300    |
| Perimeter                   | Bin Size in Voxels ▾ | / (Voxels) | 2       |
| Sphericity and Aspect Ratio | Number of Bins       | / (1)      | 49      |
| Surface and Contact         | Number of Bins ▾     | / (1)      | 49      |
| Surface-to-Volume Ratio     | Bin Size in Units ▾  | / (1/nm)   | 0.00038 |
| Surface Smoothness          | Bin Size in Units ▾  | / (1)      | 0.15    |
| Mass                        | Number of Bins ▾     | / (1)      | 10      |
| Moment of Inertia           | Number of Bins ▾     | / (1)      | 10      |

The bin size can correspond to one single plot or multiple plots are changed at once:

- The selection made under **Volume** changes the bin size for the plot under the **Volume** tab.
- The selection made under **Diameter** changes the bin size for all plots under the **Diameters** tab.
- The selection made under **Perimeter** changes the bin size for the plot under the **Perimeter** tab.
- The selection under **Sphericity and Aspect Ratio** cannot be changed, this affects the bin size for the plots under the **Sphericities** tab and the plot under the **Aspect Ratio** tab.
- The selection made under **Surface and Contact** changes the bin size for the Surfaces and Contacts plots under the **Surfaces And Contacts** tab.
- The selection made under **Surface-to-Volume Ratio** changes the bin size for the **Surface-to-Volume Ratios plot** under the **Surfaces And Contacts** tab.
- The selection made under **Surface Smoothness** changes the bin size for the **Surface Smoothnesses plot** under the **Surfaces And Contacts** tab.
- The selection made under **Mass** changes the bin size for the plot under the **Mass** tab.
- The selection made under **Moment of Inertia** changes the bin size for the plot under the **Moment of Inertia** tab.

## Grain Visualization

In the **Grain Visualization** tab you can import saved structures and computed volume fields which illustrate the grain identification process and its results.

Domain Size: 100 x 100 x 100    Voxel Length: 698.302 nm    Load Structure

Input Map    Log Map    Post Map    Results    Grain Visualization    Create Videos    Metadata

**Grain-Segmentation Result**

|                                     |            |
|-------------------------------------|------------|
| Load Grains as Index Image          | Load *.g32 |
| Load Grain-Size Distribution        | Load *.gsd |
| Load Grain-Orientation Distribution | Load *.gof |
| Load Grain-Contacts Structure       | Load *.gdt |
| Load Grain-Network Structure        | Load *.gad |

**Thresholding Result**

|                           |            |
|---------------------------|------------|
| Load Grain-Type Structure | Load *.gdt |
| Load Grain-Type Structure | Load *.gad |

**Shape-Analysis Result**

|                                                    |            |
|----------------------------------------------------|------------|
| Load Grain Fit Shapes                              | Load *.gad |
| Load Comparison of Segmented Grains and their Fits | Load *.gdt |
| Load Euclidean Distance Transform per Grain        | Load *.dst |

**Intermediate Results**

|                                                            |            |
|------------------------------------------------------------|------------|
| Load Grains from Step 1 (Result of Watershed)              | Load *.gdt |
| Load Grains from Step 2 (Result of Grain Reconnection)     | Load *.gdt |
| Load Grains from Step 3 (Result of Boundary-Grain Removal) | Load *.gdt |

Several options are available for the visualization of the different steps of **Identify Grains** and for the evaluation of the quality of the results. Some options might be unavailable, depending on the previously chosen parameters in the **Identify Grains** dialog ([Output Options tab](#)<sup>[28]</sup>). The visualization options are grouped into panels.



**Note!** For both the 3D and 2D visualization of the volume fields, reduce the visibility (in the View Controls) to the [Material to Analyze](#)<sup>[15]</sup> (which is Material ID 01 in this example) because most values in the other parts are zero.

Visible on Material IDs

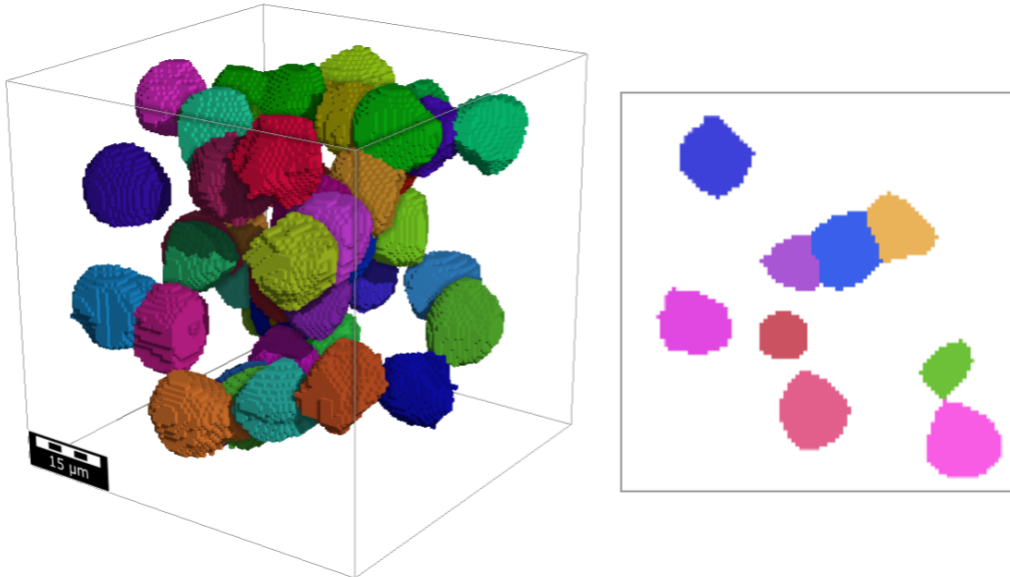
|                                     |    |          |
|-------------------------------------|----|----------|
| 1                                   | 00 | Air      |
| <input checked="" type="checkbox"/> | 01 | Calcite  |
| <input type="checkbox"/>            | 02 | Quartz   |
| <input type="checkbox"/>            | 03 | Feldspar |

## Grain-Segmentation Result

In the first panel, several options for the analysis of the identified grain shapes are available.

### ✓ Load Grains as Index Image

With **Load Grains as Index Image**, all identified grains are assigned to a unique 32-bit color and can be investigated in the Visualization area. The 2D-view of \*.g32 files is particularly suited for visual analysis of the correct segmentation.

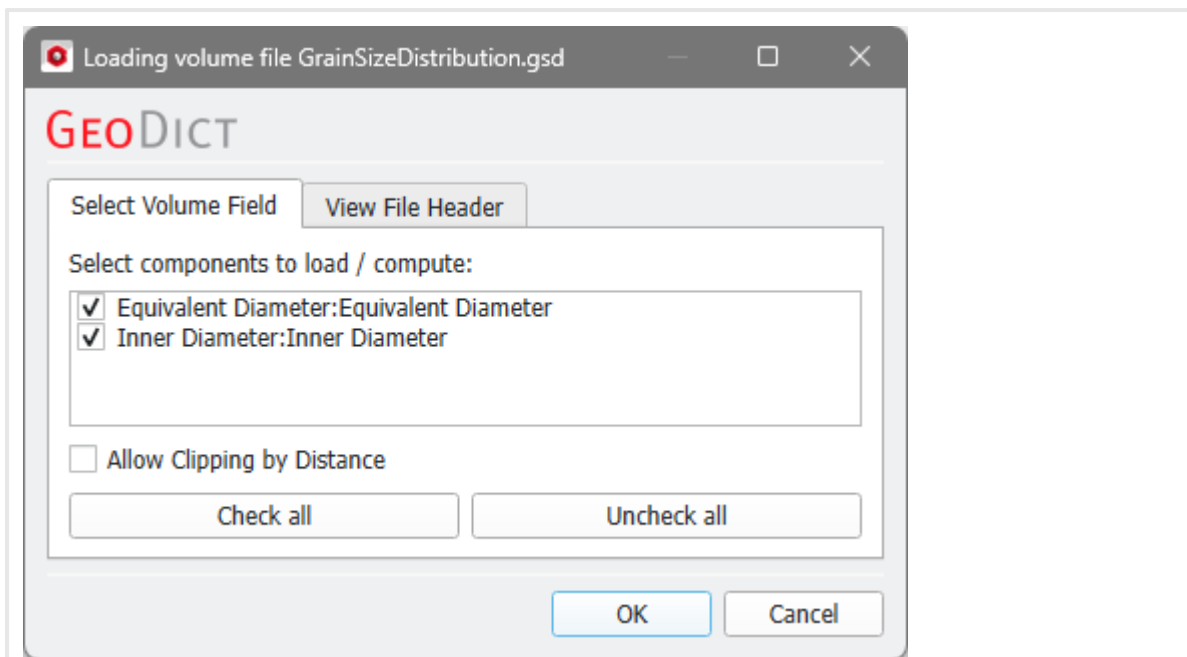


### ✓ Load Grain-Size Distribution

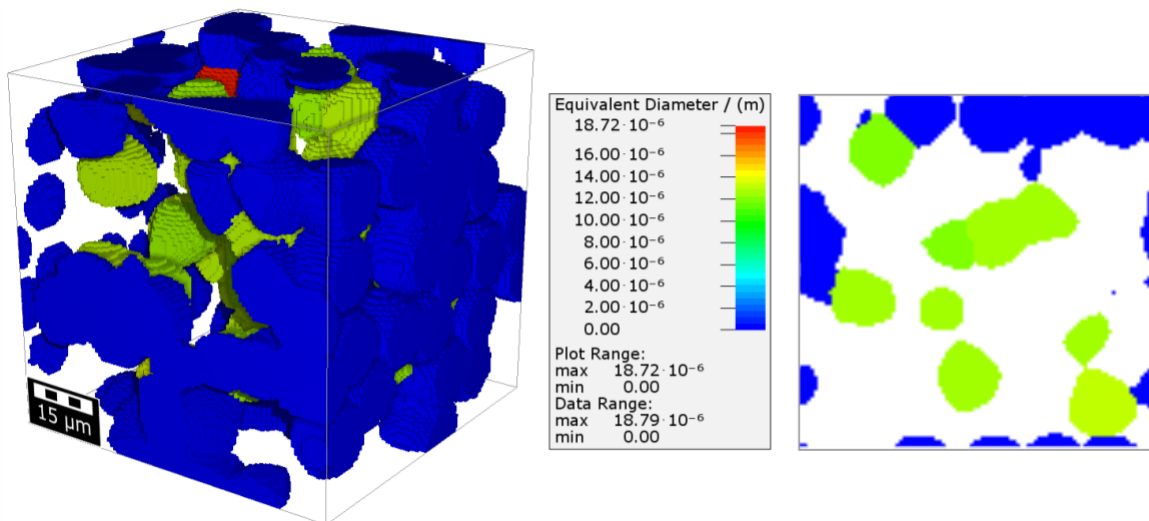
This file is only available if **Save Grain-Size Distribution (Volume-Equivalent Diameter)** as \*.gsd has been checked in the [Output Options](#) <sup>28</sup> tab and contains by default the **Equivalent Diameter** field, which is the diameter of a sphere with the same volume as the grain.

If **Save Inscribed-Sphere Diameters and Sheppard Sphericities** was checked, the \*.gsd file additionally contains the fields of the **Inner Diameter**, which is the diameter of the largest sphere that can be fitted inside the grain.





In the example below, the [Boundary-Grain Removal](#)<sup>22</sup> was activated, thus the grains touching the domain boundary have diameter zero as they are excluded from the analysis.

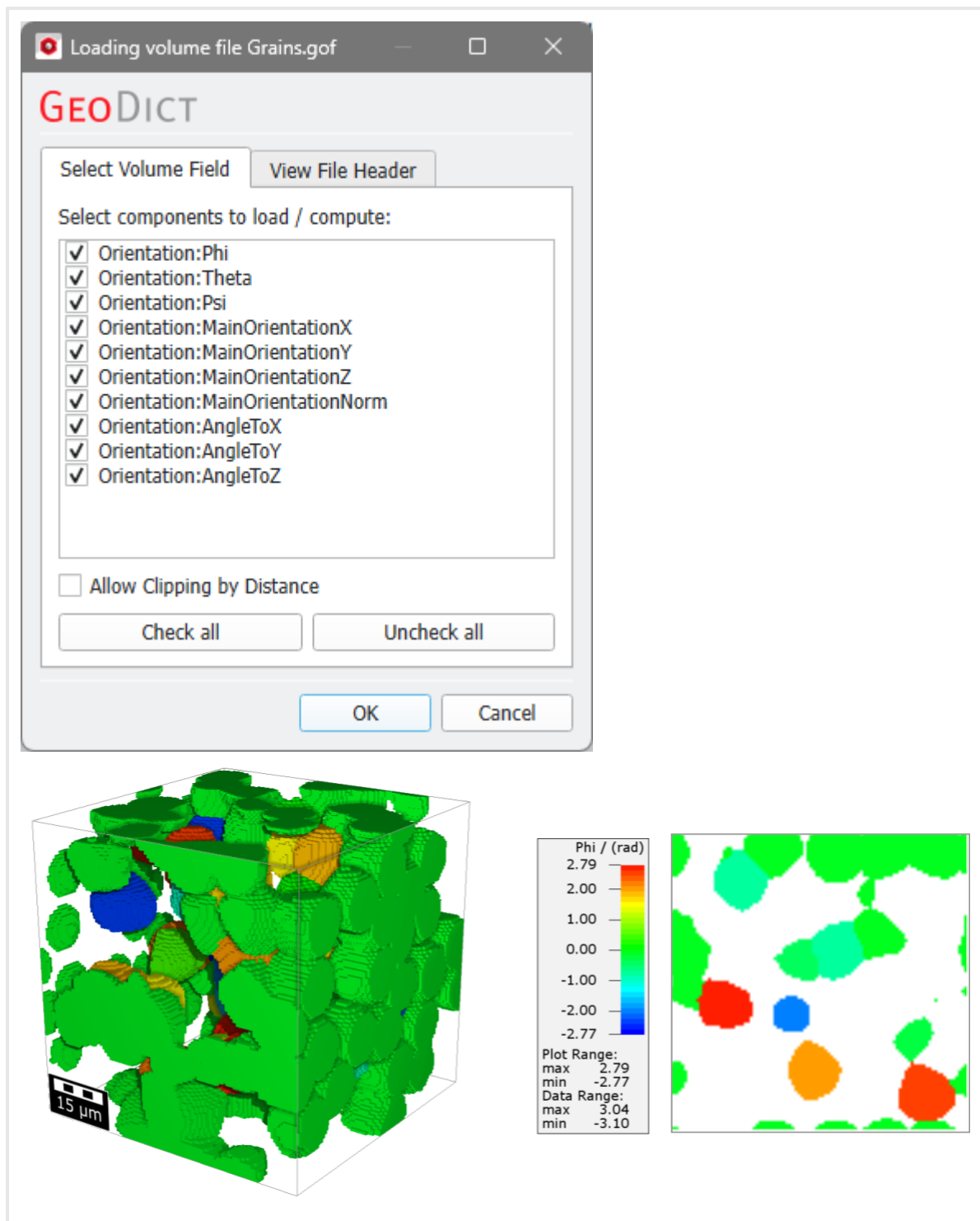


**Note!** When you selected scalar values under [GSD Field Choices](#)<sup>34</sup> in the post-processing widget, you can load the created \*.gsd file here. Depending on the choices, the file might contain additional or other fields.

## ✓ Load Grain-Orientation Distribution

This file is only available if **Save Grain-Orientation Distribution as \*.gof** has been checked in the [Output Options](#)<sup>28</sup> tab.

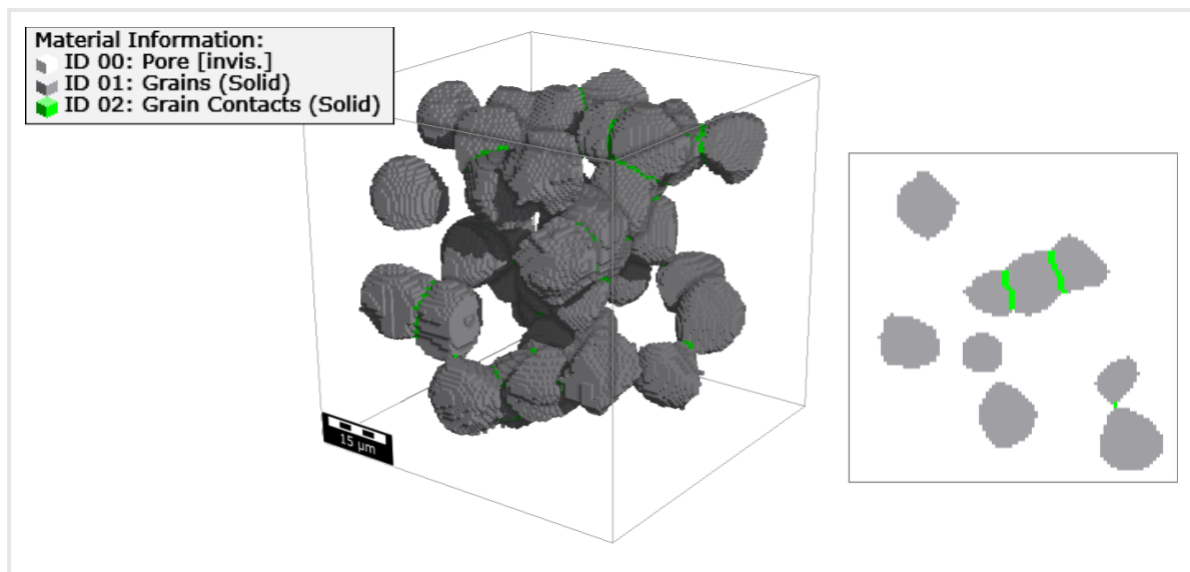
Several fields are saved in this file, e.g., the [Euler Angles](#) are available.



### ✓ Load Grain-Contacts Structure

This file is only available if **Save Grain-Contacts as \*.gdt** has been checked in the [Output Options](#) <sup>28</sup> tab.

The grains have Material ID 01, while the contacts have Material ID 02.

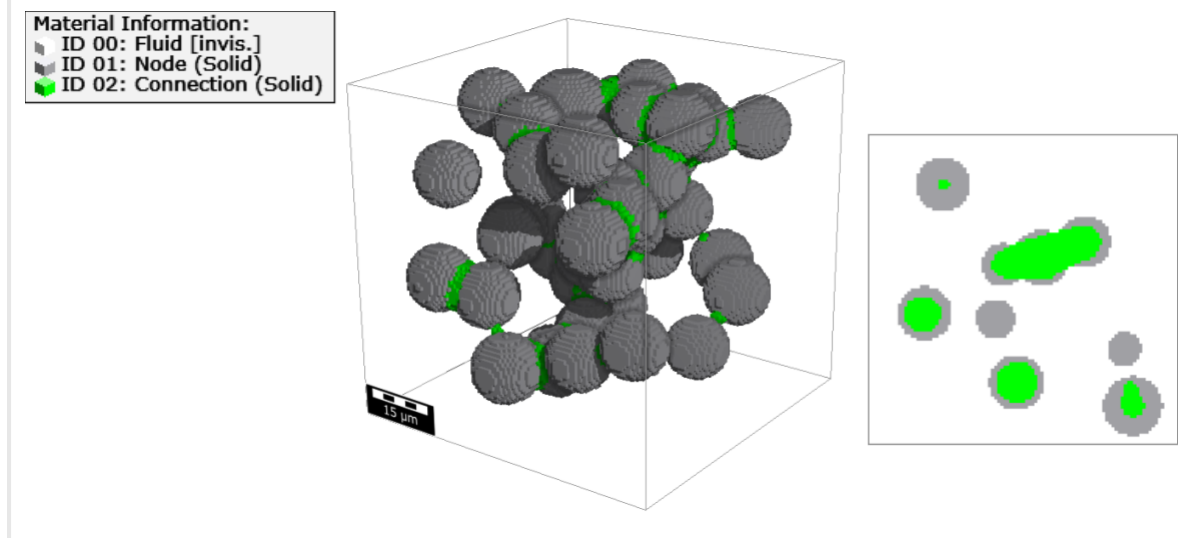


### ✓ Load Grain-Network Structure

This file is only available if **Save Grain-Network Model as \*.gad** has been checked in the [Output Options](#)  tab.

The grains (nodes) have Material ID 01, while the connections between them have Material ID 02.

The \*.gad file is generated from the fitted shapes. Grains are represented by spheres. The sphere centers are equal to the centers of the fit objects and their diameter equals the **Equivalent Diameter** (diameter of volume-equivalent sphere). The grain contacts are represented by short cylindrical fibers between the center points of the spheres. The cross-sectional area of the cylinders equals the contact area between the corresponding grains.



## Thresholding Result

As explained in the previous topic, you can classify the grains by [Thresholding](#)<sup>39</sup> a scalar value. For this example the grains are separated by their Coordination Number into grains with only few contacts to other grains (low coordination number) and many contacts to other grains (higher coordination number).

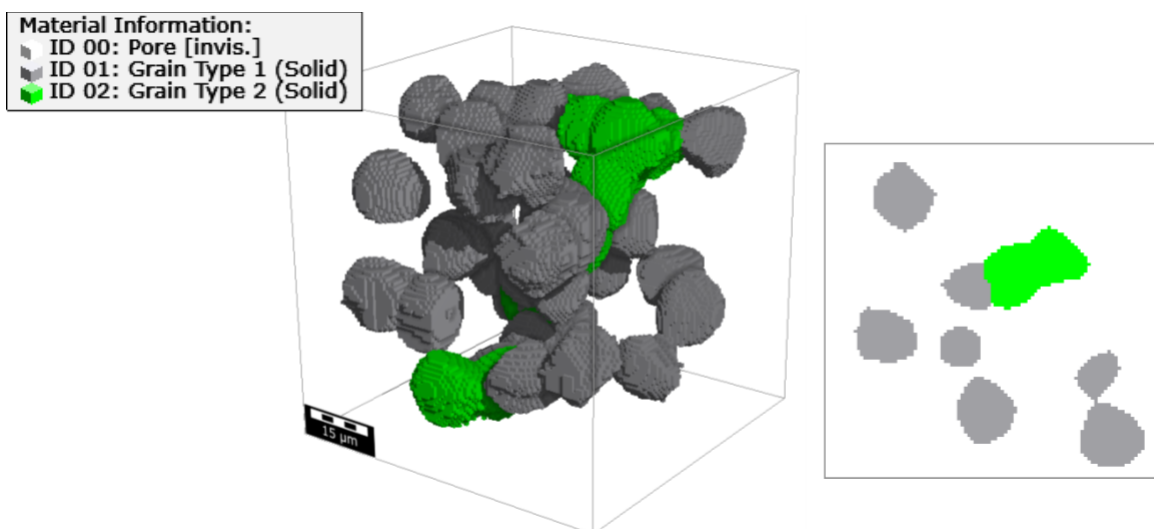
**Threshold by Scalar Value**

|                       |                     |
|-----------------------|---------------------|
| Scalar Value          | Coordination Number |
| Number of Bins        | 10                  |
| Thresholding Method   | k-Means             |
| Number of Grain Types | 2                   |

If you change the threshold settings, the grain-type structure will be recomputed.

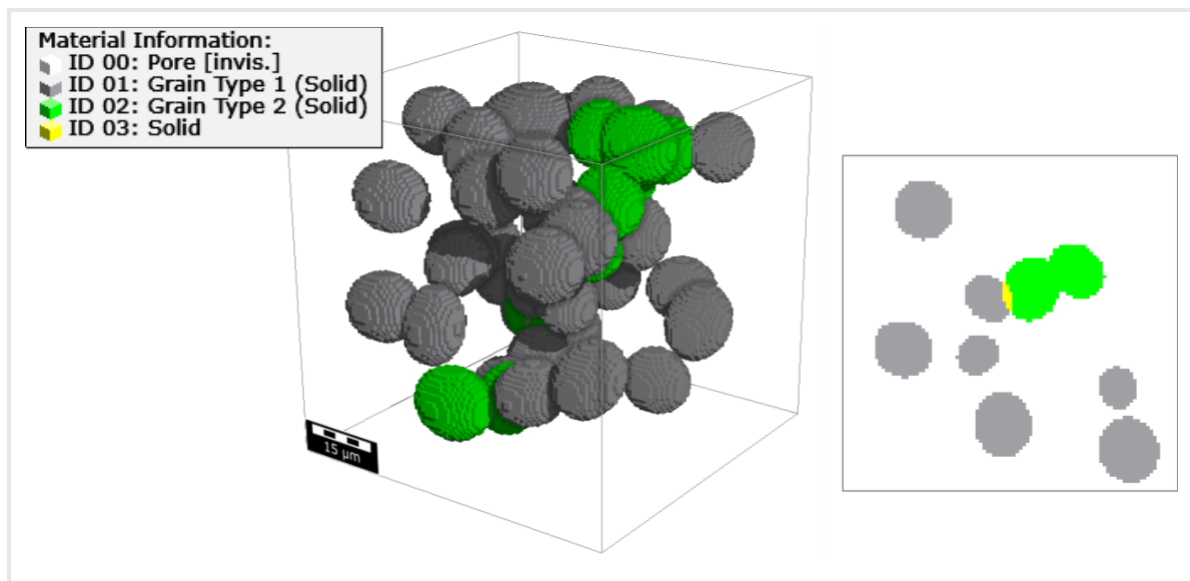
### ✓ Load Grain-Type Structure as \*.gdt

The grain-type structure saved in \*.gdt format contains the identified grains with different Material IDs for the different grain types. The grains with a scalar value below the threshold are assigned to Material ID 01 and the grains with a larger scalar value are assigned to Material ID 02.



### ✓ Load Grain-Type Structure as \*.gad

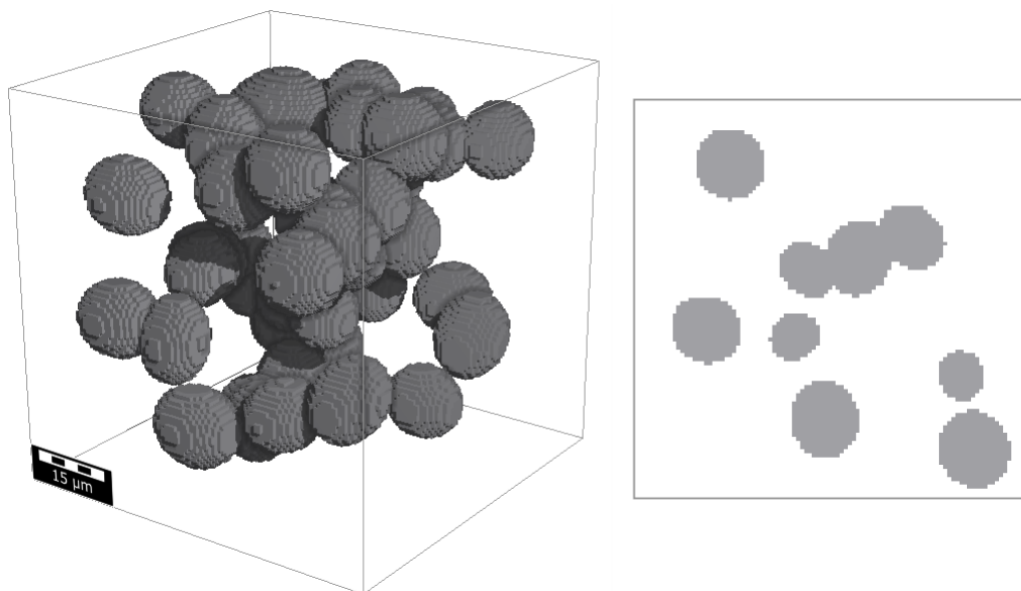
The grain-type structure saved in \*.gad format contains the fitted shapes with different Material IDs for the different grain types. Again, the grains with a scalar value below the threshold are assigned to Material ID 01 and the grains with a larger scalar value are assigned to Material ID 02.



## Shape-Analysis Result

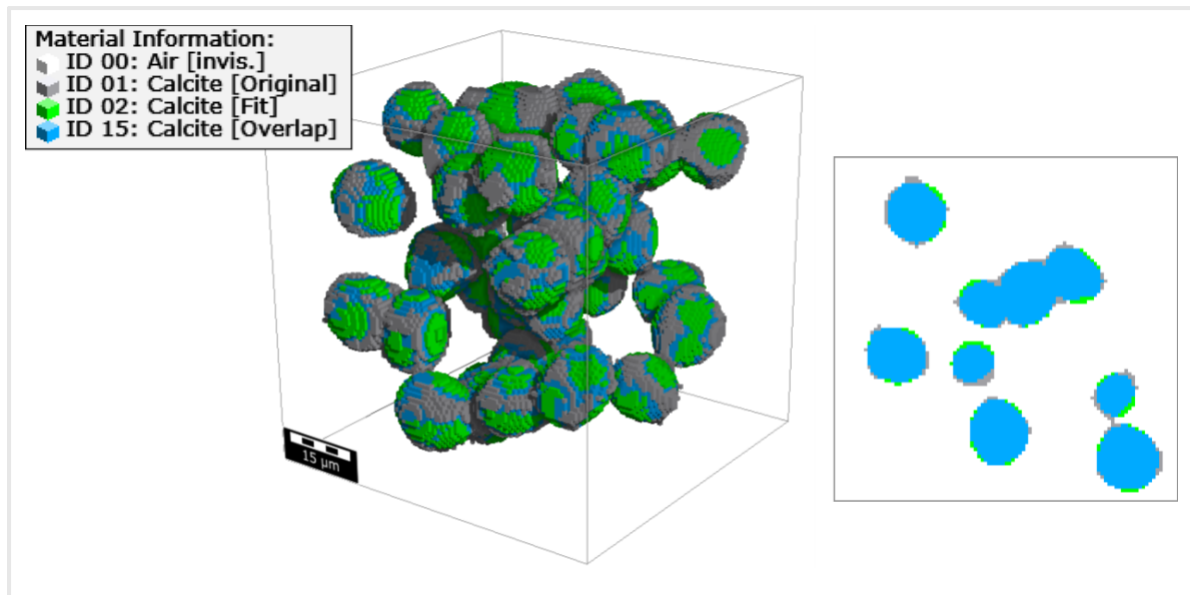
### ✓ Load Grain Fit Shapes

With **Load Grain Fit Shapes**, load the \*.gad file of the fitted shapes for the individual grains.



### ✓ Load Comparison of Segmented Grains and their Fits

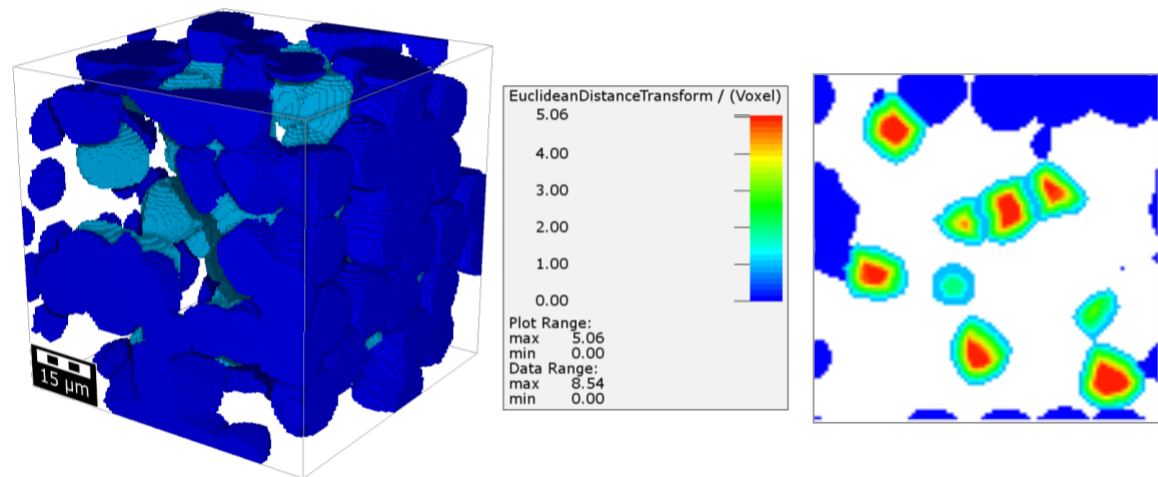
To evaluate the performance of the grain identification with the chosen options use **Load Comparison of Segmented Grains and their Fits**. The identified grains, their best-fit shapes, and their overlap are shown as different Material IDs (**Original**, **Fit**, and **Overlap**). Also have a look at the example in the topic [Grain Shape Analysis](#)<sup>23</sup>.



## ✓ Load Euclidean Distance Transform per Grain

This file is only available if **Save Euclidean Distance Transform per Grain as \*.dst** has been checked in the [Output Options](#) <sup>28</sup> tab.

During the Identify Grains algorithm, first a Euclidean Distance Transform (EDT) and based on the results of a Watershed transformation are performed. You can load the result of the EDT as volume file by clicking **Load \*.dst**.



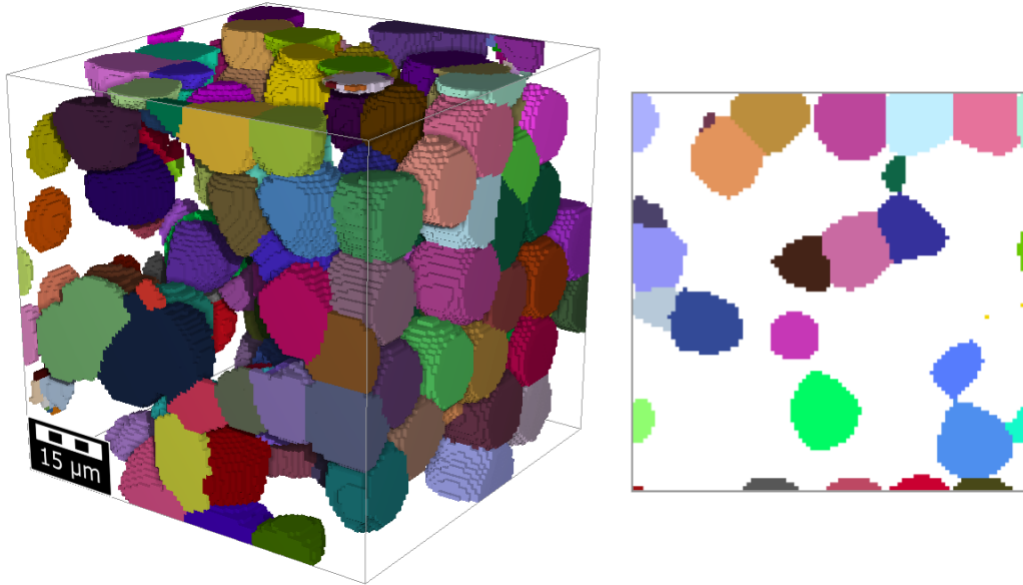
## Intermediate Results

Results from the identification steps are loaded in the **Intermediate Results** panel.

## ✓ Load Grains from Step 1 (Result of Watershed)

With **Load Grains from Step 1 (Result of Watershed)**, the segmented grains after the

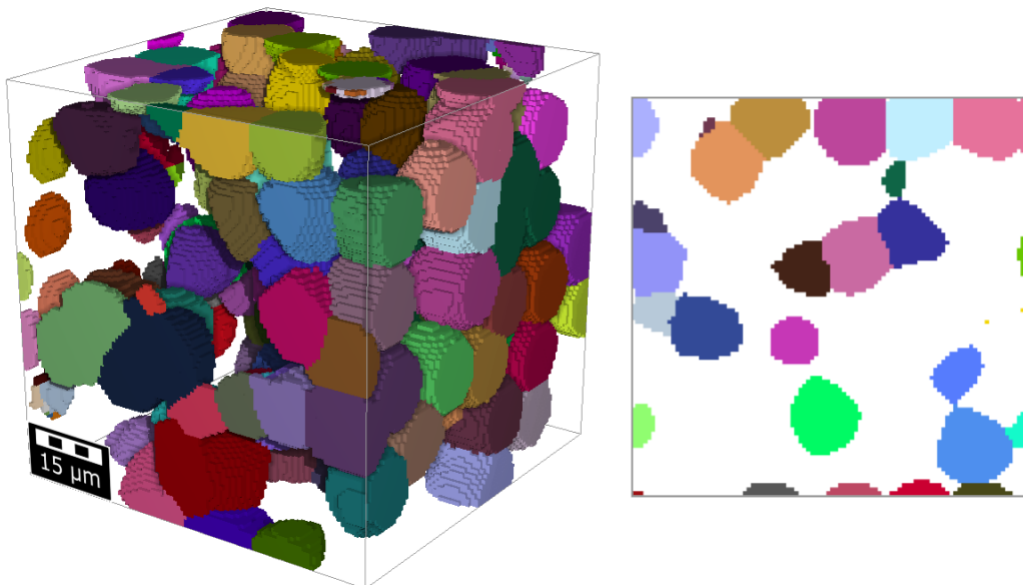
Watershed transform are shown without any post-processing. Depending on the structure and the chosen [Minimal Grain Diameter](#)<sup>[15]</sup>, this step might already be good enough to identify the grains. Otherwise, this option is useful to check the initialization options – mainly if the **Minimal Grain Diameter** was chosen correctly for the analyzed grains.



#### ✓ Load Grains from Step 2 (Result of Grain Reconnection)

This file is only available if [Reconnect Fragmented Grains](#)<sup>[19]</sup> has been checked in the **Grain Segmentation** tab.

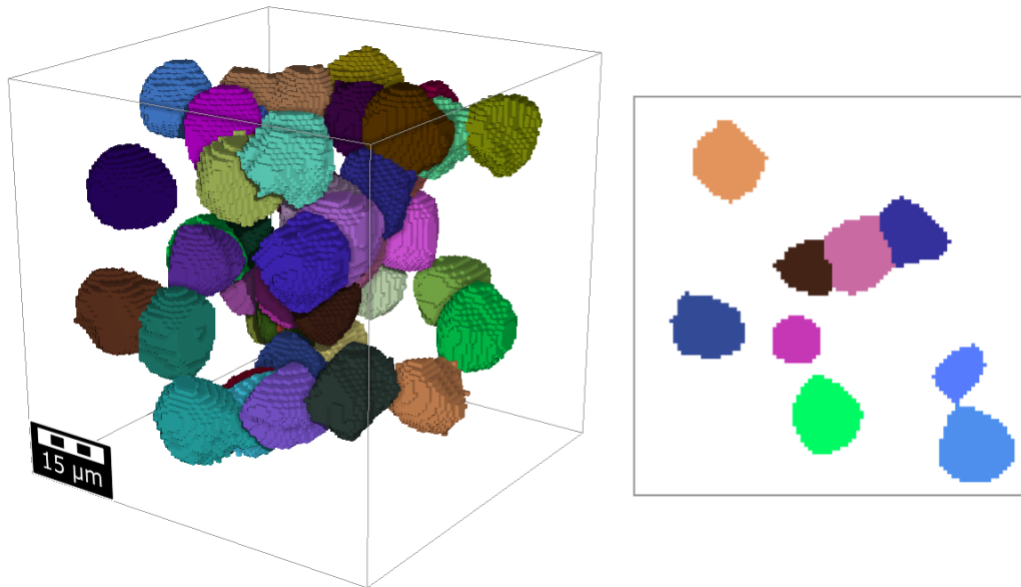
By clicking **Load Grains from Step 2 (Result of Grain Reconnection)**, the grains after the Grain-Fragment Reconnection are loaded in GeoDict. This way it can be assessed whether the chosen value for **Interface Threshold** suits the analyzed grains.



### ✓ Load Grains from Step 3 (Result of Boundary-Grain Removal)

This file is only available if [Remove Grain Fragments at Domain Boundary](#)<sup>[22]</sup> has been checked in the **Grain Segmentation** tab.

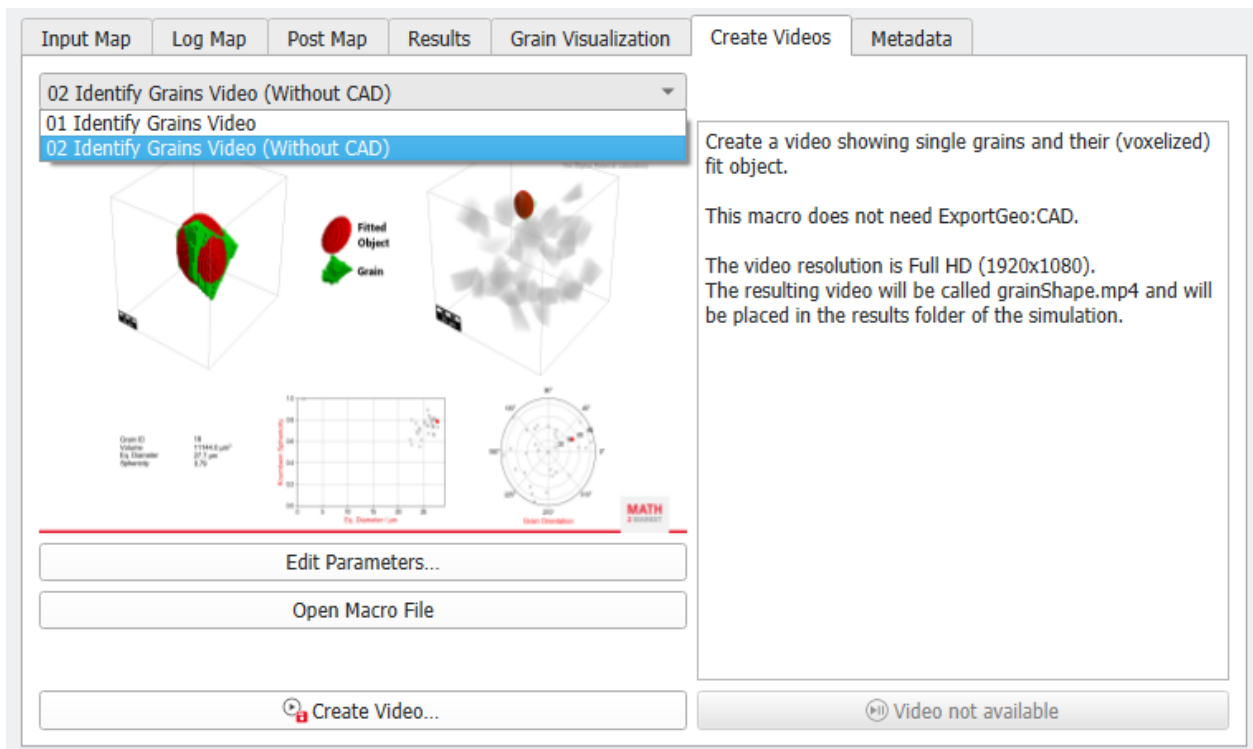
Click **Load Grains from Step 3 (Result of Boundary-Grain Removal)** to import the identified grains resulting from the removal of grain fragments at the domain boundary. This will be the basis structure for the fitting of the fit objects.



## Create Videos

Generate a video showing the largest identified grains compared to their fit shapes from the **Create Videos** tab. The exemplary video shows which information will be shown in the video. At the top right the current grain and its fit in the whole structure is highlighted. At the top left, a crop to the single grain overlayed with its fit is shown. At the bottom left, the **Grain ID**, **Volume**, **Equivalent Diameter**, and **Sphericity** are displayed. In the bottom middle, the corresponding marker in the Equivalent Diameter - Krumbein Sphericity Scatter Plot is highlighted. At the bottom right, you can find the grain orientation highlighted in the orientation polar plot.



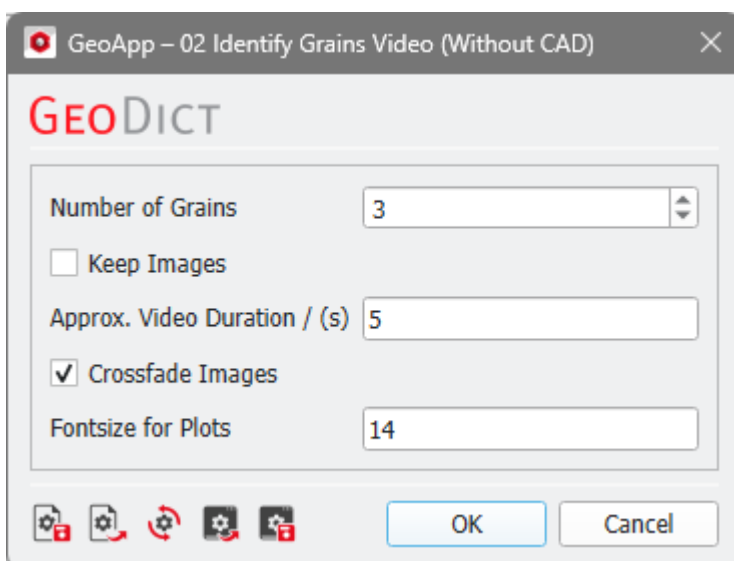


Above the exemplary video, choose from the drop-down menu if you want to create the video with or without CAD.

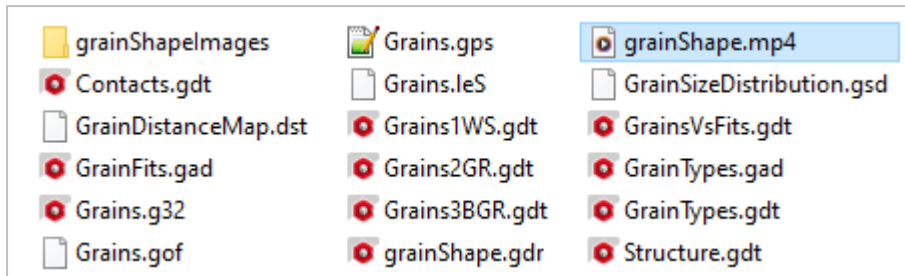


**Important!** You need an ExportGeo-CAD license to create the video with CAD! The version without CAD works in any case.

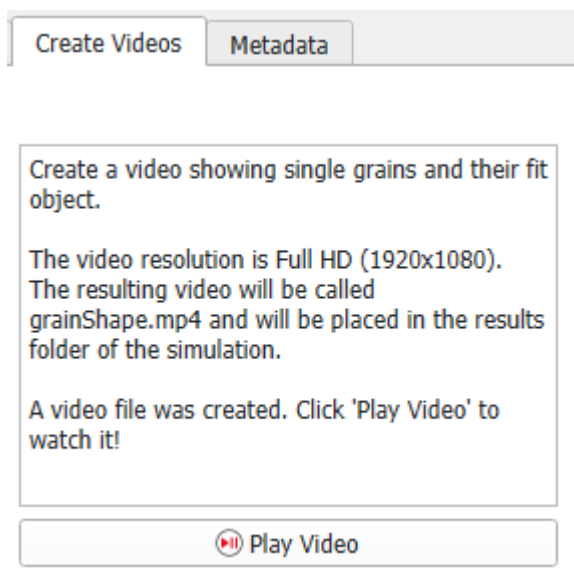
Click **Edit Parameters...** to choose the **Number of Grains** that should appear in the video. Additionally, you can edit the **Approx. Video Duration** and the **Fontsize for Plots** and their labels. Check **Keep Images** if you want to save the single images of the video. In the upper right corner of the video, the position of the currently shown grain and its fit in the whole structure is shown. If you want a smooth transition from grain to its fit, you can check **Crossfade Images**. Click OK to save the parameters and close the dialog.



To start the creation of the video click the **Create Video...** button. The video and the additional files are saved in the results folder belonging to the loaded \*.gdr file. Open the result folder by right-clicking on the file name or file path in the Result Viewer Header section and choose **Open Result Folder**.



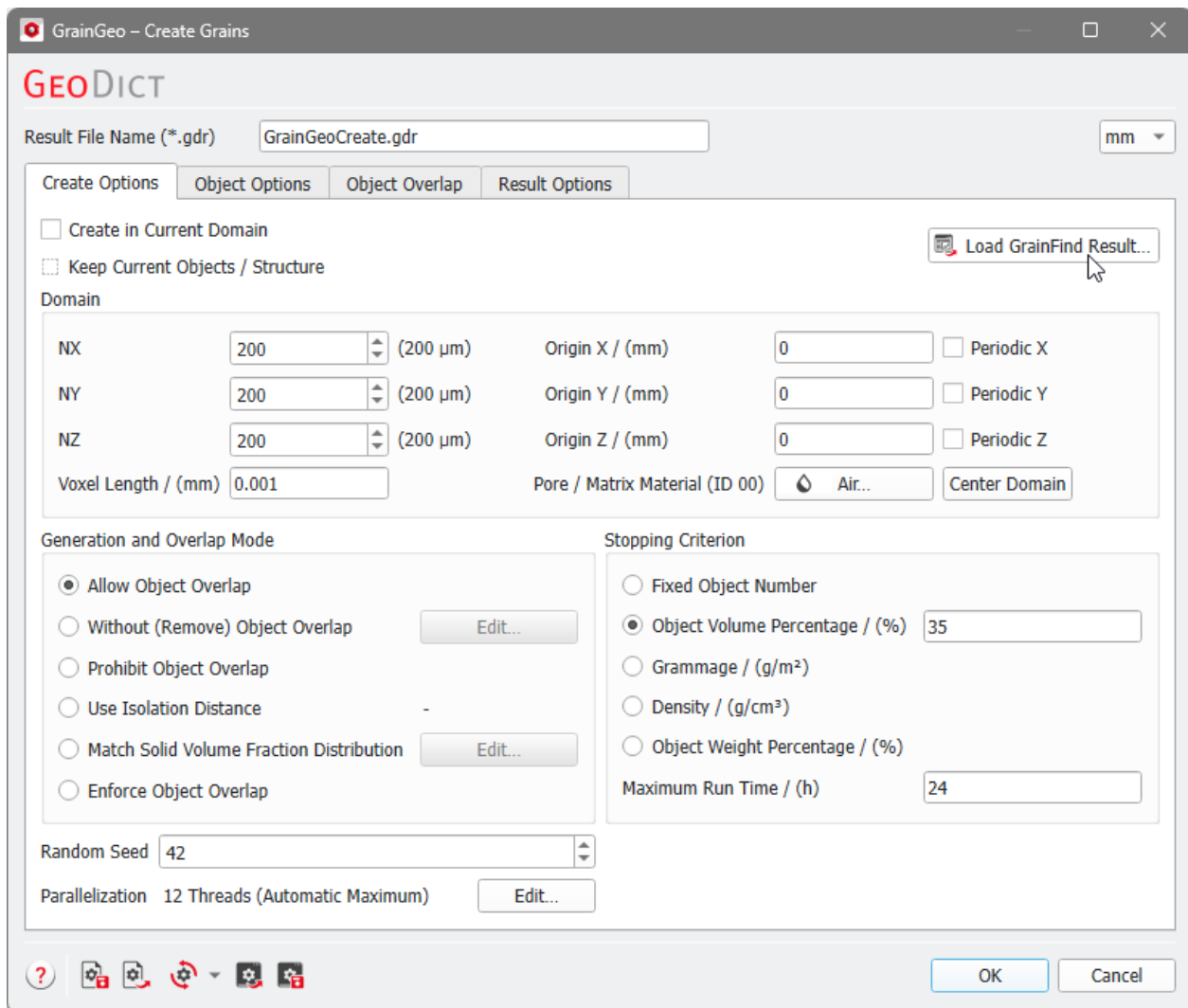
Click **Play Video** on the bottom right opens the video file in the default video player.



### 1.1.4 Connecting GrainFind analysis results with GrainGeo

Use the results of an **Identify Grains** run in GrainGeo to create a “digital twin” of the material, which is a structure with similar properties.

Start GrainGeo by selecting **Model** → **GrainGeo** in the menu bar and choose **Create Grains** from the pull-down menu. Click the **Edit...** button. In the upper right of the **GrainGeo Create Options** dialog, click **Load GrainFind Result...** and select a GeoDict result file (\*.gdr) from a GrainFind run.



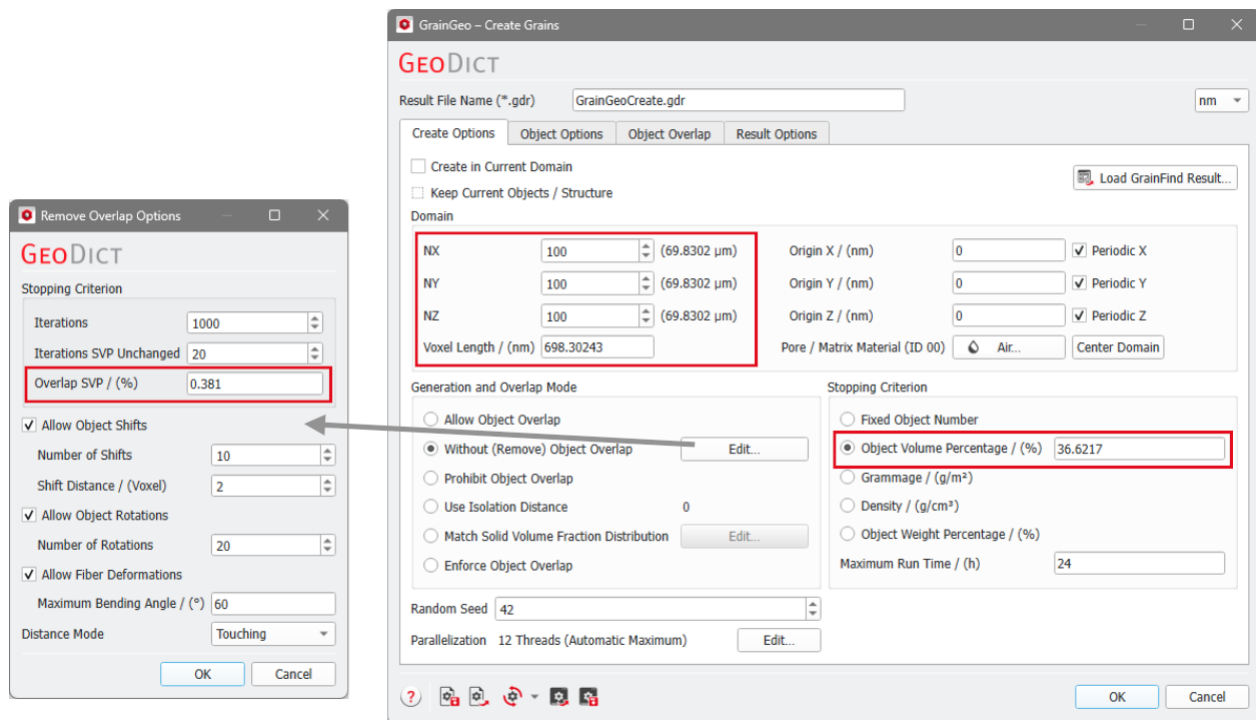
The data from the \*.gdr file is now directly loaded into the GrainGeo dialog. In the figures below, the parameters directly imported from the GrainFind result are displayed under the **Create Options** tab and the **Object Options** tab in the **GrainGeo Create Options** dialog.

The GrainFind results are automatically entered in the **Domain** parameters, the **Generation and Overlap Mode (Overlap SVP in the options of Without (Remove) Object Overlap)**, and in the **Object Volume Percentage** of the structure under the Create Options tab.

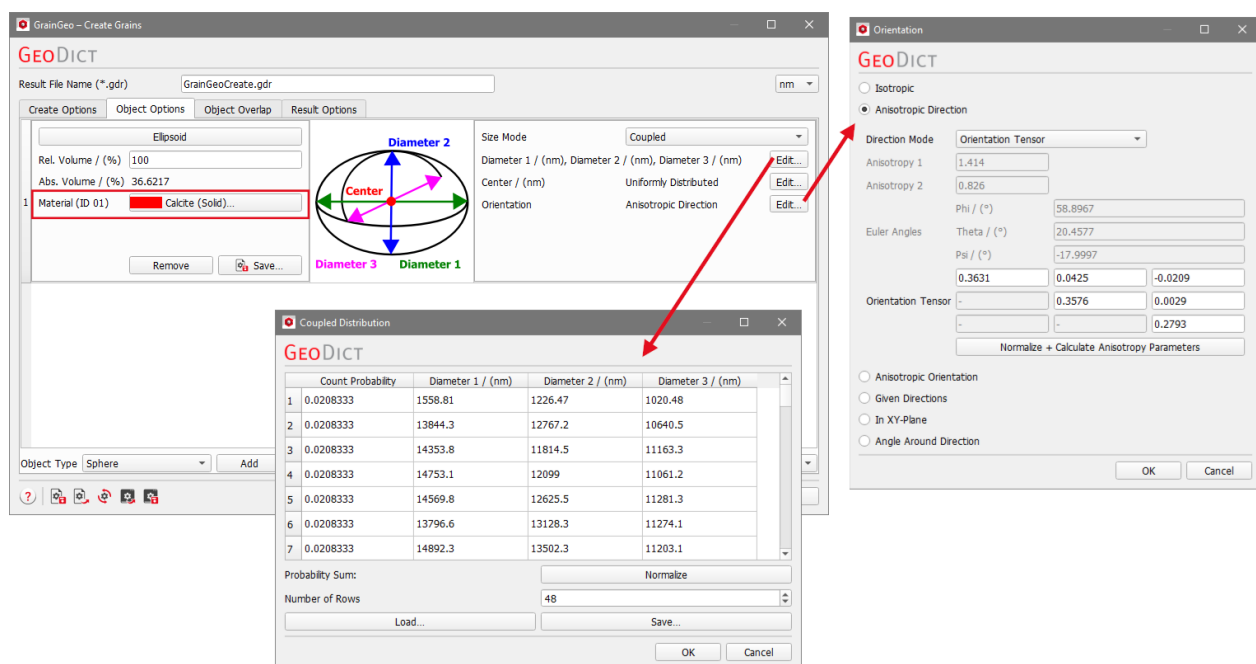


**Know how!** In the Domain panel, the **Periodicity** in all directions is automatically selected, even if the original structure was not periodic. This is done, because the **Remove Overlap** algorithm works best with periodic domains.

## GrainFind: Identify Grains



The identification analysis also automatically delivers the **Material** of the identified objects (for example, Calcite), the **Diameter** size and the **Orientation** parameters of the grains under the Object Options tab.

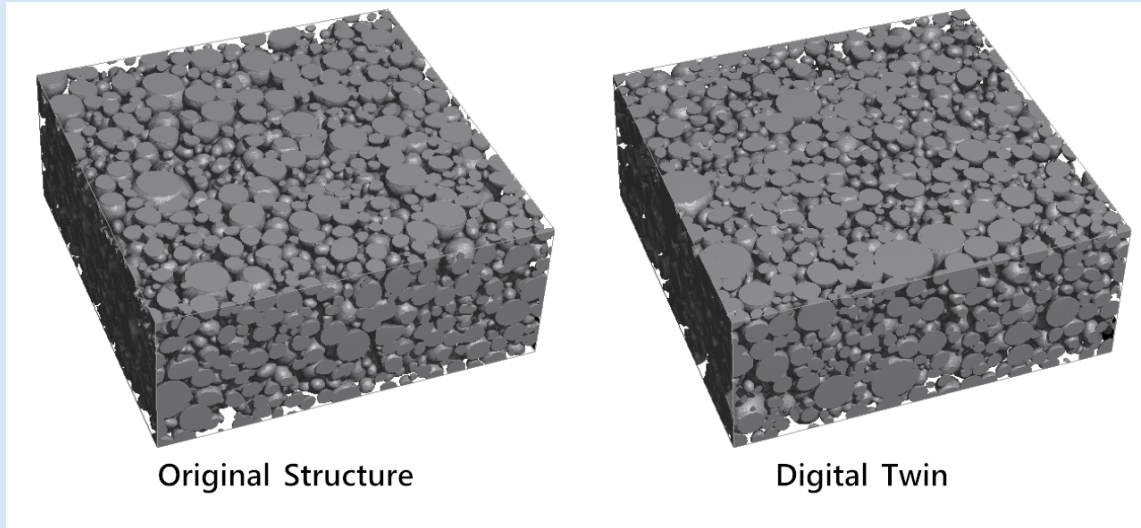


Click **Generate** in the **GrainGeo** section to generate a structure with the parameters obtained from GrainFind with GrainGeo. In the example below, on the left side the original structure (this structure is analyzed with GrainFind) and on the right side a structure based on the GrainFind parameters are shown.



### Example: Digital Twin of a 3D-Scan

With GrainFind and GrainGeo you can also create digital twins of large segmented scans, like the NMC cathode structure provided by the ETH Zurich [published by Ebner et. al.](#)<sup>[92]</sup>, which can be seen below. For more details, please have a look at our tutorial "[Building a statistical Digital Twin of a cathode](#)".

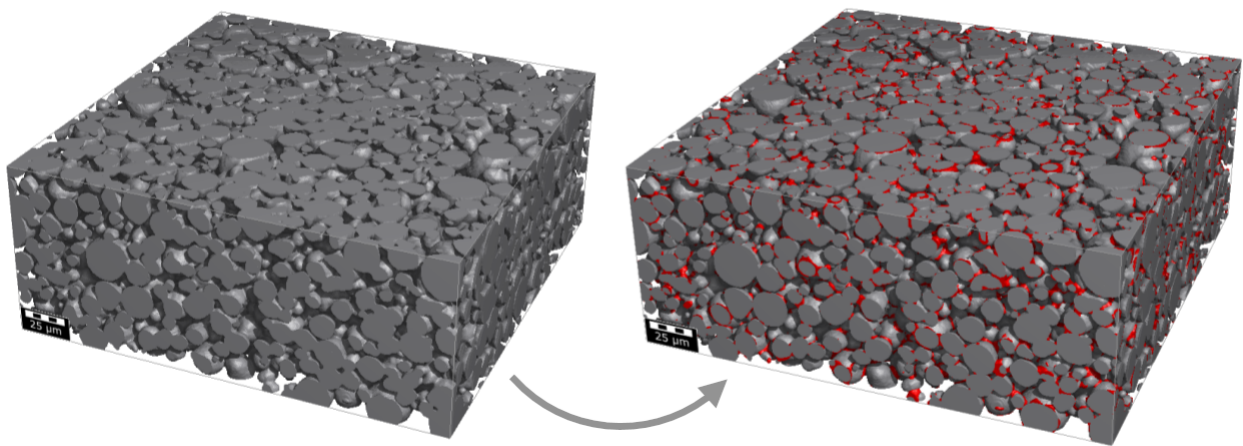


### 1.2 Identify Binder (AI)

While the separation of solid materials and pores of a structure can easily be done using image processing methods in ImportGeo-Vol, the separation of binder from grains is often not possible since they have similar gray values in the scan.

If you want to separate binder from the grains, you can use the **Identify Binder (AI)** command from GrainFind. In this command, a trained neural network is applied to the structure and its output determines whether a solid voxel is binder or not.

The structure used for the explanations is a segmented sample of a NMC cathode structure from the Laboratory for Nanoelectronics, ETH Zurich [published by Ebner et. al.](#) <sup>92</sup>.



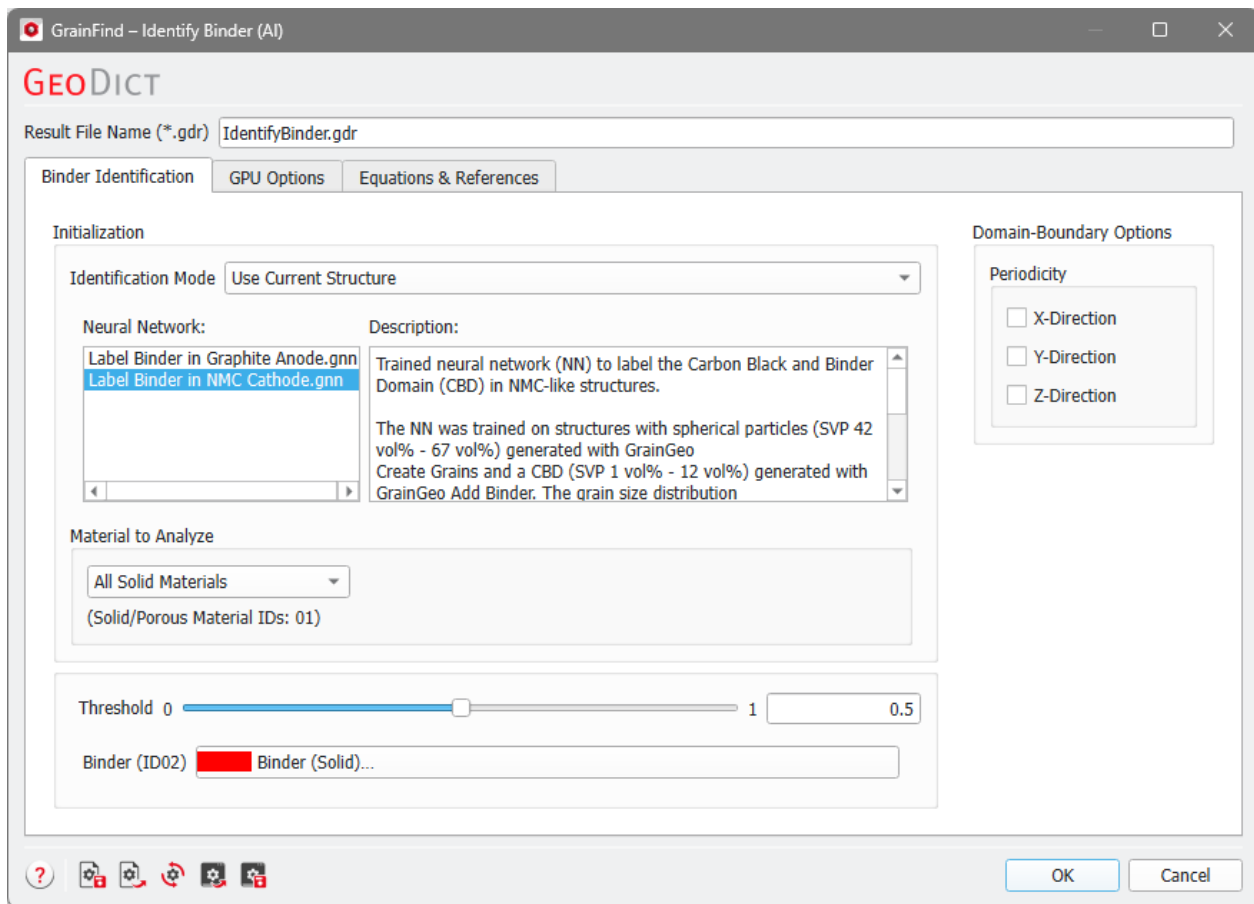
The **Identify Binder (AI)** command:

- [Options](#) <sup>66</sup>  
Set the parameters for the identification.
- [Results](#) <sup>72</sup>  
View the computed results.

#### 1.2.1 Options

The **Identify Binder (AI)** dialog opens when clicking the **Edit...** button and includes the **Binder Identification** tab, the **GPU Options** tab and the **Equations & References** tab, which cites several [references](#) <sup>92</sup>.

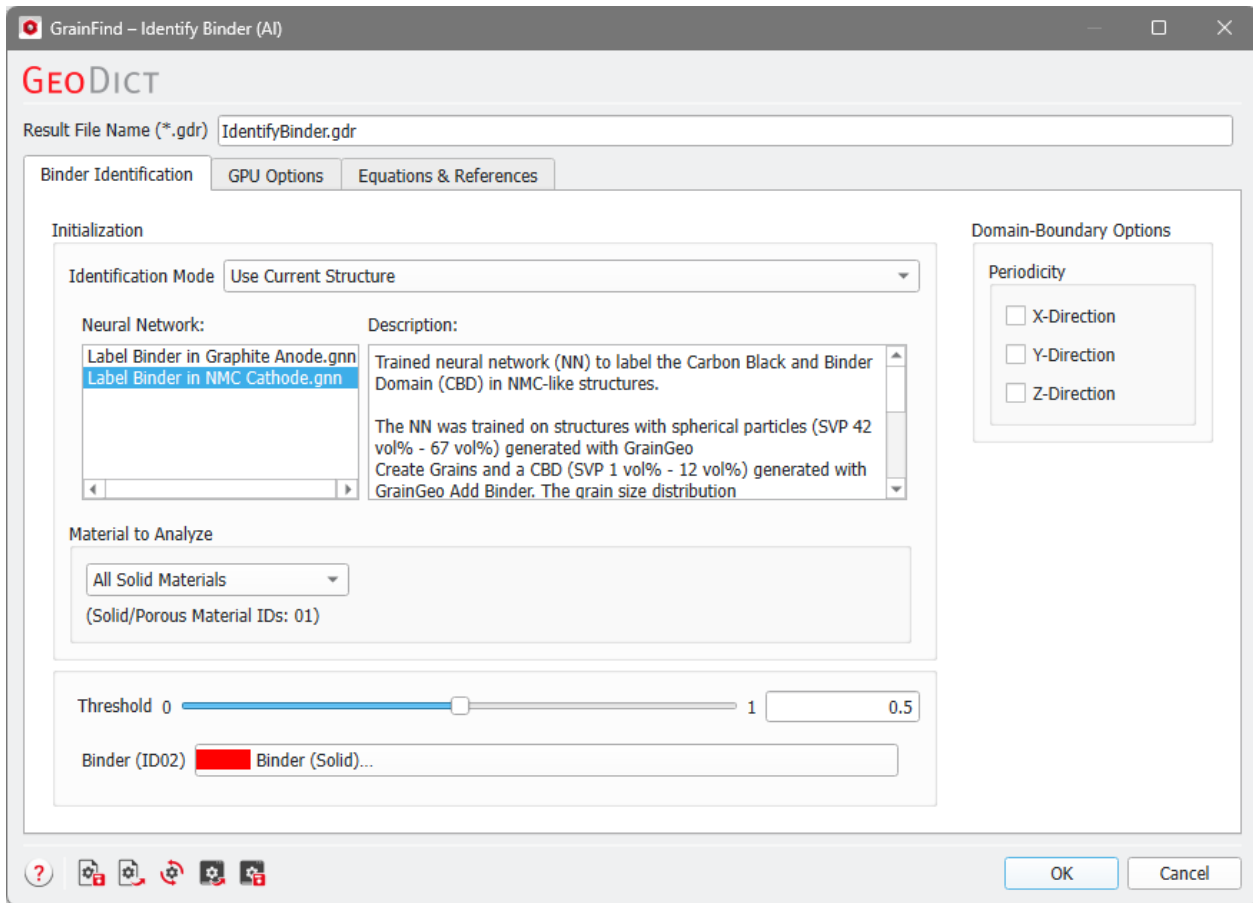
At the top of the dialog, enter the **Result File Name**. The result file is saved in the chosen project folder (**File** → **Choose Project Folder** in the menu bar).



### Identify Binder (AI) Options:

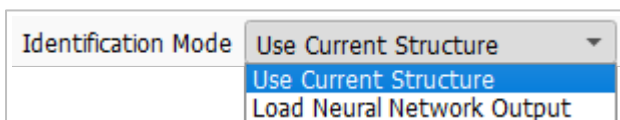
- [Binder Identification](#)<sup>68</sup>
- [GPU Options](#)<sup>72</sup>

## Binder Identification



### Initialization

Select if you want to **Use Current Structure** (recommended for first analysis) or **Load Neural Network Output** as **Identification Mode**.



#### ✓ Use Current Structure

The default **Use Current Structure** applies the binder identification to the structure currently available in the GeoDict memory.

Select one of the neural networks available under **Neural Network**. Currently two \*.gnn (**GeoDict neural network parameter**) files are delivered with GrainFind, making it possible to select the best suitable one for the structure under consideration.



| Neural Network:                                                                          | Description:                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
|------------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <div>Label Binder in Graphite Anode.gnn</div> <div>Label Binder in NMC Cathode.gnn</div> | <p>Trained neural network (NN) to label the Carbon Black and Binder Domain (CBD) in NMC-like structures.</p> <p>The NN was trained on structures with spherical particles (SVP 42 vol% - 67 vol%) generated with GrainGeo Create Grains and a CBD (SVP 1 vol% - 12 vol%) generated with GrainGeo Add Binder. The grain size distribution used for generating the training structures was obtained by analyzing the CT scan of a NMC cathode with GrainFind Identify Grains. This work has been conducted within the</p> |

In the **Description**, the current constraints for the application of the chosen neural network are listed, like the grain shape and size for that the neural network was trained. To ensure that the grains in the present structure fit to these conditions, we recommended to use [Estimate Grain Diameter](#) before running the binder identification.

Neural networks trained with GeoDict-AI can be used by copying the corresponding .gnn-file into the installation directory for **Identify Binder (AI)** (e.g., in c:\Program Files\Math2Market GmbH\GeoDict 2026\GrainFind\IdentifyBinder). Then, these neural networks appear as further options in the **Neural Network** field.

### ✓ Load Neural Network Output

In case you want to change only some of the parameters, choose the option **Load Neural Network Output**. Here, you do not have to run the identification for each voxel with the neural network again, which speeds up the analysis.

Identification Mode

Load Neural Network Output

Segmented Material Phase Image (\*.npz)

NeuralNetworkOutput.npz

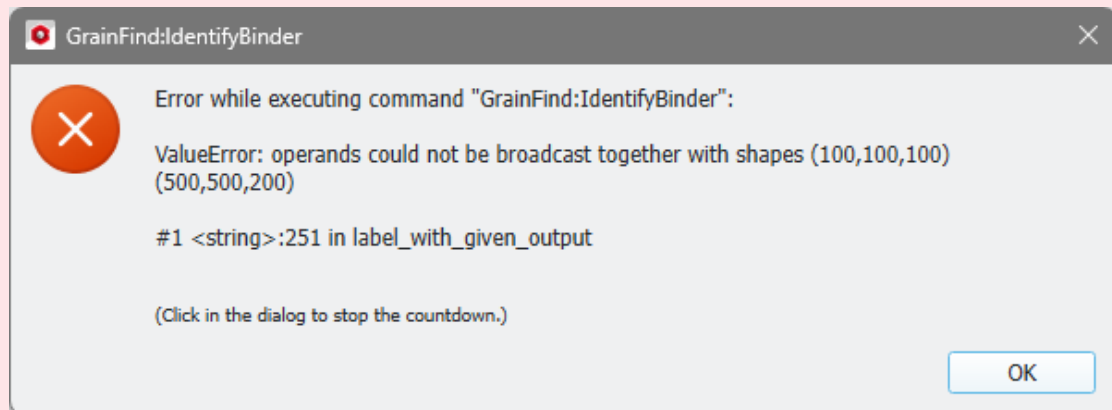
Browse...

Browse to a GeoDict result folder of a previous run of GrainFind-Identify Binder (AI) and select a **nnOutput.npz** file from that folder.

No selection of **Neural Network** is possible since already the output of the neural network is used in this case.

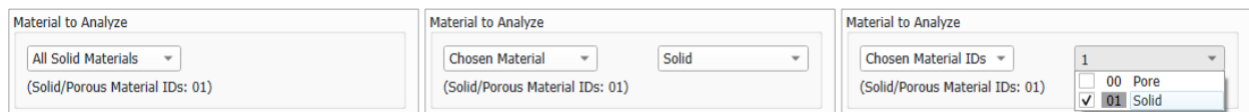


**Important!** The currently loaded structure needs to be the same with which the neural network was trained. Otherwise an error message appears.



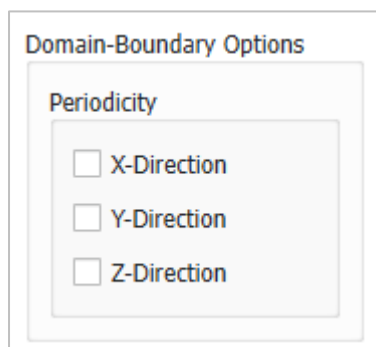
Also, make the same selection for **Material to Analyze** (see below).

Under **Material to Analyze**, define the part of the structure to be considered in the analysis. Either the complete structure can be analyzed (**All Solid Materials**), an individual material can be selected (**Chosen Material**) or a choice of Material IDs can be made (**Chosen Material IDs**). If the selection includes multiple Material IDs they are combined and analyzed as one single material.



## Domain-Boundary Options

If you have a periodic structure, you can check the boxes for periodicity in the individual directions to apply periodic domain boundary conditions. However, periodicity is unusual for most 3D scans and this setting is rarely activated.



## Additional Parameters

✓ Threshold

The neural network provides a probability whether a solid voxel is binder or not for every voxel. The **Threshold** defines the limit for labeling a voxel as binder. It is recommended to keep the default value of 0.5 for the first run.

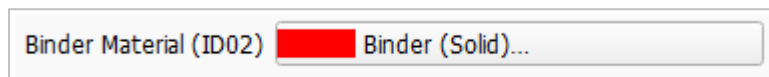


Threshold 0  1

You can load a volume field of the computed probabilities in the Result Viewer from the [Binder Visualization](#) <sup>75</sup> tab, which helps you to decide on a suited **Threshold**.

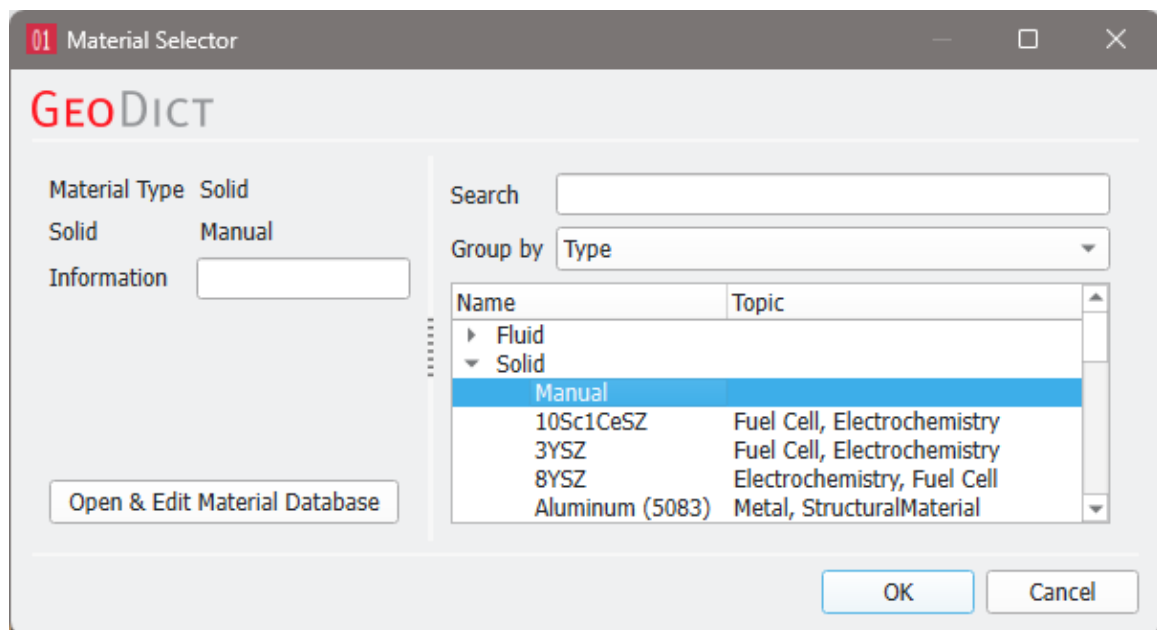
## ✓ Binder Material

Select the material assigned to the recognized binder. Click on the default material to select a new one from the Material Selector.



Binder Material (ID02) Binder (Solid)...

The pull-down menu gives access to selecting the desired material from the GeoDict **Material Database**. When none of the materials available in the database fit the preferred specifications, **Manual** should be chosen. Alternatively, a new material with the desired specifications can be added to the **Material Database** (see the Material Database chapter).



To match realistic material colors for visualization in a certain application, the default material colors can be changed through the **Color & Visibility** tab of the GUI sidebar. For more visualization options, see the Visualization chapter.

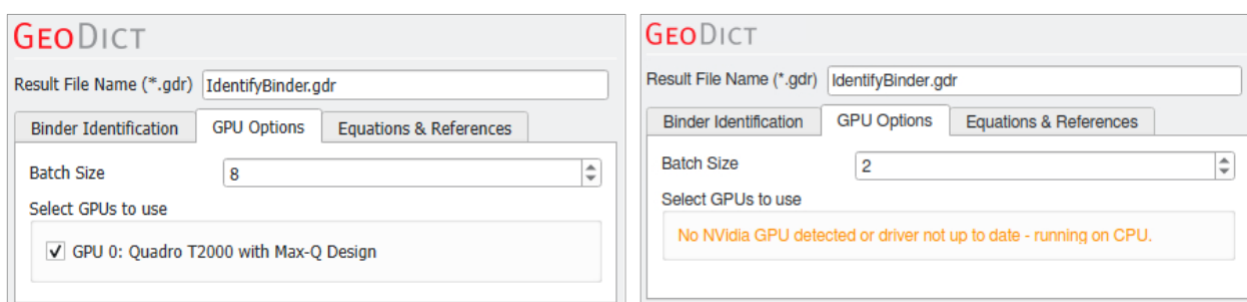
You can also set the color of the **Binder Material ID** (which is the first unused Material ID) to a color different from the color of any solid or pore material present in the original structure. This makes distinguishing the binder from the other materials much

easier. In the example structure only Material ID 00 (invisible) and Material ID 01 (gray) are present. Thus, the binder Material ID 02 is set to red.

Load the Structure with the labeled binder from the [Binder Visualization](#)  tab.

## GPU Options

Identify Binder (AI) can run in GPU mode using a suitable graphic card or in CPU mode. All suitable graphic cards detected during installation of GeoDict are displayed in the **GPU Options** tab. Use the checkboxes to select the graphic card you want to use for the computation. If no graphic card is found during installation a message appears and the run is performed on the CPU.

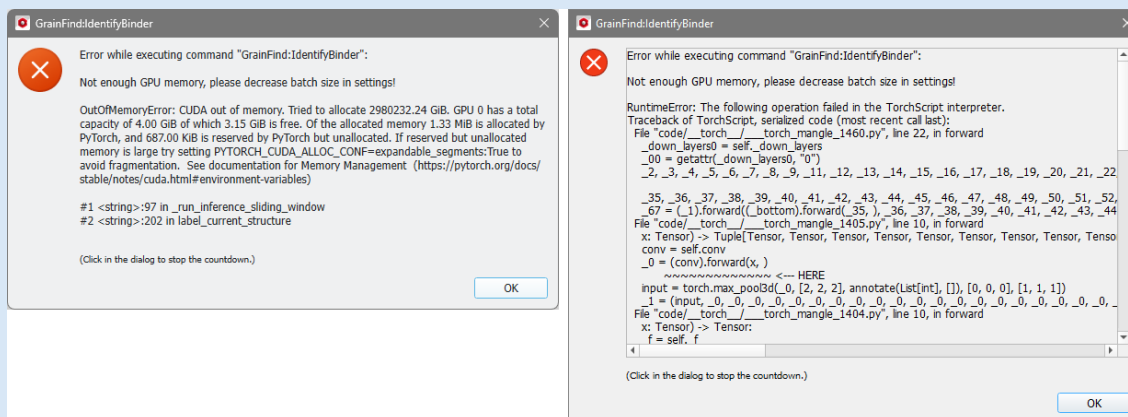


The choice for **Batch Size** is related to the memory available on the graphics card (GPU). Thus, for CPU-based computations, the choice of batch size is not needed and can be left at the default.

Conceptually, the algorithm loads the graphics card with portions of work called **batches**. The higher the number of batches, the faster the computation will be. Currently, the selection must be made manually, and the parameter is set following the value entered in **Batch Size**.



**Note!** The batch size might be chosen too large for the graphics card. In this case, an error message appears and the number of batches needs to be reduced.



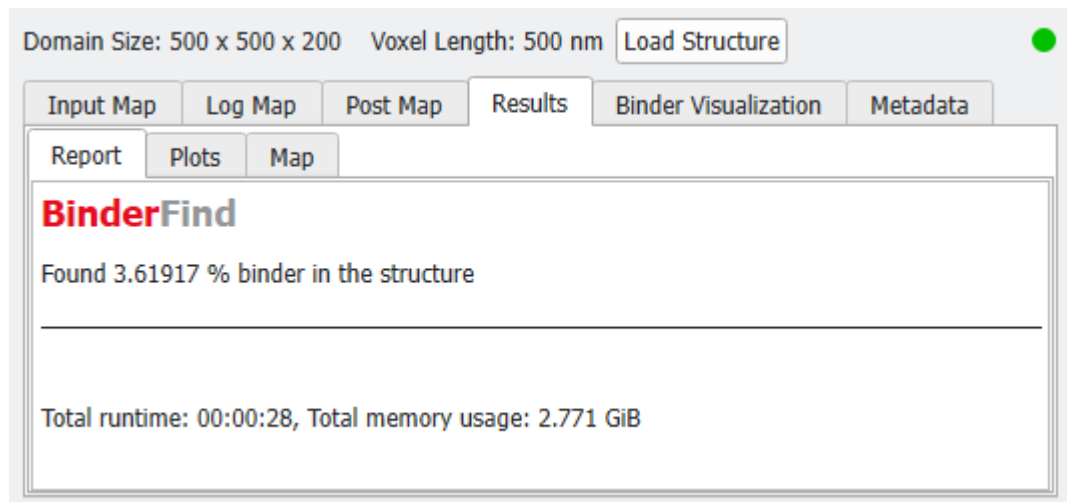
## 1.2.2 Results

After the **Identify Binder (AI)** calculation is finished, the resulting files are saved in the project

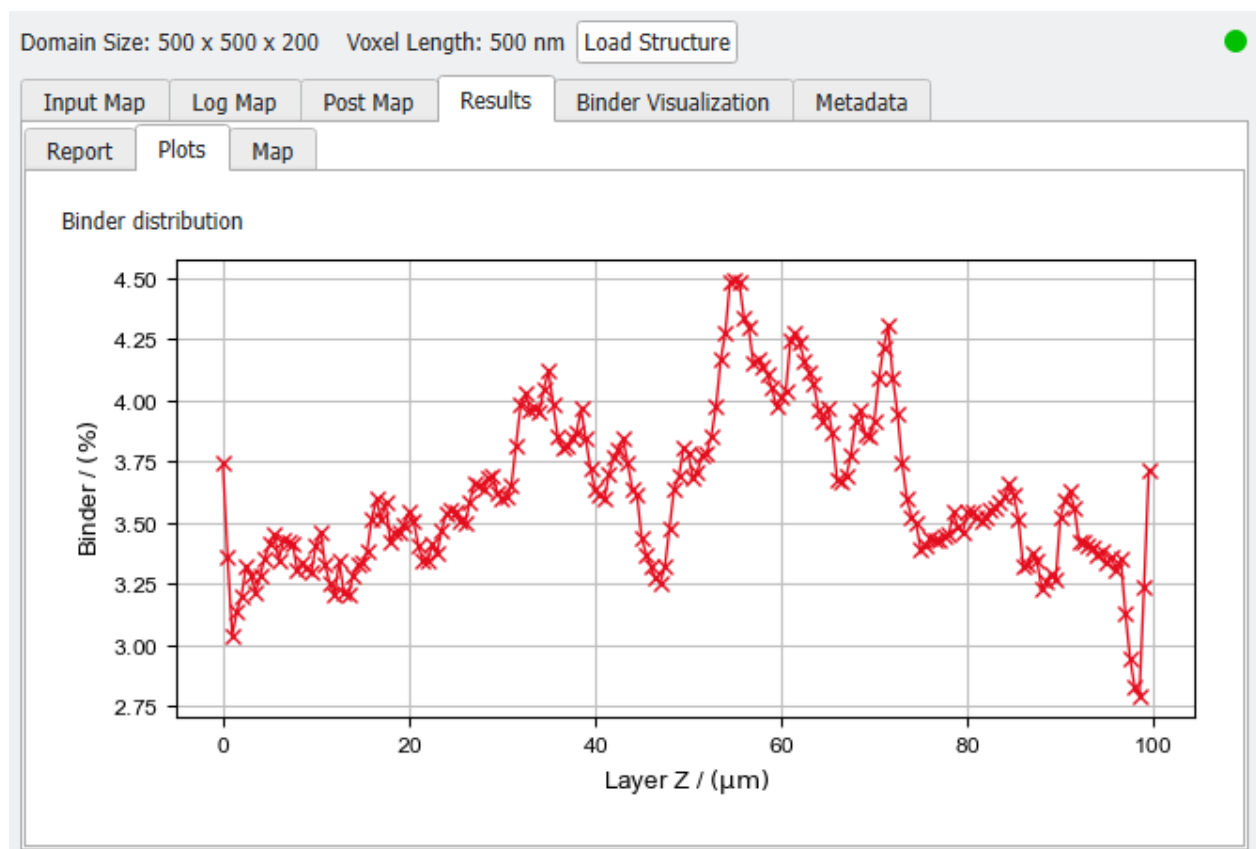
folder and a Result Viewer with the GeoDict result file opens automatically. The created GeoDict result file (\*.gdr) contains six tabs. The computational results are shown under the **Results** tab, and can be loaded for visualization via the **Binder Visualization** tab. The other four tabs (**Input Map**, **Log Map**, **Post Map**, and **Metadata**) display additional information about the computation.

Find more details on the general functionalities in the Result Viewer user guide.

Under the **Results - Report** tab, the percentage of solid voxels identified as binder is shown.



In the **Results - Plots** subtab, the **Binder distribution** in the different Z-Layers is shown.

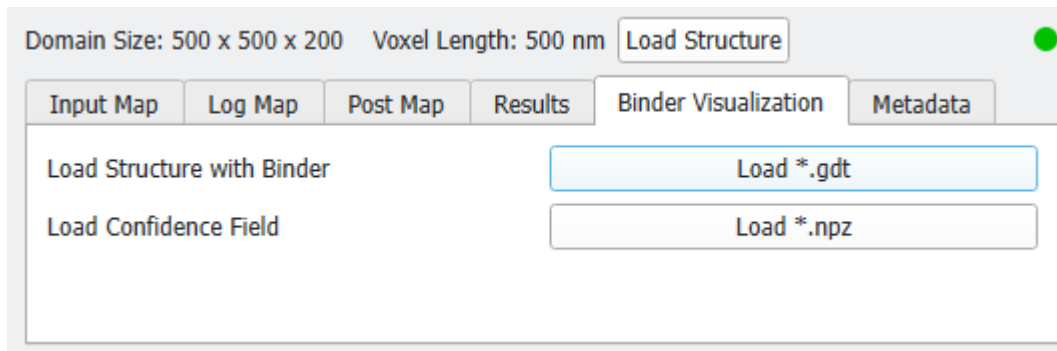


### Identify Binder (AI) Results:

- [Binder Visualization](#)<sup>74</sup>  
Load results for a graphical visualization.

## Binder Visualization

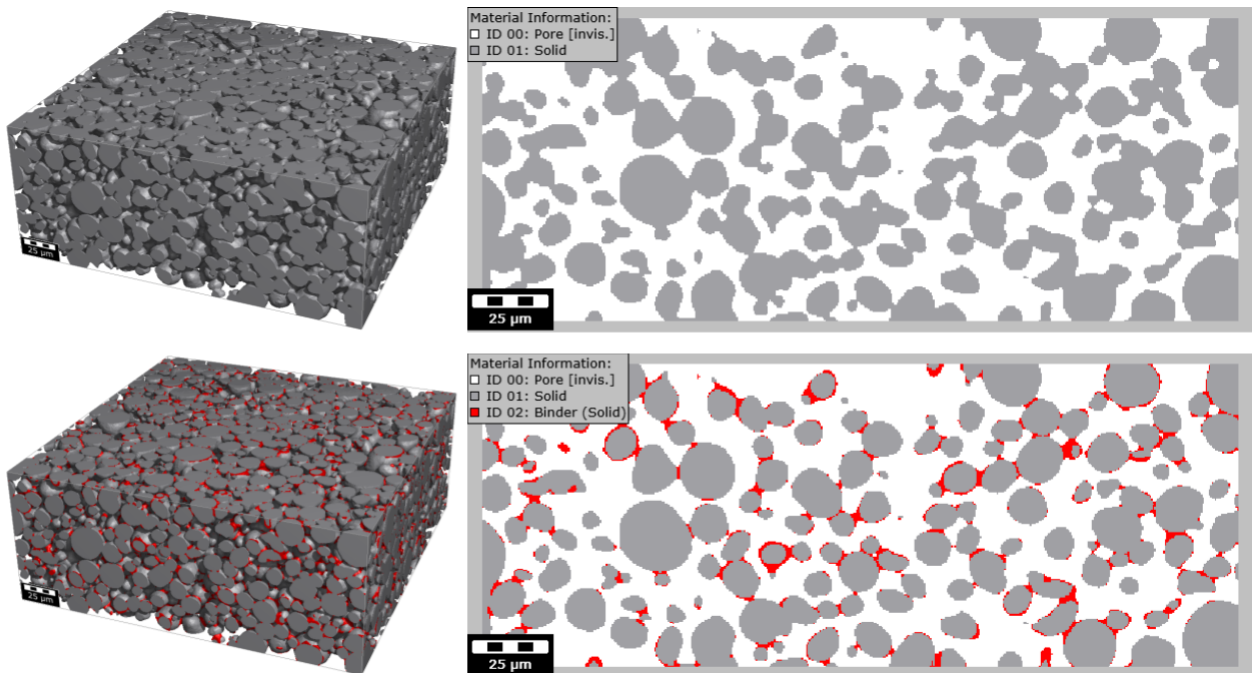
In the **Binder Visualization** tab you can import saved structures and computed volume fields which illustrate the binder identification process and its results.



### Load Structure with Binder

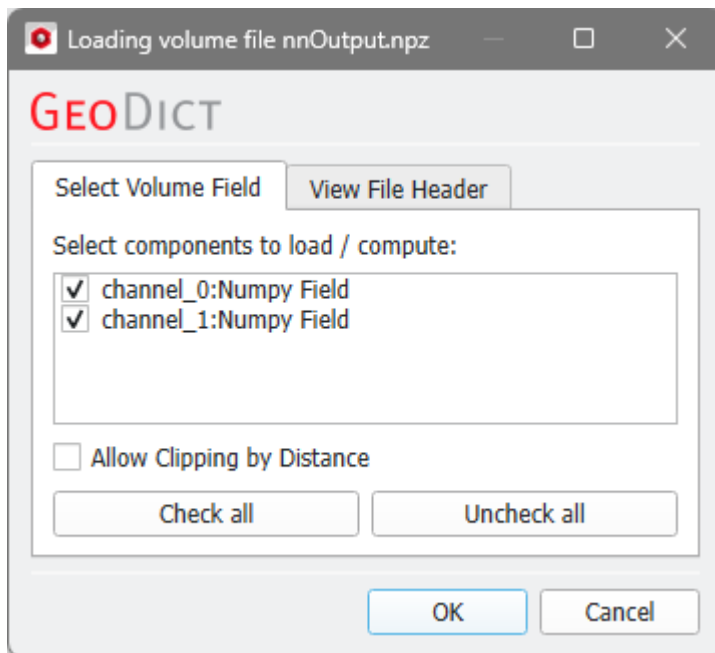
Click **Load \*.gdt** to load the structure of the identified binder labeled with a different Material ID.

In the 3D visualization, the distribution of binder between the grains is visible for the whole domain. In the 2D view you can evaluate the result of the binder identification in more detail, as seen in the example below (top: original structure, bottom: with labeled binder).



## Load Confidence Field

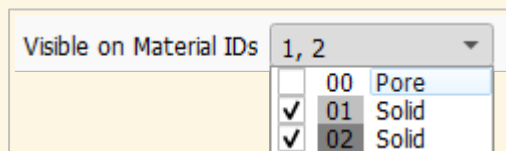
During the identification, the solid voxels are separated into two classes, binder and grain, based on the selected [Threshold](#)<sub>70</sub>. The confidence field contains the unsegmented result of the binder identification, i.e., a probability for each voxel to belong to one of the classes. Select **Load \*.npz** to view this volume file in GeoDict.



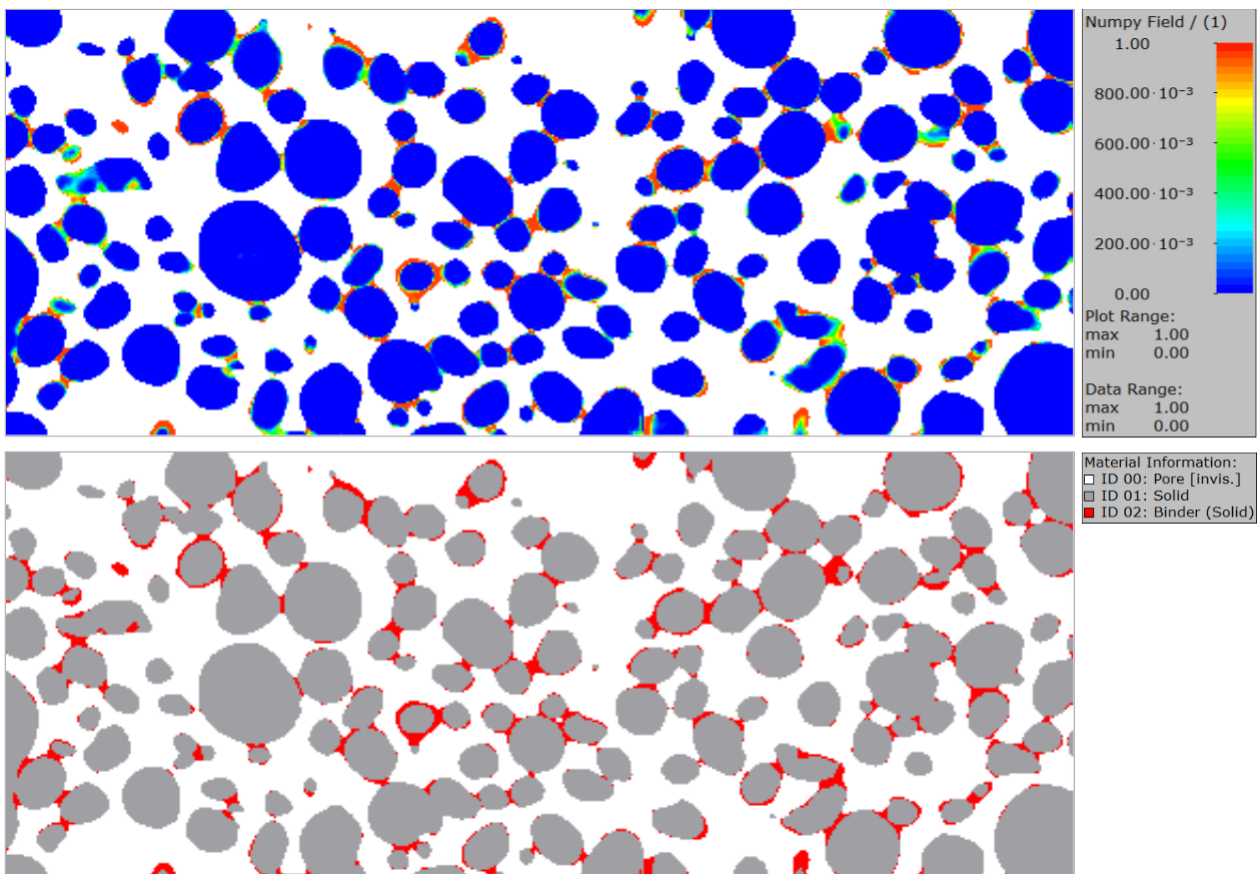
Two fields are available, where the first field contains the probability for a solid voxel to belong to the first class (which is grain) and the second field shows the probability of a voxel to be binder.



**Know how!** The values in the pore voxels are not used for the identification and can be ignored. Turn off the visibility of the confidence field in the pore voxels by disabling the visualization in the pore Material ID in the View Controls panel.



For the visualization below, the second field *channel\_1:Numpy Field* was loaded and you can observe easily where the neural network is confident of the choice and where it is uncertain: The dark blue areas are clearly marked as grain, the red areas are clearly marked as binder, and the values in between (bright blue to orange) are uncertain. In this case, the chosen [Threshold](#)<sub>70</sub> decides if the voxel is labeled as solid (confidence value below threshold) or as binder (confidence value above threshold).



**Know how!** If the segmentation results are not satisfying you can try another threshold and use the [Identification Mode](#) <sup>68</sup> **Load Neural Network Output.**



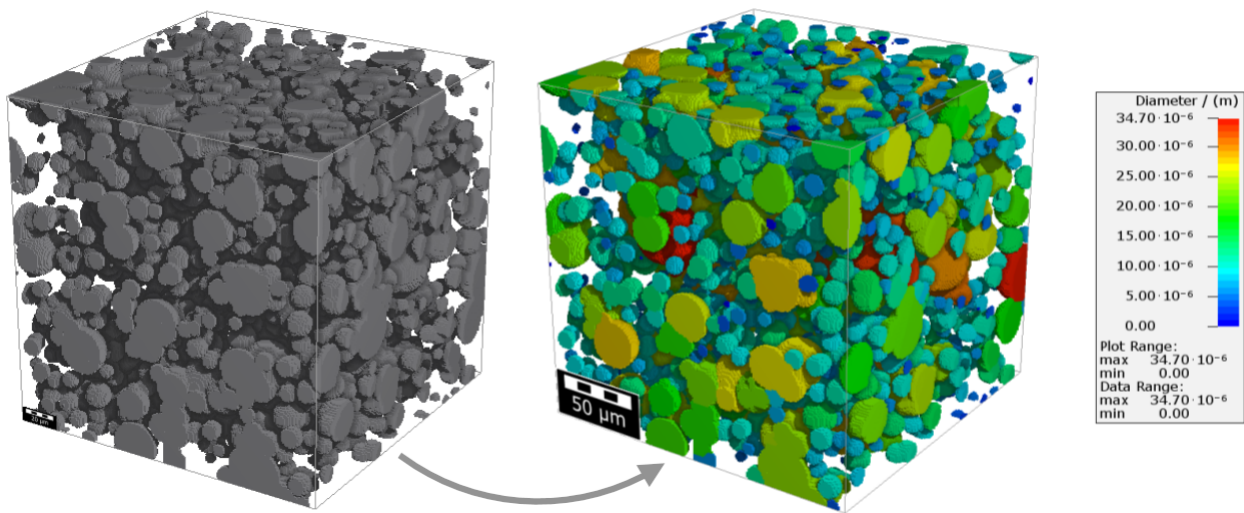
## 1.3 Estimate Grain Diameters

**Estimate Grain Diameters** gives an estimate of the grain sizes in the structure by fitting spheres into the structure and evaluating their diameters.

The algorithm is faster than [Identify Grains](#)<sup>[5]</sup> but it does not provide any information about the single grains in the structure.

During the post-processing, you can identify different diameter classes and segment the structure with respect to them.

The example structure used to explain the parameters and show the results was created with GrainGeo.



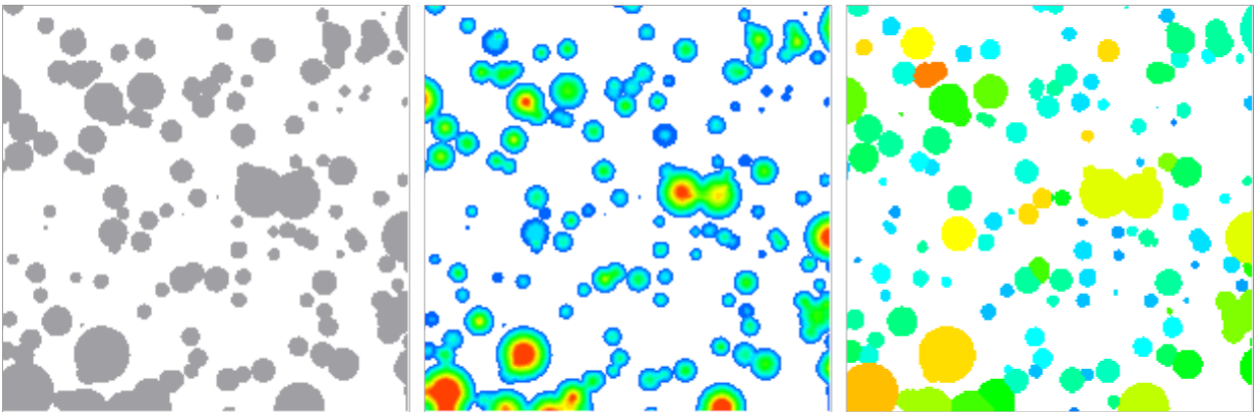
The Estimate Grain Diameters command:

- [Theoretical Background](#)<sup>[77]</sup>  
Learn more about the theory behind the grain diameter estimation.
- [Options](#)<sup>[79]</sup>  
Set the parameters for the estimation.
- [Results](#)<sup>[82]</sup>  
View the computed results.

### 1.3.1 Theoretical Background

The algorithm behind **Estimate Grain Diameters** works as follows: At the start, each voxel gets assigned a Grain Diameter of 0 voxels. Then, spheres are successively fitted into the geometry, starting at the largest possible sphere.

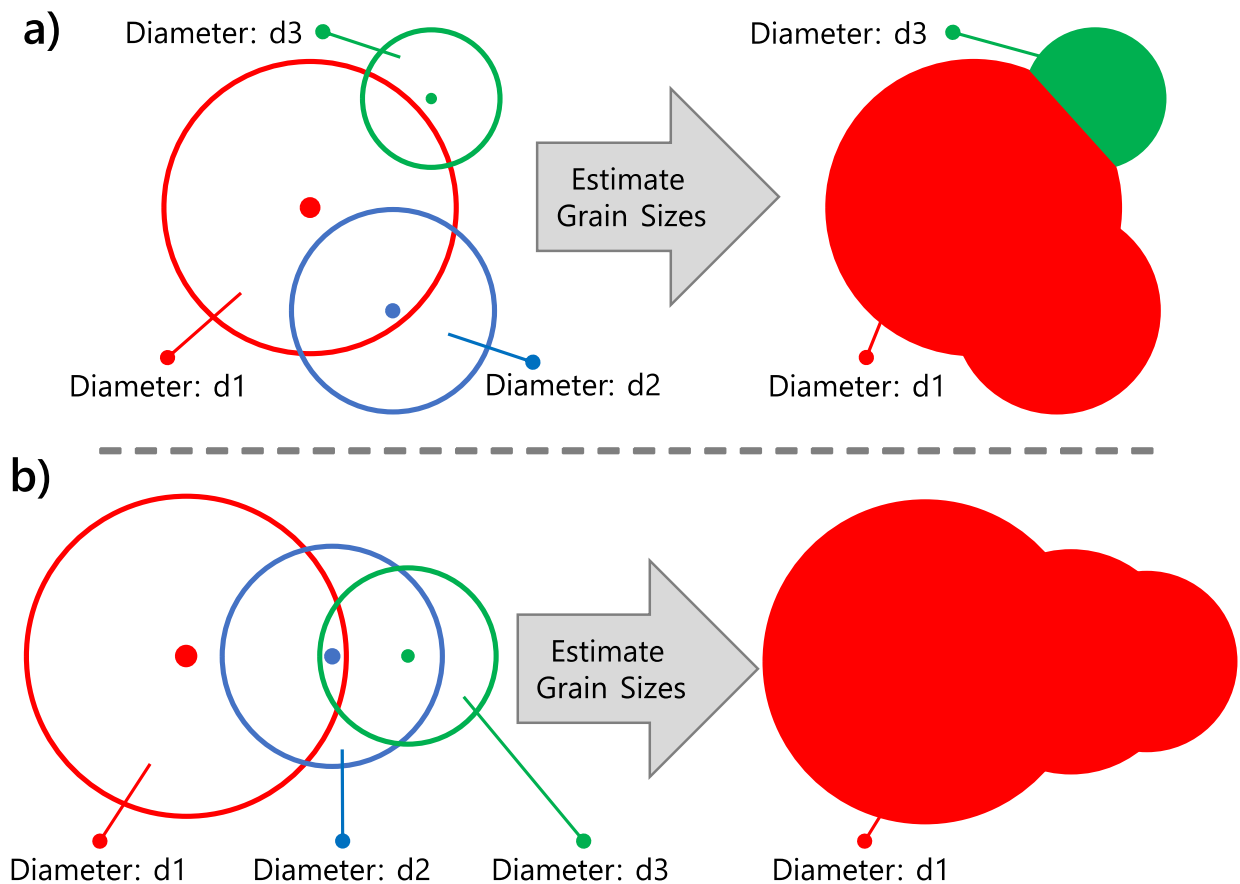
In the figure below, the process of estimating the grain size is illustrated on an example structure. On the left, the original structure (the gray grains are analyzed) is shown. In the next step (middle), an EDT is calculated to find the maximal fitting sphere at every point. On the right, the resulting [size distribution file](#)<sup>[88]</sup> of **Estimate Grain Diameters** is displayed.



If a sphere fits inside a grain and a voxel has still a diameter of 0 assigned to it yet, the diameter of the fitting sphere is assigned to all voxels contained in the sphere.

If a voxel is contained in multiple spheres, there are two options:

- The center of a smaller sphere lies inside a larger sphere. Then, the diameter value of the larger sphere is assigned to all voxels in the smaller sphere (in the figures below, see **a)** red and blue spheres and **b)** all three spheres).
- The center of a smaller sphere does not lie inside a larger sphere. Then, the overlapping area between both spheres is partitioned between both diameters (in the figures below, see **a)** red and green spheres).

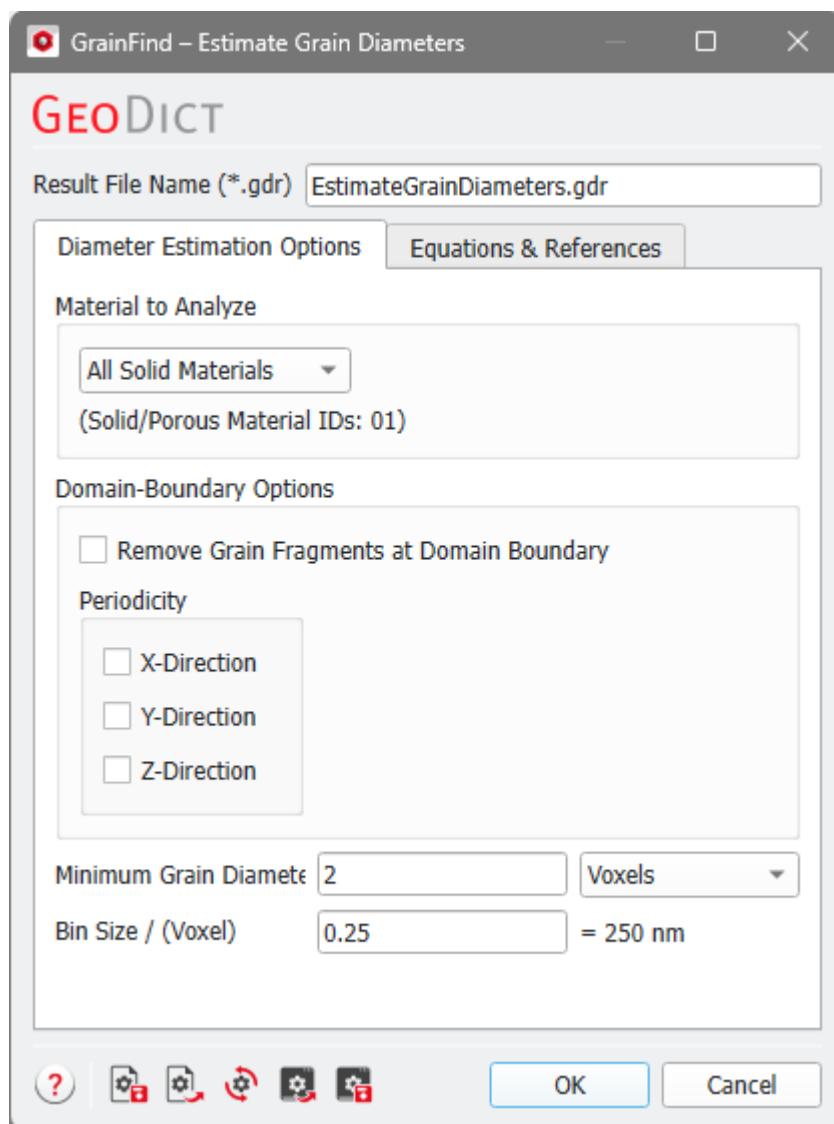


This algorithm ensures that non-spherical grains get assigned the diameter of the largest inscribed sphere.

### 1.3.2 Options

The **Estimate Grain Diameters** dialog opens when clicking the **Edit...** button and includes the **Diameter Estimation Options** tab and the **Equations & References** tab, which cites several [references](#) <sup>92</sup>.

At the top of the dialog, enter the **Result File Name**. The result file is saved in the chosen project folder (**File** → **Choose Project Folder** in the menu bar).



### Material to Analyze

Under **Material to Analyze**, define the part of the structure to be considered in the analysis. Either the complete structure can be analyzed (**All Solid Materials**), an individual material can be selected (**Chosen Material**) or a choice of Material IDs can be made (**Chosen Material**

**IDs**). If the selection includes multiple Material IDs they are combined and analyzed as one single material.

The figure shows three sequential screenshots of the 'Material to Analyze' interface. The first screenshot shows a dropdown menu with 'All Solid Materials' selected. The second screenshot shows the 'Chosen Material' dropdown set to 'Glass'. The third screenshot shows the 'Chosen Material IDs' dropdown with a list of material IDs: '00 Air' and '01 Glass'. The '01 Glass' option is selected, indicated by a checkmark.

## Domain-Boundary Options

### ✓ Remove Grain Fragments at Domain Boundary

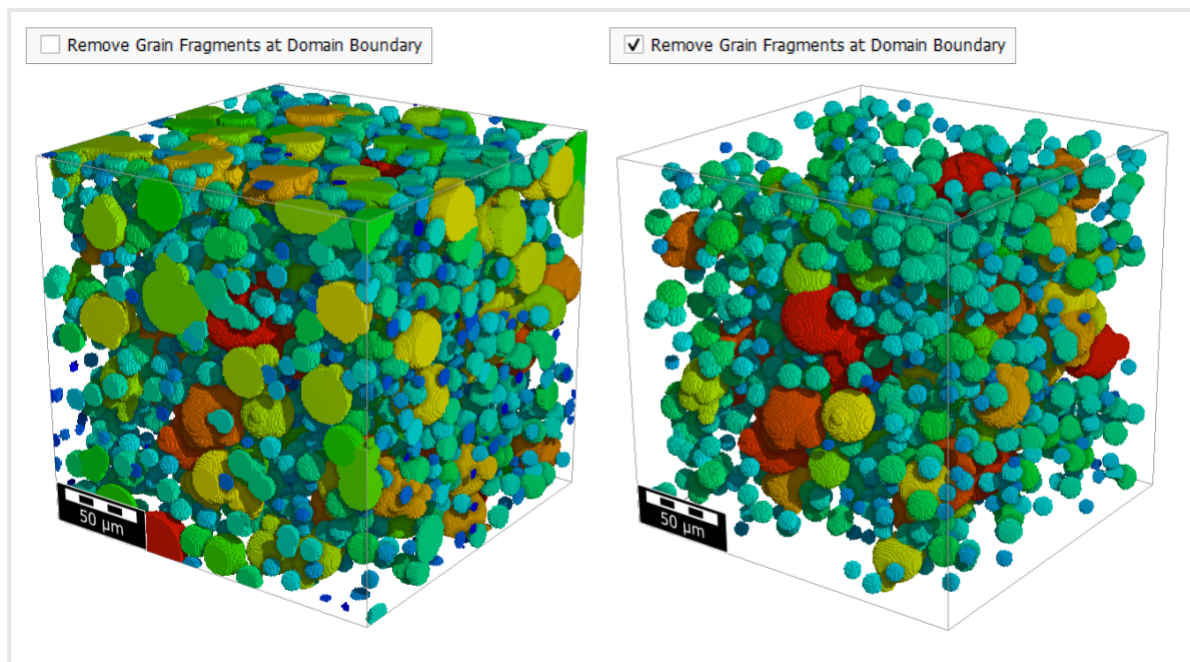
The first option is to **Remove Grain Fragments at Domain Boundary**. A grain fragment in this context is a connected component, where all voxels have the same assigned diameter value.

The figure shows a screenshot of the 'Domain-Boundary Options' dialog box. The 'Remove Grain Fragments at Domain Boundary' checkbox is checked. Below it, the 'Periodicity' section has three unchecked checkboxes: 'X-Direction', 'Y-Direction', and 'Z-Direction'.

The boundaries can have a critical influence on the results, and it must be carefully evaluated if **Remove Grain Fragments at Domain Boundary** should be used or not.

Grains at the boundary might corrupt the grain diameter estimation, as you don't know how many of the grains are completely in the domain or are cut at the domain boundary.

Nevertheless, removing the boundary grains also influences the diameter distribution: Larger grains have a higher probability to touch the boundary, and therefore also have a higher probability to be removed. Thus, large grains might be underrepresented in the diameter distribution.



## ✓ Periodicity

When **Remove Grain Fragments at Domain Boundary** is unchecked, the **Periodicity** options become available. By checking the X-, Y-, or Z-Direction checkboxes, the grain space is treated as periodic in the chosen direction(s) before the grain segmentation. Otherwise, when **Periodicity** is not chosen in a direction, the structure is assumed to be symmetric at the domain boundary.

**Domain-Boundary Options**

☐ Remove Grain Fragments at Domain Boundary

**Periodicity**

☒ X-Direction  
☒ Y-Direction  
☒ Z-Direction



**Important!** Periodicity should only be chosen for real periodic structures, otherwise it might lead to strange results (with grains which are treated as connected but are distant from each other in reality).

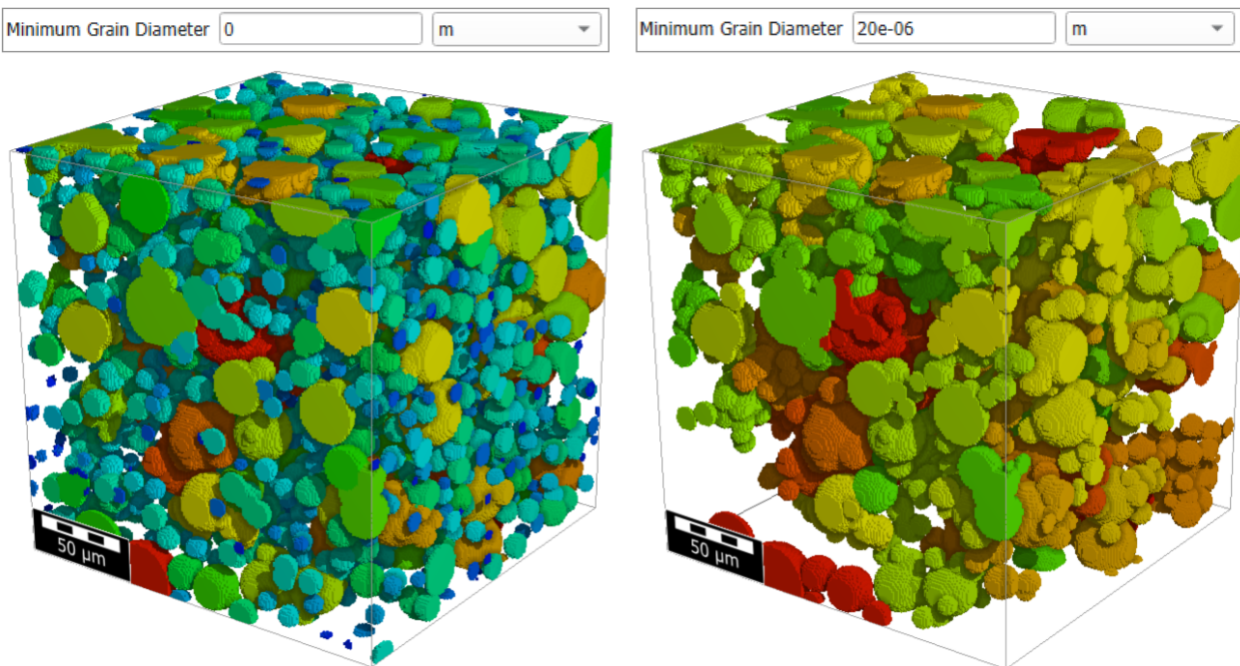
## Minimum Grain Diameter

All grain fragments with an assigned diameter value lower than the **Minimum Grain Diameter** are neglected. If they are connected to other grain fragments with a larger diameter value, the

fragments are merged and get assigned the larger diameter value. If they are not connected to any other fragments, they are set to diameter 0 voxels. The **Minimum Grain Diameter** can be entered in units of meters or voxels.

In the figure below, the behavior of the algorithm can be observed. For both visualizations, a threshold for the [\\*.gsd volume field](#)<sup>88</sup> was used to remove all voxels with diameter 0 from the visualization.

On the left, the **Minimum Grain Diameter** is set to 0  $\mu\text{m}$ , so all grain fragments are kept independent of their assigned diameter. On the right, the **Minimum Grain Diameter** is set to 20  $\mu\text{m}$  and all fragments with an assigned diameter lower than 20  $\mu\text{m}$ , which are not merged to larger grain fragments, are set to diameter 0.



## Bin Size

The **Bin Size** is the step size between following sphere diameters, which are fitted in the structure. It must be entered in voxels, but the step size is also shown in metrical units.

|                    |                                   |          |
|--------------------|-----------------------------------|----------|
| Bin Size / (Voxel) | <input type="text" value="0.25"/> | = 250 nm |
|--------------------|-----------------------------------|----------|

The choice of the Bin Size is important for the post processing. If it was not chosen as desired, the value for the **Bin Size** can be changed later in the [Post-Processing Widget](#)<sup>86</sup> in the Result Viewer.

### 1.3.3 Results

After the **Estimate Grain Diameters** calculation is finished, the resulting files are saved in the project folder and a Result Viewer with the GeoDict result file opens automatically. The created GeoDict result file (\*.gdr) contains six tabs. The computational results are shown under

the **Results** tab, and can be loaded for visualization via the **Data Visualization** tab. The other four tabs (**Input Map**, **Log Map**, **Post Map**, and **Metadata**) display additional information about the computation.

Find more details on the general functionalities in the Result Viewer user guide.

The **Results** tab is the central point for the analysis of the identified grains. It is grouped in three subtabs: **Report**, **Plots** and **Map**. The **Report** tab shows statistics about the estimated grain diameters and the **Plots** tab contains a histogram of the estimated grain diameters. The **Map** tab contains all resulting data from the **Estimate Grain Diameters** run. This data is the basis for the tables in the **Report** tab and for the plot in the **Plots** tab. On the left, the [Post-Processing Widget](#)<sup>[86]</sup> allows you to classify the grains into the specified **Number of Grain Types** by fitting a Gauss function to the estimated diameters. Collapse the **Post-Processing Widget** by pulling it to the left.

Domain Size: 200 x 200 x 200    Voxel Length: 1  $\mu\text{m}$     Load Structure

Input Map   Log Map   Post Map   **Results**   Data Visualization   Metadata

Bin Size / (Voxel)    0.25

Thresholding Method    k-Means

Number of Grain Types    2

Apply

☒ Back-up result file

Report   Plots   Map

### GrainFind

**General analysis of the size distribution (\*.gsd):**

Average inner diameter: 19.9773  $\mu\text{m}$   
Standard deviation: 8.22319  $\mu\text{m}$

**Grain type analysis:**

Specified number of types: 2

|        | Average inner diameter / ( $\mu\text{m}$ ) | Standard deviation / ( $\mu\text{m}$ ) | Median diameter / ( $\mu\text{m}$ ) | Volume fraction / (%) |
|--------|--------------------------------------------|----------------------------------------|-------------------------------------|-----------------------|
| Type 1 | 11.2128                                    | 2.65767                                | 11.375                              | 41.9615               |
| Type 2 | 26.2969                                    | 4.0067                                 | 26.375                              | 58.0385               |

Type threshold 1: 18.5  $\mu\text{m}$   
(result depends on the post-processing bin-size)

**Characteristic diameters:**

D 10: 9.28009e-06 m  
D 50: 2.17473e-05 m  
D 90: 3.07572e-05 m

**Histogram:**

| Min. diameter / ( $\mu\text{m}$ ) | Max. diameter / ( $\mu\text{m}$ ) | Volume fraction / (%) |
|-----------------------------------|-----------------------------------|-----------------------|
| 0                                 | 0.25                              | 0                     |

Plot Options

#### Estimate Grain Diameters Results:

- [Report](#)<sup>[84]</sup>  
See the computed results.
- [Plots](#)<sup>[85]</sup>  
View result plots.
- [Data Visualization](#)<sup>[88]</sup>  
Load results for a graphical visualization.



## Report

The **Report** tab shows statistics about the estimated grain diameters.

Domain Size: 200 x 200 x 200    Voxel Length: 1  $\mu\text{m}$     [Load Structure](#)

Input Map    Log Map    Post Map    **Results**    Data Visualization    Metadata

Report    Plots    Map

### GrainFind

#### General analysis of the size distribution (\*.gsd):

Average inner diameter: 19.9773  $\mu\text{m}$   
Standard deviation: 8.22319  $\mu\text{m}$

#### Grain type analysis:

Specified number of types: 2

|        | Average inner diameter / ( $\mu\text{m}$ ) | Standard deviation / ( $\mu\text{m}$ ) | Median diameter / ( $\mu\text{m}$ ) | Volume fraction / (%) |
|--------|--------------------------------------------|----------------------------------------|-------------------------------------|-----------------------|
| Type 1 | 11.2128                                    | 2.65767                                | 11.375                              | 41.9615               |
| Type 2 | 26.2969                                    | 4.0067                                 | 26.375                              | 58.0385               |

Type threshold 1: 18.5  $\mu\text{m}$   
(result depends on the post-processing bin-size)

#### Characteristic diameters:

D 10: 9.28009e-06 m  
D 50: 2.17473e-05 m  
D 90: 3.07572e-05 m

#### Histogram:

| Min. diameter / ( $\mu\text{m}$ ) | Max. diameter / ( $\mu\text{m}$ ) | Volume fraction / (%) |
|-----------------------------------|-----------------------------------|-----------------------|
| 0                                 | 0.25                              | 0                     |
| 0.25                              | 0.5                               | 0                     |

### ✓ General analysis of the size distribution (\*.gsd)

Here, the computed **Average inner diameter** of all grains and the **Standard deviation** are given. Both values are computed from the values in the **GeoDict size distribution** (gsd) file, where only the analyzed materials are taken into account. You can load the \*.gsd file from the [Data Visualization](#) <sup>88</sup> tab.

### ✓ Grain type analysis

The statistical parameters (Average inner diameter, Standard deviation, and Median diameter) of the fitted Gauss function for each class are displayed in this table.



Additionally, the volume fraction for each class is given.

If more than one class is reported, the [Threshold\(s\)](#)<sup>[87]</sup> used to determine the types are given below the table.



**Note!** These values depend on the entered [Bin Size](#)<sup>[86]</sup>!

### ✓ Characteristic diameters

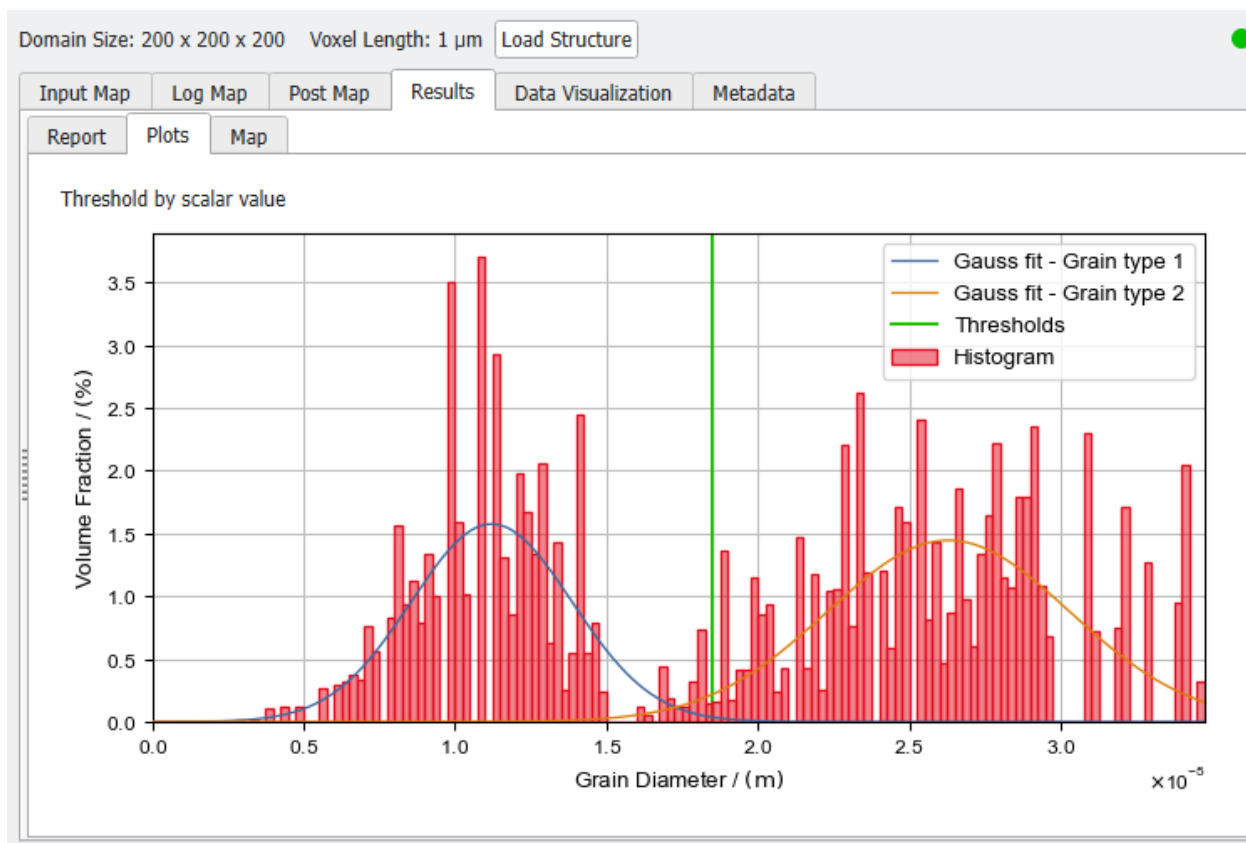
The characteristic diameters D10, D50, and D90 are the diameters such that 10%, 50%, or 90% of all grains have a smaller estimated diameter than the corresponding value.

### ✓ Histogram

The histogram table contains the values from the [histogram plot](#)<sup>[85]</sup>, where each row contains the data of one bin. The diameter of the grains in one bin is between the minimum and maximum diameter. The volume fraction shows how many grains are contained in a bin. Of course, the data in the table changes when entering another [Bin Size](#)<sup>[86]</sup>.

## Plots

The **Plots** tab shows the histogram of the estimated grain diameters. Additionally, the fitted Gauss functions for the different classes are plotted.



## Post-processing widget

In the post-processing panel on the left, you can choose the **Bin Size** to define the granularity of the histogram. Use the **Thresholding Methods** and **Number of Grain Types** to classify the grains into different classes based on their diameter by fitting a Gauss function to the estimated diameters. Clicking **Apply** immediately changes the results in the **Map** subtab, and therefore the tables in the **Report** subtab and the histogram in the **Plots** subtab. Collapse the **Post-Processing Widget** by pulling it to the left.

Bin Size / (Voxel)

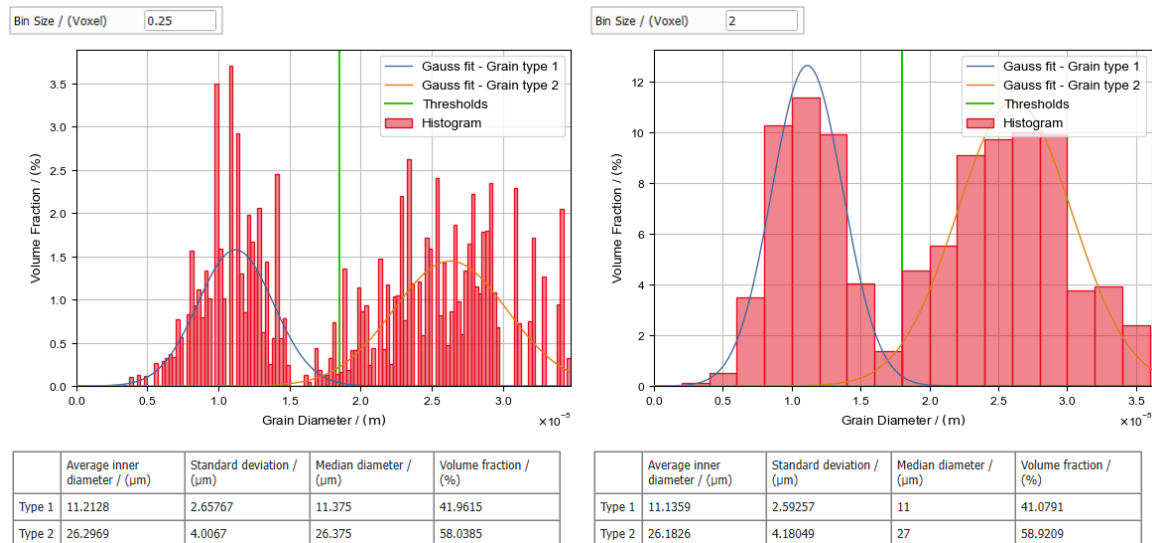
Thresholding Method

Number of Grain Types

### ✓ Bin Size

Changing the **Bin Size** affects the resolution of the histogram in the **Plots** tab and the histogram table in the **Report** tab. A too large **Bin Size** leads to a “blocky” histogram, while a too small **Bin Size** leads to a volatile and noisy histogram. The **Bin Size** should

be chosen so that the histogram is smooth and detailed. The effect of the Bin Size on the histogram is illustrated below.



## ✓ Thresholding Method and Number of Grain Types

You can classify the grains in the structure into different types based on the estimated diameter.

Thresholding Method k-Means

Number of Grain Types 2

To determine the threshold value, three **Thresholding Methods** are available:

Thresholding Method k-Means

k-Means

Otsu

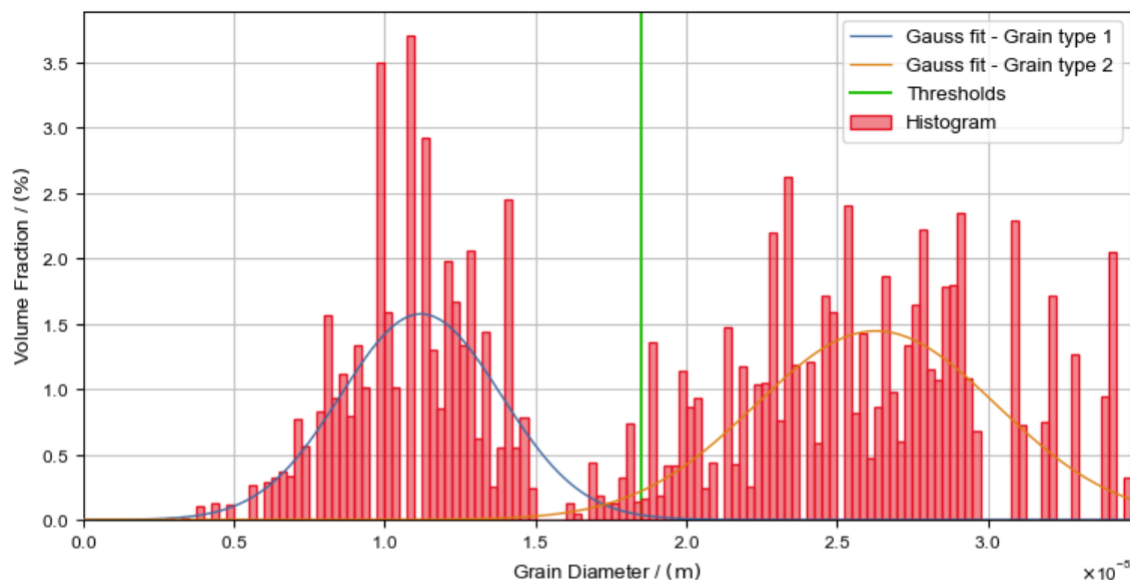
Manual

- **k-Means:** uses the k-Means algorithm to find thresholds for the chosen **Number of Enter value Types**.
- **Otsu:** uses the Otsu algorithm to find thresholds for the chosen **Number of Enter value Types**.
- **Manual:** define your own thresholds by writing a comma-separated list of thresholds into **Threshold(s)**. You implicitly define the number of Enter value types by the number of thresholds you enter, e.g, if you enter two threshold values this will result in three Enter value types.

Thresholding Method Manual

Threshold(s) / ( $\text{m}^3$ )

After clicking **Apply**, the **Grain Type Analysis** table is updated and shows for each type the relevant parameters. In the **Plot** tab, the Gauss fit of each grain type and the threshold values are added to the histogram plot. This allows you to control if the computed thresholds fit to the grain diameter distribution or need to be adapted.



#### Grain type analysis:

Specified number of types: 2

|        | Average inner diameter / ( $\mu\text{m}$ ) | Standard deviation / ( $\mu\text{m}$ ) | Median diameter / ( $\mu\text{m}$ ) | Volume fraction / (%) |
|--------|--------------------------------------------|----------------------------------------|-------------------------------------|-----------------------|
| Type 1 | 11.2128                                    | 2.65767                                | 11.375                              | 41.9615               |
| Type 2 | 26.2969                                    | 4.0067                                 | 26.375                              | 58.0385               |

Type threshold 1: 18.5  $\mu\text{m}$

Based on these diameter classes, the structure is automatically segmented and can be loaded from the [Data Visualization](#)  tab

## Data Visualization

In the **Data Visualization** tab you can import the computed volume field of the estimated grain diameters and the structure with the segmented grain types.

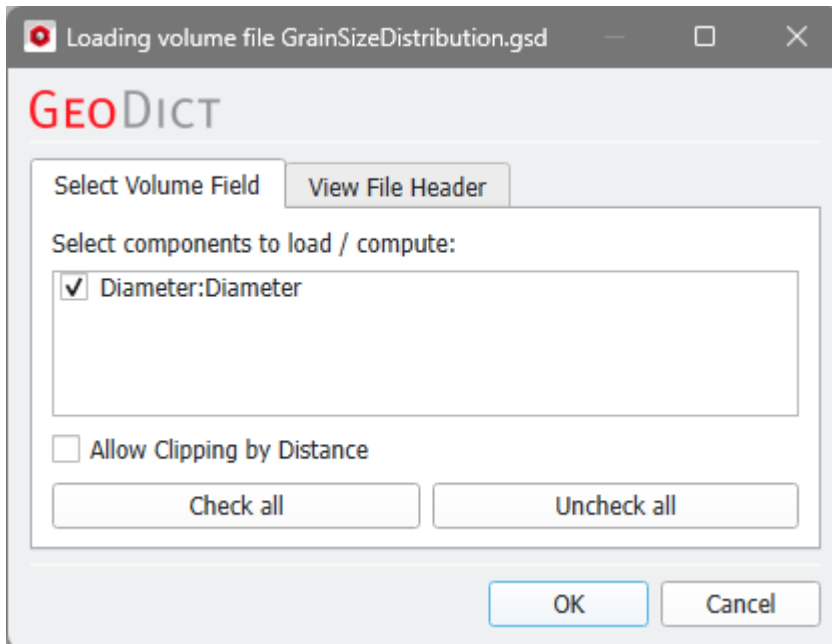
Domain Size: 200 x 200 x 200    Voxel Length: 1  $\mu\text{m}$      

Grain Diameter Distribution   

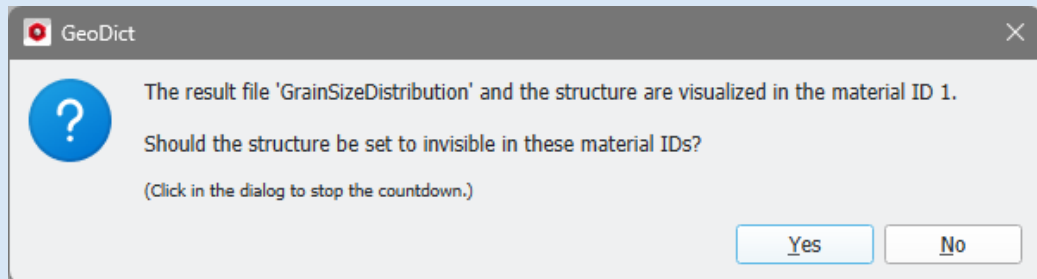
Grain Type Structure   

✓ Grain Diameter Distribution

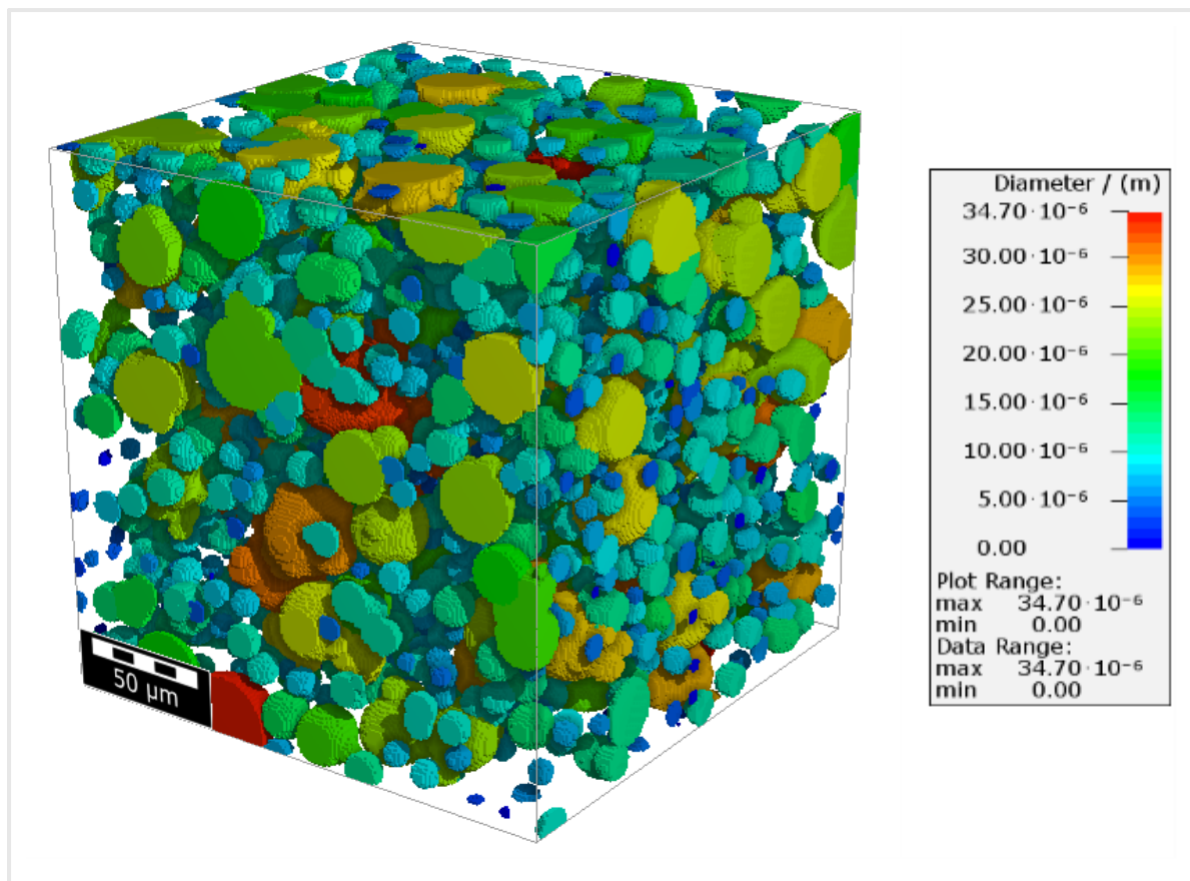
Click on **Load GeoDict Size Distribution (\*.gsd)** to load the volume file with the estimated diameters for each voxel.



**Note!** In an opening message you may be asked if the structure should be set to invisible for certain Material IDs. We recommend choosing **Yes**, because the volume field will be visualized in the same Material ID as the grains in the structure.

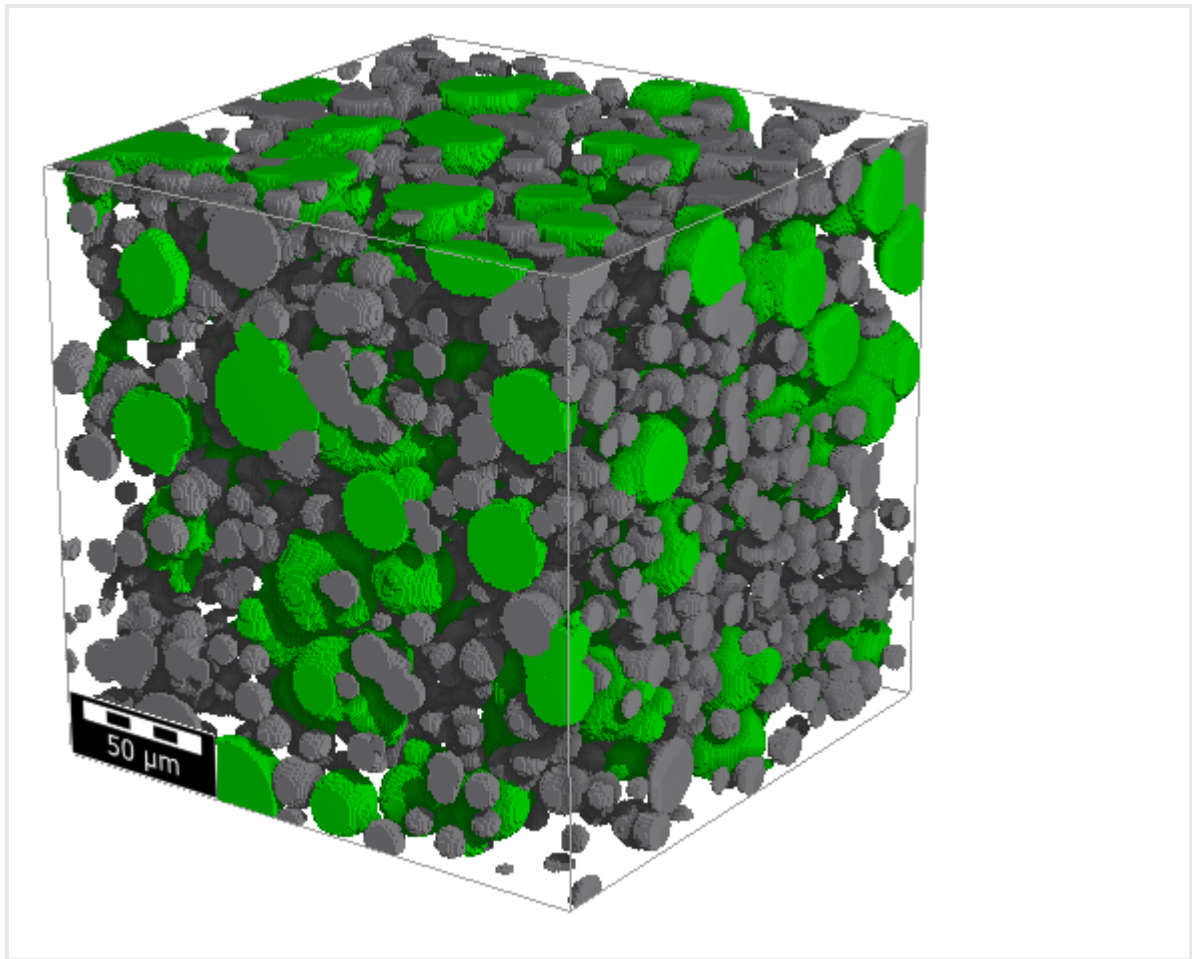


The visualization with the default settings is shown here. Find out more about the visualization settings in the Visualization chapter.



## ✓ Grain Type Structure

Click **Load \*.gdt** to load the segmented structure, based on the entered **Number of Grain Types** and the computed **Threshold** in the [post-processing widget](#)<sup>87</sup>. Each grain type is assigned its own Material ID, so all grains of the same type have the same Material ID.



## 1.4 References

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interface ratio 19

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