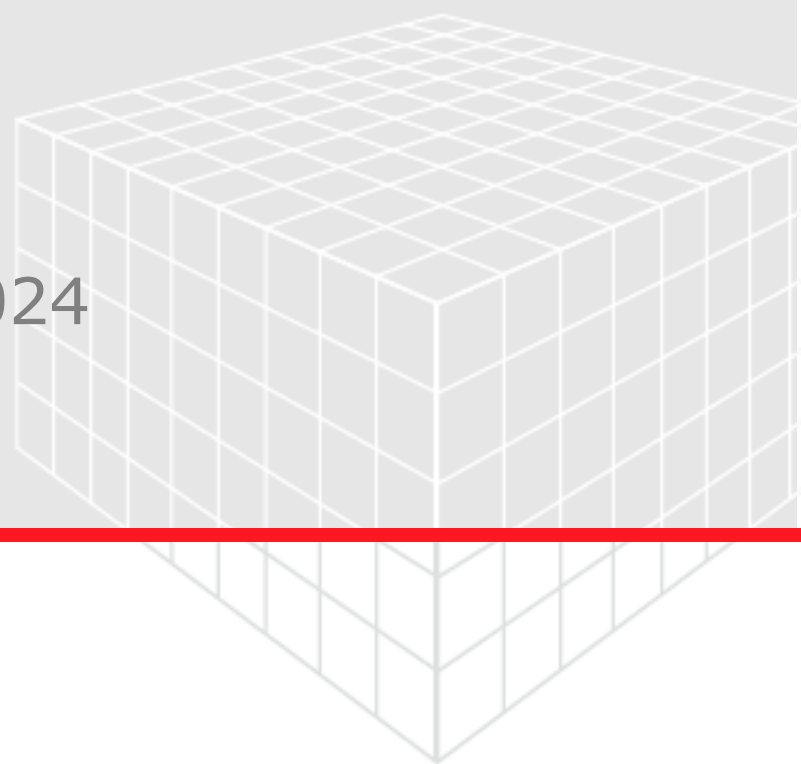


GRAINFIND

User Guide

GeoDict release 2024

Published: April 22, 2024



GEO DICT

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

© Math2Market GmbH 2024

Citation:

Anne Blumer, Jürgen Becker, Barbara Planas. GeoDict 2024 User Guide. GrainFind handbook. Math2Market GmbH, Germany, doi.org/10.30423/userguide.geodict

All rights reserved. It is not permitted to reproduce the book or parts thereof in any form by photocopy, microfilm or other methods or to transfer it into a language suitable for machines, in particular data processing systems, without the express permission of the publisher. The same applies to the right of public reproduction.

The handbooks in the User Guide series of Math2Market GmbH can be obtained from:

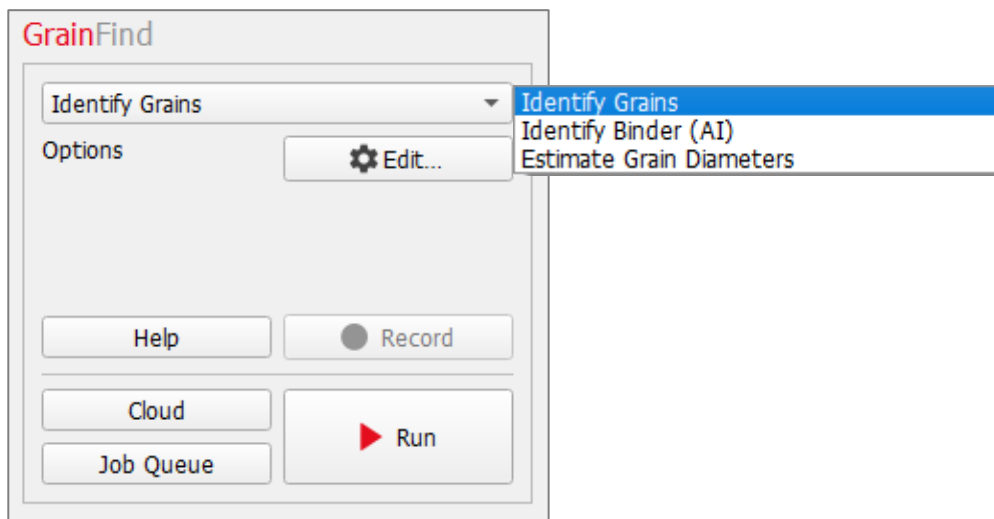
Math2Market GmbH
Richard-Wagner-Strasse 1
67655 Kaiserslautern
Germany

Phone: +49 631 205 605 0
Fax: +49 631 205 605 99
Email: info@math2market.de
Web: www.math2market.de

GRAIN ANALYSIS WITH GRAINFIND	1
IDENTIFY GRAINS	3
HOW DOES IDENTIFY GRAINS WORK?	3
Euclidean Distance Transform	4
Watershed Algorithm	5
Sphericity parameters	5
SETTING PARAMETERS FOR GRAIN IDENTIFICATION WITH GRAINFIND	7
Grain Segmentation	7
Output Options	14
Constituent Materials	15
GRAIN IDENTIFICATION RESULTS	17
Results	17
Grain Visualization	26
Create Videos	28
CONNECTING GRAINFIND ANALYSIS RESULTS WITH GRAINGEO	29
Example: Digital Twin of a 3D-Scan	32
IDENTIFY BINDER (AI)	33
BINDER IDENTIFICATION SETTINGS	34
Binder Identification tab	34
Solver Options tab	36
Equations & References	37
BINDER IDENTIFICATION RESULTS	37
ESTIMATE GRAIN DIAMETERS	41
ESTIMATE GRAIN DIAMETERS OPTIONS	43
GRAIN DIAMETER ESTIMATION RESULTS	46
REFERENCES	51

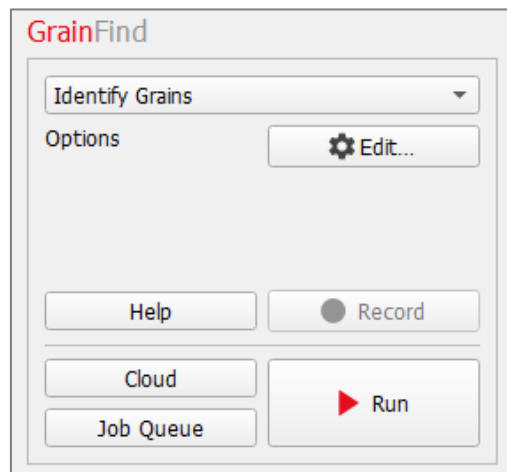
Additional to the grain identification, it is also possible to **Identify Binder (AI)** using machine learning technologies. Please note that for this feature a special license is required.

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



IDENTIFY GRAINS

With **GrainFind** - Identify Grains, individual grains are identified and analyzed in a given structure. The analysis includes the determination of 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 in **GrainGeo**.



Select **Identify Grains** from the pull-down menu in the **GrainFind** module section at the bottom-left of the GUI. The parameters needed by the **GrainFind** algorithm can be entered in the **Identify Grains** dialog, that is opened by clicking the Options' **Edit...** button. Before describing the needed parameters in detail, we investigate the method behind the identifying algorithm.

HOW DOES IDENTIFY GRAINS WORK?

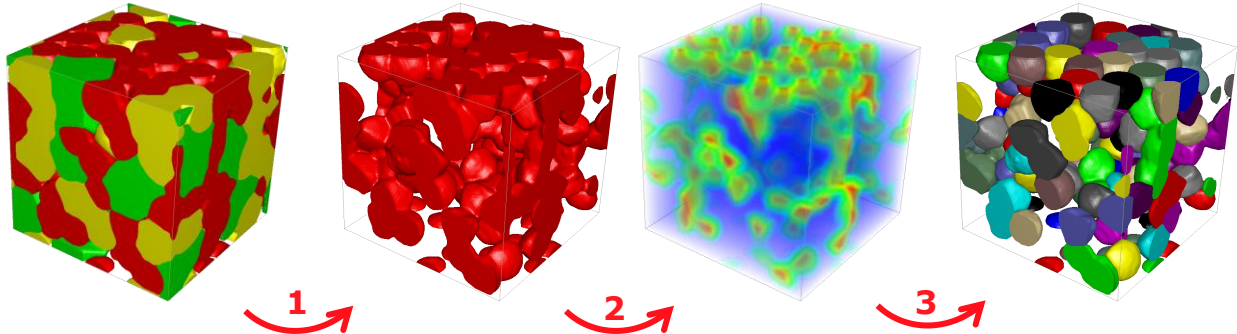
The grain identification process in **GrainFind** is mainly based on the **Watershed algorithm** (WA, [https://en.wikipedia.org/wiki/Watershed_\(image_processing\)](https://en.wikipedia.org/wiki/Watershed_(image_processing))) that is widely used for the segmentation of image data. The challenge of identifying 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 minimal grain diameter) and the post-processing (reconnection of grain fragments, boundary grain handling 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 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.

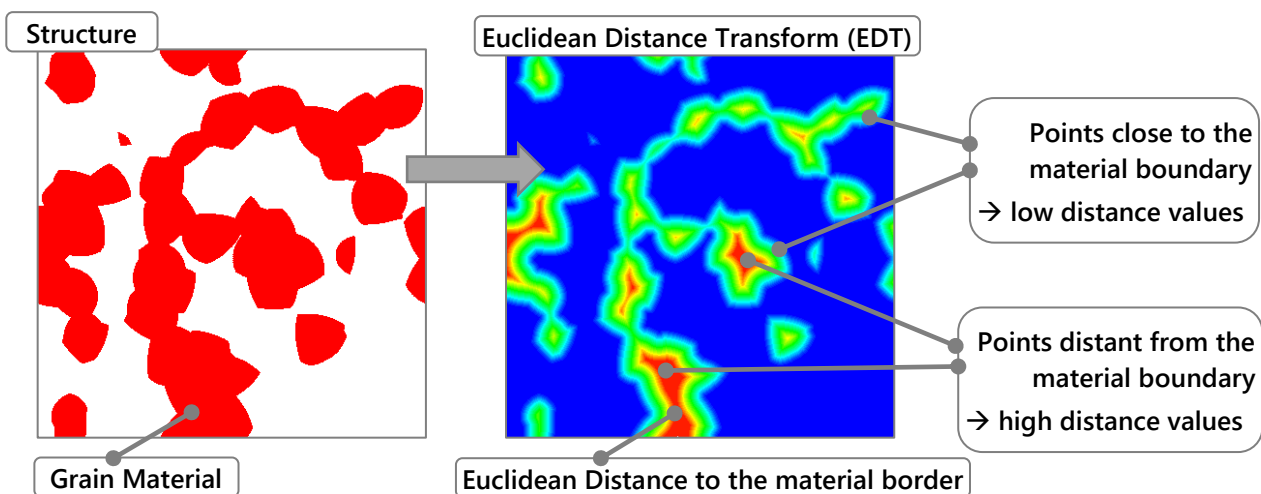


In many cases, the result of the watershed transform is enough to identify the grains. Otherwise, further steps are required.

EUCLIDEAN DISTANCE TRANSFORM

For a given material in a structure, a distance transform computes the distance to the boundary of the material for every point (voxel) in the structure (https://en.wikipedia.org/wiki/Distance_transform). Points close to the material boundary get assigned low distance values, whereas points deeper in the material get assigned larger distance values. The larger the value of the Euclidean Distance Transform, the larger the sphere which can be inscribed in the structure. The EDT is therefore a measure for the grain sizes.

In the figure below, the EDT is illustrated in a simple 2D example. On the left side, a structure of several overlapping grains is shown. On the right, the resulting EDT is shown. Points close to the material boundary are marked in green, and points distant to the material boundary are marked in red.

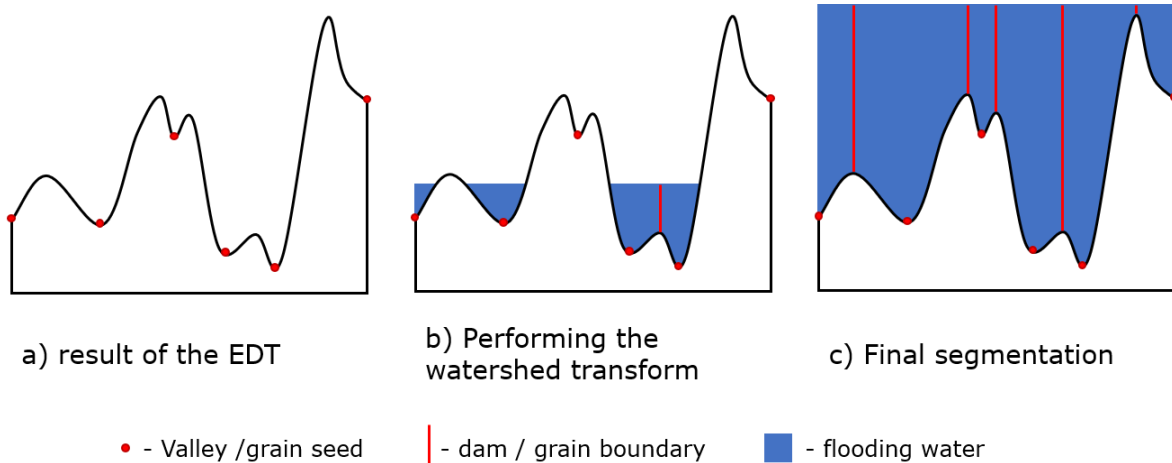


WATERSHED ALGORITHM

The watershed algorithm (WA) is a segmentation algorithm commonly used in image processing. The WA is based on the 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

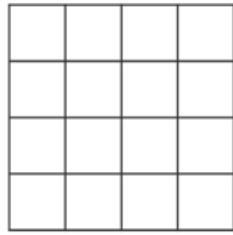
While there are many definitions of sphericity, the two sphericity indices given in the **GrainFind** output are those defined by Sheppard (2006) (optional) and Krumbein (1941). See the references on page [51](#).

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

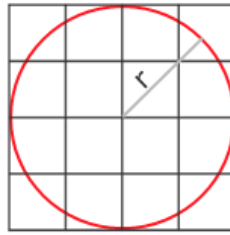
$$P_s = \frac{R_i}{R_e} \quad (1)$$

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 EDT.

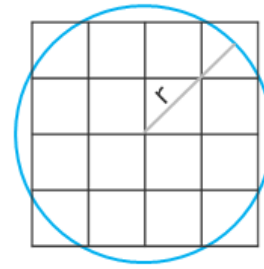
Sphericity values range between 0 and 1. The more the grain resembles a sphere, the higher is the sphericity value. A value of 1 marks a perfect spherical grain.



Grain geometry



Inner radius
r=2 voxel



Equivalent radius
r=2.26 voxel

Illustration of a 2D grain geometry and its inner and equivalent radii.

To calculate sphericity based on Krumbein, three principal axes (a , b , c) are measured by fitting an ellipsoid into the grain. The Krumbein sphericity P_K is then calculated using the length of the axes

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

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

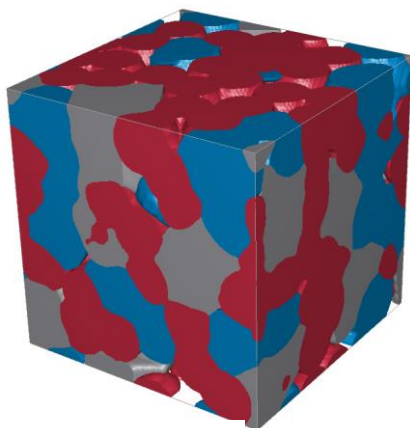
Analogously to the Sheppard sphericity, the values for the Krumbein sphericity range between 0 and 1, with 1 characterizing perfectly spherical grains.

SETTING PARAMETERS FOR GRAIN IDENTIFICATION WITH GRAINFIND

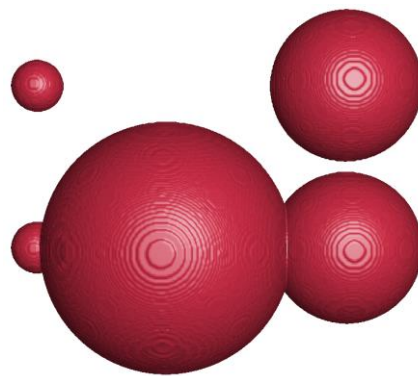
In the **Identify Grains** dialog window, enter the **Result File Name (*.gdr)** under which the results are saved in the chosen project folder.

The Identify Grains dialog consists of three tabs. In the **Grain Segmentation** tab the parameters for the segmentation can be entered. In the next tab the **Output Options** can be defined and in the **Constituent Materials** tab material specific properties like the density can be set.

The two structures used to explain these parameters are shown below: A structure with sintered grains, generated with **GrainGeo (Sinter)**, and a simple structure with overlapping spheres (**Spheres**), generated with **GadGeo**.



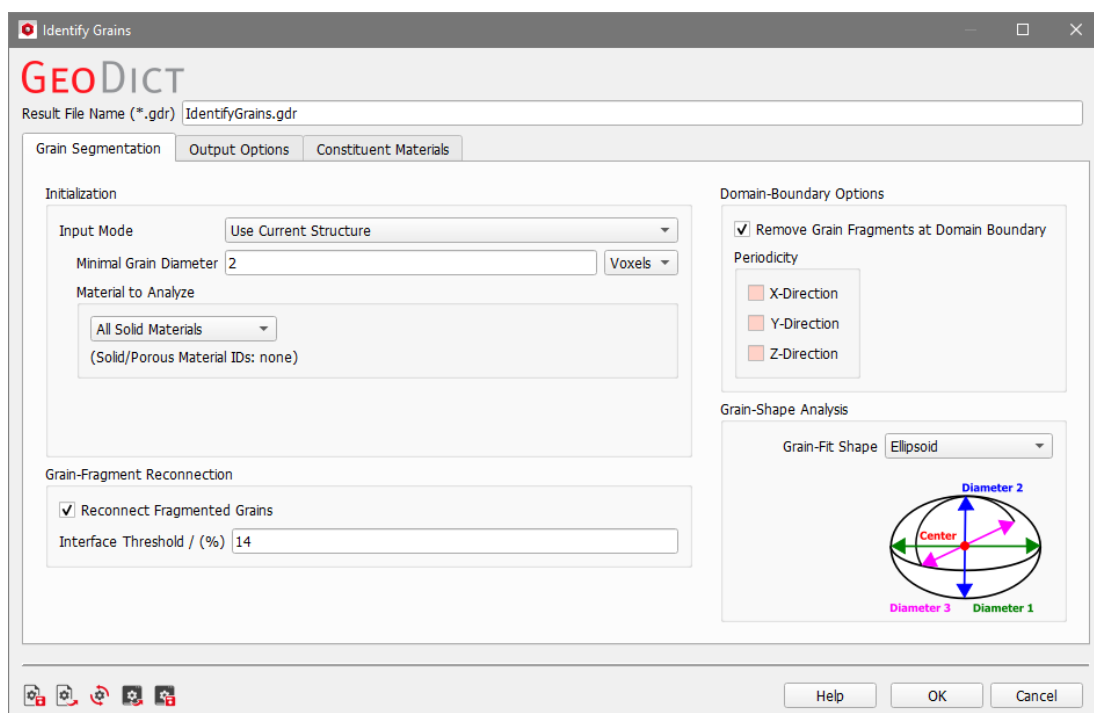
Sinter



Spheres

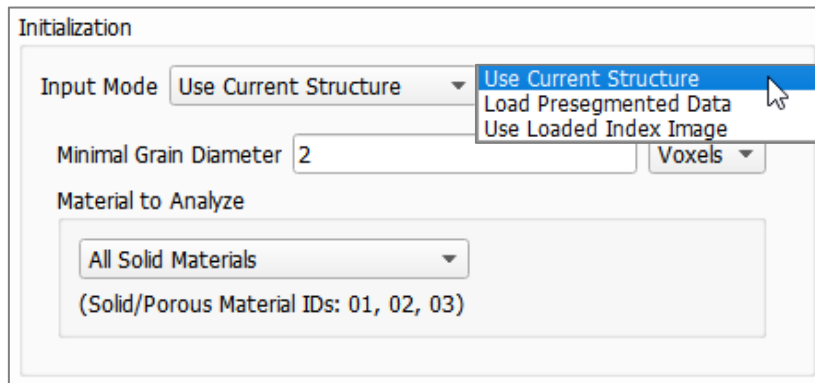
GRAIN SEGMENTATION

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



INITIALIZATION

The parameters in the **Initialization** panel define the basis for the analysis. Depending on the choice made for the **Input Mode** different parameters are available.



For the **Input Mode**, three options are available:

- Use the structure currently in memory (**Use Current Structure**)
- Import already segmented data from an index-image file *.g32 or *.leS (**Load Presegmented Data**)
- Use the currently loaded *.g32 file (**Use Loaded Index Image**)

The initialization (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, where the initialization is kept unchanged while other parameters are varied. So, the segmentation results from previous GrainFind runs can be used.

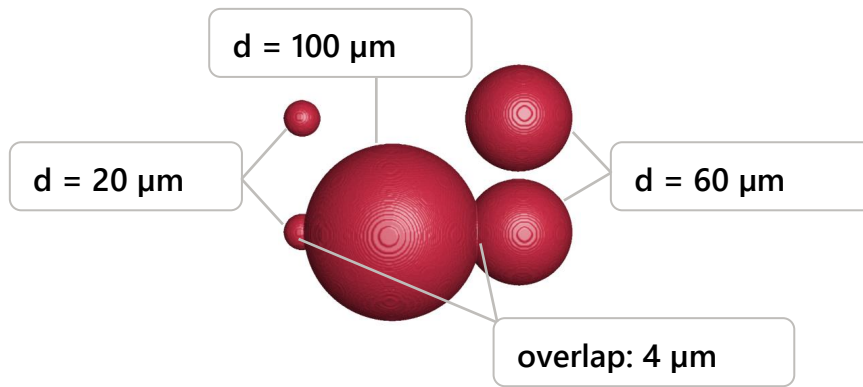
Use Current Structure

When **Use Current Structure** is used as **Input Mode**, the parameters for the watershed segmentation need to be defined. The **Minimal Grain Diameter** defines the minimal size an individual grain must have for the GrainFind analysis. This parameter determines which grains to keep and which grains to neglect or merge with others. If smaller grains exist which are connected to larger grains, these grains are merged. Single grains (i.e. which are unconnected to other grains) with a diameter smaller than **Minimal Grain Diameter** are neglected.



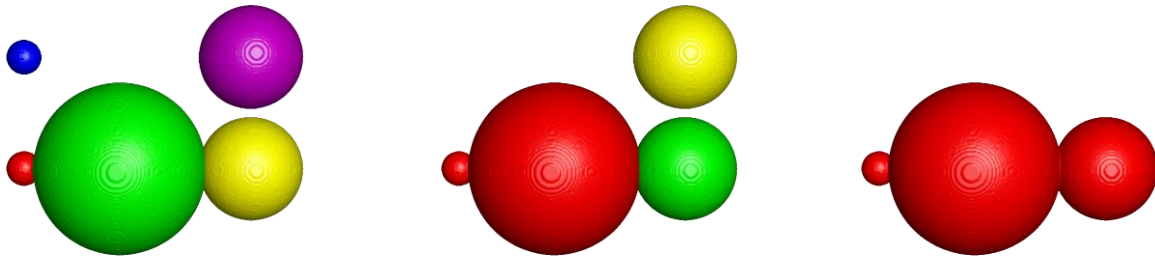
The **Minimal Grain Diameter** can be entered in unit of voxels or in unit of meters. The default value of 2 voxels works well in most cases and should therefore be left unchanged if a good estimation is unknown. The unit of the **Minimal Grain Diameter** can be changed through the pull-down menu next to the value box.

The effect of the choice for **Minimal Grain Diameter** is illustrated below. The figures show the result of the initialization step (of the watershed algorithm). The original structure has a voxel length of 1 μm and contains spheres with diameters 100 μm , 60 μm , and 20 μm , and some of the grains overlap.

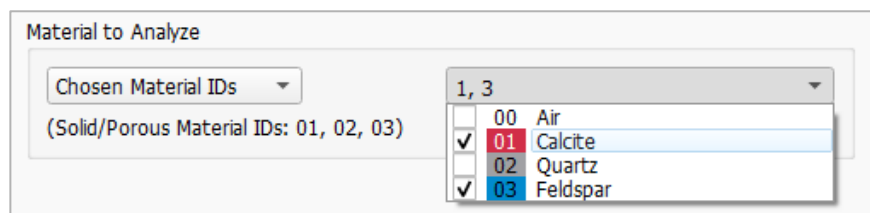
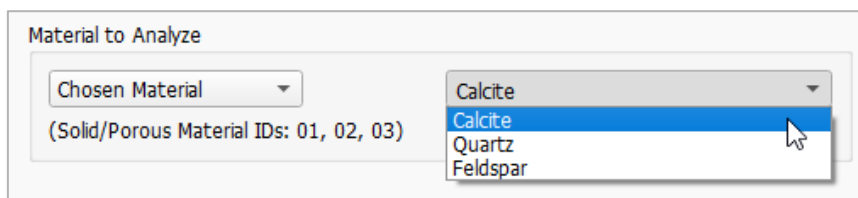


With **Minimal Grain Diameter** set to zero, all five spheres are identified as single grains and labelled in different colors. When setting the **Minimal Grain Diameter** to $25 \mu\text{m}$ (25 voxel), the single $20 \mu\text{m}$ sphere (top left) is neglected, while the $20 \mu\text{m}$ sphere connected to the larger sphere is merged. Analogously, for a choice of $65 \mu\text{m}$, only one single merged grain is kept while the smaller spheres are neglected. The effect of removing small objects from the structure is suitable for denoising.

Minimal Grain Diameter Voxels Minimal Grain Diameter Voxels Minimal Grain Diameter Voxels

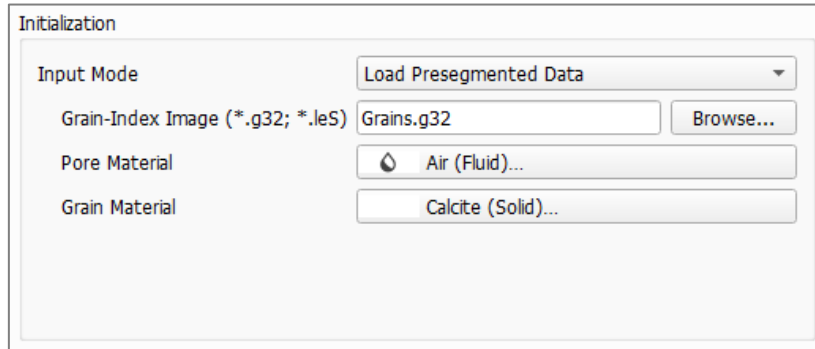


Under **Material to Analyze**, the user defines the part of the structure to be considered. Either the complete structure can be analyzed (**All Solid Materials**), an individual material can be selected (**Chosen Material**) or a choice of material IDs can be made (**Chosen Material IDs**). With **Chosen Material IDs**, one or multiple IDs can be chosen, which are then combined and analyzed as one single material.



Load Presegmented Data

For **Load Presegmented Data**, the data needs to be available as a **GeoDict** index image. An index image is a voxel image, where each voxel is assigned to an object ID. Such an image can e.g. be obtained from a previous **GrainFind** run. The file containing this index image can be selected with the **Browse...** button (*.g32 and *.leS files are allowed).

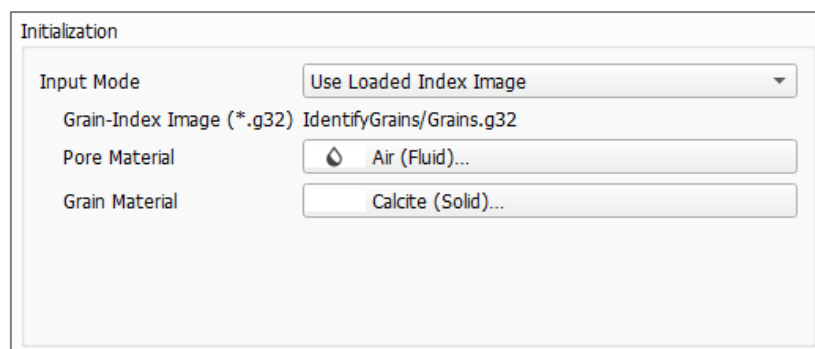


The difference between the *.g32 and *.leS formats is that *.g32 is a binary format, which produces comparatively smaller files but is not human readable, and *.leS is an ASCII-format which is human-readable, but produces larger files. Furthermore, loading a *.g32 file into **GeoDict** is much faster than loading a *.leS file. Therefore, we recommend to use the *.g32 option when possible.

GeoDict index images contain no material information. Therefore, a **Pore Material** and **Grain Material** must be selected. The material info is used in the Results Viewer to compute the grain mass and the moment of inertia.

Use Loaded Index Image

This mode works analogously to **Load Presegmented Data**. The only difference is that the index image must be already in memory. This is especially useful when an index image is created in **GeoDict**, but not yet saved to a file.



GRAIN-FRAGMENT RECONNECTION

In some cases (e.g. for complex grain shapes), the watershed algorithm in step 1 tends to over-segment the structure. This means, that some grains are identified as multiple grains ("*Fragmented Grains*") when, in fact, they may be a single grain with a complex shape. With **Reconnect Fragmented Grains**, it is possible to handle this over-segmentation by merging grains depending on the size of their shared interface.

Activate the checkbox **Reconnect Fragmented Grains** to merge connected grains depending on the value chosen for **Interface Threshold**.

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.

$$\text{interface ratio} = \frac{\text{interface of the touching grain fragments}}{\min(\text{surface of grain 1, surface of grain 2})} \quad (3)$$

For the computation of the interface ratio, the grain surfaces and interfaces need to be computed. The surface area estimation is based on MatDict's "[Estimate Surface Area](#)" (see Ohser, Mücklich [3]).

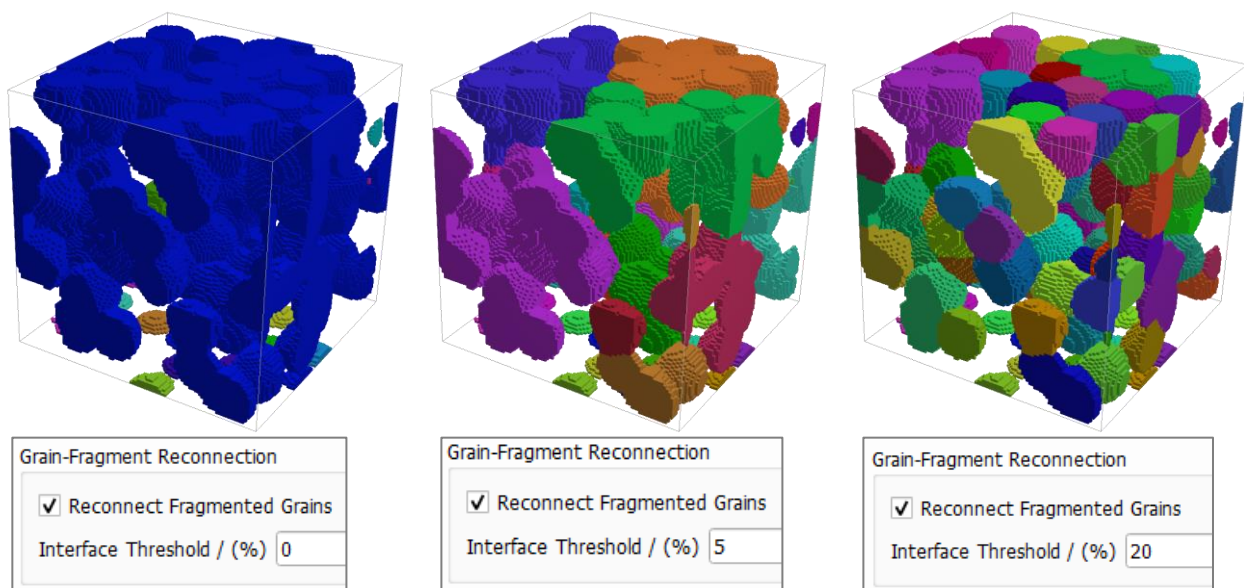
If the *interface ratio* is larger than the percentage chosen for the **Interface Threshold**, the two grain fragments are merged. For example, if the **Interface Threshold** is set to **14%**, then all grain fragments with an *interface ratio* larger than 14% are merged.

Grain-Fragment Reconnection

Reconnect Fragmented Grains

Interface Threshold / (%)

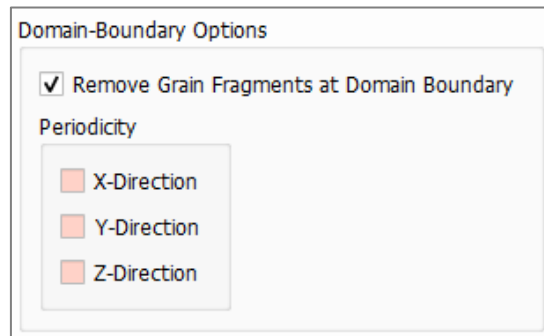
The value for the **Interface Threshold** must be chosen carefully depending on the structure. The smaller the threshold, the more grains are merged. In the figure below, observe the effect of different choices for the **Interface Threshold**. For the extreme value 0 %, all connected grains fragments are merged to one. For a value of 5 %, several large and complex grains are detected in the structure, and for a value of 20 %, many small grains are detected. The choice of the **Interface Threshold** must be adapted to the expected grain shapes for the structure type. To help the user finding the correct **Interface Threshold** for the structure, the **Reconnection Indicators** histogram under the **Results** → **Plots** subtab in the Result Viewer can be used.



DOMAIN-BOUNDARY OPTIONS

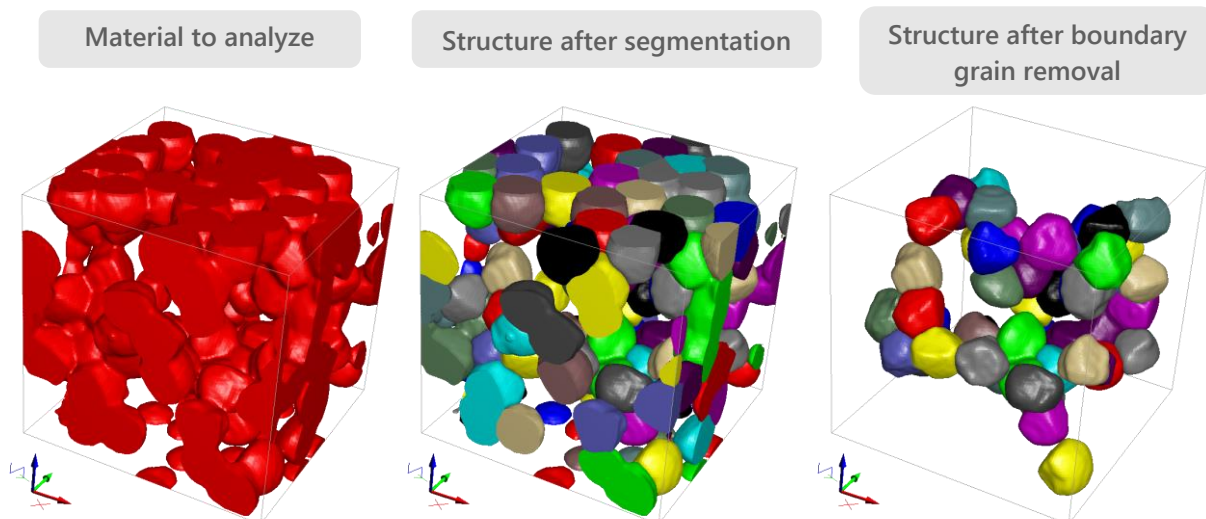
In the **Domain-Boundary Options** panel, the handling of boundary grains is defined. When **Remove Grain Fragments at Domain Boundary** is checked, all grains touching the domain boundary, after the initialization and the grain-fragment reconnection are done, are removed.

This is especially useful if the goal is to estimate the grain shapes and sphericity parameters in the structure: Boundary grains which lay not completely in the structure might lead to wrong estimates for the grain shapes. Nevertheless, also removing the boundary grains influences the results. See page [44](#) for an example and further explanations.



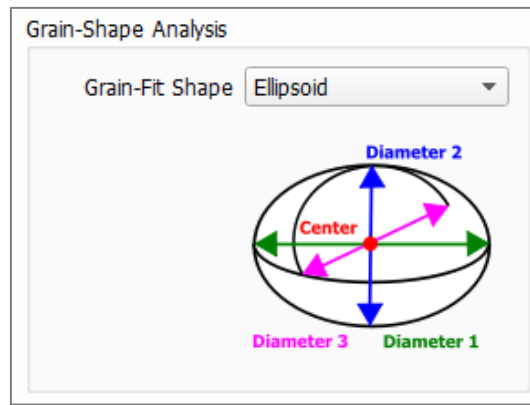
When **Remove Grain Fragments at Domain Boundary** is unchecked, the **Periodicity** options become available. By checking the X-, Y-, or Z-Direction checkboxes, the structure is treated as periodic in the chosen direction(s) before the segmentation.

This option should only be chosen if the investigated structure is really periodic, otherwise it might lead to strange results (with grains which are treated as connected but are distant from each other in reality). Otherwise, when **Periodicity** is not chosen in a direction, the structure is analyzed with encased boundary conditions (i.e. empty space around the domain) in this direction.

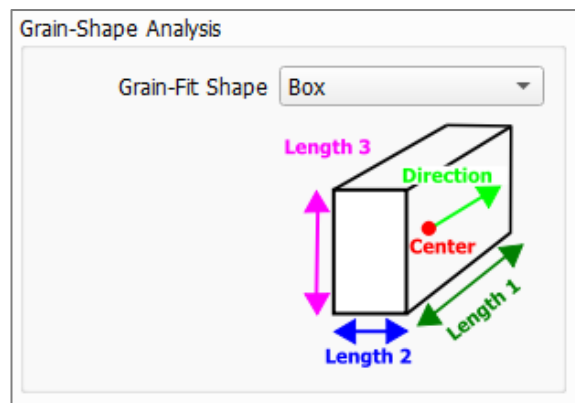
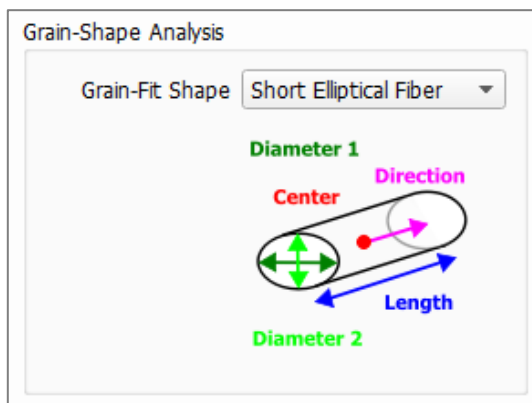


GRAIN-SHAPE ANALYSIS

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 with the help of best-fit shapes.



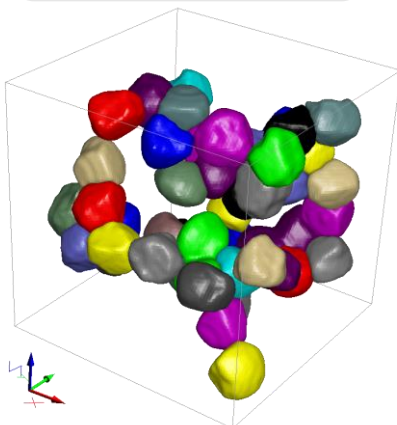
There are three options available for the **Grain-Fit Shape**: Either an **Ellipsoid**, a **Short Elliptical Fiber** or a **Box** can be chosen. The Grain-Fit Shape should be chosen depending on the grain shape appearing in the analyzed structure.



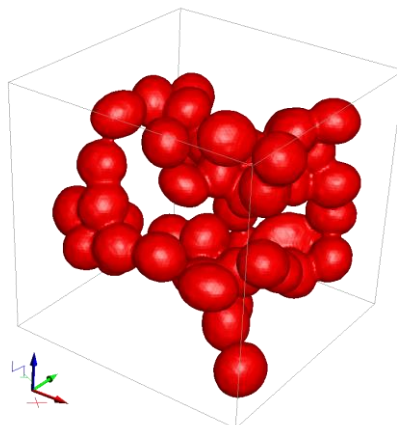
In the figure below, the results of the **Grain-Shape Analysis** are shown. These visualizations are loaded from the Results Viewer of the *.gdr result file (under the **Grain Visualization** tab), see page [17](#) for more information.

The structure after Boundary-Grain Removal is shown on the left. In the middle, the grain-fit shapes are shown (here, **Ellipsoid** was chosen as the **Grain-Fit Shape**) and on the right, a comparison between the identified grains (red) and their fit shapes (green) is shown, where the matching voxels are shown in grey.

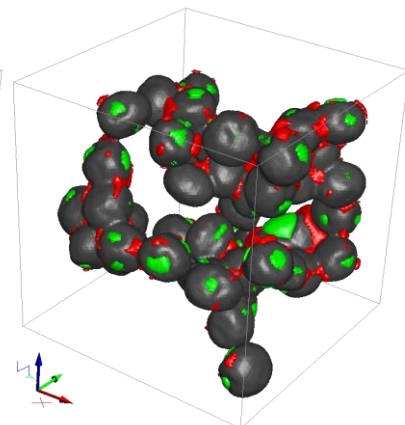
Load Grains from Step 3
(Result of Boundary Grain
Removal)



Load Grain Fit Shapes



Load Comparison of Segmented
Grains and their Fits



OUTPUT OPTIONS

Under the **Output Options** tab, some additional results to be computed and saved can be chosen. They are displayed later for visualization in the Result Viewer under the **Grain Visualization** tab. Some of these options need an additional computing effort and are unchecked by default.

- Choose **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 (see page [26](#)) or for further analysis with Python.

- With **Save Inscribed-Sphere Diameters and Sheppard Sphericities** checked, the diameter of the inscribed sphere for every grain is calculated and the Sheppard sphericity is computed according to [\(1\)](#).

The Sheppard sphericities and the inscribed sphere diameters can be found in the Result Viewer (Results – Plots – Sphericities tab and Diameters tab, see page [18](#)). Both options need additional computing effort and are unchecked by default.

- **Save Grain-Orientation Distribution as *.gof** to 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.

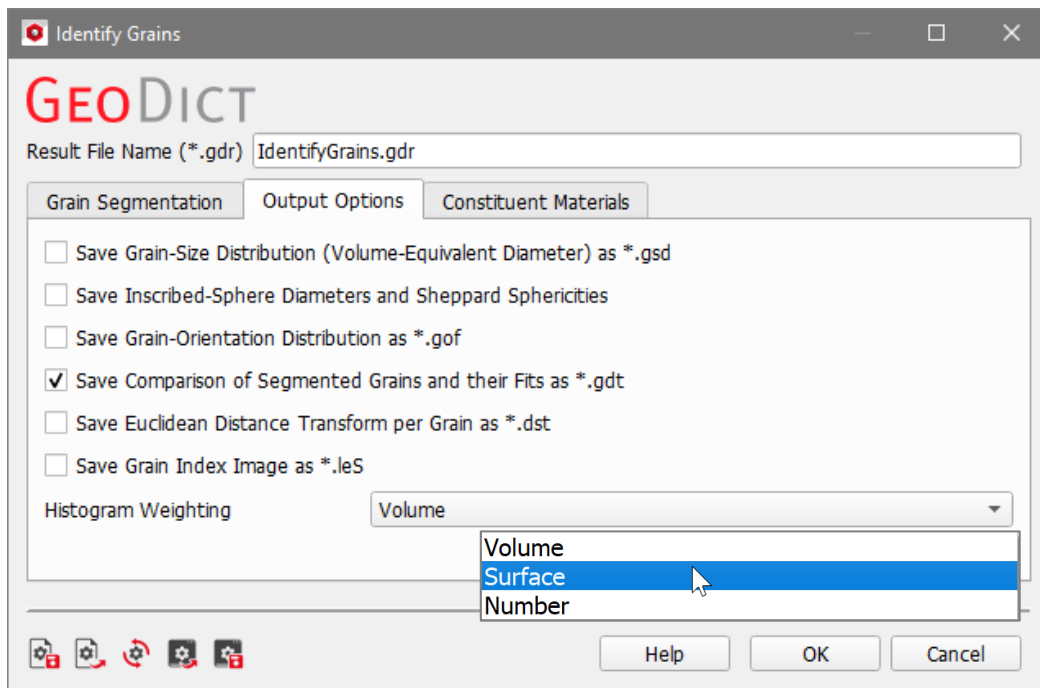
- The checked-by-default option **Save Comparison of Segmented Grains and their Fits as *.gdt** is useful to evaluate the quality of the computed **Grain-Fit Shapes** (Ellipsoids, Short Elliptical Fibers or Boxes, see page [13](#)).

A good accordance of the grain fit shapes and the identified grains is important as a basis for generating good digital twins of the structure with **GrainGeo Create – Load GrainFind Result** (See page [29](#)).

- With **Save Euclidean Distance Transform per Grain as *.dst**, the Euclidean distance transform for every grain is calculated individually and the result is saved in one single *.dst file. This option needs additional computing effort and is unchecked by default.

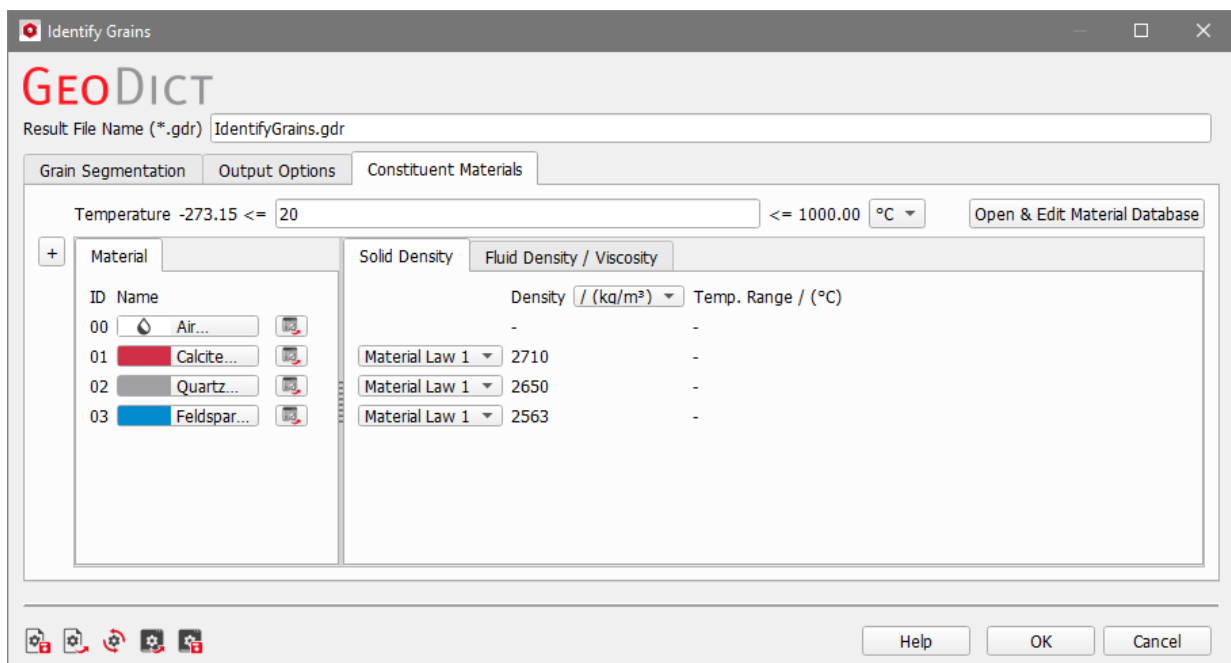
- The resulting grain index image is saved by default in the binary *.g32 format. With **Save Grain Index Image as *.leS**, it can be additionally saved as an ASCII file. This format takes more space and needs longer to write and load into **GeoDict**, but it is human-readable and can easily be imported 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 result viewer after the simulation has been run.

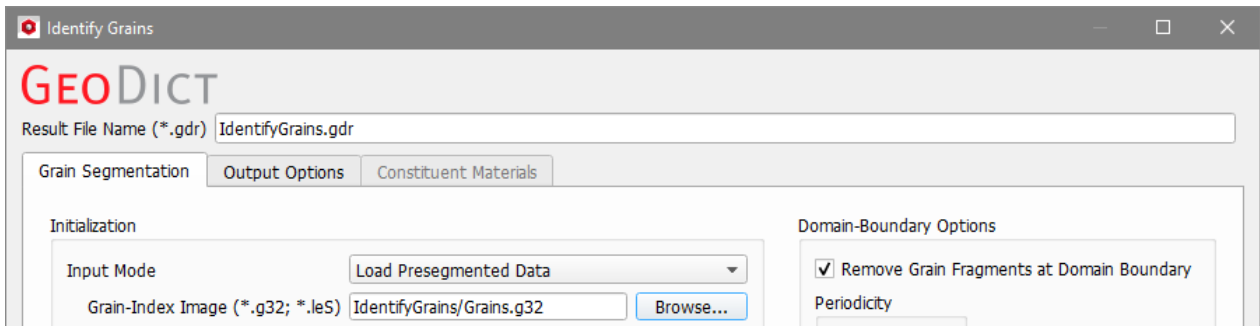


CONSTITUENT MATERIALS

In the constituent materials tab, a material from the **GeoDict** material database can be assigned to each material phase in the structure. Alternatively, manual materials can be defined. In **GrainFind-Identify Grains**, the density of the grain materials is used to compute the mass and moment of inertia of the grains. For further information about material in **GeoDict**, see the [GeoDict Material Database](#) handbook of the User Guide.



The **Constituent Materials** tab is only available if **Use Current Structure** is chosen as input under the **Grain Segmentation** tab. In the other cases, no material IDs exist to which the materials could be assigned, and the tab is greyed out.



GRAIN IDENTIFICATION RESULTS

After performing the **GrainFind** analysis, the results are saved in a **GeoDict** result file (*.gdr) with the given Result File Name. When the analysis is finished the **Result Viewer** opens automatically. For more information about the GeoDict **Result Viewer**, refer to the [Result Viewer](#) handbook of the User Guide

The **Result Viewer** contains several tabs. The **Results** tab shows the report of the run as well as several plots, which are described in the [Results](#) section below. In the **Grain Visualization** tab, additional result files can be loaded depending on the choice made in the Output Options. A video of single grains and their fit object can be generated in the **Create Videos** tab.

RESULTS

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** subtab shows statistics about the identified grains. The **Plots** subtab contains different plot options for the analysis of the results. The **Map** subtab contains all resulting data from the **Identify Grains** run. This data is the basis for the tables in the **Report** subtab and for the plots in the **Plots** tab. The **Report** subtab for the example is shown below.

The screenshot shows the **Result Viewer** window. At the top, there is a file list with columns for File, Module, and Command. The selected file is `.../IdentifyGrains.gdr` from the `GrainFind` module, with the command `IdentifyGrains`. Below the file list, there are buttons for `Open...`, `Up`, `Down`, `Swap Selected`, and a checkbox for `Synchronize Tabs`. The main window title is `Mo Aug 28 2023 (2024 Build 67482)` and the file path is `.../GrainFind2024/IdentifyGrains.gdr`. The domain size is `100 x 100 x 100` and the voxel length is `698.302 nm`. The `Load Structure` button is visible. The **Results** tab is active, with subtabs for `Report`, `Plots`, and `Map`. The `Report` subtab is selected, showing the **GrainFind** main results and statistics.

GrainFind Main results

- Number of grains: **48**.
- Number of grain contacts: **63** (total grain contact area: 2737.01 μm^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

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

The interface also includes a histogram weighting control panel on the left with options for `Number` and `Relative` weighting, `Scatter Plot` options for `Vertical Axis (y-Axis)` (Krumbein Sphericities) and `Horizontal Axis (x-Axis)` (Equivalent Diameters), `Threshold by Scalar Value` options for `Scalar Value` (Volume), `Number of Bins` (10), `Thresholding Method` (k-Means), and `Number of Grain Types` (2). There are also `GSD Field Choices` (Equivalent Diameter), `Apply...` button, `Back-up result file` checkbox, and `Plot Options` dropdown. At the bottom, there are buttons for `Manage Data`, `Load Input Parameters`, `Export`, and `Close`.

First, it shows the number of grains and grain contacts that were found. The **Grain volume percentage statistics** table shows the grain volume percentage after each step performed: initial structure, after the watershed transformation, after the reconnection and after the boundary grain removal. The **Grain volume statistics**, **Grain sphericity statistics**, **Grain diameter statistics**, and **Coordination number statistics** tables, each show the minimal and maximal value, the mean value and the standard deviation. For the grain diameters, also the D10, D50, and D90 values are given. At the end of the report tab, the **Grain Orientation tensor** is displayed.

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, **Orientation** polar plot and **Reconnection Indicators** histogram.

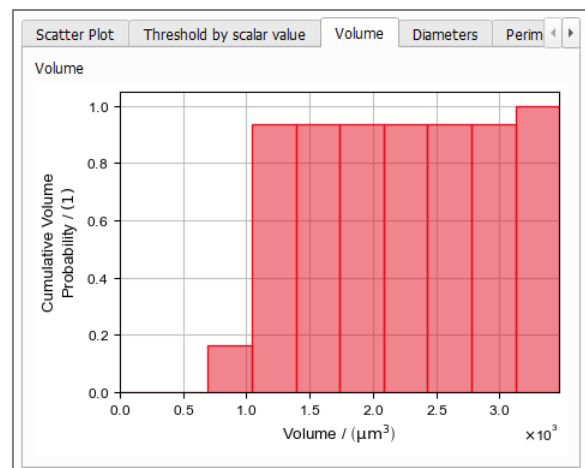
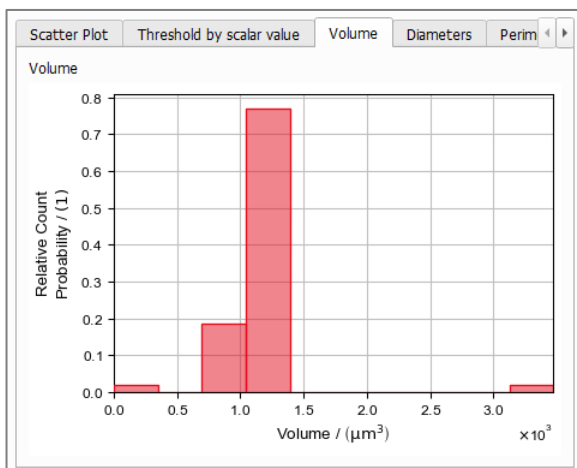
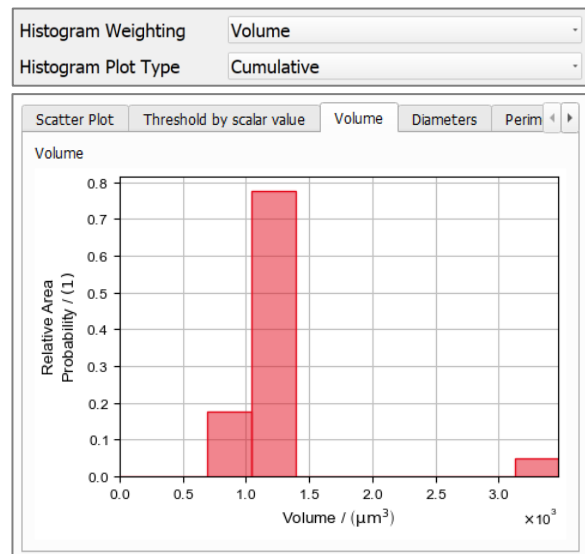
Settings for these plots can be selected in the panel at the left side of the **Plots** tab. After changes are made, click **Apply...** to use the new values. The changes are also applied to the tables under the **Report** subtab.

Plot Options Panel

Histogram Weighting and Histogram Plot Type

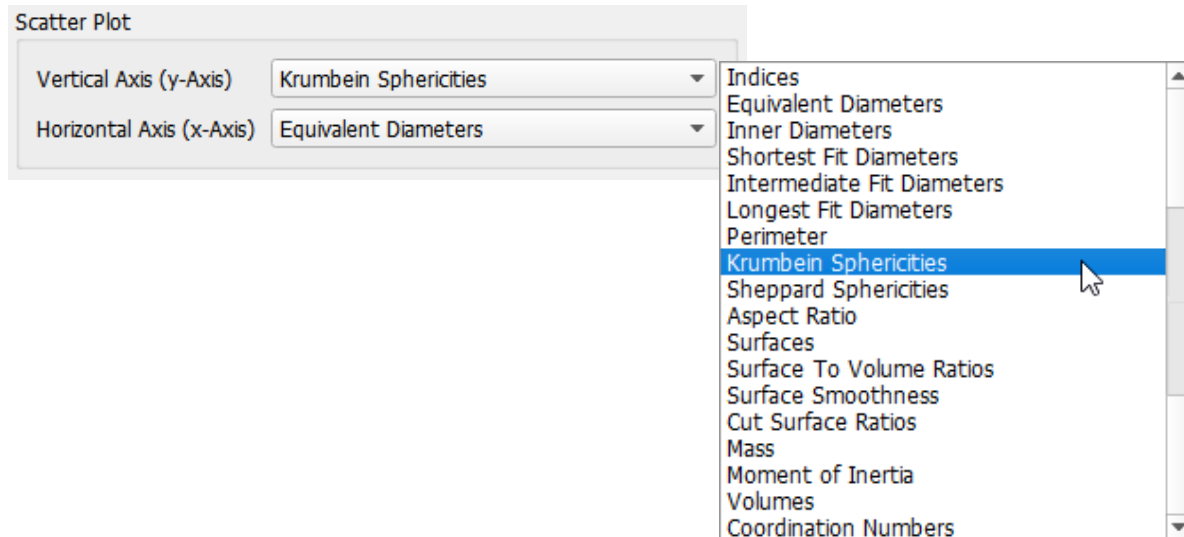
The values on the Y-axes of the histograms in all plots (except **Scatter Plot**, **Threshold by scalar value**, **Orientation** and **Reconnection Indicators**) show Count Probability (weighting by **Number**), Area Probability (weighting by **Surface**) or Volume Probability (weighting by **Volume**), as a **Relative** or **Cumulative** plot. This can be set by adjusting the **Histogram Weighting** and **Histogram Plot Type**.

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.

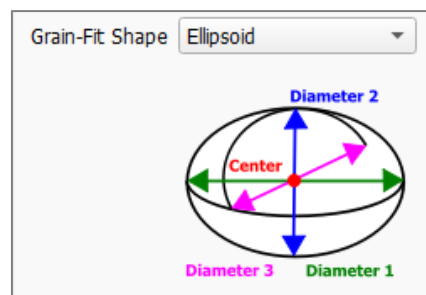


Scatter Plot

Under **Scatter Plot**, the variables for the X- and Y-axis in the scatter plot can be chosen. The variable **Indices** refers to the index of the identified grains and is the same as in the *.g32 file (see page [26](#)). More on the variables can be found in the next section.



The Scatter Plot, as well as the Orientation plot, distinguish between four possible shapes for the **Ellipsoids** that are fitted to the grains. To define such an ellipsoid, a center point and three diameters are needed.

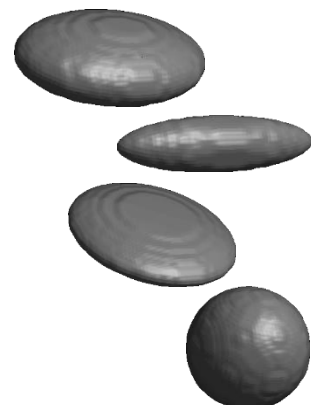


In the following, we set

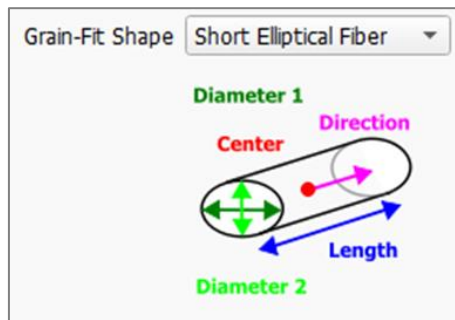
- a to be the length of the longest of the three diameters,
- b to be length of the medium diameter,
- c to be length of the shortest diameter.

Listed below are the four possible shapes for the ellipsoids that are fitted to the grains:

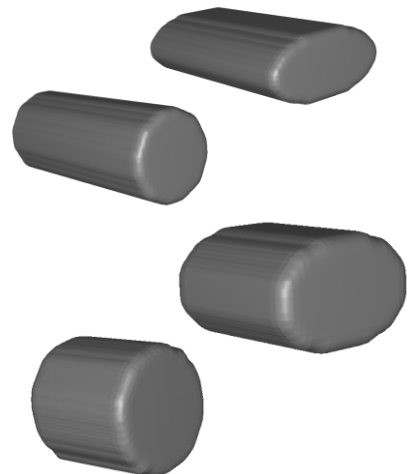
- An ellipsoid is formed as a **Flat Bar**, if all three diameters a , b , and c differ much from each other.
- A **Prolate Spheroid** has one bigger diameter, a , and the two smaller diameters, b and c , are similar to each other. Its shape is similar to a cigar.
- The two bigger diameters (a and b) 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.



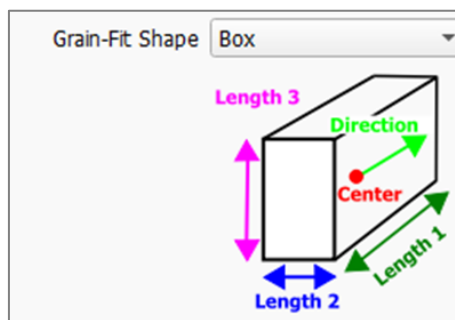
For the shape **Short Elliptical Fiber**, a center point, two diameters and a length are needed to describe one of the following four shapes:



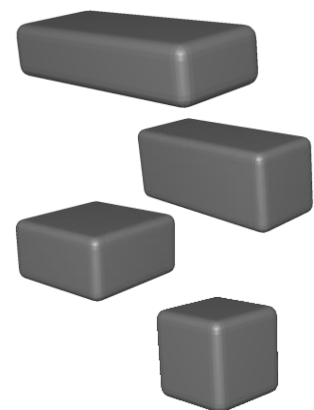
- A fiber is **Elliptical**, if the two diameters are different.
- It is **Circular**, if the two diameters are the same.
- An **Elliptical Stub** has at least one diameter larger than the length and the diameters are different.
- The **Circular Stub** is the same as above, but with equal diameters.



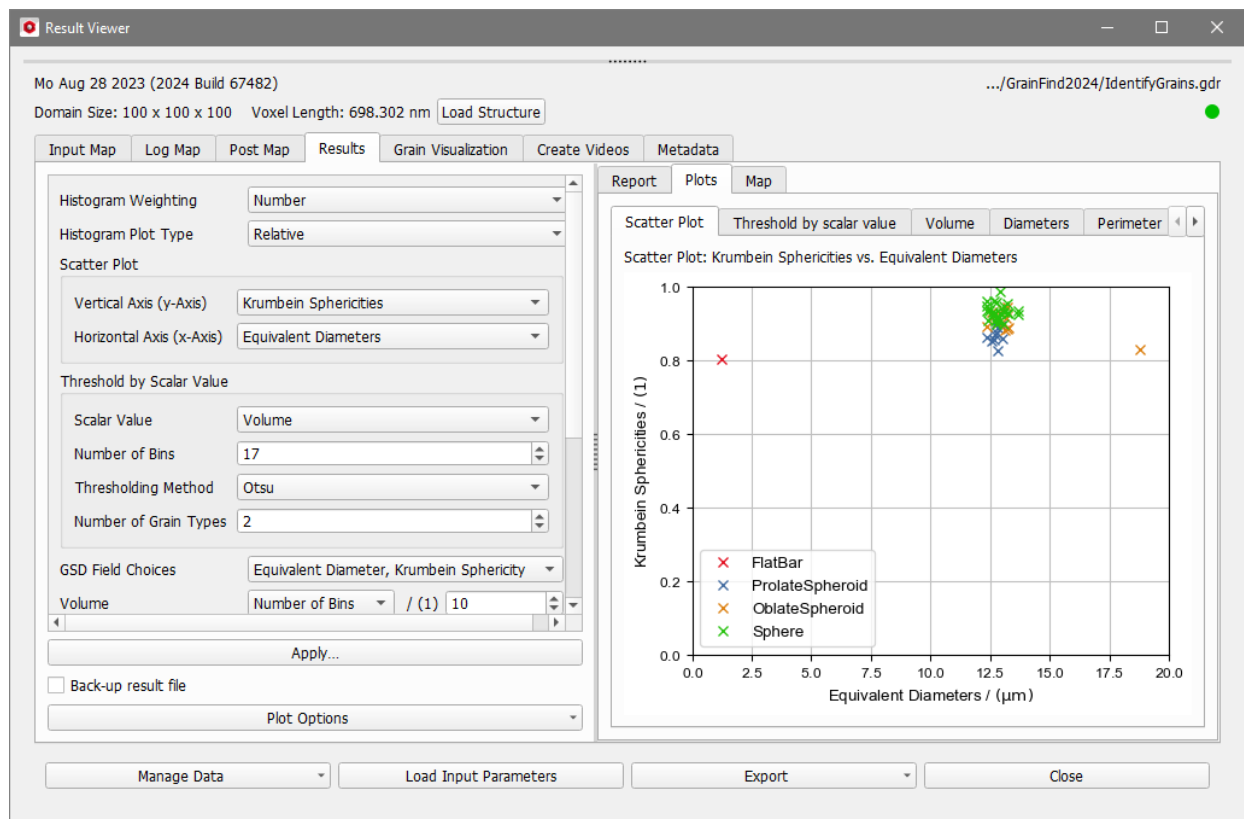
For the shape **Box**, a center point and three diameters are needed to describe the following shapes:



- If 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**.



In the example below, 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 μm , except of two outliers.



Threshold by Scalar Value

The **Threshold by scalar value** plot helps to classify the identified grains based on the computed results. Additionally, a structure containing the materials of the thresholded grains will be created, that can be accessed through the **Grain Visualization** tab → **Load Grain-Type Structure** → click **Load *.gdt** or **Load *.gad** button. In the panel on the left side, several options for thresholding the structure depending on the results are available. First, the **Scalar Value** to determine a threshold for must be selected from the drop-down list. The default scalar value is **Volume**. The choice of the **Scalar Value** affects the plot that is created under the **Plots - Threshold by scalar value** subtab. The following **Scalar Values** are available for thresholding:

- **Equivalent Diameter:** The equivalent diameter is the diameter of the sphere which has the same volume as the grain.
- **Inner Diameter:** The inner diameter is the diameter of the largest sphere that can be inscribed into the grain.
- **Shortest Fit Diameter:** This is the shortest diameter of the shape (ellipsoid, box, short fiber) fitted to the grain.
- **Intermediate Fit Diameter:** This is intermediate diameter of the shape (ellipsoid, box, short fiber) fitted to the grain.
- **Longest Fit Diameter:** This is the longest diameter of the shape (ellipsoid, box, short fiber) fitted to the grain.

- **Perimeter:** The computed perimeter is the shortest perimeter around the shape. For a fitted ellipsoid, it is computed as the perimeter of the ellipse formed from the two smallest of the three diameters, that define the ellipsoid.
- **Krumbein Sphericity:** The Krumbein Sphericity is a measure for the sphericity of the grain, based on the grain fit (see equation (2)).
- **Sheppard Sphericity:** The Sheppard Sphericity is defined as the diameter of the inscribed sphere divided by the diameter of the volume-equivalent sphere (see equation (1)).
- **Aspect Ratio:** The aspect ratio is the shortest diameter of the shape divided by the largest diameter of the shape.
- **Surface Area:** The surface of the grains is estimated by an algorithm based on MatDict's **Estimate Surface Area** command (see [3] and MatDict handbook of the User Guide). 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.
- **Surface-to-Volume Ratio:** The estimated surface area of the grain is divided by the volume of the grain.
- **Surface Smoothness:** This is the surface of a fitted shape divided by the estimated surface of the grain. Usually the estimated 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.
- **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.

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 (page 12), then the cut surface ratio is zero, too, because there will be no grains left that have an interface with the domain boundaries.

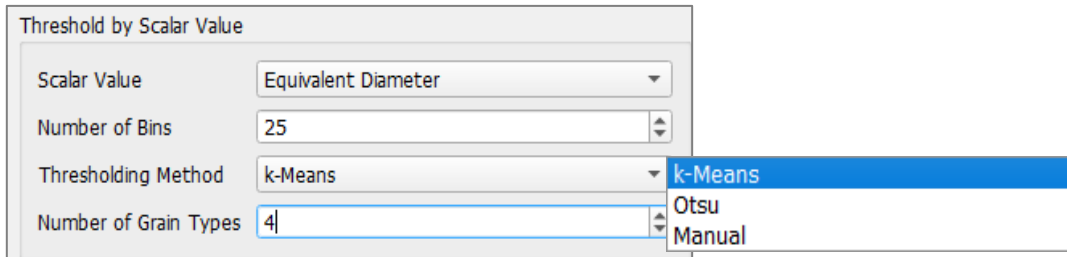
- **Mass:** If a density is assigned to the solid materials, each grain has a mass which can be calculated from its volume.
- **Moment of Inertia:** The moment of inertia is computed based on the grain shape and the density of the grain material.
- **Volume:** The volume of the grain is simply determined by the number of voxels the grain contains. To get a volume in metrical units, it is multiplied by the cubed voxel length:

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

- **Coordination Number:** This is the number of contacts of a grain to other grains.

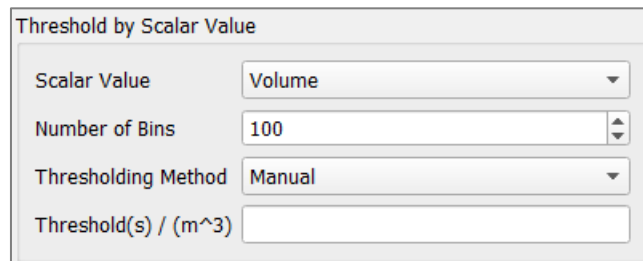
NOTE that the choice of **Inner Diameter** and **Sheppard Sphericity** are only available if the option **Save Inscribed-Sphere Diameter and Sheppard Sphericities** was checked in the **Output Options** of the grain-identification options (page [14](#)).

The **Number of Bins** defines how many bins the histogram **Threshold by scalar value** has.



The following **Thresholding Methods** are available:

- **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)**. They will then be applied to the computed grain index image.



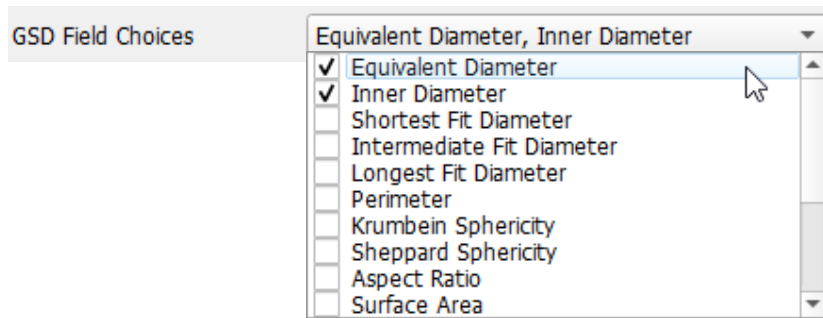
GSD Field Choices

The **GeoDict** size distribution (GSD) files allow to visualize the various scalar grain properties that are a result of the grain identification.

See the options for the configuration of a **GeoDict** size distribution (GSD) file in the figure below. For every chosen grain property, a volume field is created containing the 3D distribution of this grain property. These volume fields are saved together in a GSD file (*.gsd), which can be accessed through the **Grain-Visualization** tab → **Load Grain-Size Distribution** → click **Load *.gsd** button.

For example, by choosing **Equivalent Diameter** and **Inner Diameter**, the *.gsd file will contain two volume fields: one with the size distribution of the diameters of volume-equivalent spheres, and one with the distribution of the inner diameters.

The same parameters to assemble a customized size distribution are available as for the thresholding (see page [21](#)).



Histogram Bin Sizes

The bin sizes used in the plotted histograms can be customized.

Volume	Number of Bins	/ (1)	10
Diameter	Number of Bins	/ (1)	50
Perimeter	Bin Size in Voxels	/ (Voxels)	1
Sphericity and Aspect Ratio	Number of Bins	/ (1)	50
Surface and Contact	Number of Bins	/ (1)	54
Surface-to-Volume Ratio	Bin Size in Units	/ (1/nm)	0.00038
Surface Smoothness	Number of Bins	/ (1)	50
Mass	Number of Bins	/ (1)	10
Moment of Inertia	Number of Bins	/ (1)	25

In general, it is possible to 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 appropriate unit (m, μm , nm, 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.

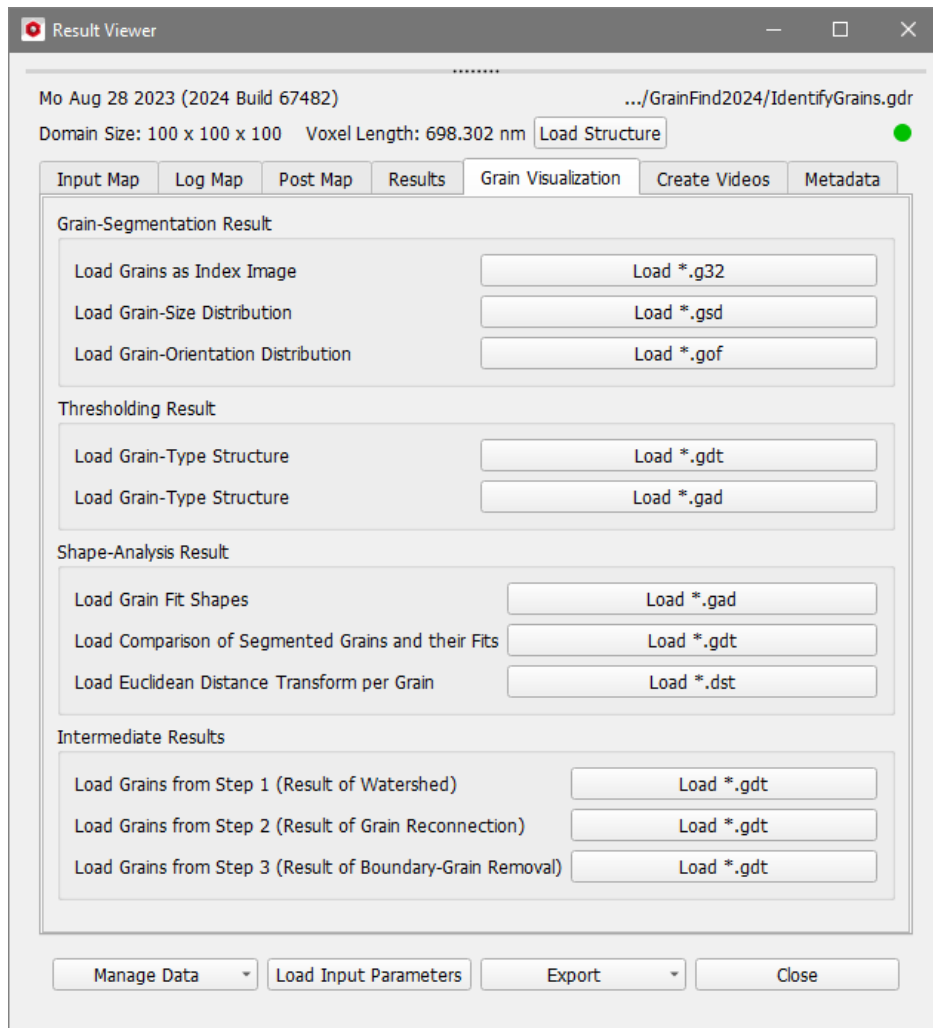
- The selection made under **Volume** changes the bin size for the plot under the **Volume** tab.
- The selection made under **Diameter** changes the bin size for all plots under the **Diameters** tab.
- The selection made under **Perimeter** changes the bin size for the plot under the **Perimeter** 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 for **Mass** changes the bin size for the **Mass** histogram.
- The selection made for **Moment of Inertia** changes the bin size for the **Moment of Inertia** histogram.

GRAIN VISUALIZATION

The **Grain Visualization** tab is used to import structures and computed volume fields which illustrate the grain identification process and its results.

There are several options available for the visualization of the different steps of **Identify Grains** and for the evaluation of the quality of the results. Some options in the **Grain Visualization** tab might be unavailable, depending on the parameters chosen in the **Identify Grains dialog** (Output Options tab, see page [14](#)). The visualization options are grouped into panels.



GRAIN-SEGMENTATION RESULT

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

The **Load Grain-Size Distribution** and the **Load Grain-Orientation Distribution** are greyed out when the corresponding option has not been previously checked under the **Output Options** tab of the **Identify Pores** dialog (see page [14](#)).

As mentioned above in [GSD Field Choices](#), the option **Load Grain-Size Distribution** loads the Grain-Size Distribution file (*.gsd), that contains the 3D distributions of the grain properties chosen in the **Results** tab (page [Error! Bookmark not defined.](#)).

Load Grain-Orientation Distribution loads the orientation distribution file (*.gof) of the grains found by the grain identification process.

THRESHOLDING RESULT

The structure that contains the thresholded grain materials is loaded by clicking the **Load Grain-Type Structure** button. Here, either **Load *.gdt** or **Load *.gad** can be chosen. The options for the thresholding can be found in the **Results** tab as mentioned above in [Thresholding](#).

SHAPE-ANALYSIS RESULTS

Several options for the analysis of the identified grain shapes are available in the **Shape-Analysis Results** panel. With **Load Grain Fit Shapes**, the best-fit shapes for the individual grains are imported into GeoDict as *.gad file and can be visualized.

The option to **Load Comparison of Segmented Grains and their Fits** is closely related to **Load Grain Fit Shapes**. The identified grains and their best-fit shapes are both imported into GeoDict and shown as different materials (**Original** and **Fit**). This visualization is useful to check if the chosen best-fit shape type suits the grain structure. It is also a good indicator to evaluate the performance of GrainFind with the chosen options (compare the figure on page [13](#) for reference).

With **Load Euclidean Distance Transform per Grain**, the results of the Euclidean Distance Transform for each grain can be imported if **Save Euclidean Distance Transform per Pore as *.dst** was previously checked under the **Output Options** tab of the **Identify Pores** dialog (see page [14](#)).

INTERMEDIATE RESULTS

In the **Intermediate Results** panel, results from the identification steps can be loaded.

With **Load Grains from Step 1 (Result of Watershed)**, the segmented structure after the watershed transform is shown without any post-processing. Depending on the structure and the chosen **Minimal Grain Diameter**, this step might already suffice for identifying the grains. Otherwise, this option is useful for checking the initialization options – mainly if the **Minimal Grain Diameter** was chosen correctly for the investigated structure.

By clicking **Load Grains from Step 2 (Result of Grain Reconnection)**, the structure after the Grain-Fragment Reconnection is loaded in GeoDict. This way it can be investigated if the chosen value for the **Interface Threshold** suits the analyzed structure. This is only available if **Reconnect Fragmented Grains** was checked in the **Grain Segmentation** tab of the **Identify Grains** dialog (see page [10](#)).

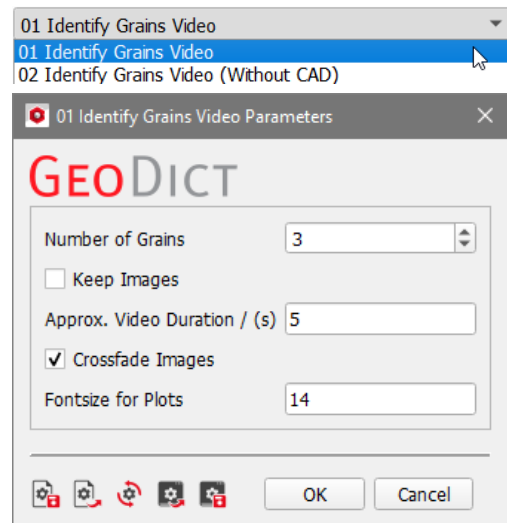
Load Grains from Step 3 (Result of Boundary-Grain Removal) imports the structure after the steps defined in the **Domain-Boundary options** are evaluated. This is only available if **Remove Grain Fragments at Domain Boundary** was checked in the **Grain Segmentation** tab of the **Identify Grain** dialog (see page [12](#)).

For the visualization of the identified grains, remember that the visibility of all material IDs must be set to visible in **Settings** → **Color & Visibility Settings** → **visible**. The identified grains are assigned up to 255 random colors, which are unrelated to their size. The visibility of the pore space (ID 00) should remain unchecked and thus it will not be rendered.

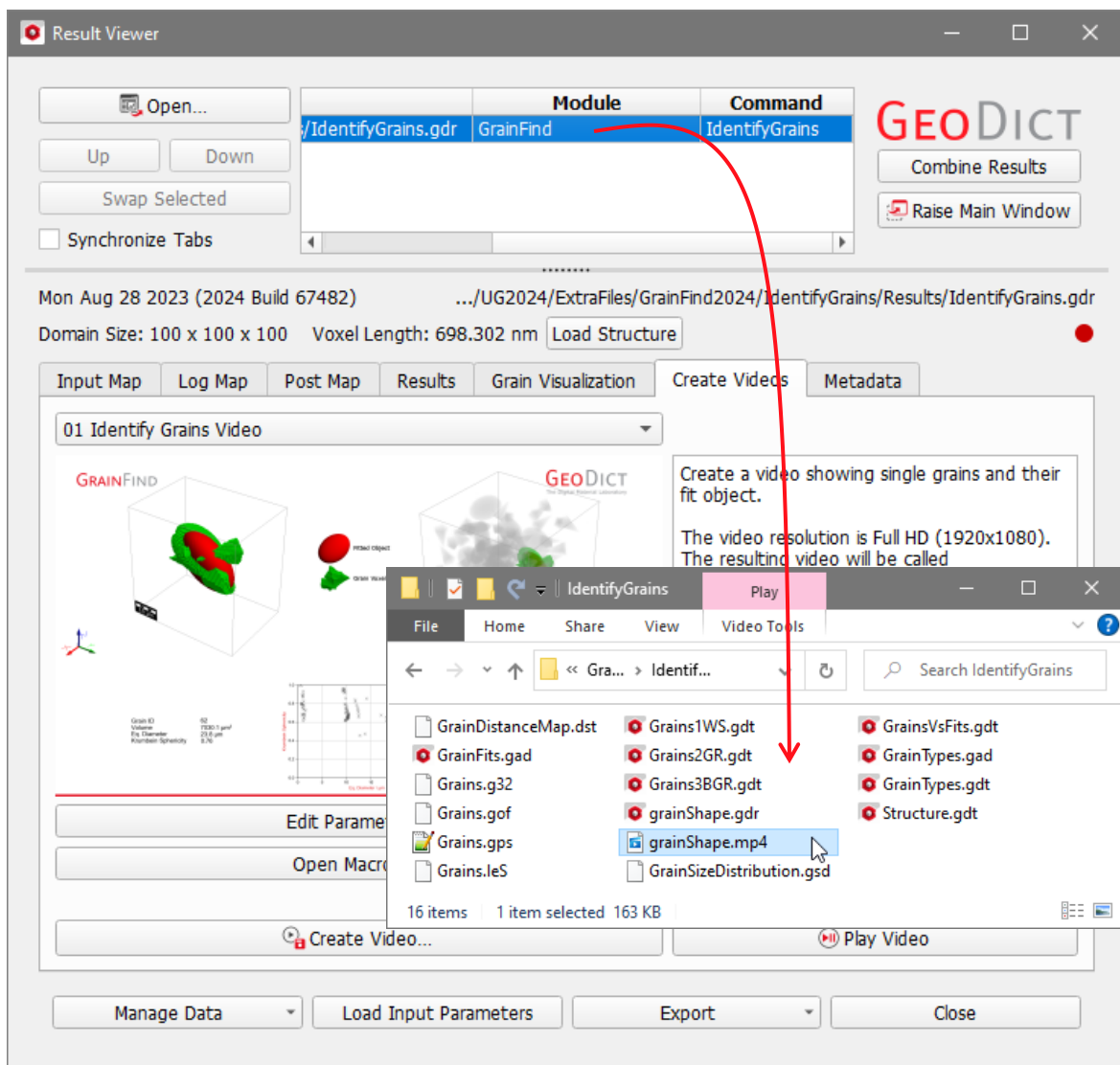
CREATE VIDEOS

With **Create Videos**, it is possible to automatically generate a video showing the largest identified grains compared to their fit shapes. During the creation, **ExportGeo-CAD** is used to create a smooth surface for the visualized grains. Note that a special license is required to use this feature. Alternatively, in the drop-down menu there is the option to choose the video generation without the module **ExportGeo-CAD** by choosing **Identify Grains Video (Without CAD)**.

Click **Edit Parameters...** to choose the number of grains that should appear in the video. Additionally, the video duration and the fontsize for the plot labels can be edited.



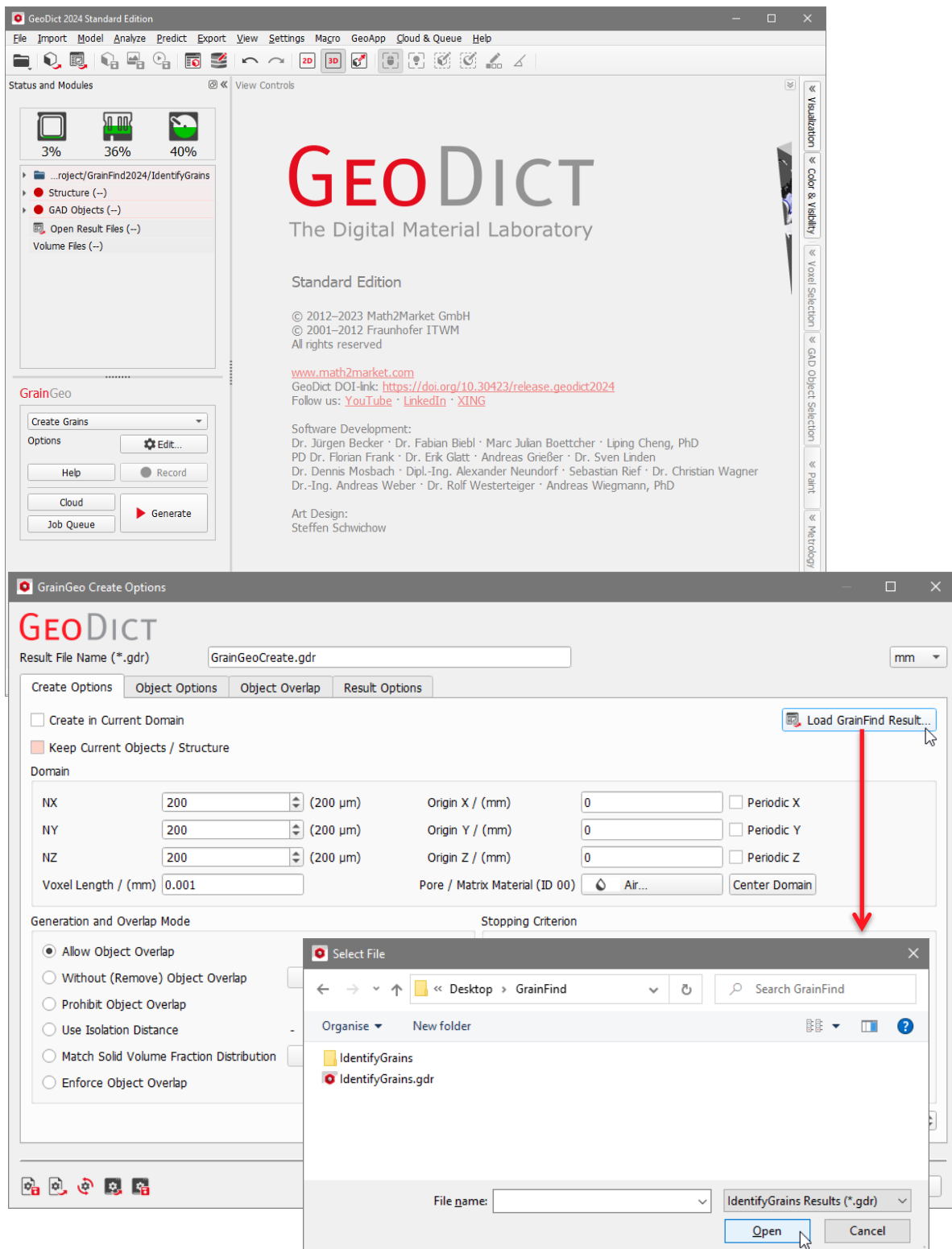
Clicking the **Create Video ...** button starts the creation of the video. When the video is finished, the video file is saved in the results folder belonging to the loaded *.gdr file. The result folder can be opened by right-clicking on the file name and path in the Result Viewer Header section box and choosing **Open Result Folder**.



CONNECTING GRAINFIND ANALYSIS RESULTS WITH GRAINGEO

The results of a **GrainFind** run can be used to generate structures with similar properties in **GrainGeo** – a “digital twin” of the material can be created. Here, this procedure is shown with the structure used for the examples above.

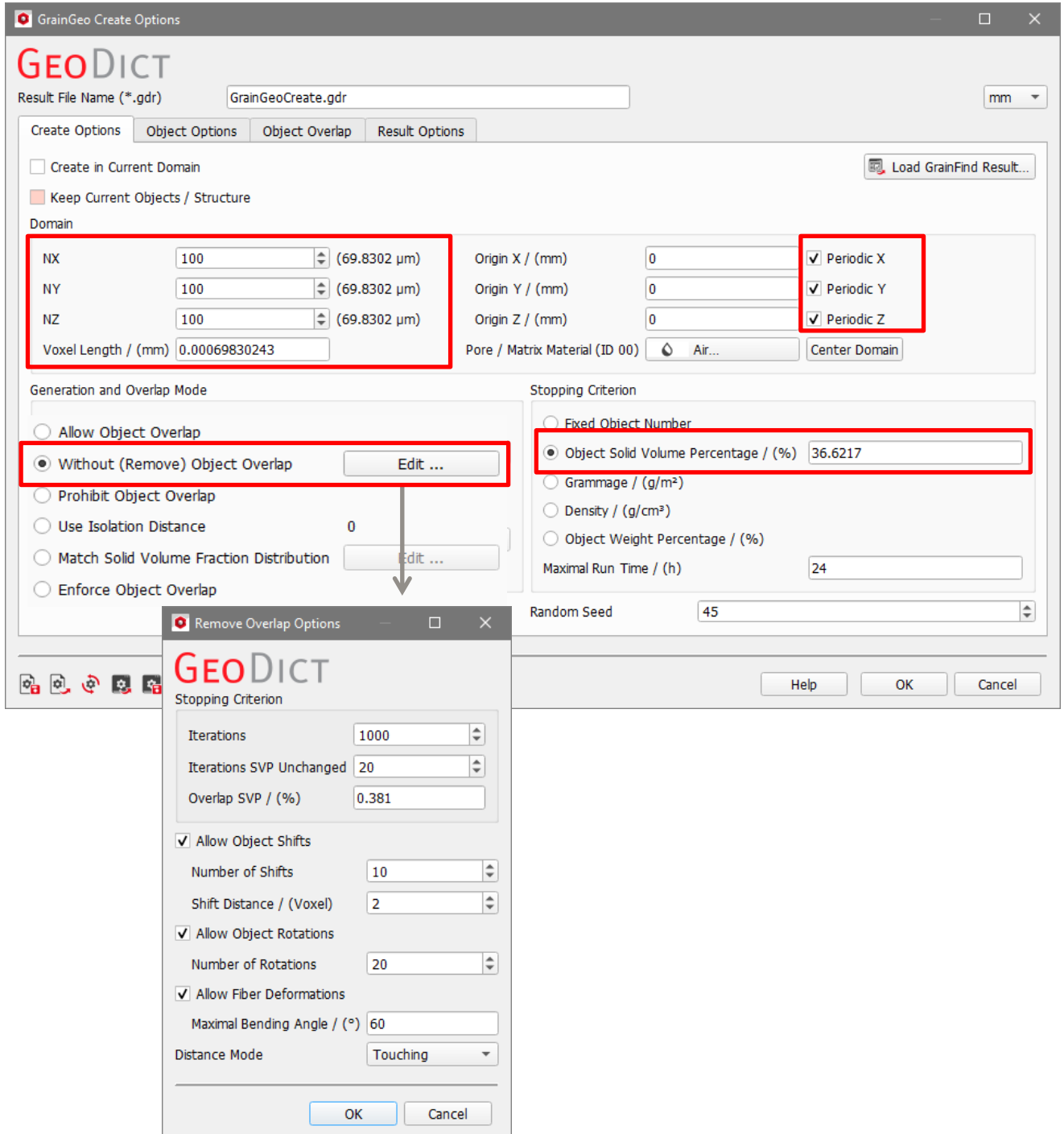
Start **GrainGeo** by selecting **Model** → **GrainGeo** in the menu bar and choose **Create Grains** from the pull-down menu. Click the **Edit...** button. In the upper right of the **GrainGeo Create Options** dialog, click **Load GrainFind Result ...** and select a **GeoDict** result file (*.gdr) from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



The data from the *.gdr file is now directly loaded into GrainGeo.

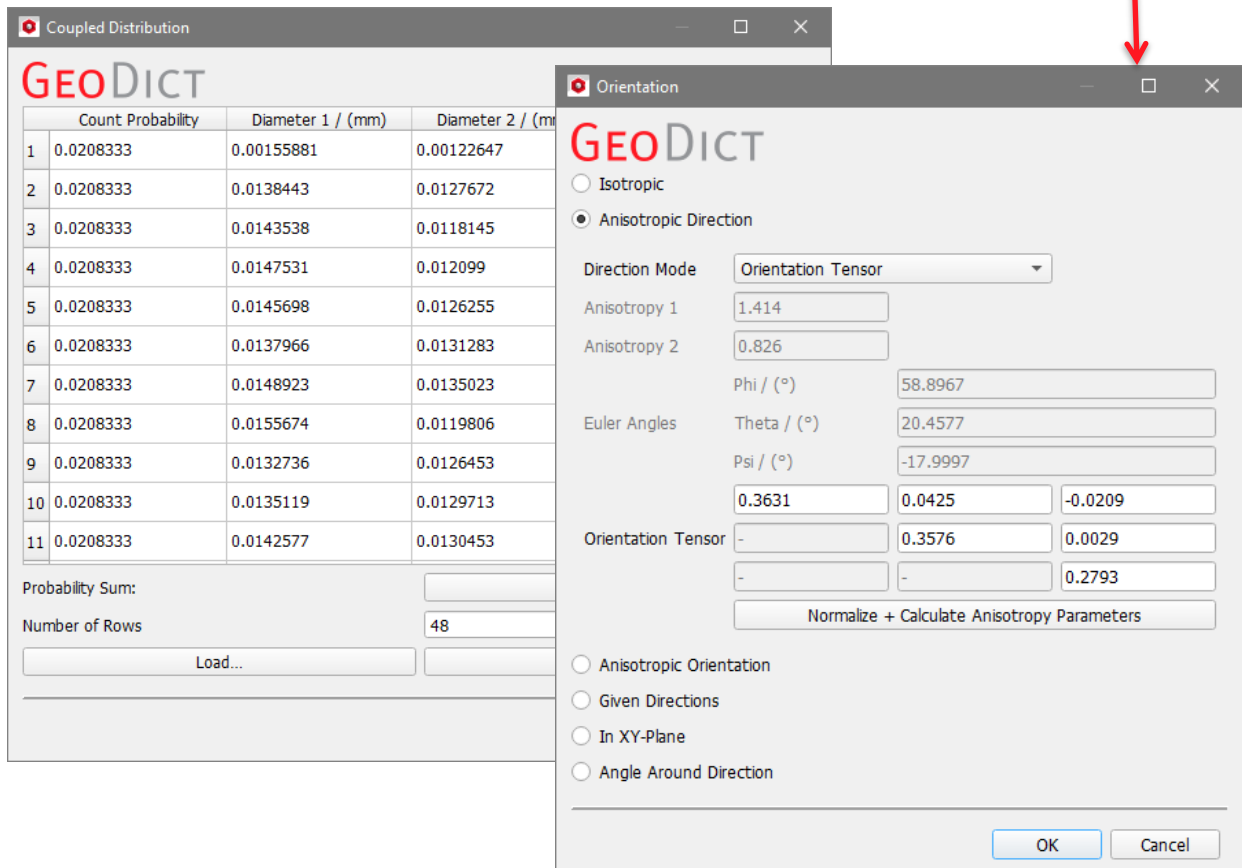
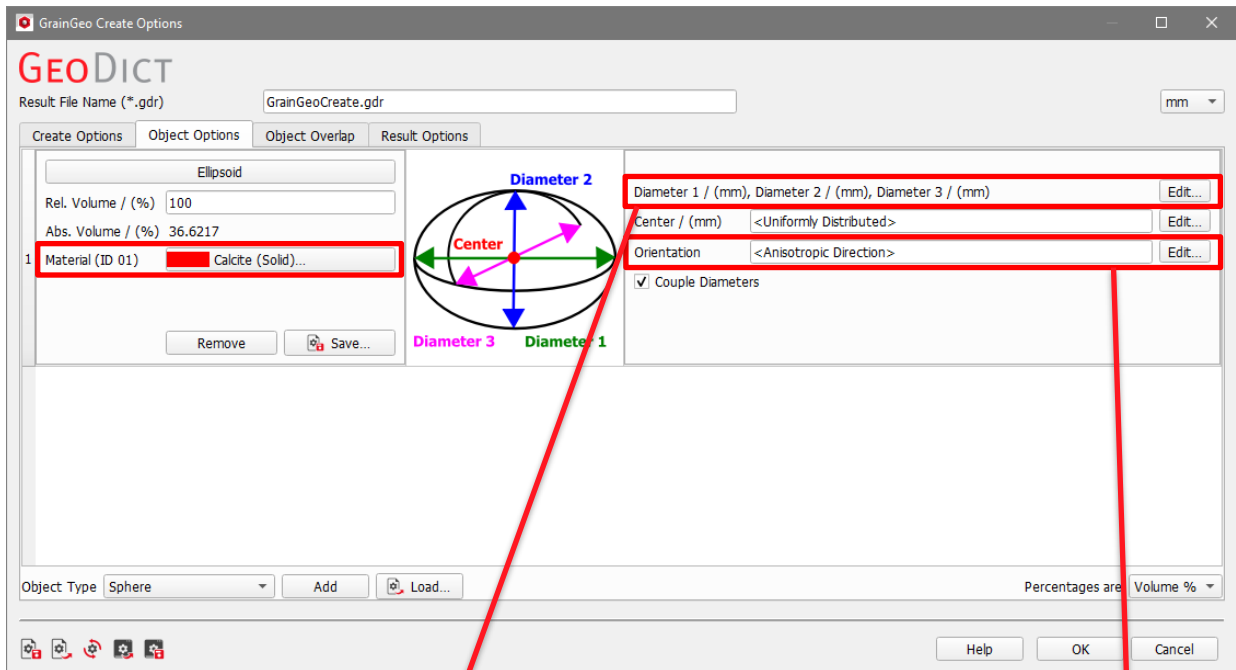
In the figure below, the parameters directly imported from the GrainFind result are displayed under the **Create Options** tab and the **Object Options** tab in the **GrainGeo Create Options** dialog.

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 **Solid Volume Percentage** of the structure under the Create Options tab.

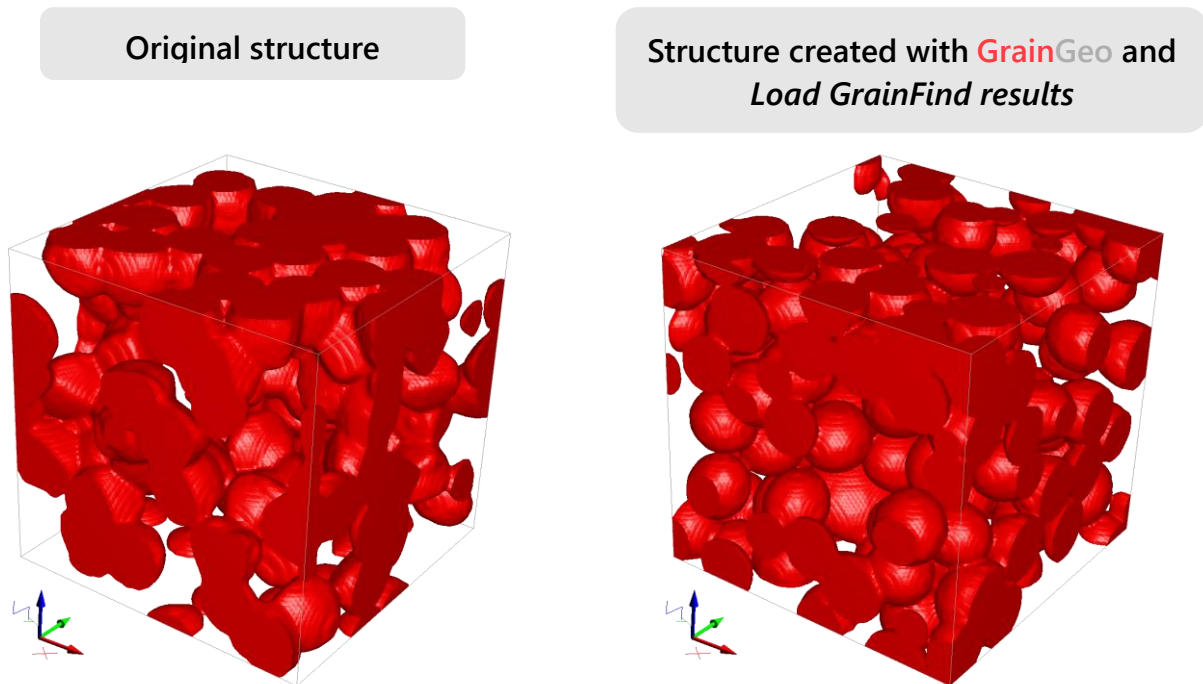


Identify grains – Connecting GrainFind with GrainGeo

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.

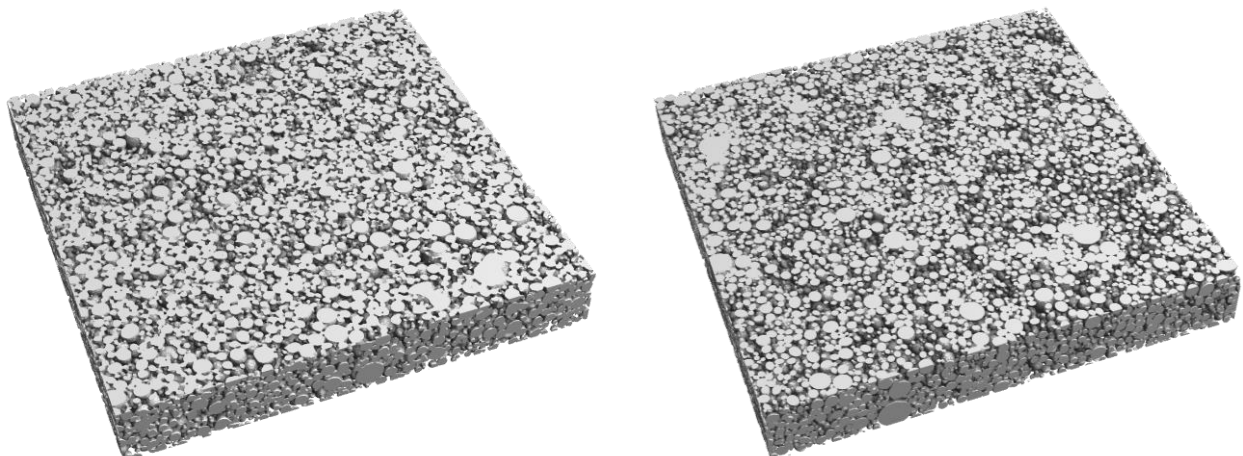


By clicking **Generate** in the **GrainGeo** section, a structure with the parameters obtained from **GrainFind** is created in **GrainGeo**. In the example below, on the left side the original structure (this structure is analyzed with **GrainFind**) and a structure based on the **GrainFind** parameters 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, which can be seen below. For more details, please have a look at our tutorial "[Building a statistical Digital Twin of a cathode](#)".



Segmented NMC cathode structure. Data provided by the Laboratory for Nanoelectronics, ETH Zurich.

See M. Ebner et al., Tortuosity Anisotropy in Lithium-Ion Battery Electrodes, Advanced Energy Materials, Volume 4, Issue 5, April 2, 2014. This structure is also used in the GrainFind tutorial.

Structure created with GrainGeo and "Load GrainFind Results"

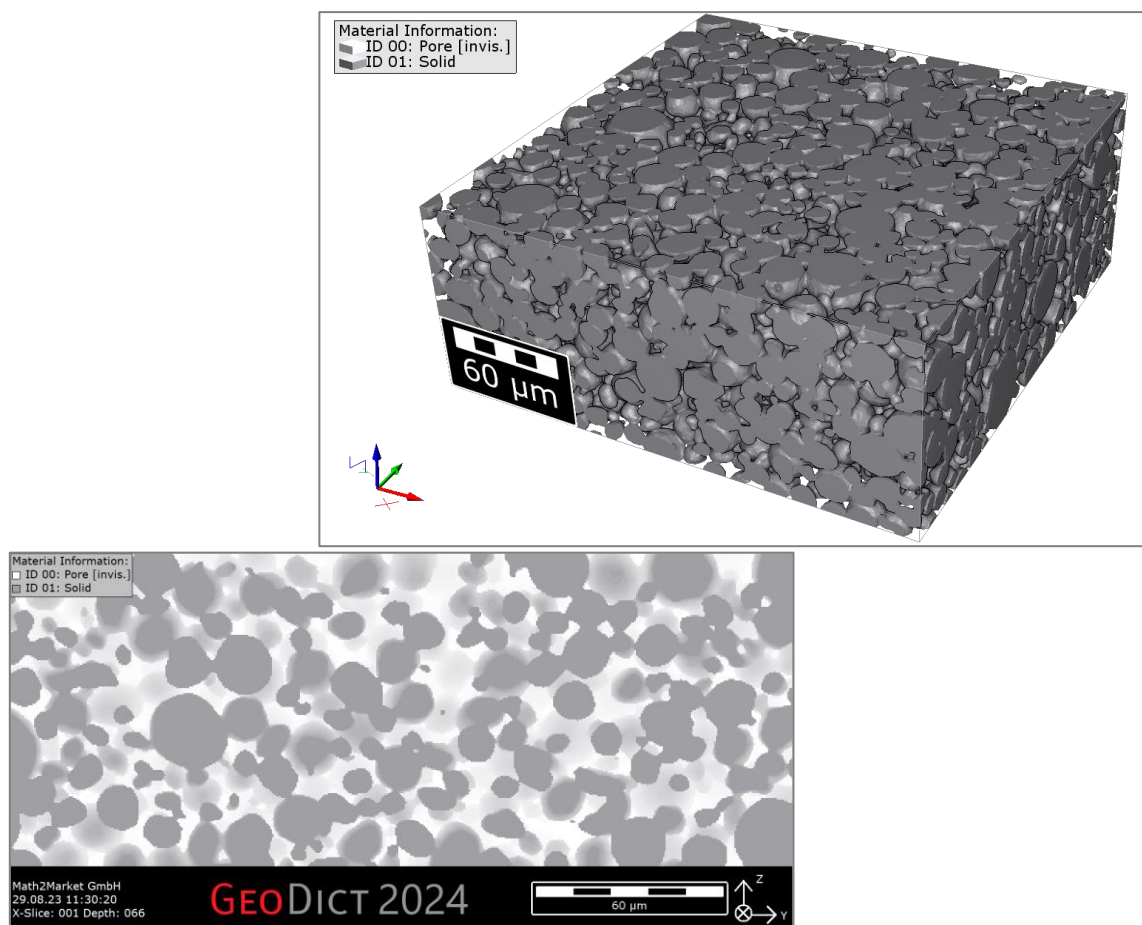
For more information, check the "[Building a statistical Digital Twin of a cathode material with GrainFind and GrainGeo](#)" tutorial

IDENTIFY BINDER (AI)

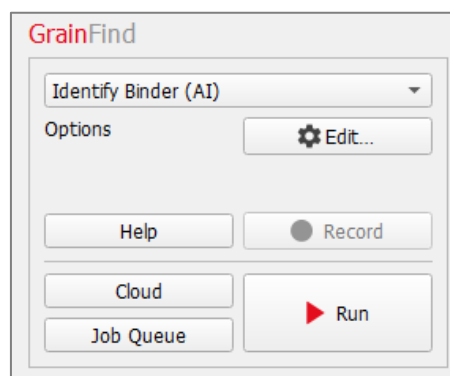
To use the **Identify Binder (AI)** functionality, a **GrainFind-AI** license is required.

The separation between solid and pores of a structure can usually be done using image processing methods during the import of the scanned data sets (see the [ImportGeo-Vol](#) handbook of the User Guide for more details). However, the separation of binder from grains is often not possible since they have similar gray values in the scan.

The structure shown here is a segmented sample of a NMC cathode structure from the Laboratory for Nanoelectronics, ETH Zurich (See page [32](#) for reference).



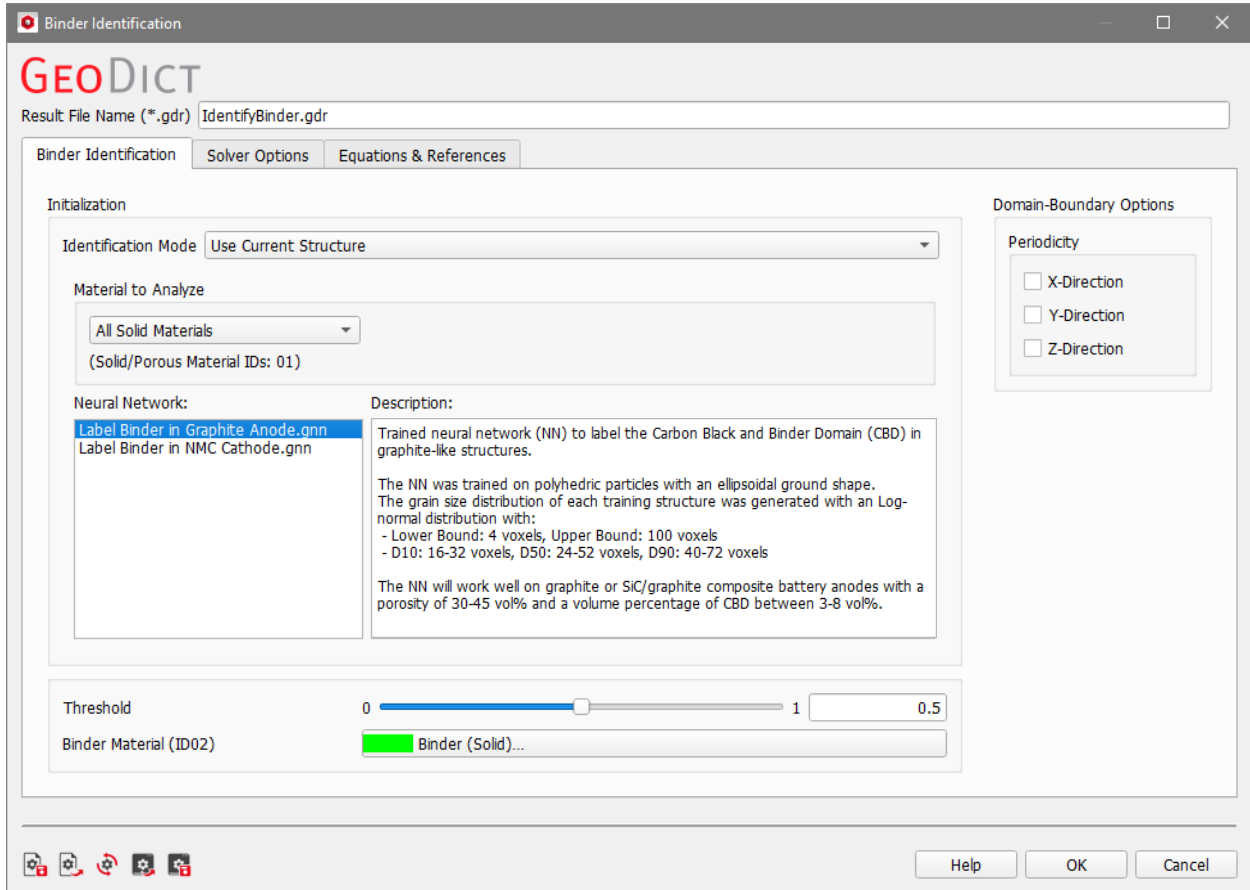
To start, select **Analyze** → **GrainFind** from the menu bar and, in the **GrainFind** section, select **Identify Binder (AI)** from the pull-down menu. Click the **Options' Edit...** button.



BINDER IDENTIFICATION SETTINGS

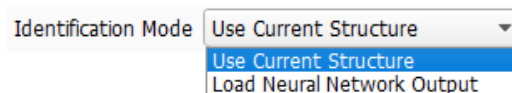
The **Binder Identification** dialog that opens includes the **Binder Identification** tab, the **Solver Options** tab and the **Equations & References** tab.

At the top, enter the **Result File Name (*.gdr)** under which the results are saved in the chosen project folder.



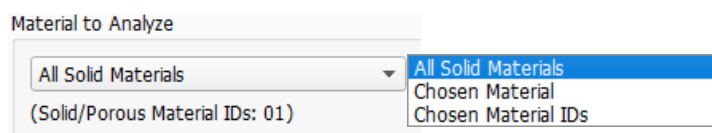
BINDER IDENTIFICATION TAB

Two choices are available as **Identification Mode: Use Current Structure** and **Load Neural Network Output**.



The default **Use Current Structure** applies the binder identification to the structure currently available in the GeoDict memory. This is the common use case for Identify Binder.

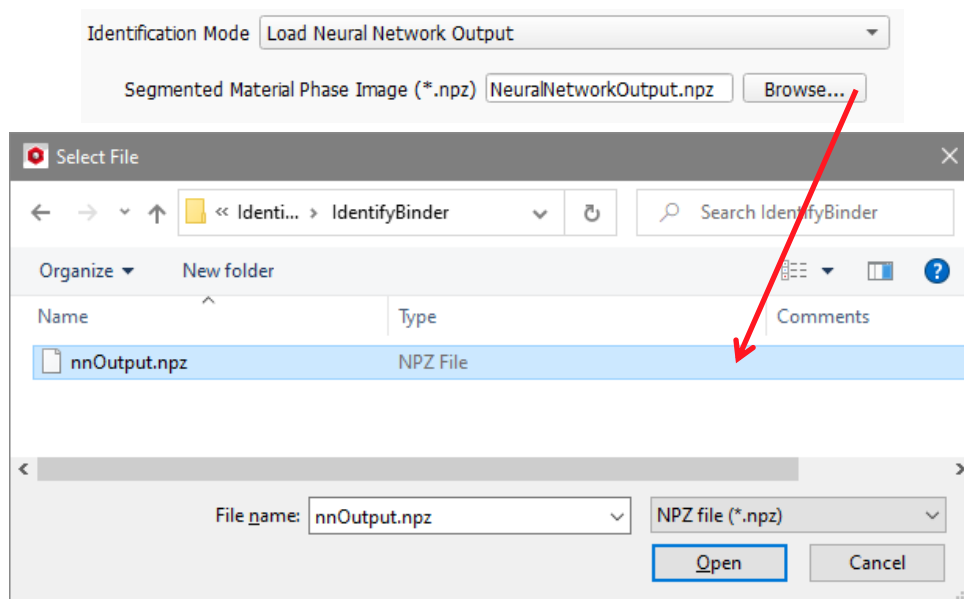
The **Material to Analyze** panel offers the choice of whether GrainFind-Identify Binder (AI) should be applied to all solids in the structure or only on a subset, defined either by choosing a material or several material IDs.



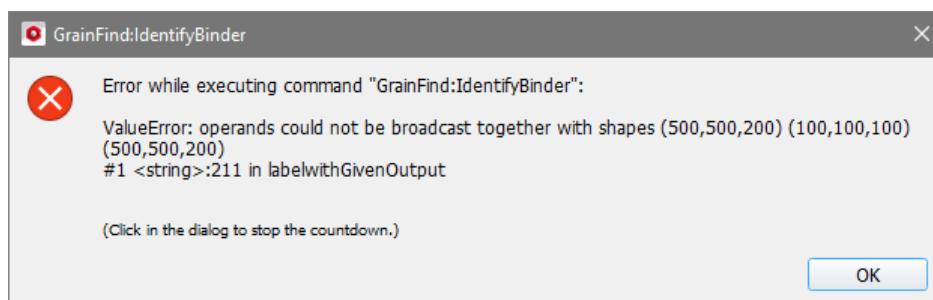
Next, select one of the neural networks available under **Neural Network**. Since **GeoDict 2023**, more than one neural network (.gnn stands for **GeoDict neural network parameter file**) is provided, making it possible to select the best suitable one for the structure under consideration.

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. In order ensure that the grains in the present structure fit to the grains with which the neural network was trained, it is recommended to use [Estimate Grain Diameter](#) before running the binder identification.

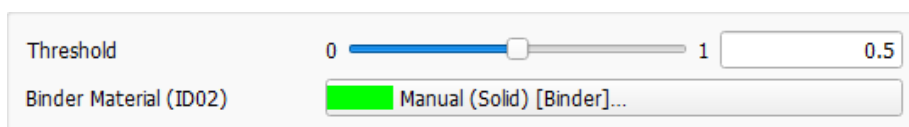
On occasion, the user may want to change some parameters, without having to run the identification for each voxel with the neural network again and in that case, the option **Load Neural Network Output** may be very useful.



Browse to a **GeoDict** result folder of a previous run of **GrainFind-Identify Binder (AI)** and select a `nnOutput.npz` file from that folder. Since already the output of the neural network is used in that case, no selection of **Material to Analyze** or **Neural Network** is possible and the currently loaded structure needs to be the same with which the neural network was trained. Otherwise an error message appears.

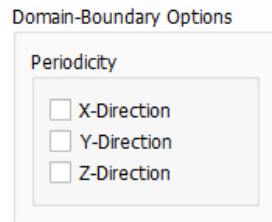


The **Threshold** is an expert parameter: The neural network provides probabilities if a solid voxel is binder or not. The **Threshold** defines the limit for labelling a voxel as binder. It is recommended to keep the default value of 0.5, since this reflects the computed probabilities correctly.



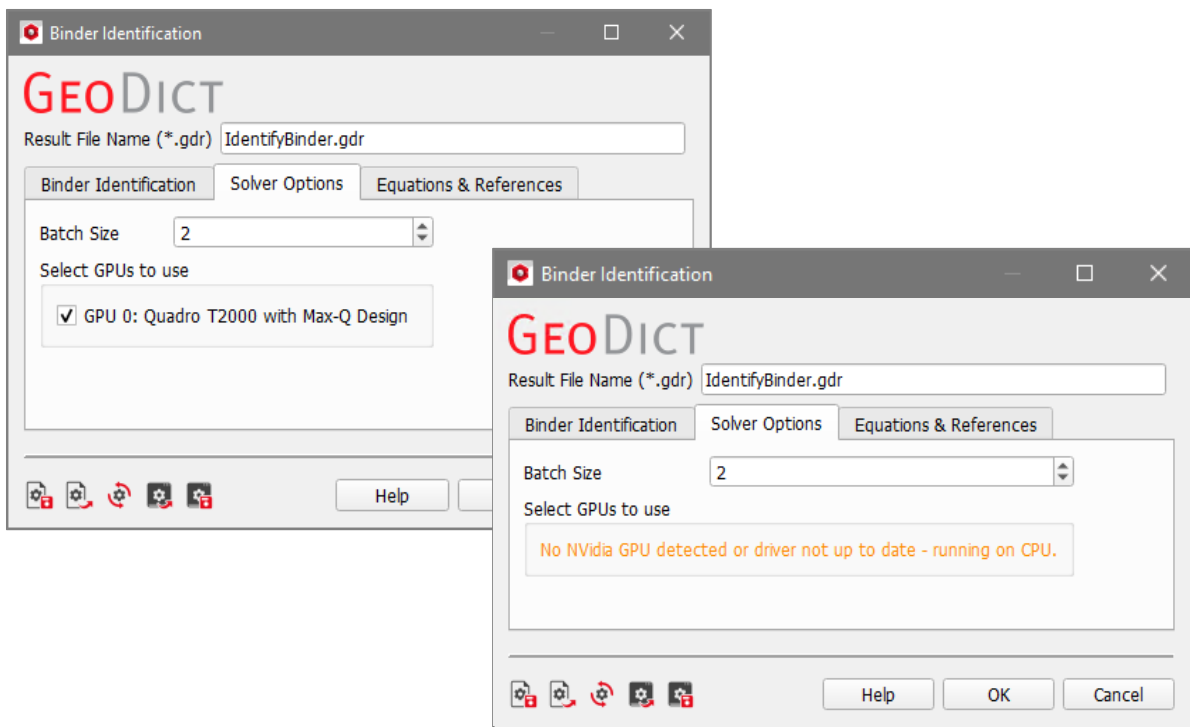
The **Binder Material ID** specifies the material ID to label the binder. The first unused material ID is used for the Binder Material. In the example below, the structure contains only material ID 00 and 01, thus the **Binder Material ID** is 02. To be able to distinguish the binder properly from the other materials, the color for this ID should be changed to a color different from the color of any solid or pore material present in the original structure after the identification has finished. This can be done under **Settings → Color & Visibility Settings....**

Select one or several boxes on the **Domain-Boundary Options** panel if the underlying structure for the binder identification is periodic in one or more directions. However, periodicity is unusual for most 3-D scans and this setting is rarely changed.



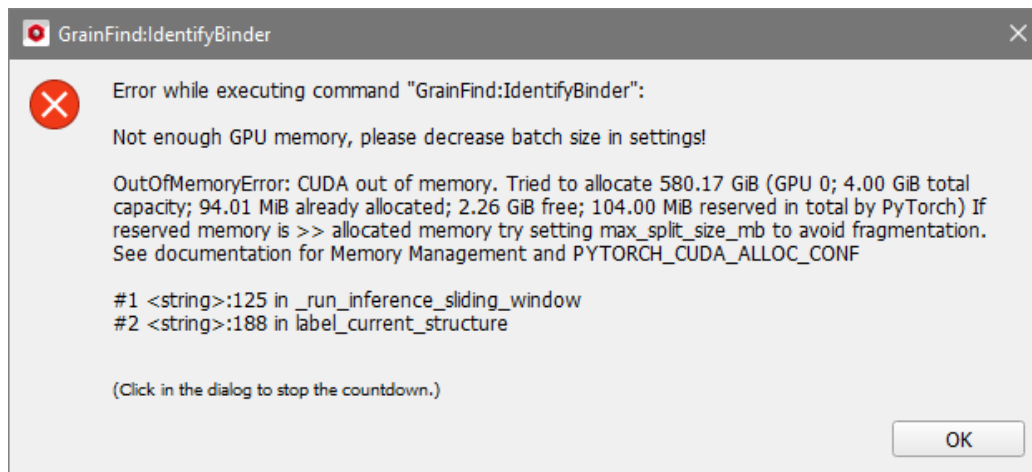
SOLVER OPTIONS TAB

GrainFind-Identify Binder (AI) can run in GPU mode by using a suitable graphic card or in CPU mode. All suitable graphic cards detected during installation of GeoDict are displayed on the **Solver Options** tab. Use the checkboxes to select the graphic card used 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). Conceptually, GrainFind-Identify Binder loads the graphics card with portions of work called **batches**. Currently, the selection must be made manually, and the parameter is set following the value entered in **Batch Size**.

The batch size might be chosen too large for what is available on the graphics card. In this case, an error message appears.



In this case, the number of batches needs to be reduced. Note that for CPU-based computation, the choice of batch size is not critical and can be left at the default.

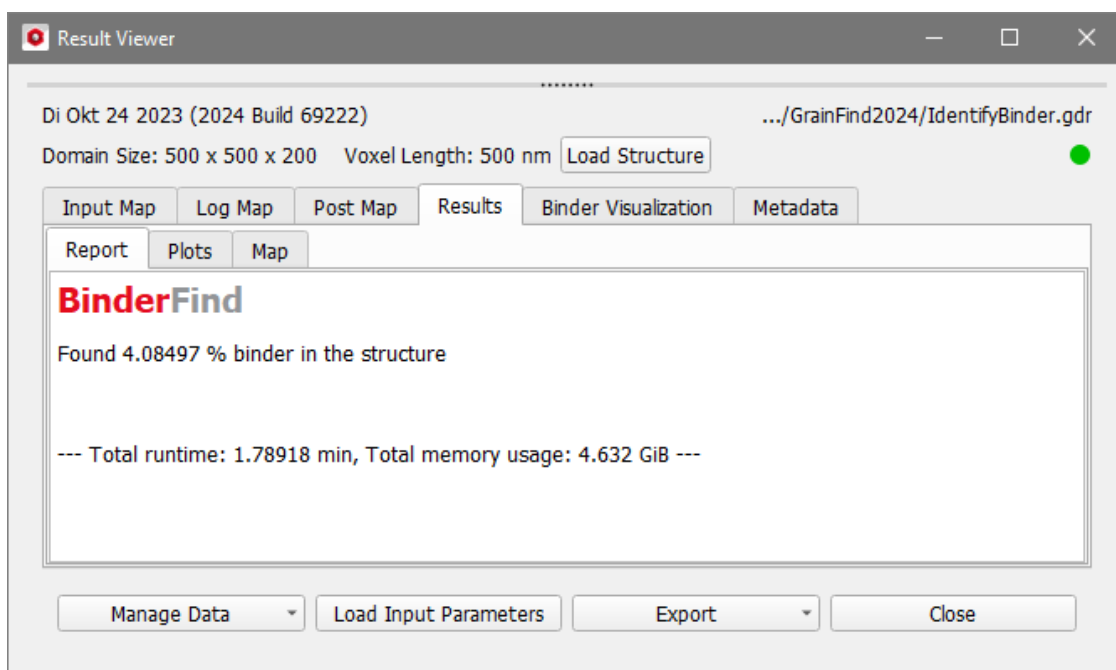
The default setting in **GrainFind-Identify Binder** for the **Batch Size** is 2, and it is recommended to keep this setting.

EQUATIONS & REFERENCES

The **Equations & References** tab provides information about the methods used during this command. The [References](#) are found also at the end of this handbook.

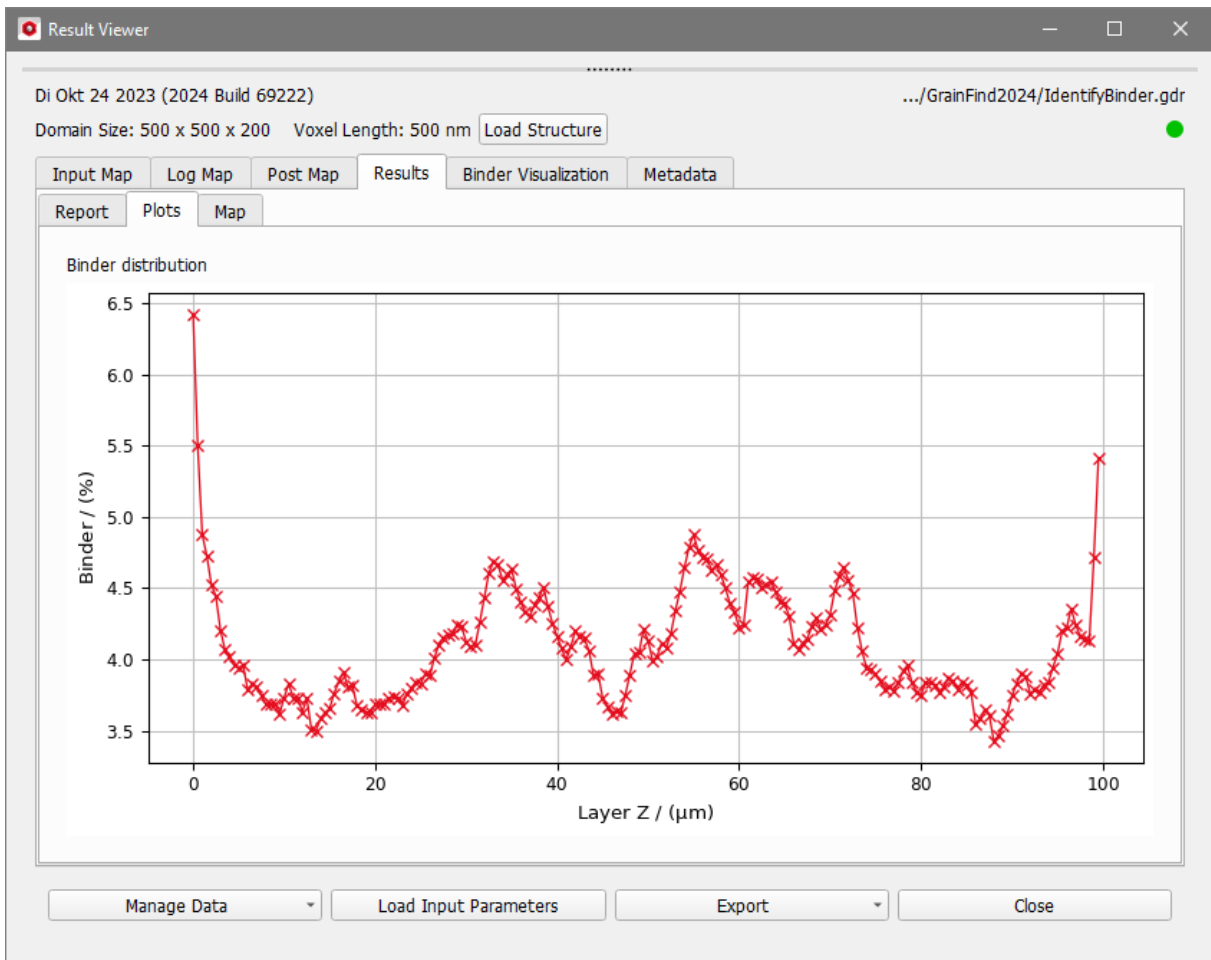
BINDER IDENTIFICATION RESULTS

After the successful binder identification, the **GeoDict Result Viewer** opens for the result file (.gdr). Under the **Results - Report** tab, the percentage of solid voxels identified as binder is shown.

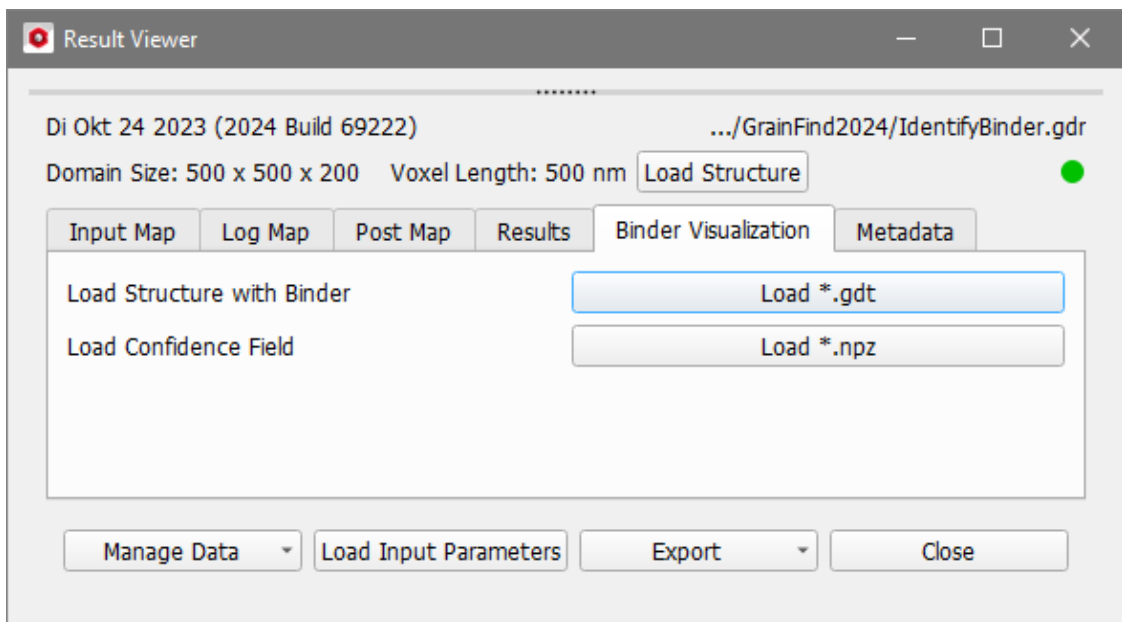


In the **Results - Plots** subtab, the **Binder distribution** in the different Z-Layers is shown. Observe, that the detected binder at the boundaries is much more than in the

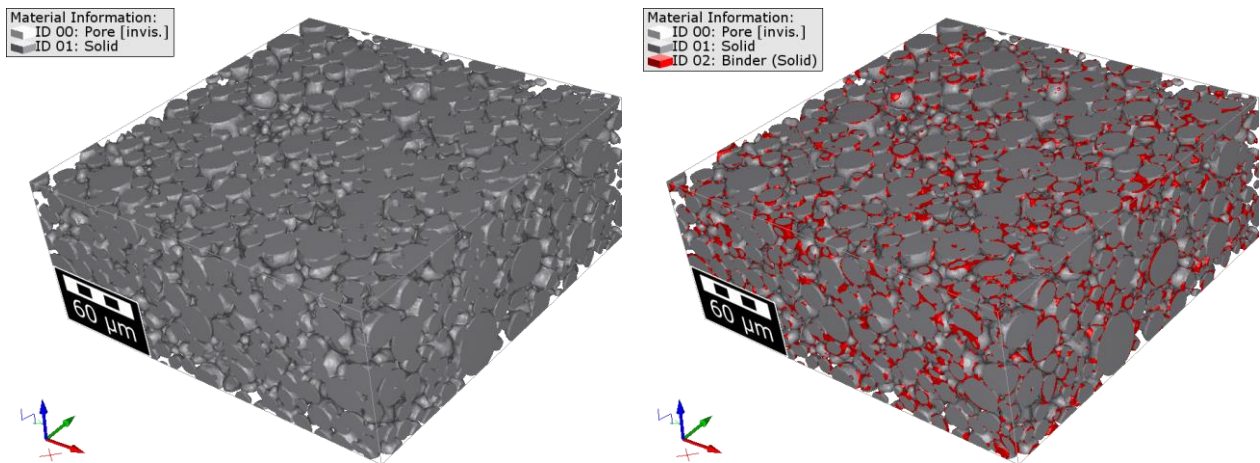
middle of the structure. This is a boundary artefact, which does not occur for periodic structures.



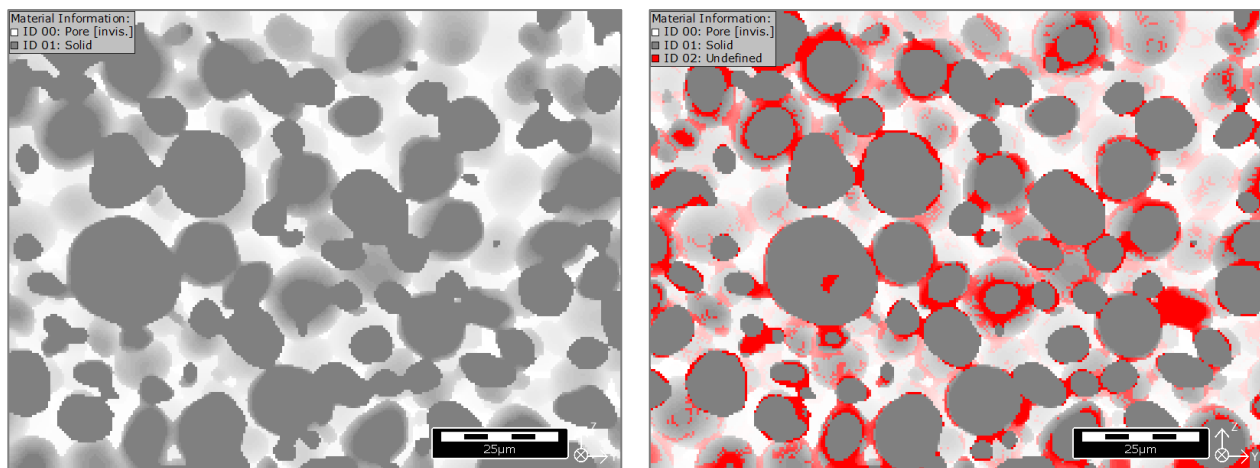
To load the structure with identified binder, click **Load *.gdt** under the **Binder Visualization** tab.



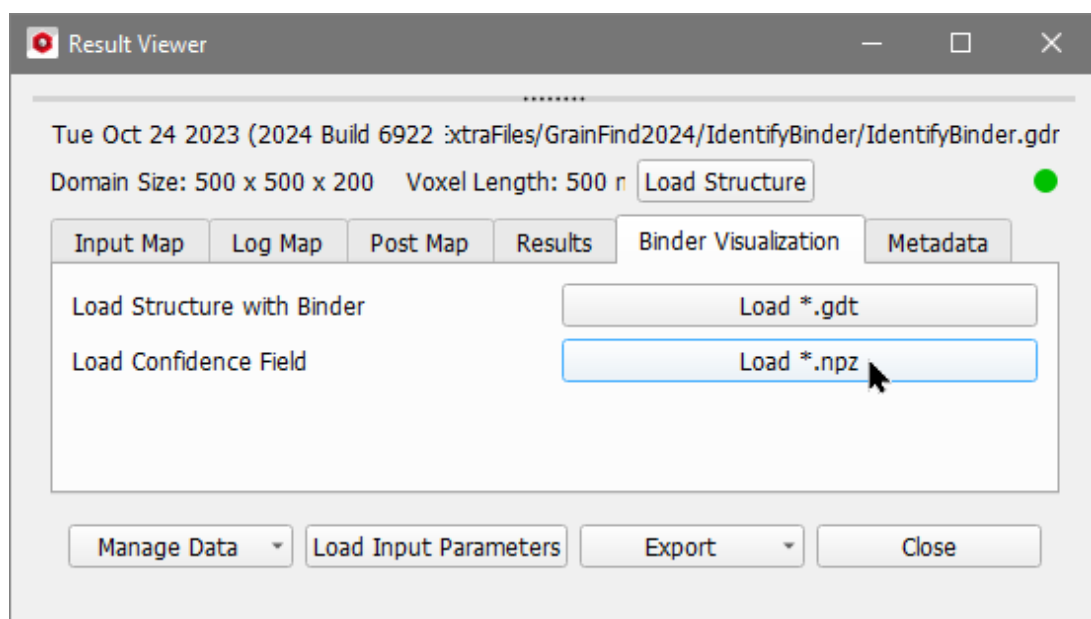
In the 3D visualization, the distribution of binder between the grains is visible for the whole domain.



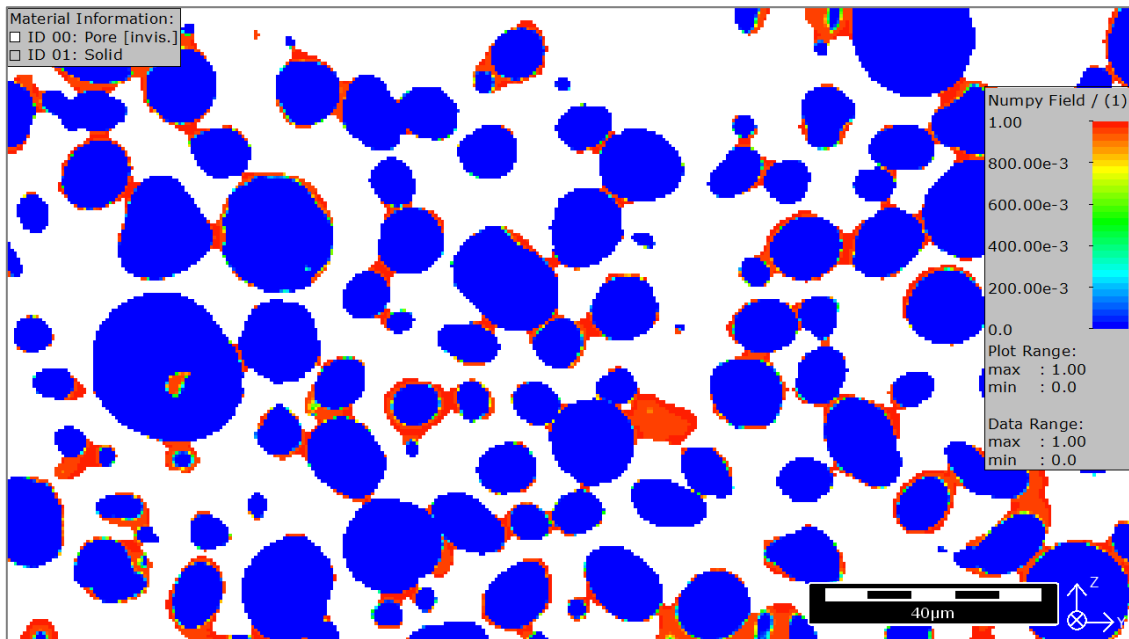
The 2D view is useful to evaluate the result of the binder identification, as seen in the example below (left: without binder identification, right: with binder identification).



Load the confidence field, by selecting **Load *.npz** under the **Binder Visualization** tab, i.e. the unsegmented result of the binder identification.



The confidence field contains the probability for each voxel to be binder. In the figure below, the field is only visible for the solid materials and it is well visible 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.

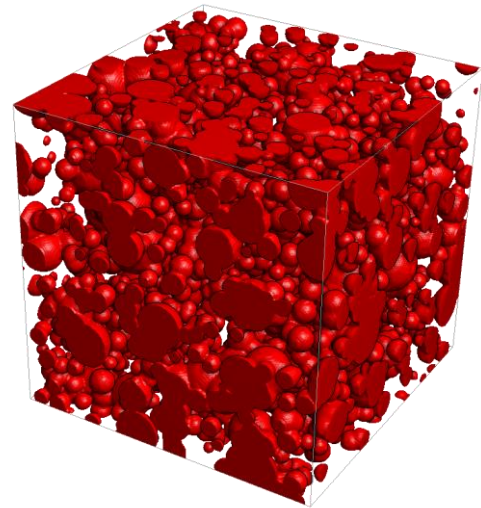


ESTIMATE GRAIN DIAMETERS

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 and it does not need any information about the single grains in the structure. In post-processing, different diameter classes can be identified, and the structure can be segmented with respect to them.

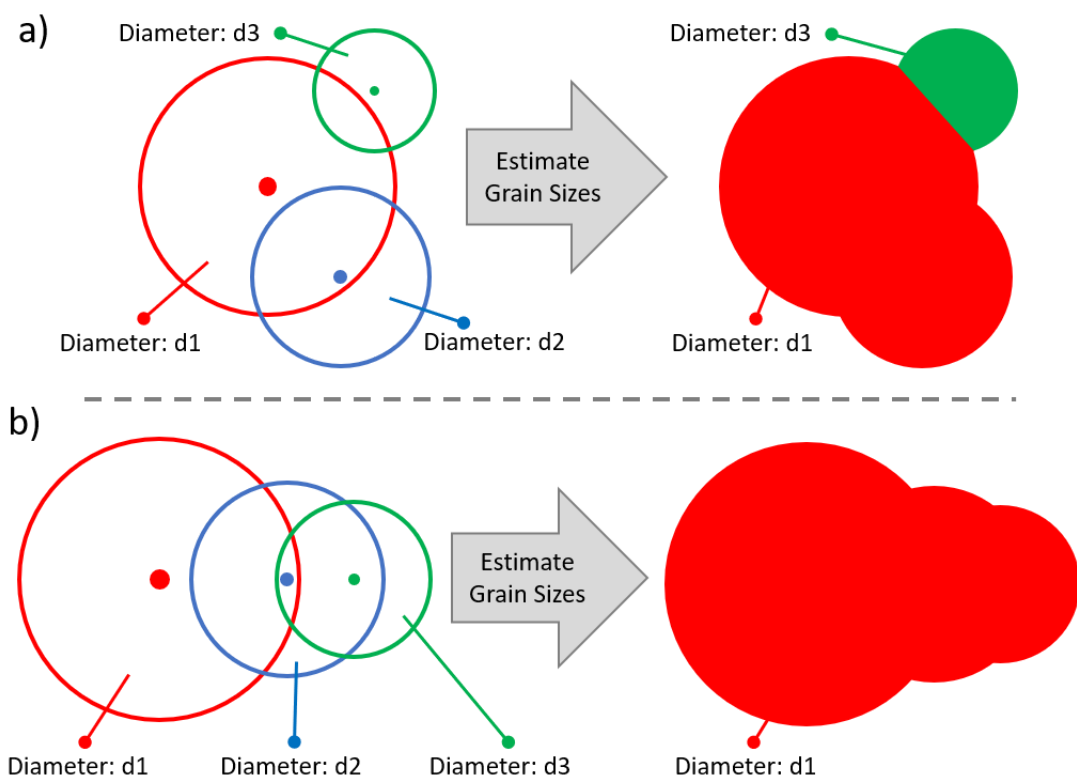
Here, the example structure created with **GrainGeo** and shown on the right is used.

The algorithm behind **Estimate Grain Diameters** works as follows: At the start, each voxel gets assigned a Grain Diameter of 0. Then, spheres are successively fitted into the geometry, starting at the largest possible sphere. If a sphere fits and a voxel has no diameter assigned to it yet, the diameter of the fitting sphere is assigned to all voxels contained in the sphere.



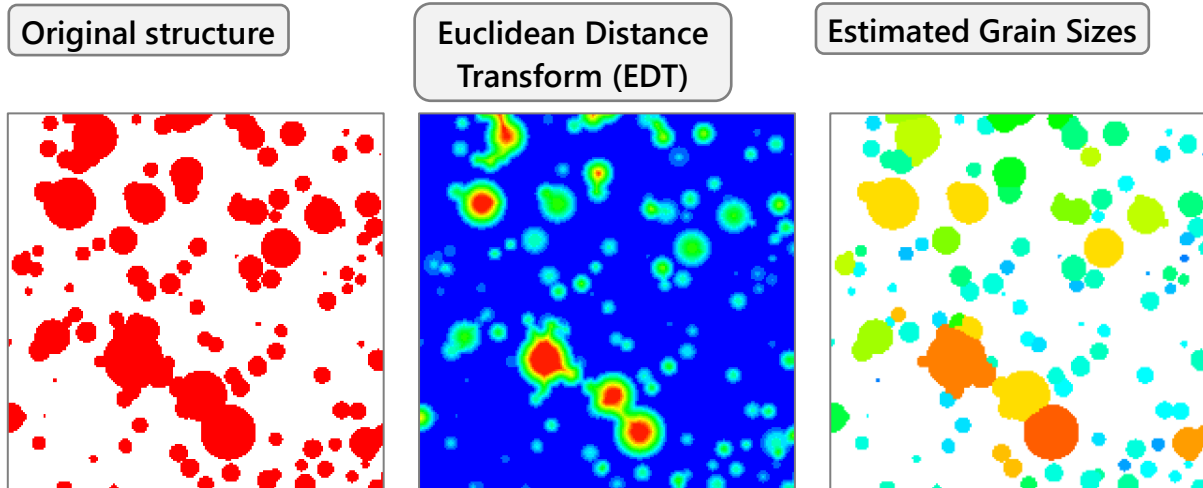
If a voxel is contained in multiple spheres, there are two options:

1. The center of a smaller sphere lays inside a larger sphere. 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)
2. The center of a smaller sphere does not lay inside a larger sphere. 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.

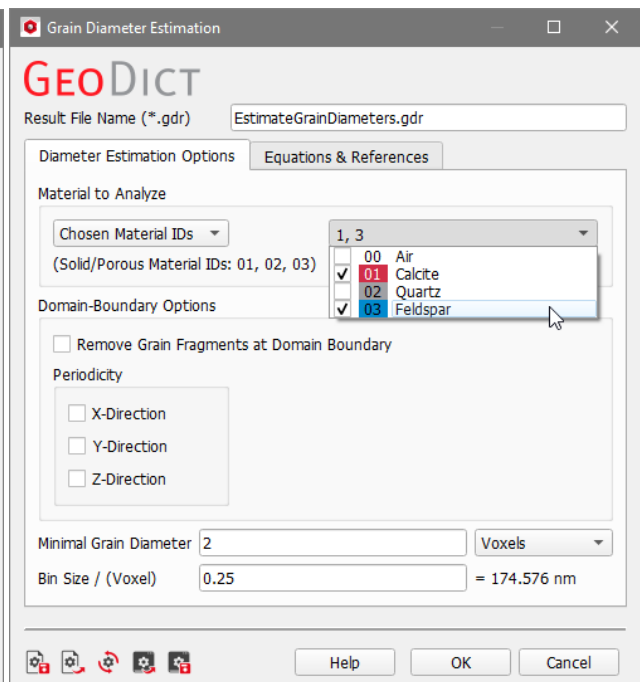
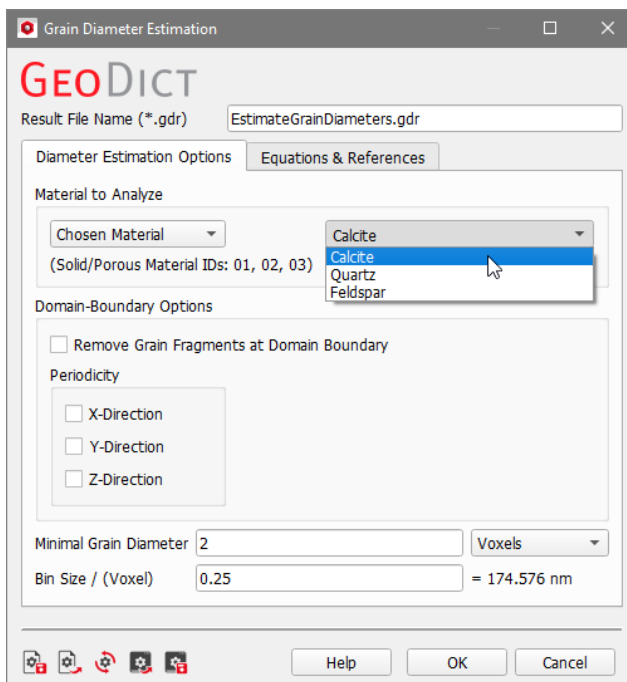
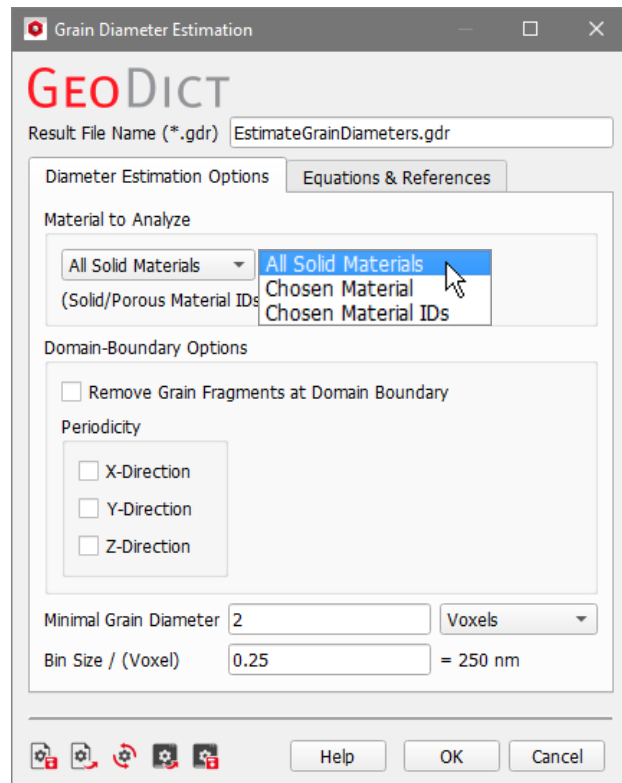
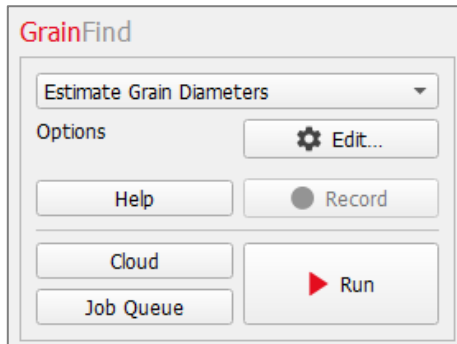
In the figure below, the process of estimating the grain size is illustrated on the example structure shown above. On the left, the original structure (the material which is selected to be analyzed) is shown. In the next step (middle), the EDT (see page [4](#)) is calculated to find the maximal fitting sphere at every point. On the right, the result of **Estimate Grain Diameters** is displayed.



ESTIMATE GRAIN DIAMETERS OPTIONS

After selecting **Analyze** → **GrainFind** from the menu bar, the **GrainFind** section opens on the left bottom of the **GeoDict** GUI. Select **Estimate Grain Diameters** from the pull-down menu and click the **Edit...** button.

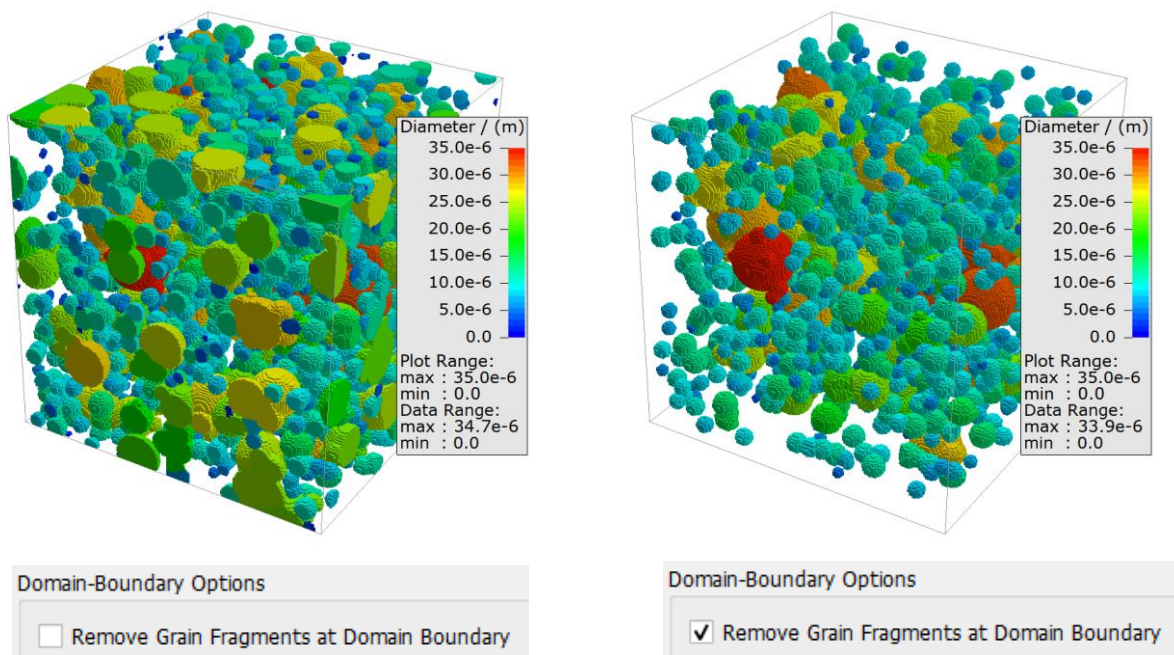
The default **Result File Name** can be kept or changed to a user-defined file name. Under **Material to Analyze**, the materials for which the grain size is estimated are chosen. The available options are **All Solid Materials**, **Chosen Material**, or **Chosen Material IDs**. The selected combination of materials (All Solid Materials or multiple material IDs) is analyzed as one.



In the Domain-Boundary Options panel, the first option is to **Remove Grain Fragments at Domain Boundary**. A grain fragment in this context is a connected area with the same assigned diameter value.

- Grain fragments at the boundary might corrupt the grain diameter estimation, since it cannot be known if the grains at the boundary lie completely in the domain or if they are cut at the domain boundary (compare the images below).
- Nevertheless, removing the boundary grains also influences the diameter distribution: Larger grains have a higher probability to touch the boundary, and therefore also a higher probability to be removed. Thus, large grains might be underrepresented in the diameter distribution.

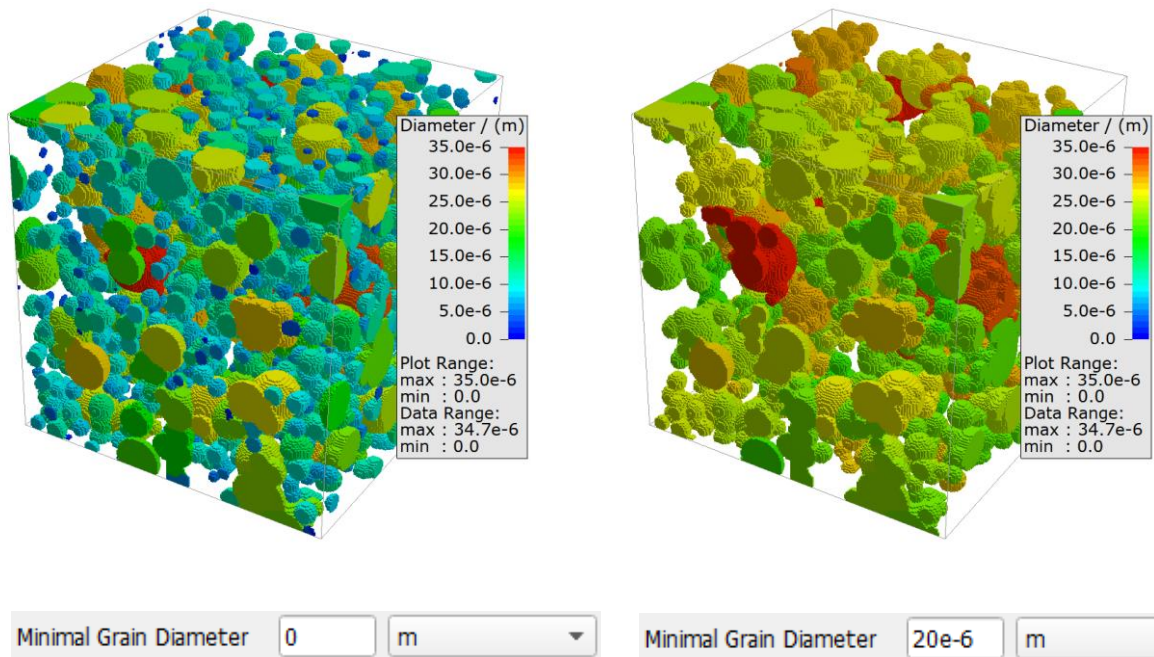
The boundaries can have a critical influence on the results, and it must be carefully evaluated if **Remove Grain Fragments at Domain Boundary** should be used or not.



With the **Periodicity** option, the handling of the structure at the domain boundary can be defined. If a direction is chosen, periodic boundary conditions are applied in this direction. Otherwise, encased boundary conditions are applied. **Periodicity** should only be chosen if the corresponding real-world structure is periodic, too. This option is important to define the handling of boundary grains, since no information is available about the structure outside of the domain.

All grain fragments with an assigned diameter value lower than the **Minimal 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 removed from the structure.

In the figure below, the behavior of the algorithm can be observed: On the left, the **Minimal Grain Diameter** is set to 0 μm , so all grain fragments are kept independent of their assigned diameter. On the right, the **Minimal Grain Diameter** is set to 20 μm and all fragments with an assigned diameter lower than 20 μm , which are not merged to larger grain fragments, are neglected.



The **Minimal Grain Diameter** can be entered in units of meters or voxels.

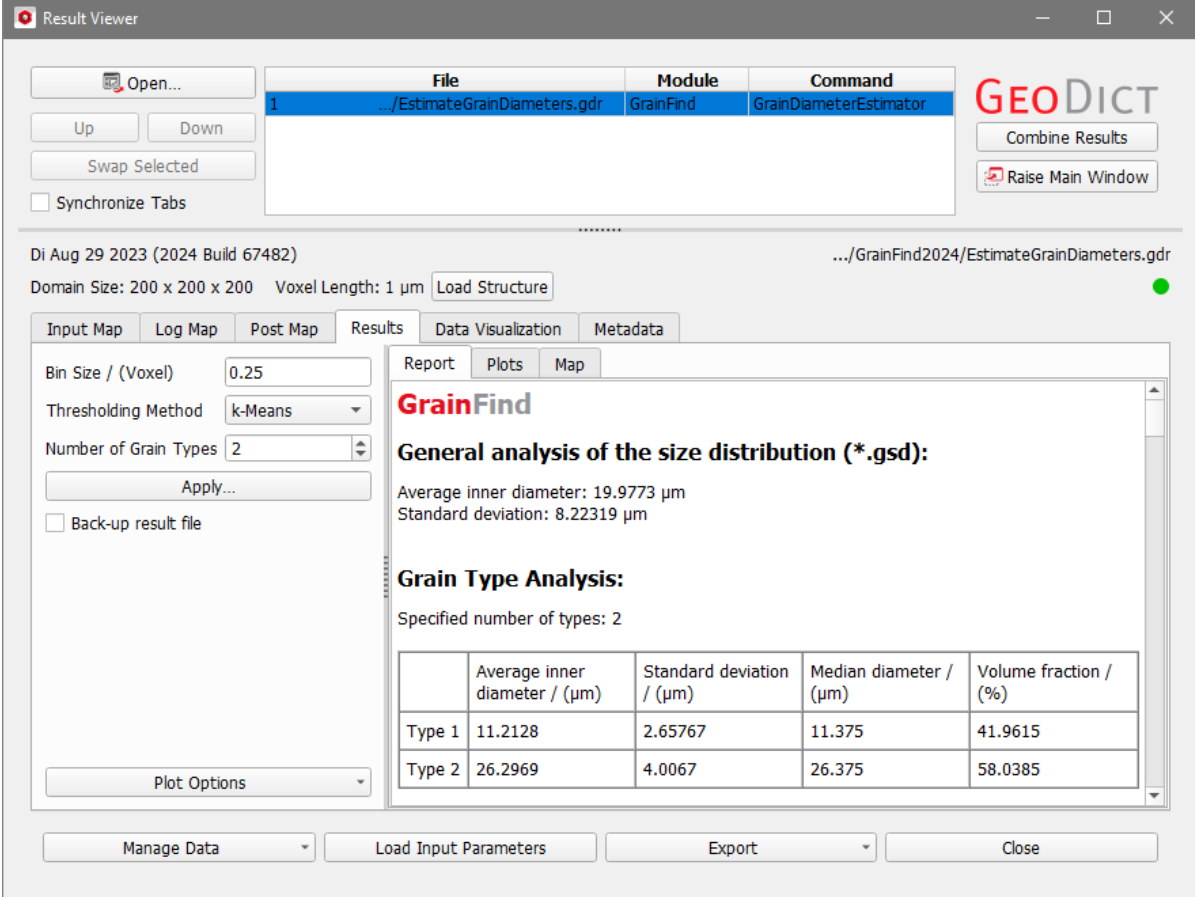
The **Bin Size** is the step size between following sphere diameters, which are fitted in the structure. It must be entered in voxels, but the step size is also shown in metrical units. The choice of the Bin Size is important in post processing. It affects the results in the *.gdr file, e.g. the Inner Grain Diameter Histogram (see page [Error! Bookmark not defined.](#)). If it was not chosen as desired, the value for the **Bin Size** can be changed later during postprocessing in the Result Viewer of the result file (under the **Results** → **Plots** subtab).

GRAIN DIAMETER ESTIMATION RESULTS

At the end of the estimations of grain diameter, the results are shown in the Result Viewer. Alternatively, they can be loaded at any time by opening the corresponding *.gdr-file in the project folder (File → Open Results (*.gdr)...).

The Result Viewer shows several tabs, but only the **Results** and **Data Visualization** tabs are explained here in detail. For the other tabs refer to the [Result Viewer](#) handbook of the User Guide.

The **Results** tab contains the **Report**, **Plots** and **Map** subtabs, which are strongly interconnected. The **Report** subtab shows the average inner diameter of all grains and the standard deviation, the results from the grain type analysis and a table with the bins for the histogram. The **Plots** subtab shows a histogram of the estimated grain diameters. The **Map** subtab contains the resulting data from Estimate Grain Diameters. This data is the basis for the tables in the **Report** subtab and for the histogram in the **Plots** subtab.



The screenshot shows the Result Viewer window with the following details:

- File List:**

File	Module	Command
1 .../EstimateGrainDiameters.gdr	GrainFind	GrainDiameterEstimator
- Settings Panel (Left):**
 - Bin Size / (Voxel): 0.25
 - Thresholding Method: k-Means
 - Number of Grain Types: 2
 - Buttons: Open..., Up, Down, Swap Selected, Synchronize Tabs, Apply..., Back-up result file
- Report Subtab (Main Area):**

GrainFind

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

Average inner diameter: 19.9773 µm
Standard deviation: 8.22319 µm

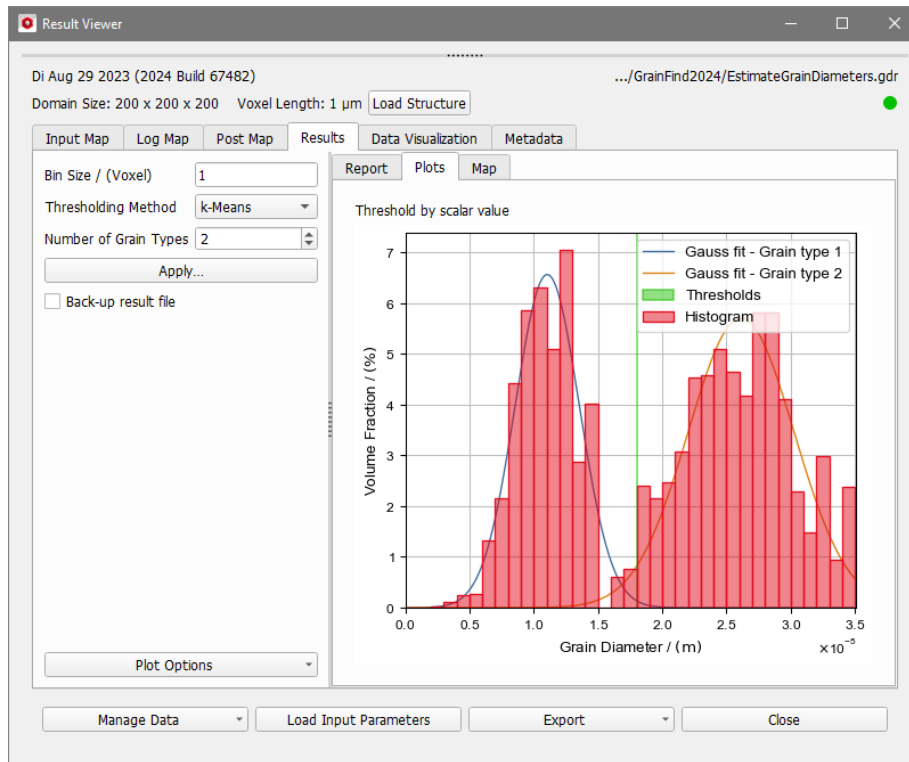
Grain Type Analysis:

Specified number of types: 2

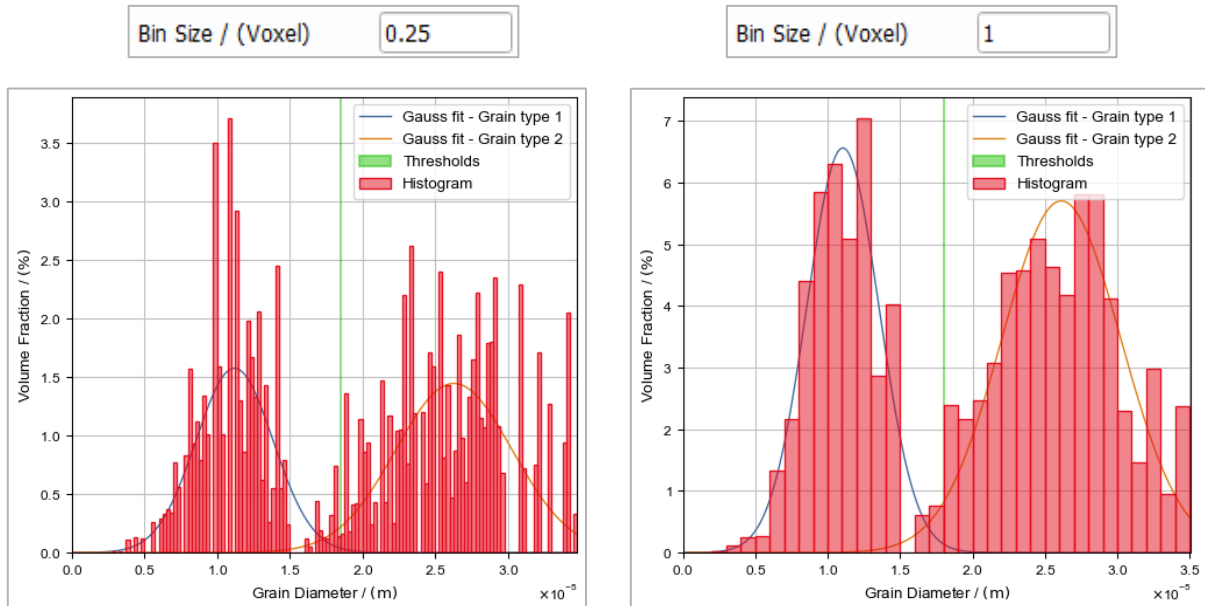
	Average inner diameter / (µm)	Standard deviation / (µm)	Median diameter / (µm)	Volume fraction / (%)
Type 1	11.2128	2.65767	11.375	41.9615
Type 2	26.2969	4.0067	26.375	58.0385

The three subtabs share the (collapsible and expandable) settings panel on the left, where the **Bin Size**, the **Thresholding Method**, and the **Number of Grain Types** can be chosen. Changing a value and 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.

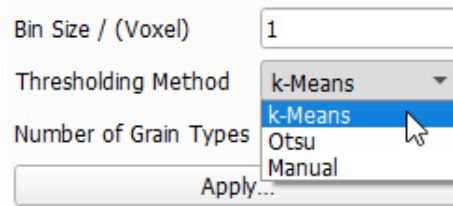
Changing the **Bin Size** effects the resolution of the histogram in the **Plots** tab and the histogram table in the **Report** tab. The histogram table contains the values from the histogram plot. Each row contains the data of one bin. The diameter of grains in one bin is between the minimum and maximum diameter. The volume fraction shows how many grains are contained in a bin.



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 in the two images below.



Use the **Thresholding Methods** and **Number of Grain Types** to classify the grains into different classes based on their diameter. The thresholding methods **k-Means**, **Otsu**, and **Manual** are the same as described on page 23.

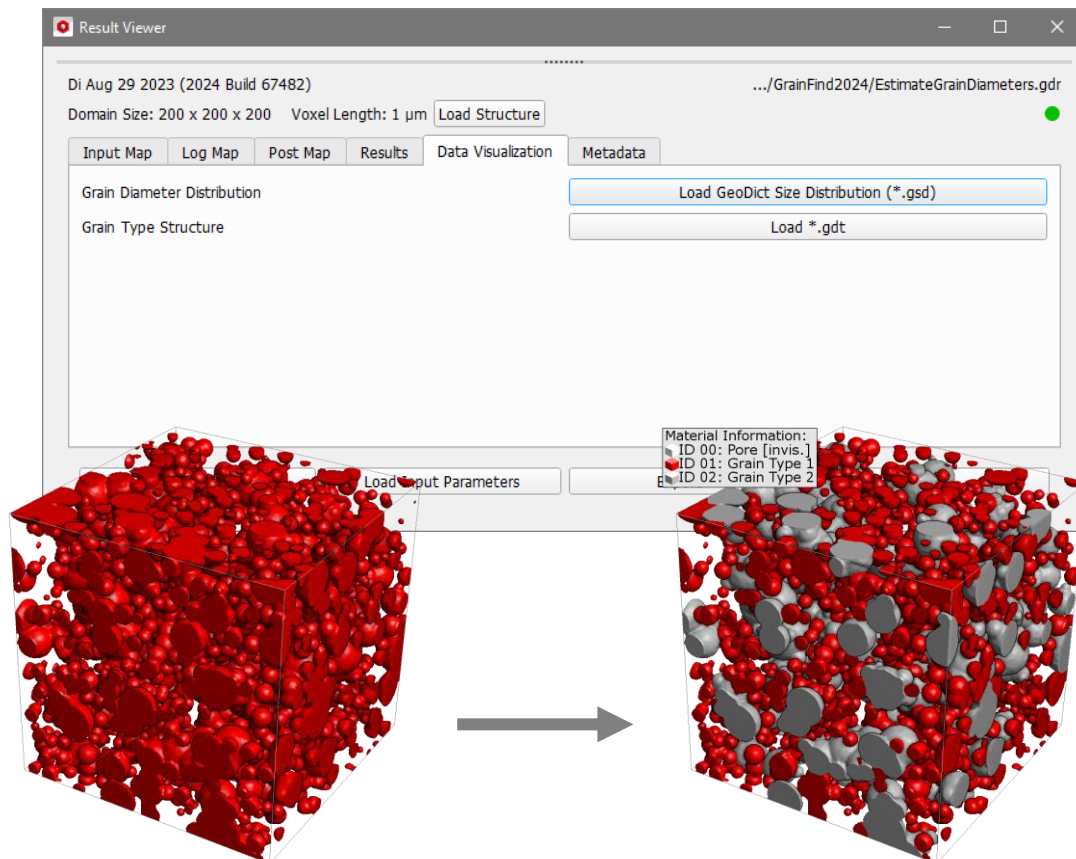


After clicking **Apply**, the **Grain Type Analysis** table is updated and shows for each type the relevant parameters. These are the average (mean) diameter of the grains of this type, the standard deviation, the median diameter of this type and the volume fraction of the grains of this type. Under the table find the threshold value(s) that were used to separate the grain types. Note, that the threshold values depend on the chosen bin size as the minimum diameter of a bin is chosen as threshold value.

In the **Plot** tab, the Gauss fit of each grain type and the threshold value(s) 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.

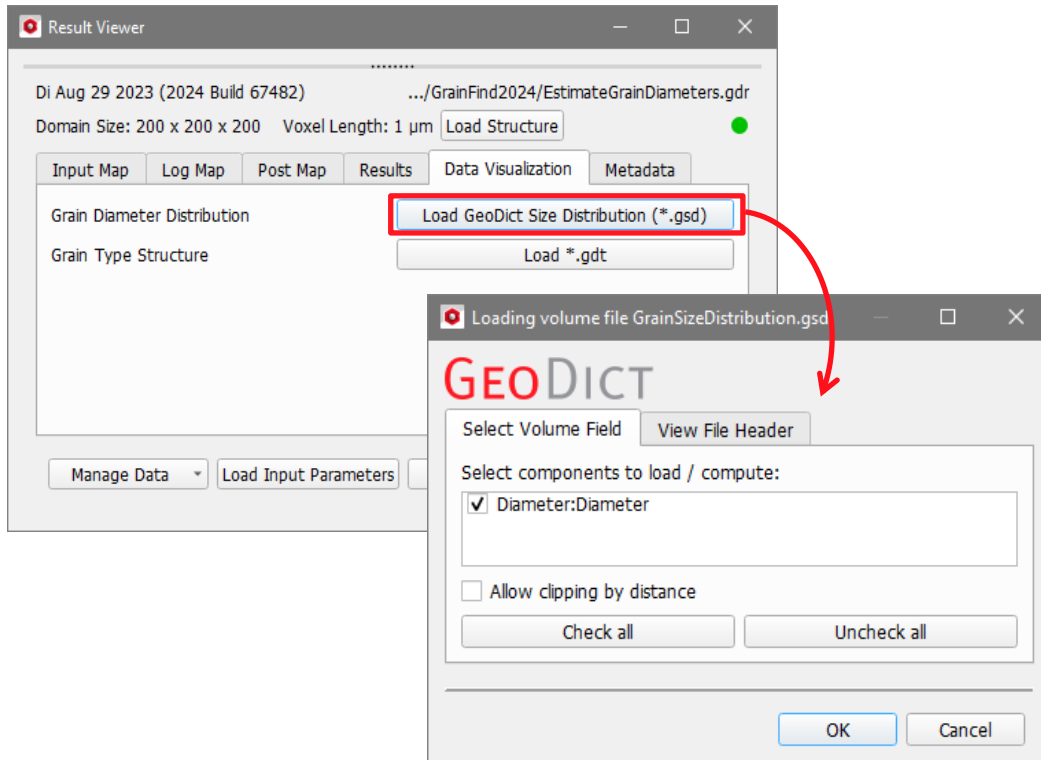
In the **Report** tab, the D10, D50, and D90 values are given. They indicate the diameters such that 10%, 50%, or 90% of the grains have a diameter smaller or equal than the corresponding value.

Based on these diameter classes, the structure is automatically segmented and the result is saved in the result folder. It can be visualized by clicking **Grain Type Structure** → **Load *.gdt** in the **Data Visualization** tab, as seen below. Each grain type is assigned its own material ID, so all grains of the same type have the same material ID.

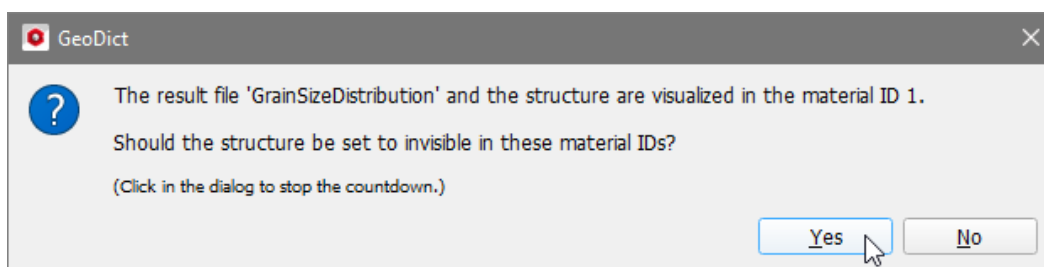


Under the **Data Visualization** tab, load the **Grain Diameter Distribution** to visualize and examine in detail the estimated grain diameters in the Visualization area of GeoDict.

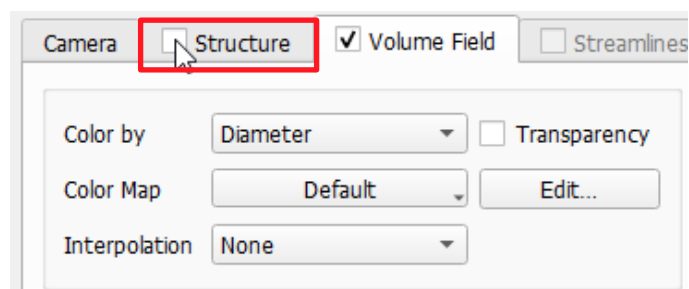
The workflow is as follows: To create images similar to those used for the illustration of the **Domain-Boundary Options** and for the **Minimal Grain Diameter** (see page [44](#)), click **Data Visualization** → **Load GeoDict Size Distribution (*.gsd)**. Click **OK** in the pop-up window.



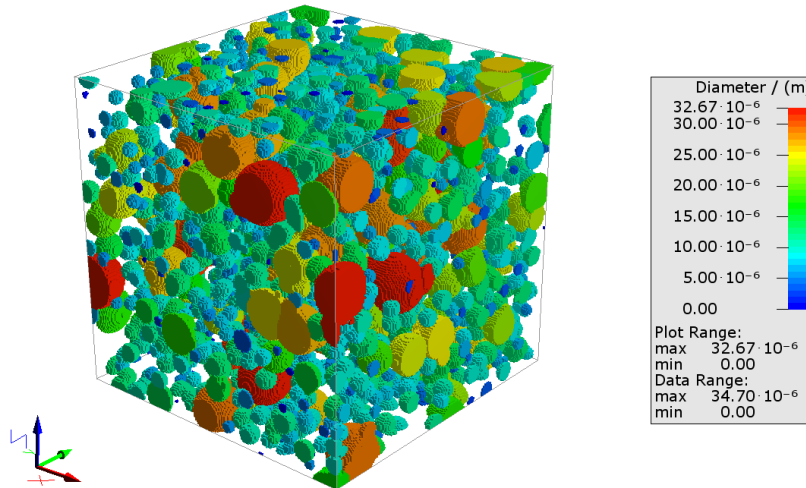
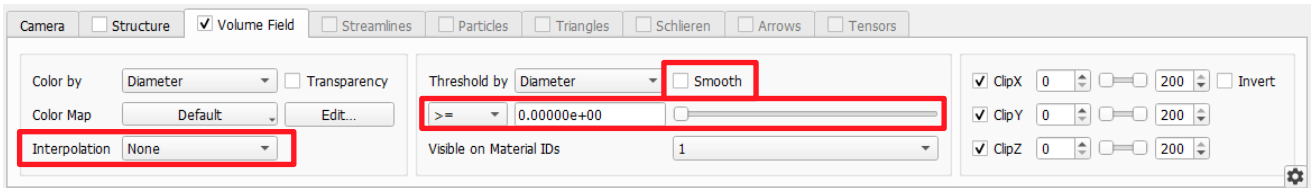
The structure is shown in the Visualization area with the default visualization settings and a message appears indicating that the visibility of the structure will be turned off (unless the user clicks No). Click **Yes**.



The visualization of the structure can also be turned off by unchecking the **Structure** tab in the Visualization panel above the Visualization area.



Next, in the **Volume Field** tab of the Visualization panel, check that **No Interpolation** is selected and **Smooth** is unchecked for **Threshold by**. Finally, if needed, use the slider for the threshold to select the grain diameters that should be displayed. Here all grain diameters are displayed by setting the **Diameter** to zero and the mode to **>=**.



REFERENCES

- [1] M. Abadi, et. al; 2015; TensorFlow: Large-scale machine learning on heterogeneous systems; tensorflow.org.
- [2] W.C. Krumbein; 1941; Measurement and geological significance of shape and roundness of sedimentary particles; Journal of Sedimentary Research 11.2.
- [3] J. Ohser, F. Mücklich; 2000; Statistical Analysis of Microstructures in Materials Science; Wiley and Sons, page 115.
- [4] M. Peterson, E. Glatt; 2021; Computation of fiber diameters from discretized binary images with detailed error estimation; Report series of Math2Market GmbH; Report No. M2M-2021-01.
- [5] O. Ronneberger, P. Fischer, T. Brox; 2015; U-Net: Convolutional Networks for Biomedical Image Segmentation; Medical Image Computing and Computer-Assisted Intervention.
- [6] A.P. Sheppard, et al; 2006; Analysis of rock microstructure using high-resolution X-ray tomography; Proceedings of the International Symposium of the Society of Core Analysts.

Technical
documentation:

Anne Blumer
Jürgen Becker
Barbara Planas

MATH
2 MARKET

Math2Market GmbH
Richard-Wagner-Str. 1, 67655 Kaiserslautern, Germany
www.geodict.com