GrainFind

User Guide

GeoDict release 2022

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GeoDict

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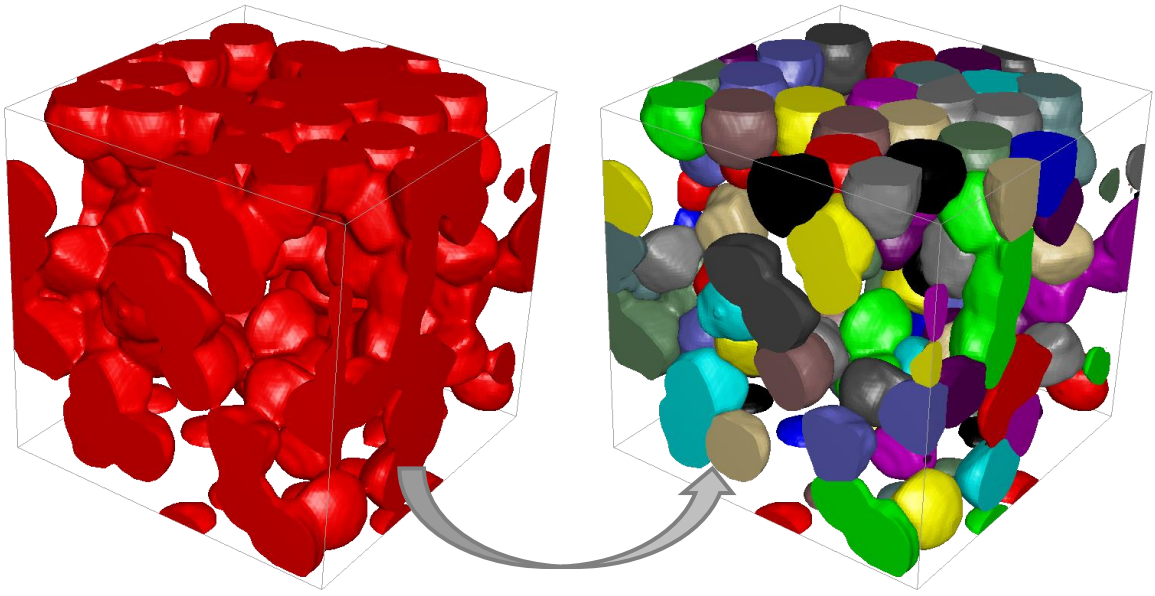
GRAIN ANALYSIS WITH GRAINFIND

With GeoDict's GrainFind module, individual grains can be identified in structures where the grain boundaries are previously unknown. For each identified grain, an individual best-fit shape is computed and its orientation in the structure is obtained.

In this way, simulations on the structure are possible which were impossible before, such as simulations of mechanical properties which depend on grain orientation. Furthermore, the structural information gained can be used to generate similar structures using the GrainGeo module – so-called *digital twins* of the structure can be modelled.

Possible applications are in the area of electrochemistry, where grains in battery electrodes can be identified, or in Digital Rock Physics, where information about individual grains fosters a thorough understanding of the rock structure. GrainFind can also be used to characterize particles in particle filtration applications.



Identify Grains

For successful GrainFind runs, the parameters for the module 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.

Additional to the **grain identification**, also 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.

HOW DOES IDENTIFY GRAINS WORK?

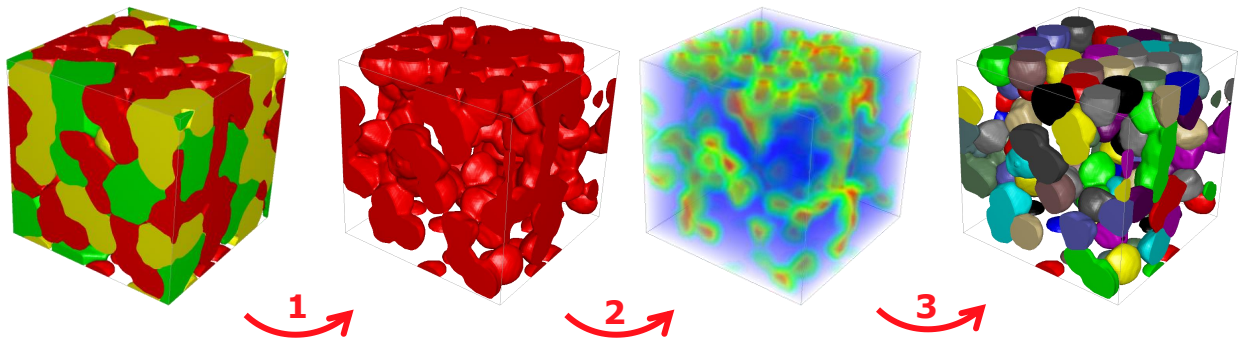
The grain identification process in GrainFind is mainly based on the **Watershed algorithm** (WA, https://en.wikipedia.org/wiki/Watershed_(image_processing)) that is widely used for the segmentation of image data. The challenge of identifying individual grains in a connected structure can be performed 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.

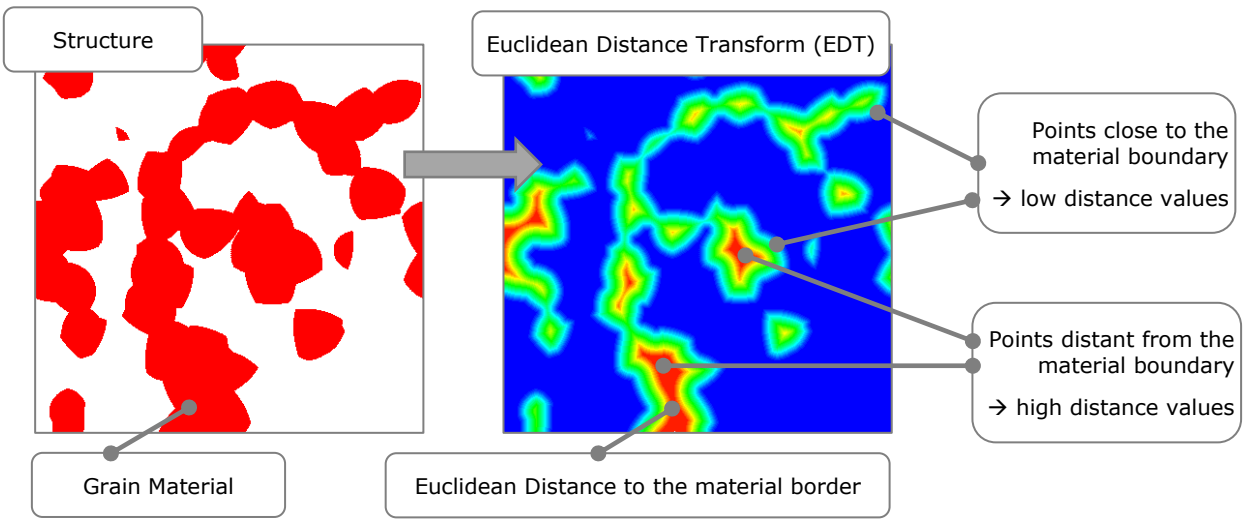


In many cases, the result of the watershed transform is enough to identify the grains. Otherwise, further steps are required.

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.

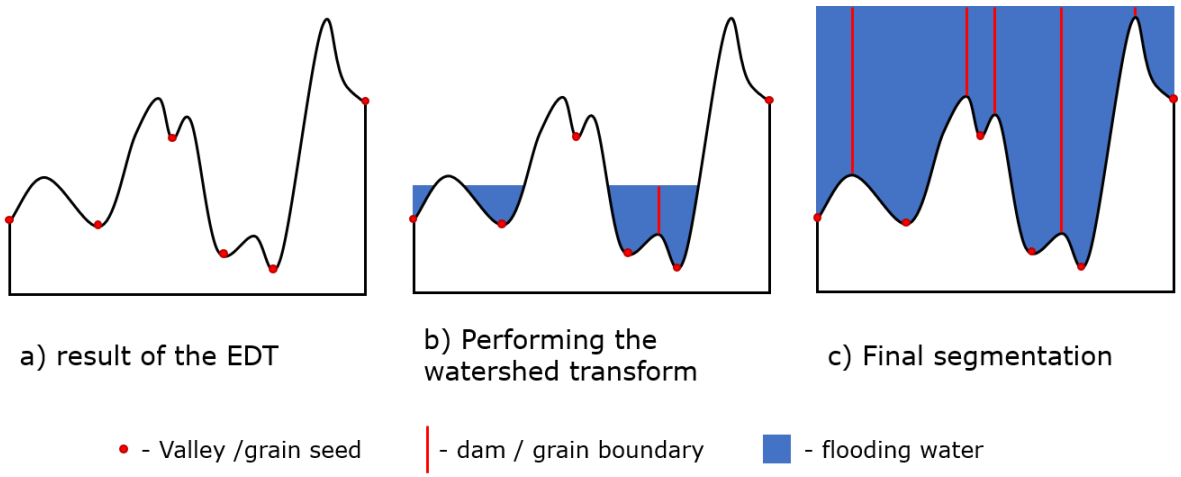


Watershed Algorithm

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 below, in page *5*.

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.

$$P_S = \frac{R_i}{R_e} \tag{2}$$

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.

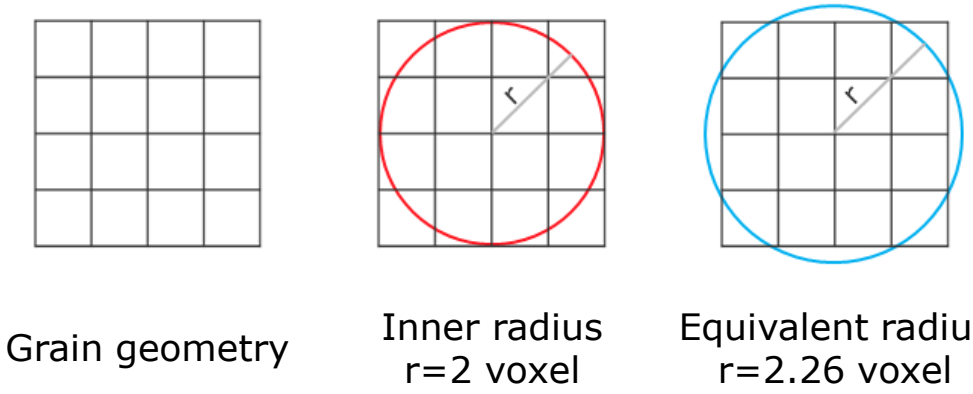


Illustration of a 2D grain geometry and its inner and equivalent radii.

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 axes' length.

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

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.

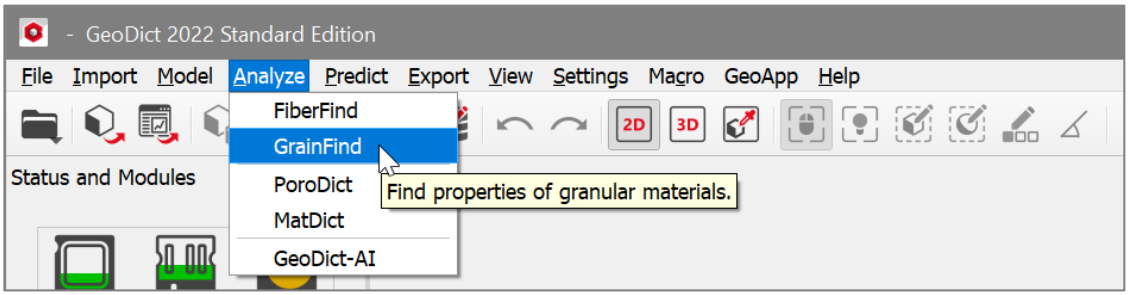
References:

W.C. Krumbein. "Measurement and geological significance of shape and roundness of sedimentary particles." *Journal of Sedimentary Research* 11.2 (1941).

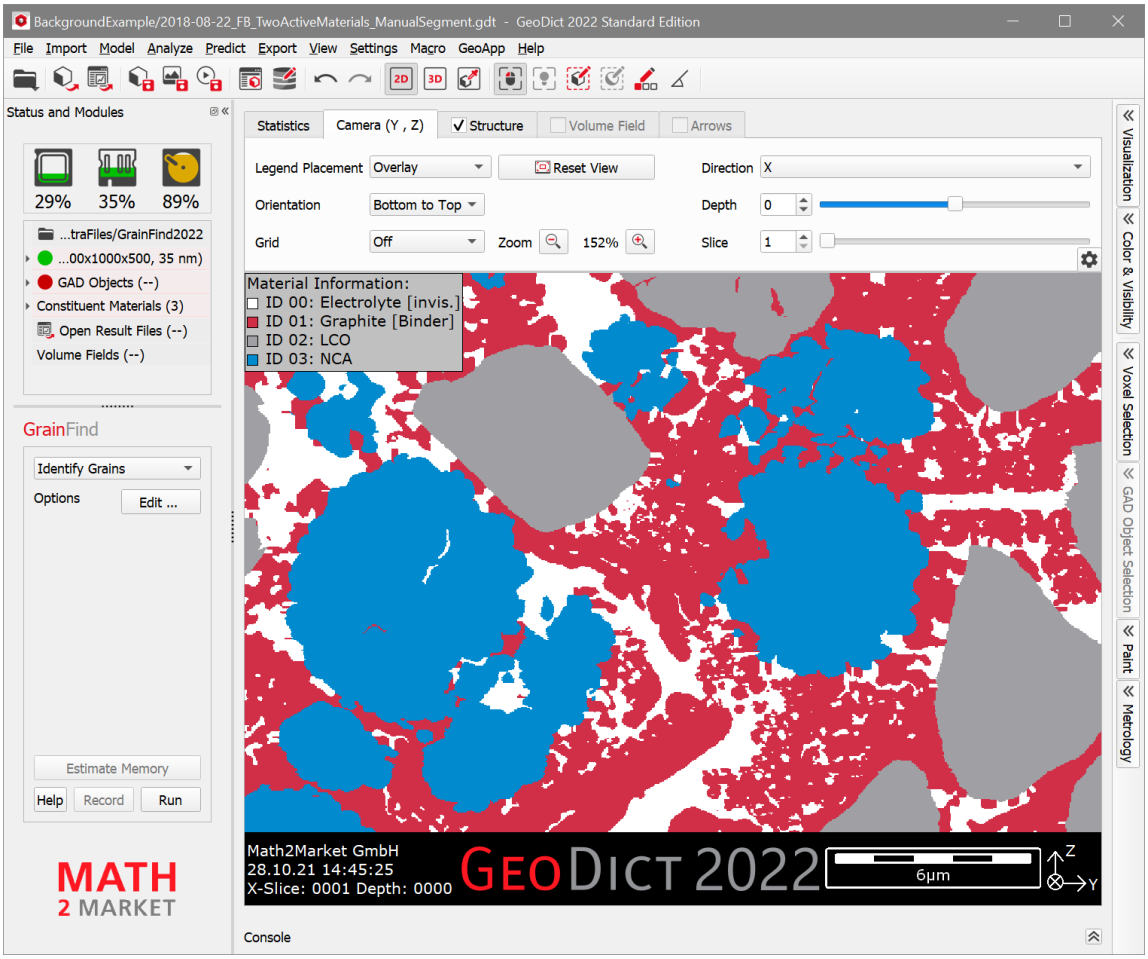
A.P. Sheppard, et al. "Analysis of rock microstructure using high-resolution X-ray tomography." *Proceedings of the International Symposium of the Society of Core Analysts*. (2006).

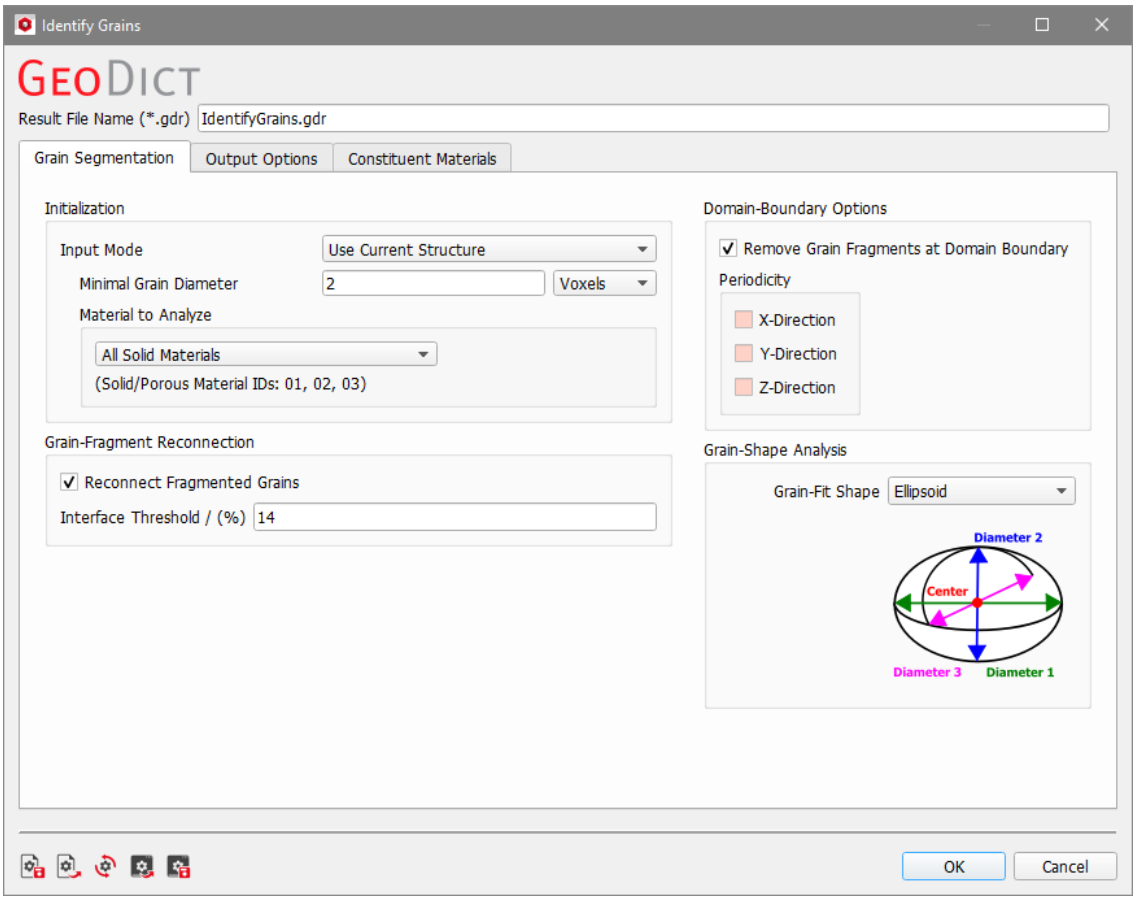
SETTING PARAMETERS FOR GRAIN IDENTIFICATION WITH GRAINFIND

To start GrainFind, select **Analyze** → **GrainFind** from the menu bar.

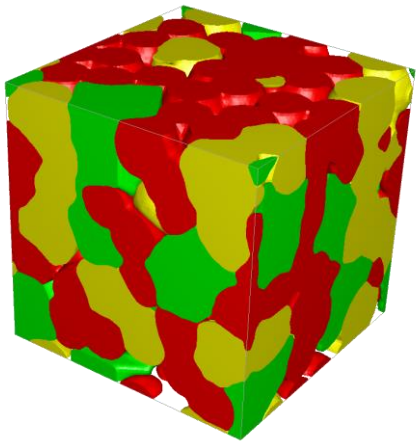


Select **Identify Grains** from the pull-down menu in the **GrainFind** module section (bottom/left of the GUI) and click **Edit ...**. The parameters needed by the GrainFind algorithm can be entered in the **Identify Grains** dialog.

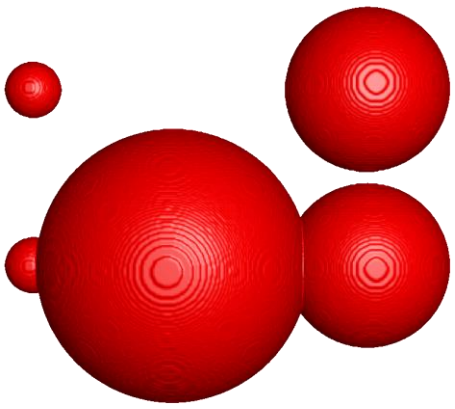




The two structures used to explain these parameters are shown below: A structure with sintered grains, generated with GrainGeo (**Sinter**), and a simple structure with overlapping spheres (**Spheres**), generated with GadGeo.



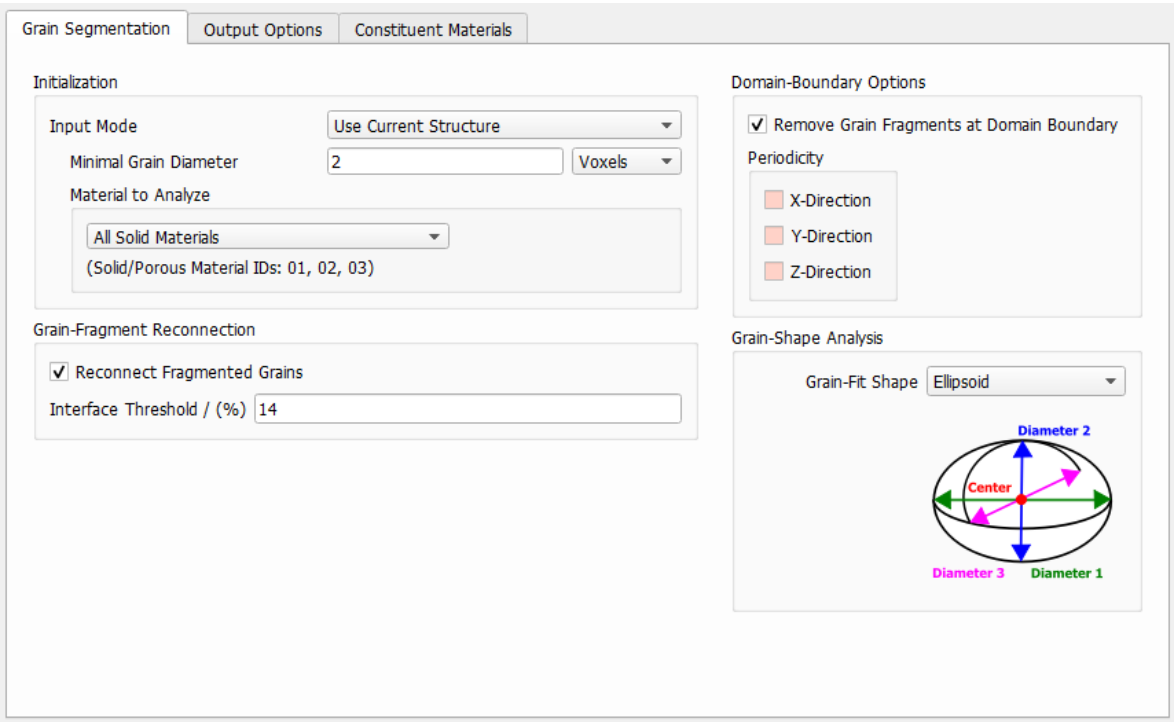
Sinter



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. The structure to be evaluated is chosen through the **Input Mode** and the material to be analyzed is selected through **Material to Analyze**.

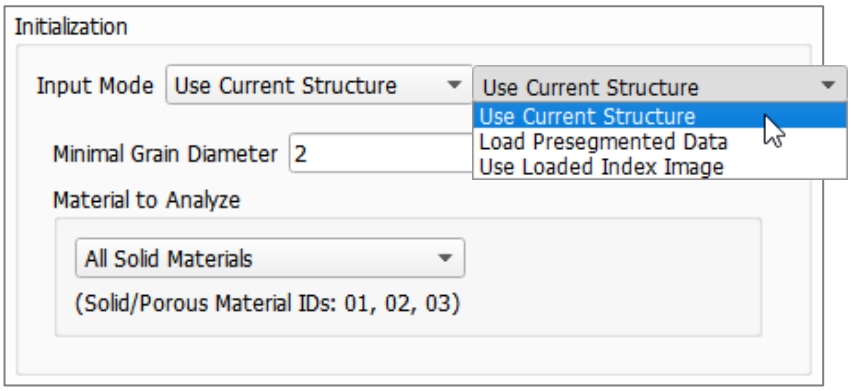
For the **Input Mode**, three options are available:

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

Only with **Use Current Structure**, the watershed algorithm is used to segment the structure. This procedure might be time-consuming for large structures. Thus, the options **Load Presegmented Data** and **Use Loaded Index Image** are useful when performing parameter studies with GrainFind, where the data is already segmented. For these options, the segmentation results from previous GrainFind runs can be used.

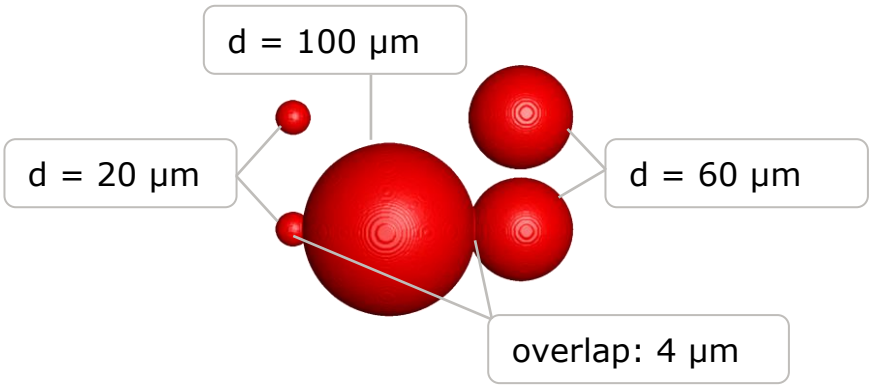
Use Current Structure

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.

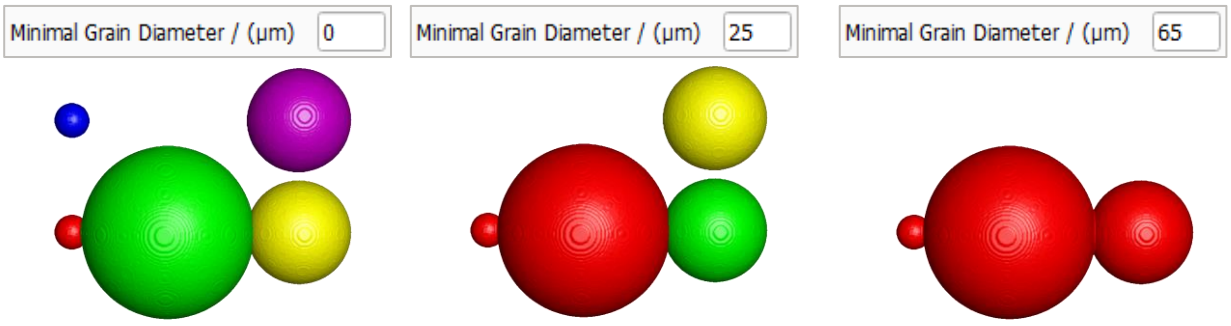


The **Minimal Grain Diameter** can be entered in unit of voxels and in unit of meters. The default value of 2 voxels works well in most cases and should therefore be left unchanged if a good estimation is unknown. The unit of the **Minimal Grain Diameter** can be changed through the pull-down menu next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

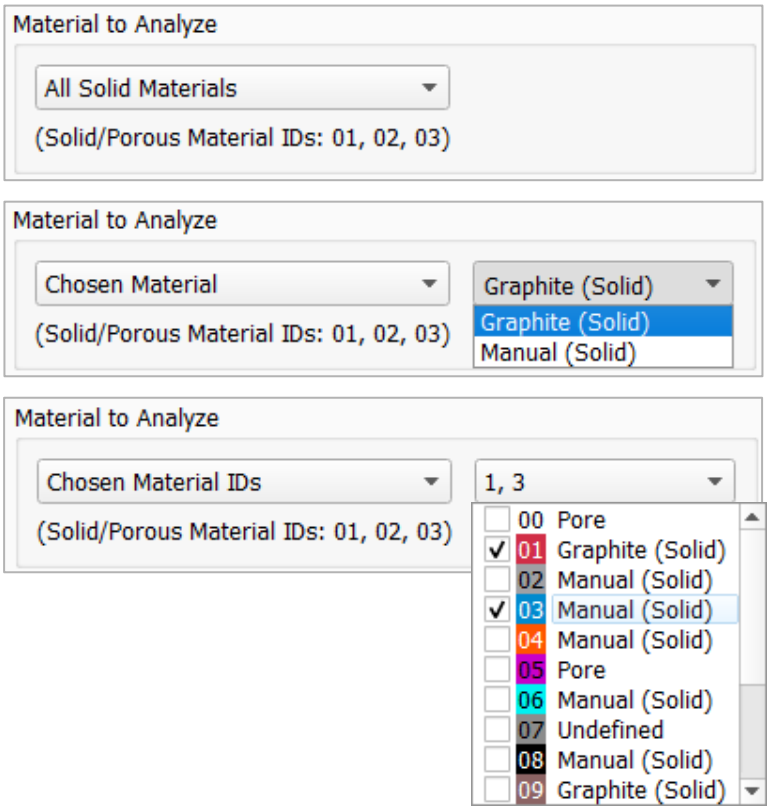
The effect of the choice for **Minimal Grain Diameter** is illustrated below. The figures show the result of the initialization step (of the watershed algorithm). The original structure contains spheres with diameters 100 µm, 60 µm, and 20 µm, and some of the grains overlap.



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

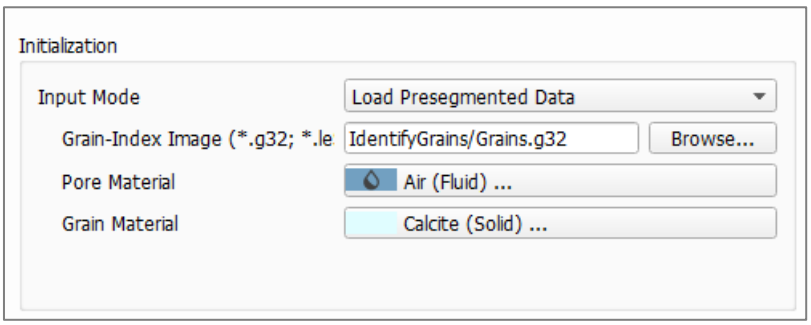


Under **Material to Analyze**, the user defines the part of the structure to be investigated. Either the complete structure can be analyzed (**All Solid Materials**), an individual material can be selected (**Chosen Material**) or a choice of material IDs can be made (**Chosen Material IDs**). With **Chosen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

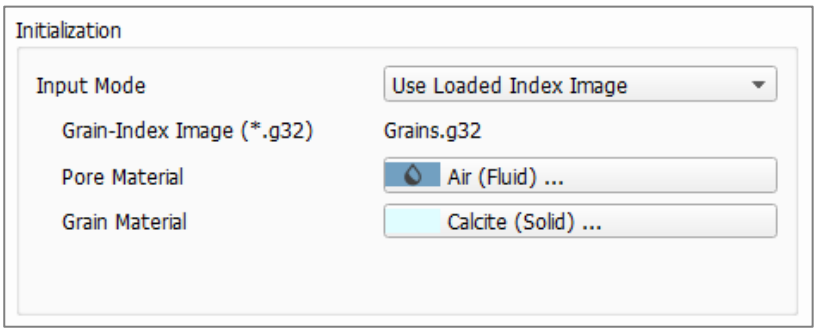


The difference between the *.g32 and *.leS formats is that *.g32 is a binary format, which produces comparatively smaller files but is not human readable, and *.leS is an ASCII-format which is human-readable, but produces larger files. Furthermore, loading a *.g32 file into GeoDict is much faster than 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*"). With **Reconnect Fragmented Grains**, it is possible to overcome this over-segmentation by merging grains depending on the size of their shared interface.

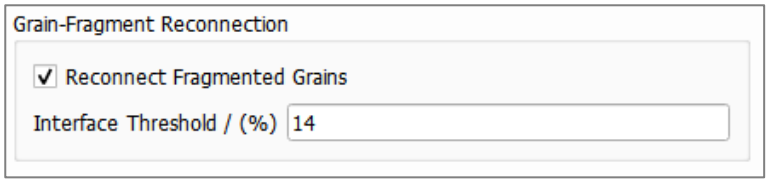
Activate the checkbox **Reconnect Fragmented Grains** to merge connected grains depending on the values chosen for **Interface Threshold** and **Reconnection Decision Mode**.

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.

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

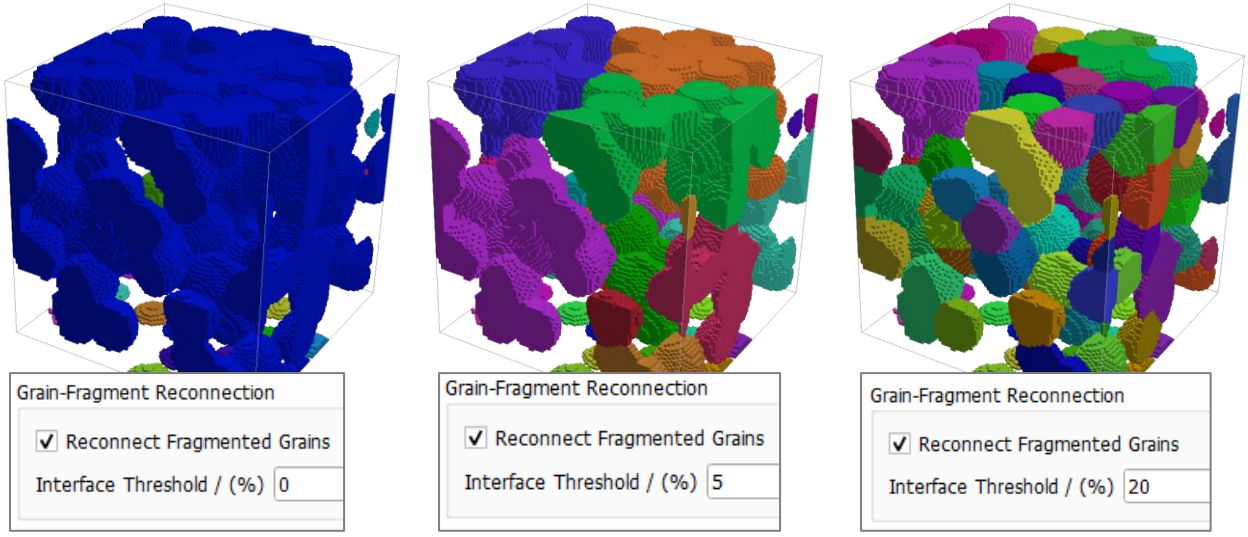
For the computation of the interface ratio, the grain surfaces and interfaces need to be computed. The surface area estimation is based on PoroDict's "Estimate Surface Area" (see J. Ohser and F. Mücklich, Statistical Analysis of Microstructures in Materials Science, Wiley and Sons, 2000, page 115).

If the *interface ratio* is larger than the percentage chosen for the **Interface Threshold**, then 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.



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

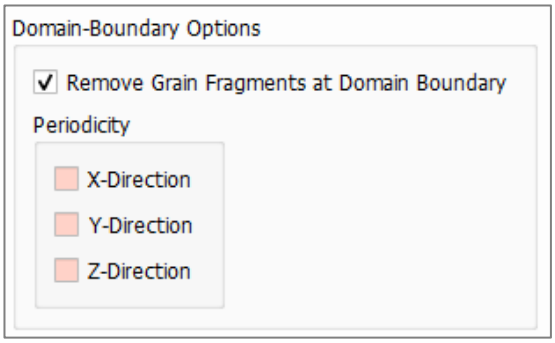
be adapted to the expected grain shapes for the structure type. Parameter studies for the **Interface Threshold** can be programmed with the help of a GeoPython script.



Domain-Boundary Options

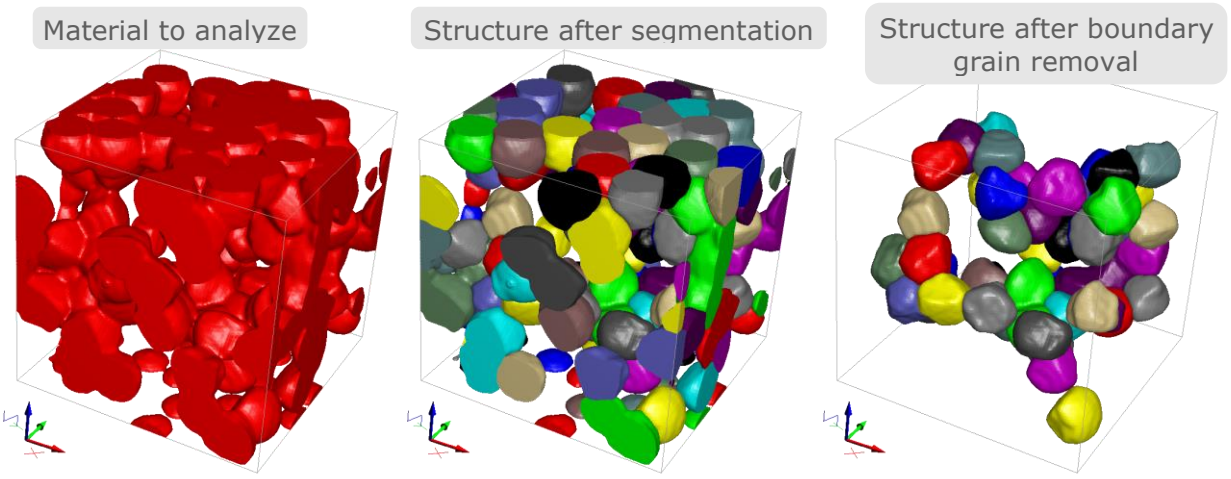
In the **Domain-Boundary Options** panel, the handling of boundary grains is defined. When **Remove Grain Fragments at Domain Boundary** is checked, all grains touching the domain boundary after the initialization and the grain-fragment reconnection are removed.

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 41 for an example and further explanations.



When **Remove Boundary Grains** 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 directions before the segmentation.

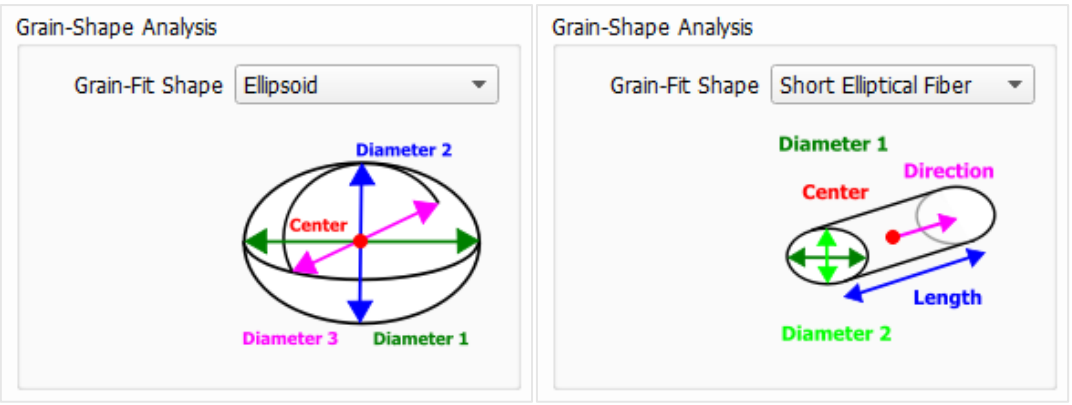
This option should only be chosen if the investigated structure is really periodic, otherwise it might lead to strange results (with grains which are treated as connected but are distant from each other in reality). Otherwise, when **Periodicity** is not chosen in a direction, the structure is analyzed with symmetric boundary conditions in this direction. This is the best option for estimating the shape of boundary grains.

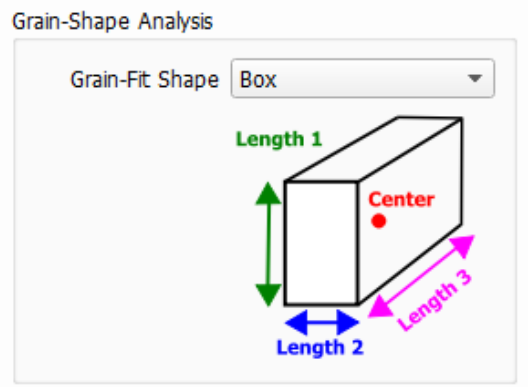


Grain-Shape Analysis

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.

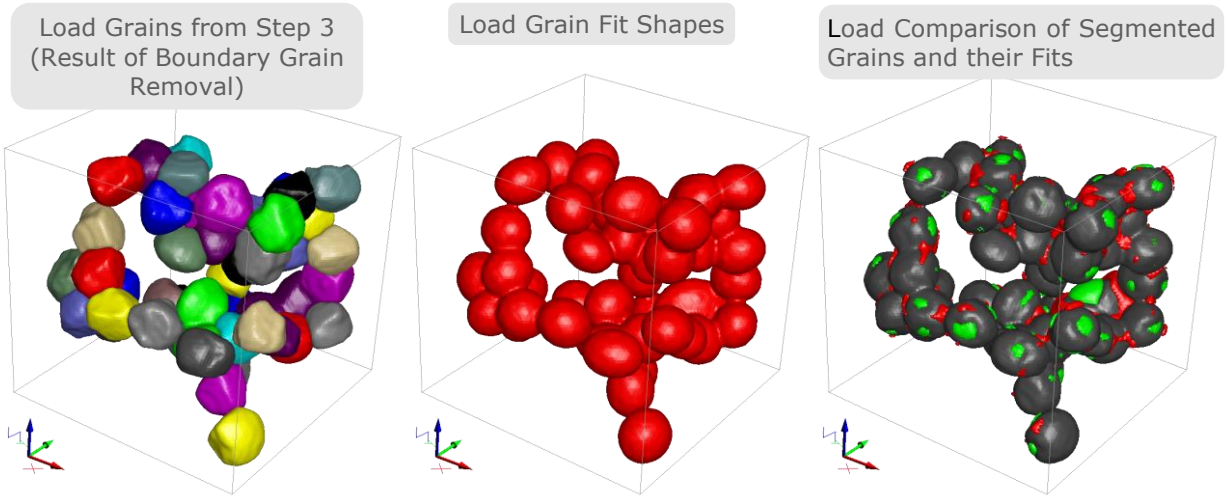
There are three options available for the **Grain-Fit Shape**: Either an **Ellipsoid**, a **Short Elliptical Fiber** or a **Box** can be chosen. The Grain-Fit Shape should be chosen depending on the grain shape appearing in the analyzed structure.





In the figure below, the results of the **Grain-Shape Analysis** are shown. The structures shown below can be loaded directly from the Result Viewer through the **Grain Visualization** tab if the corresponding results file (*.gdr) is loaded (See page 17 for more information).

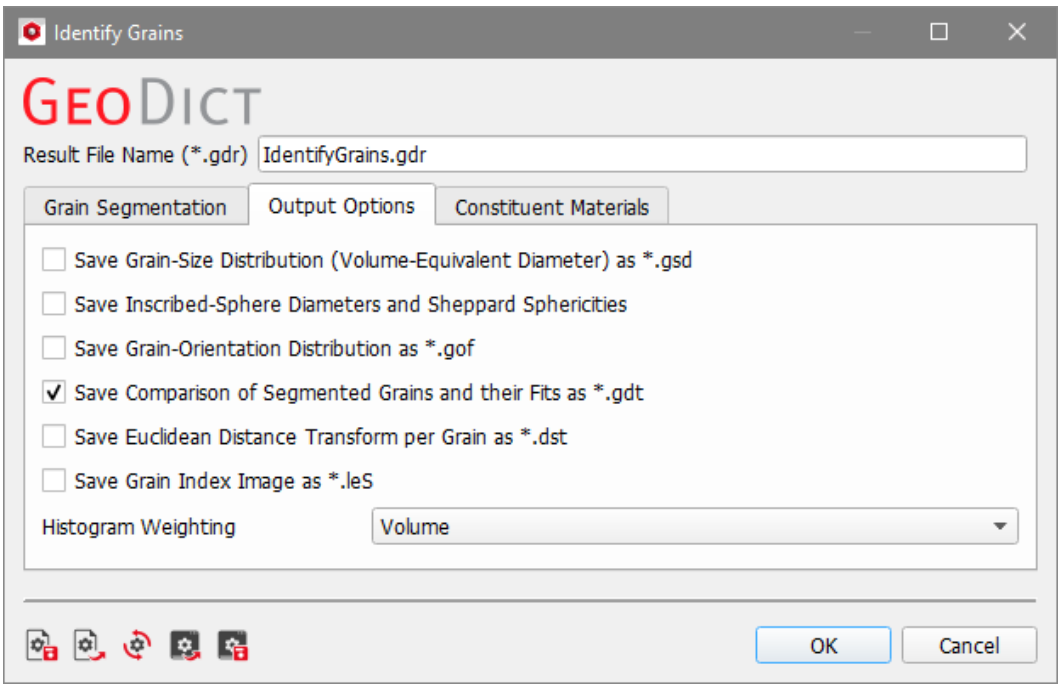
On the left, the structure after Boundary-Grain Removal is shown. In the middle, the grain-fit shapes are shown (here, **Ellipsoid** was chosen as the **Grain-Fit Shape**) and on the right, a comparison between the identified grains (red) and their fit shapes (green) is shown, where the matching voxels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



Output Options

Under the **Output Options** tab, some additional files can be selected to be saved:

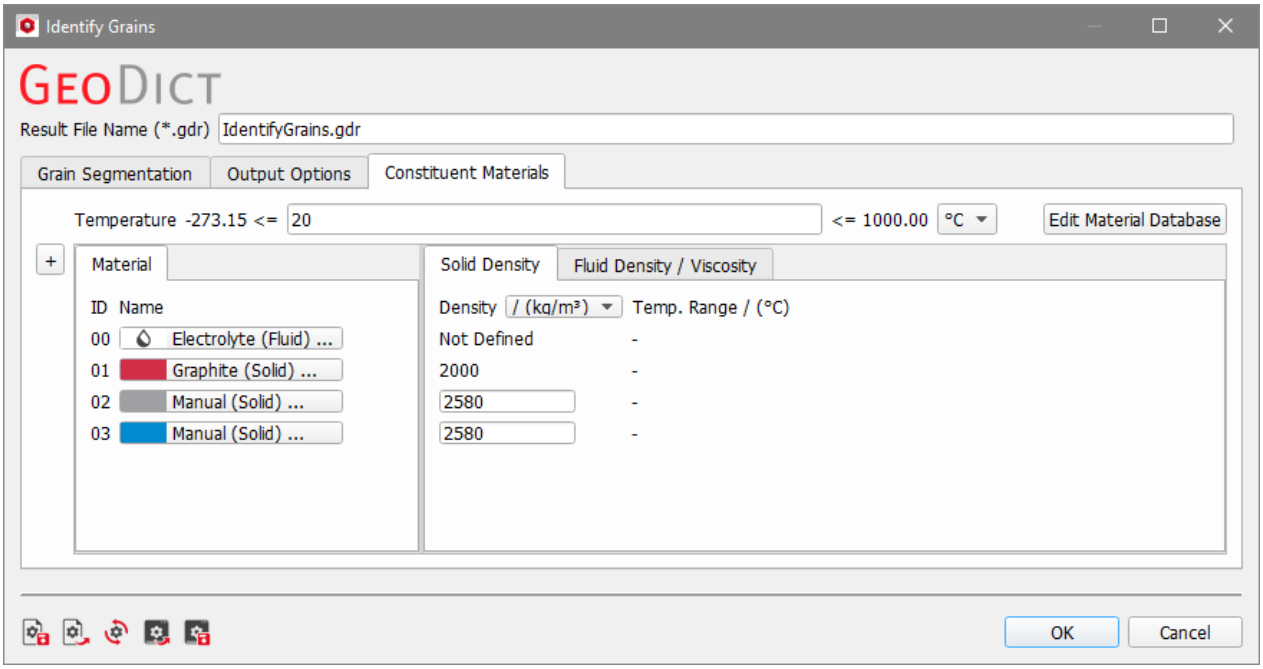
- Choose **Save Grain-Size Distribution (Volume-Equivalent Diameter) as *.gsd** to save the computed grain size distribution as a volume field. This information can be used for visualization and for further analysis.
- With **Save Inscribed-Sphere Diameters and Sheppard Sphericities** and, the mentioned parameters are calculated and shown in the results file. 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 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 14). 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 per grain is saved as *.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, but it is human readable and can easily be imported into other software.



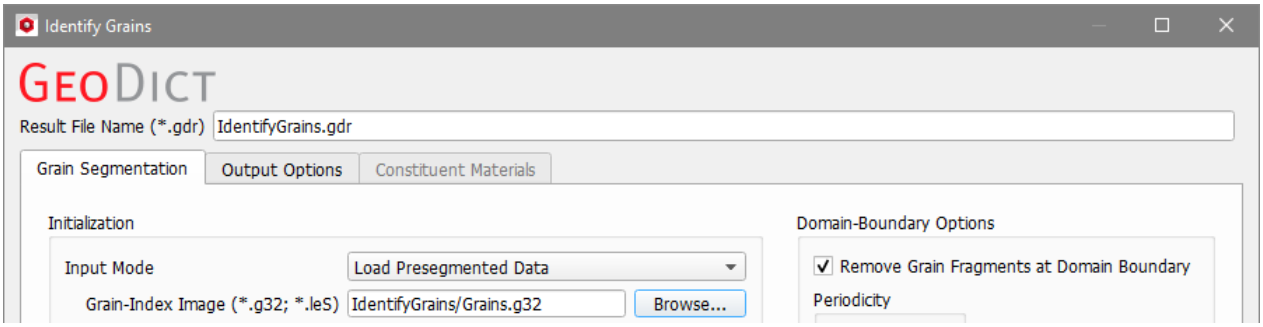
Choosing **Histogram Weighting** as **Volume**, **Surface** or **Number** changes the values on the y-axis of the resulting histogram plots. Then, either the grain volume probability, the grain surface area probability, or the grain count probability is shown. The **Histogram Weighting** can be changed 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 this User Guide



The **Constituent Materials** tab is only available if **Use Current Structure** is used 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). When the analysis is finished, the results file is automatically opened in the Result Viewer. For more information about the GeoDict **Result Viewer,** refer to the Results Viewer handbook of this User Guide

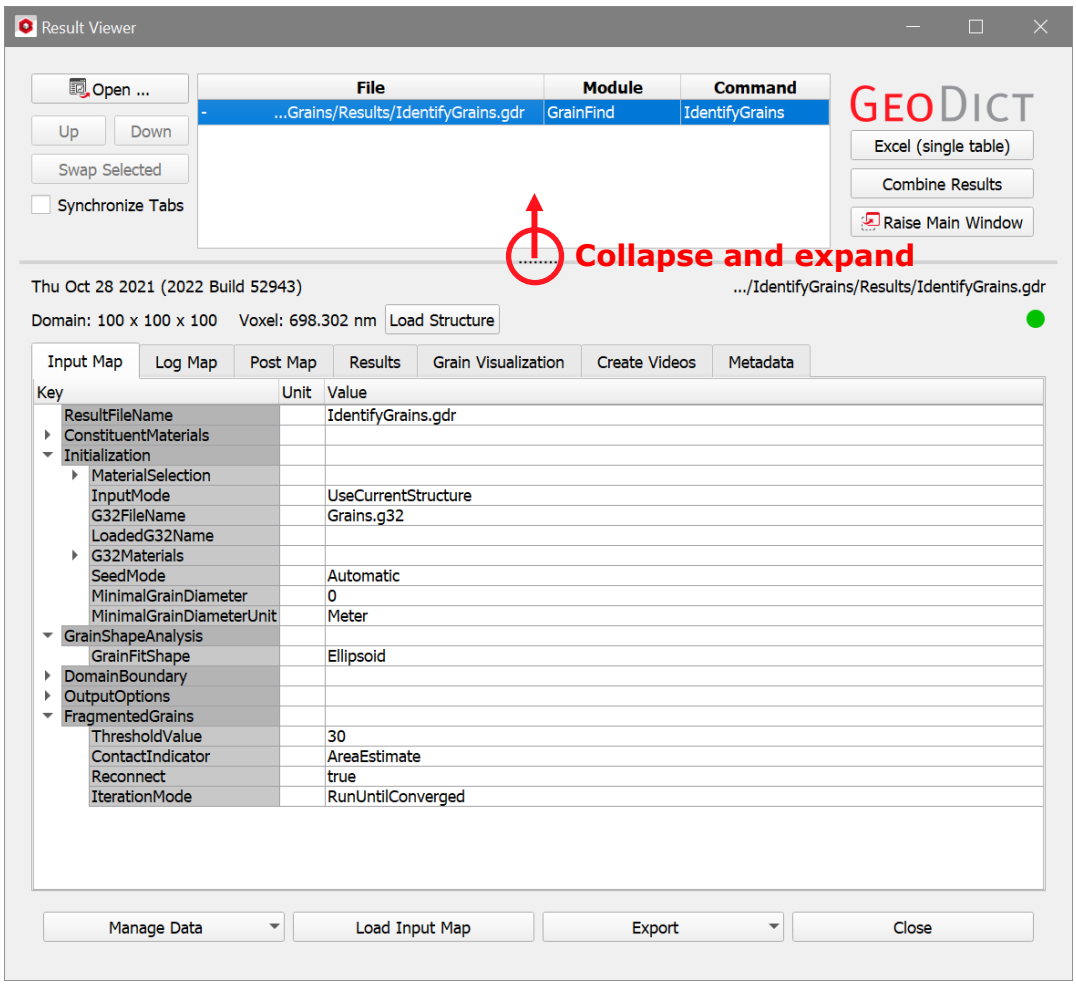
By clicking **Load Structure**, the analyzed structure can be imported into the Visualization area of the GeoDict GUI. Observe the dot at the right side of the **Load Structure** button: a green dot means that the structure currently in memory corresponds the results shown in the Result Viewer. A red dot means that the structure does not correspond to the results.

The **Result Viewer** contains several tabs. **Input Map**, **Log Map**, and **Post Map** contain the parameters concerning the GrainFind process. The **Log Map** contains information about the identification process, as e.g. the runtime and the used computer. The **Post Map** contains all information about the post-processing in the results viewer, as e.g. the chosen plots and their parameters. Only the **Input Map** is shown here in detail, the other two are structured analogously.

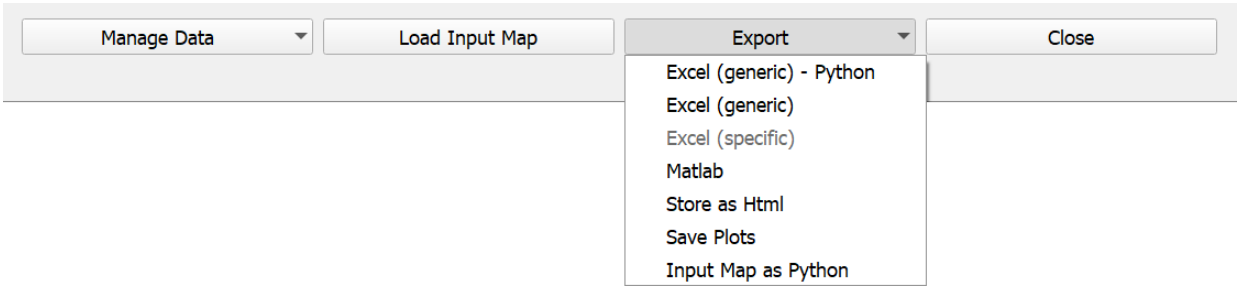
The **Metadata** tab contains some meta information about the results file.

INPUT MAP

The **Input Map** contains all chosen input parameters for **Identify Grains**. For example, in the screenshot below, it is shown that **Reconnect Fragmented Grains** was enabled (true), and that **Ellipsoid** was selected as the **Grain-Fit Shape**.



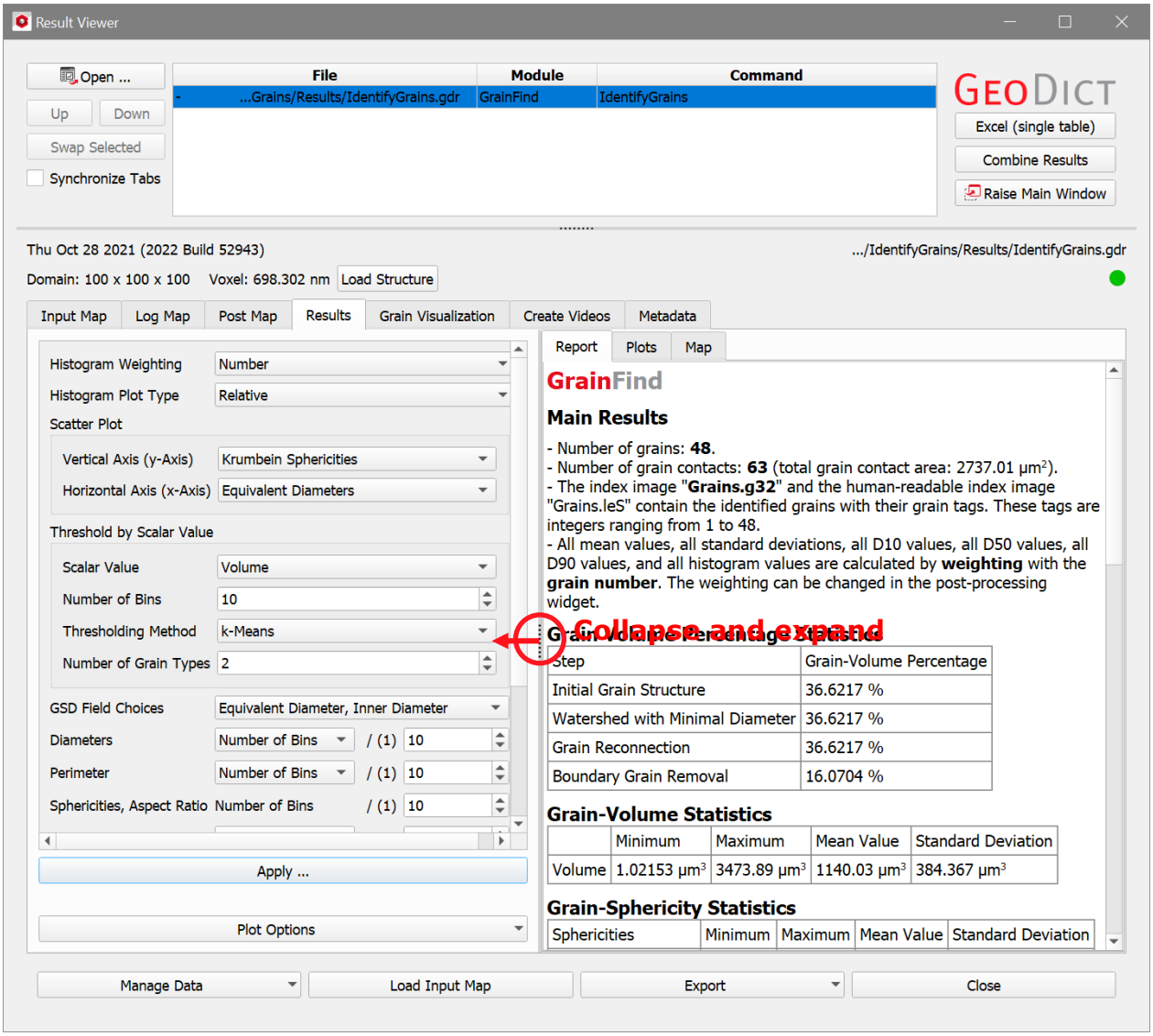
At the bottom of the Result Viewer, several buttons are available:



- With **Manage Data**, the results can be cleaned up, compressed and renamed.
- With **Load Input Map**, the parameters in the input map are loaded in the GUI and can be used to analyze different structures.
- **Export** data:
  - Analyze and plot computation results in Microsoft Excel®. Check out the GeoDexcel and Result Viewer handbooks for more information.
  - Analyze the results in MATLAB® using GeoDict's MATLAB® interface GeoLab by clicking **Matlab**. All information included in the results file is loaded into MATLAB® automatically.
  - Save the information in the result file in *.html format by clicking **Store As HTML**.
  - **Save Plots** to save images for all plots in the current results file
- Close the results file by clicking **Close**.

RESULTS

The **Results** tab is the central point after 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 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.



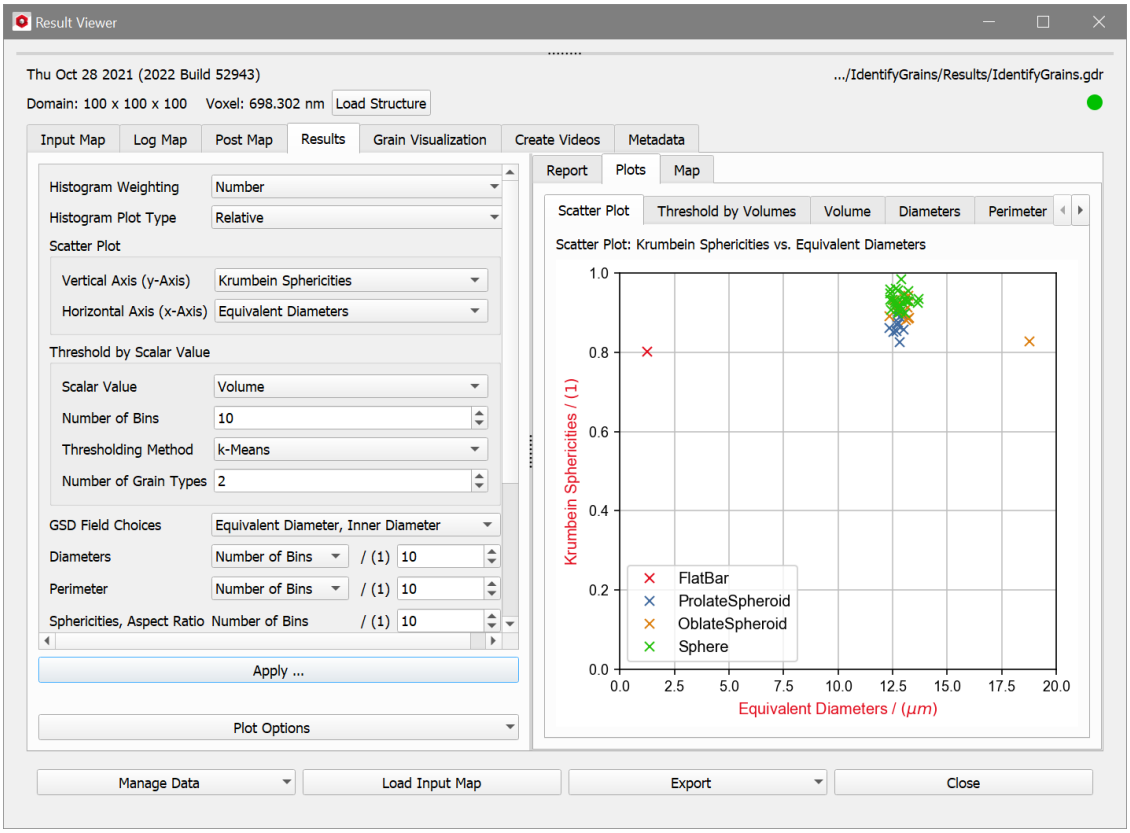
PLOTS

Under the **Plots** tab, several plots visualize the results. These plots are grouped in 12 tabs which show the relationship between grain parameters: **Scatter Plot**, **Threshold by...** histogram, **Diameters** histogram, **Perimeter** histogram, **Sphericities** histogram, **Aspect Ratio** histogram, **Surfaces and Contacts** histogram, **Mass** histogram, **Moment of inertia** histogram, **Coordination Number** histogram, **Volume** histogram, and the **Orientation** polar plot.

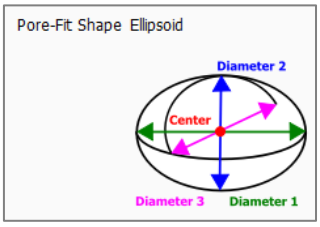
For the **Threshold by...** histogram, the threshold parameter must be selected under **Threshold by Scalar Value** on the left (See page 21 for further explanations). The default is **Threshold by Volume**.

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

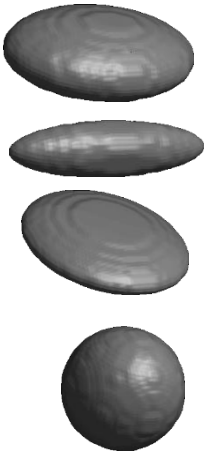
In the example below, observe in the **Scatter Plot** that all identified grains in the structure are nearly spherical (Krumbein Sphericities close to 1). Nearly all grains have an equivalent diameter around 12.5 µm, except of two outliers.



The plots Scatter Plot and Orientation distinguish between the four shapes **Flat Bar**, **Prolate Spheroid**, **Oblate Spheroid** and **Sphere**. These are the four possible shapes for the ellipsoids that are fitted into the pores.



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



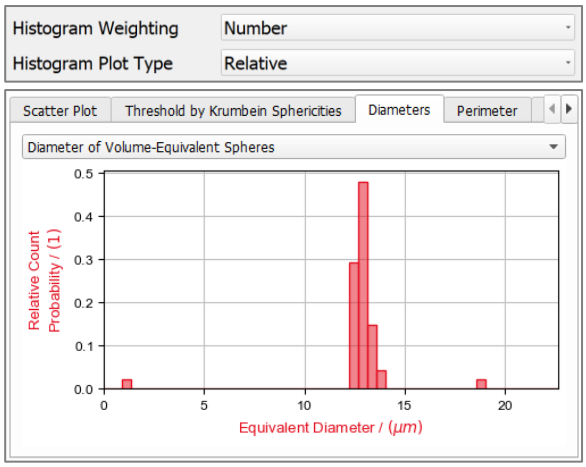
The settings for all plots are chosen in the collapse-expand panel to the left of the tabs.

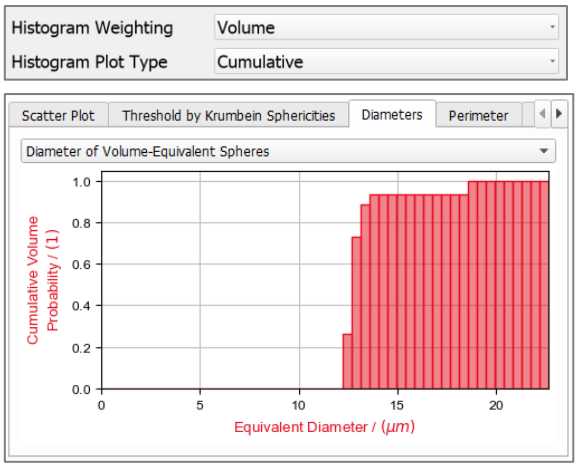
Histogram Weighting and Histogram Plot Type

The values on the Y-axes of the histograms in all plots (except **Scatter Plot**, **Threshold by...**, **Volume** and **Orientation**) can show Count Probability, Area Probability or Volume Probability, as a Relative or Cumulative plot. 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.

This can be set by adjusting the **Histogram Weighting** and **Histogram Plot Type**.

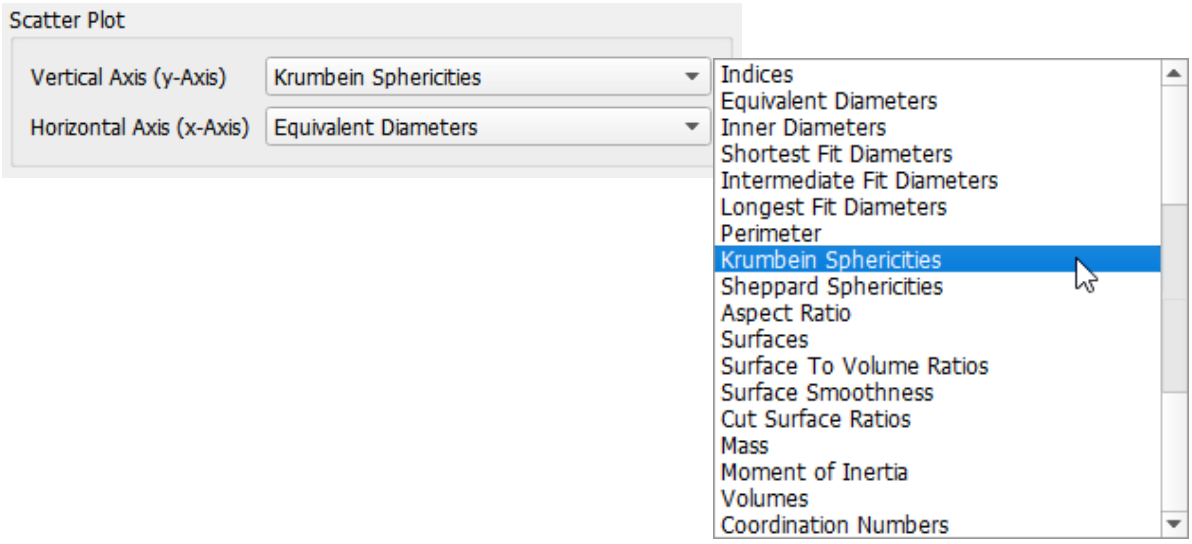




The plot under the **Volume** tab can show only Count Probability or Volume Probability, which can also be selected with the **Histogram Weighting**. If **Surface** is chosen as Histogram Weighting, Volume Probabilities will be used in the **Volume** plot.

Scatter Plot

For example, under **Scatter Plot**, the variables for the scatter plot can be chosen.

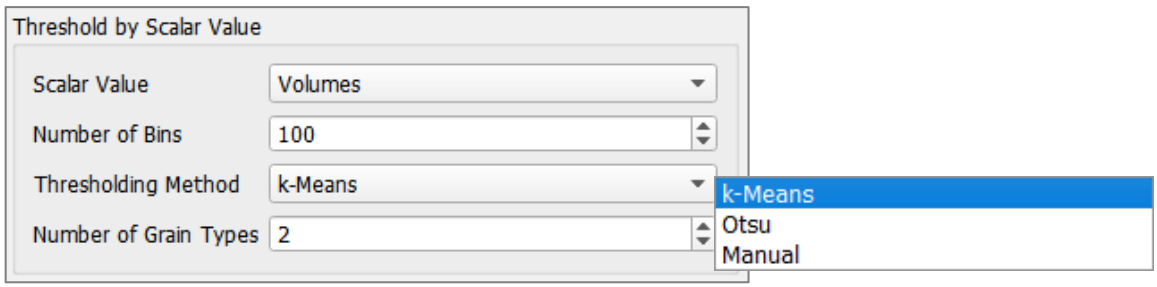


Threshold by Scalar Value

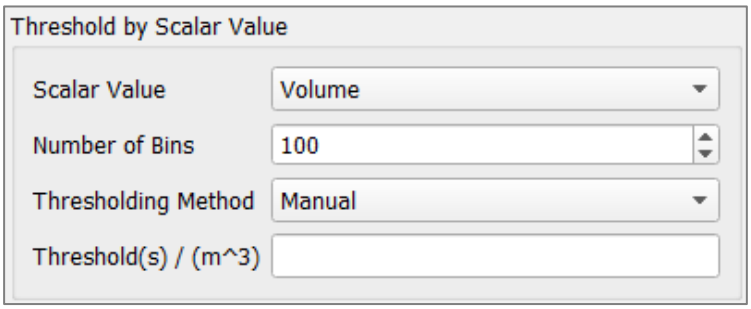
In **Threshold by Scalar Value**, several options for thresholding the structure depending on the results are available. The following **Thresholding Methods** are available:

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



In every case, a plot will be created under the **Plots** - **Thresholding by ...** subtab, and 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** button.

The following measures (scalar values) are available for thresholding:

- **Equivalent Diameter**: The diameter of the volume-equivalent sphere.
- **Inner Diameter**: The diameter of the largest sphere that can be inscribed into the grain.
- **Shortest Fit Diameter**: The shortest diameter of the shape (ellipsoid, box, short fiber) fitted onto the grain.
- **Intermediate Fit Diameter**: The intermediate diameter of the shape (ellipsoid, box, short fiber) fitted onto the grain.
- **Longest Fit Diameter**: The longest diameter of the shape (ellipsoid, box, short fiber) fitted onto the grain.
- **Perimeter**: three diameters are defined by the ellipsoid fitted into the pore. The perimeter is the shortest perimeter around this ellipsoid, computed as the perimeter of the ellipse formed from the two smallest of those three diameters.
- **Krumbein Sphericity**: A measure for the sphericity based on the grain fit (see page 4).
- **Sheppard Sphericity**: The diameter of the inscribed sphere divided by the diameter of the volume-equivalent sphere (see page 4).

- **Aspect Ratio:** three diameters are defined by the ellipsoid fitted into the pore. The aspect ratio is the shortest diameter divided by the largest of those diameters.
- **Surface**: Surface of the grains estimated by an algorithm based on PoroDict's **Estimate Surface Area** command (see J. Ohser and F. Mücklich, Statistical Analysis of Microstructures in Materials Science, Wiley and Sons, 2000, page 115)
- **Surface-to-Volume Ratio**: Estimated surface of the grain divided by the volume of the grain
- **Surface Smoothness**: The surface of a fitted ellipsoid divided by the estimated surface. Usually the estimated surface is larger than the surface of the fitted ellipsoid. Hence, the surface smoothness is usually below 1. Only if the shape of the grain is very ellipsoidal, then the surface estimation might be a little smaller than the surface of the fitted ellipsoid.
- **Cut-Surface Ratio**: The interface of the grain with the domain boundary over the remaining surface of the grain. The **Cut-Surface Ratio** measures how much of the grain surface is part of the domain boundary. 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**: The mass of the grains is computed based on their volume and the density of the grain material.
- **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.
- **Coordination Number**: 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).

GSD Field Choices

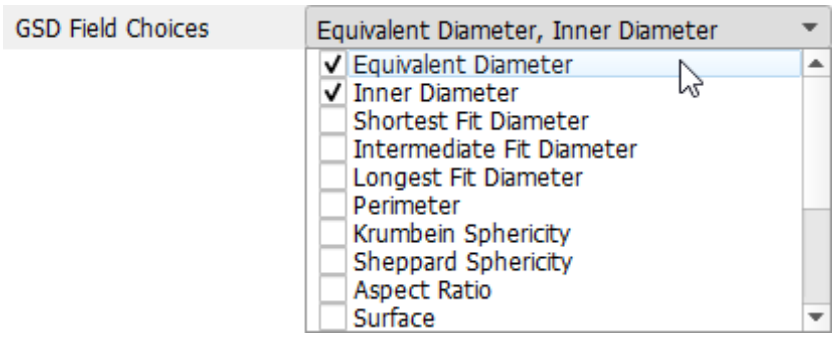
The GeoDict size distribution (GSD) files allow to visualize the various scalar grain properties that are a result of the grain identification.

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.

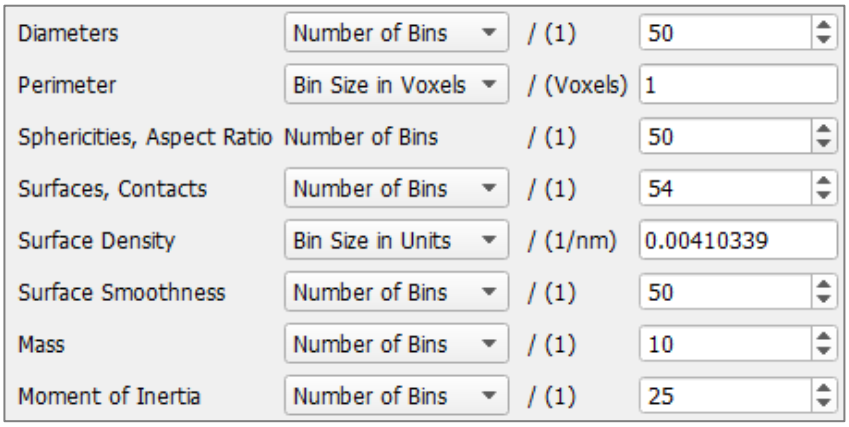
For example, by choosing **Equivalent Diameter** and **Surface**, the *.gsd file will contain two volume fields: one with the size distribution of the diameters of volume-equivalent spheres, and one with the distribution of the grain surface.

The same measures for assembling 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.



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.

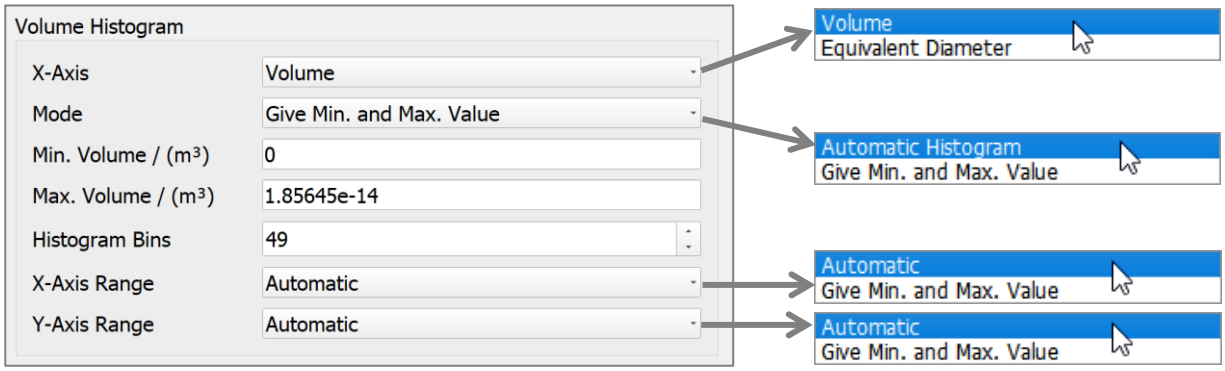
As the different histogram plots show different results, only those choices are available which make sense for the corresponding plot.

- The selection made under **Diameters** 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 made under **Sphericities, Aspect Ratio** changes the bin size for both plots under the **Sphericities** tab and the plot under the **Aspect Ratio** tab.
- The selection made under **Surfaces, Contacts** changes the bin size for the **Surfaces** and **Contacts** plots under the **Surfaces And Contacts** tab.
- The selection made under **Surface Density** changes the bin size for the **Surface-to-Volumes 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.

Volume Histogram Options

Finally, the **Volume Histogram** options change the appearance of the histogram under the **Volume** tab. (Remember, that the value shown on the Y-Axis is already defined through the **Histogram Weighting** and **Histogram Plot Type**).



Grain Visualization

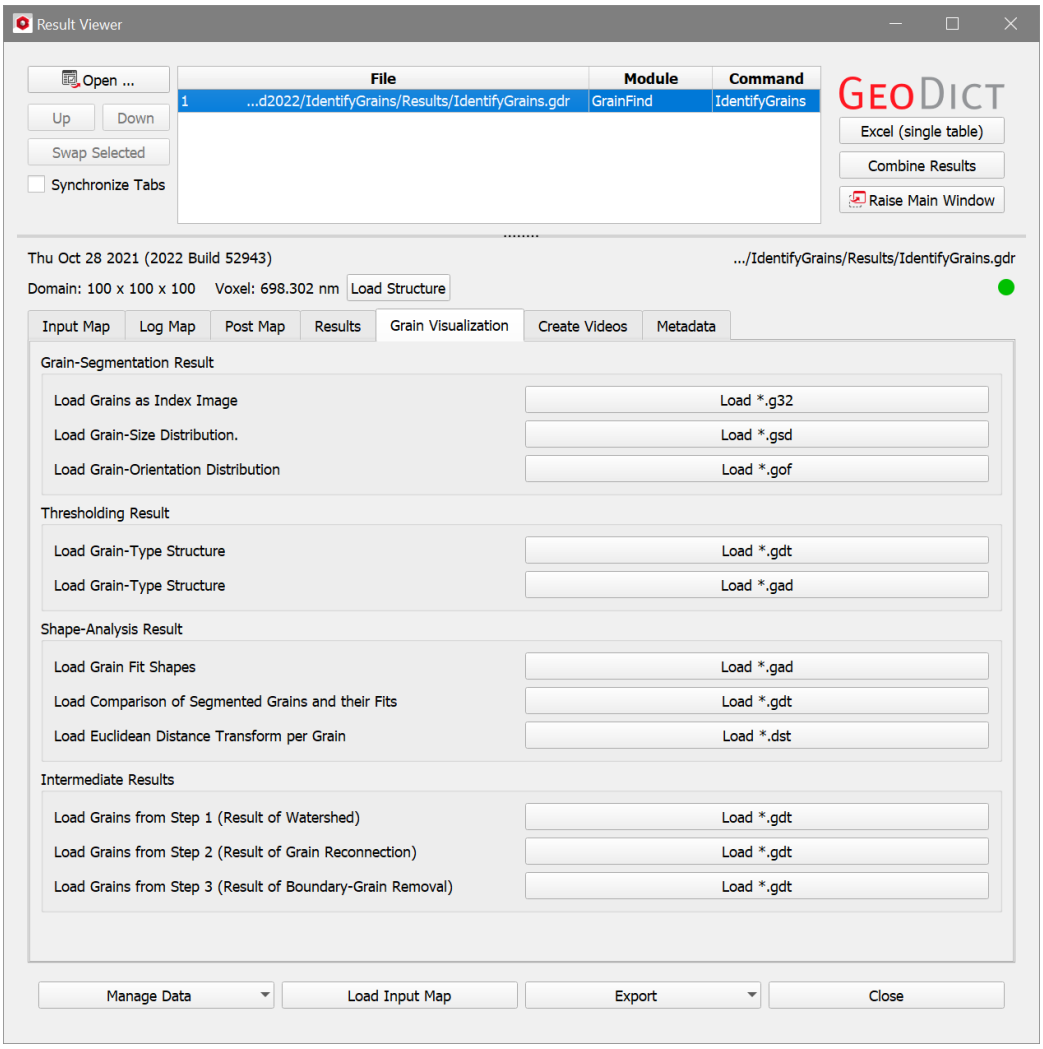
The **Grain Visualization** tab is used to import structures and volume fields which illustrate the grain identification process and its results.

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 these two options have not been previously checked under the **Output Options** tab of the **Identify Pores** dialog (see page 29).



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 24).

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

Thresholding Result

As mentioned above in Thresholding, clicking the **Load Grain-Type Structure' Load *.gdt** button loads the structure that contains the thresholded grain materials. The options for the thresholding can be found in the **Results** tab.

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.

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 14 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 29).

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** is chosen correctly for the investigated structure.

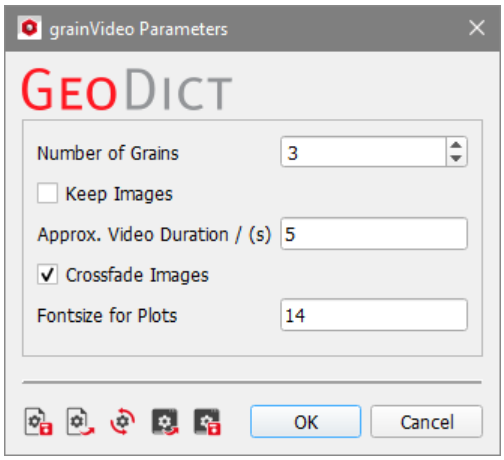
By clicking **Load Grains from Step 2 (Result of Grain Reconnection)**, the structure after the Grain-Fragment Reconnection is loaded in GeoDict. This way it can be investigated if the chosen value for the **Interface Threshold** suits the analyzed structure.

Load Grains from Step 3 (Result of Boundary-Grain Removal) imports the structure after the steps defined in the **Domain-Boundary options** are evaluated.

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 15 random colors, which are unrelated to their size. The visibility of the pore space (ID 00) should remain unchecked.

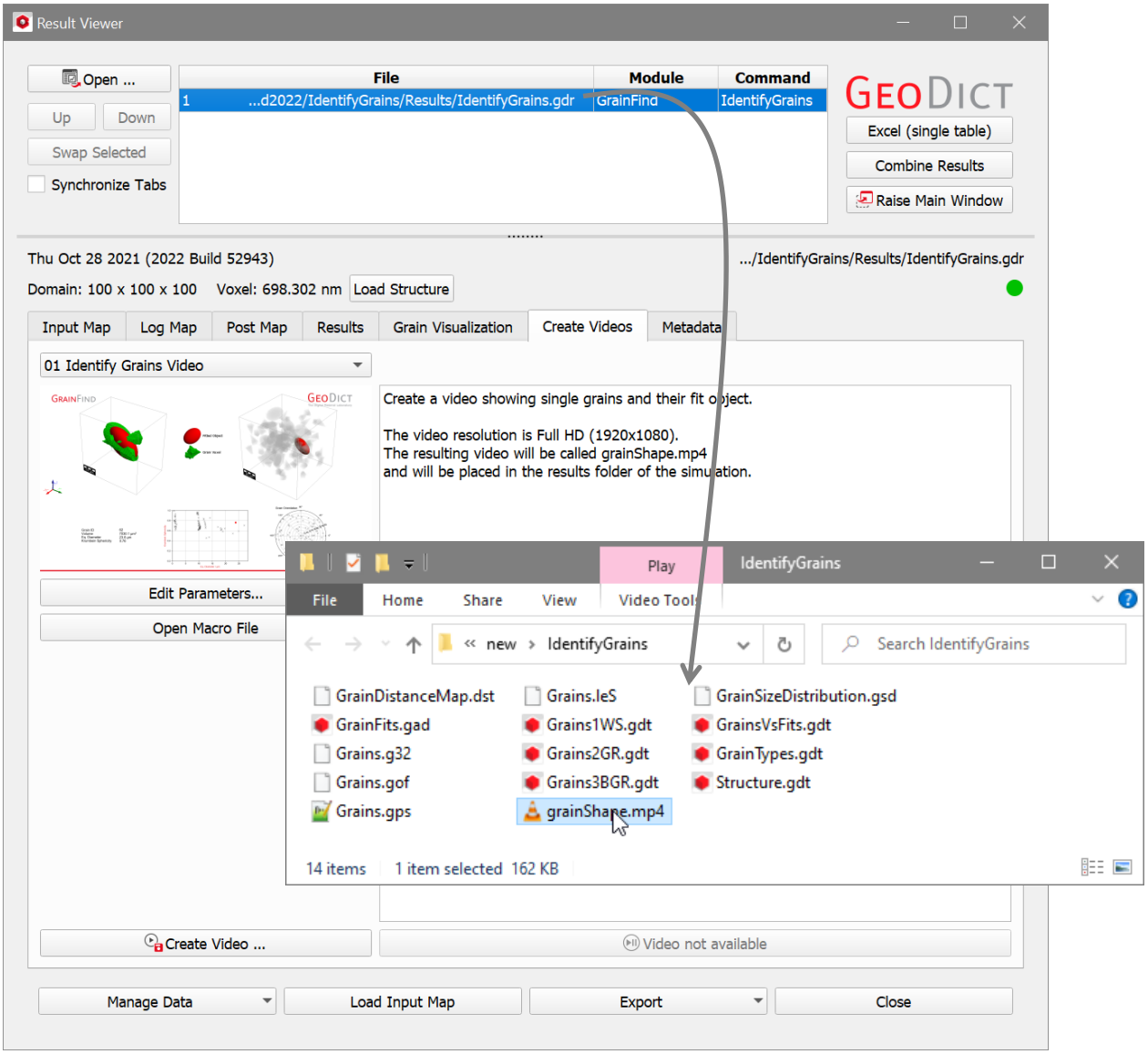
Create Videos

With **Create Videos**, it is possible to automatically generate a video showing the largest identified grains compared to their fit shapes.



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

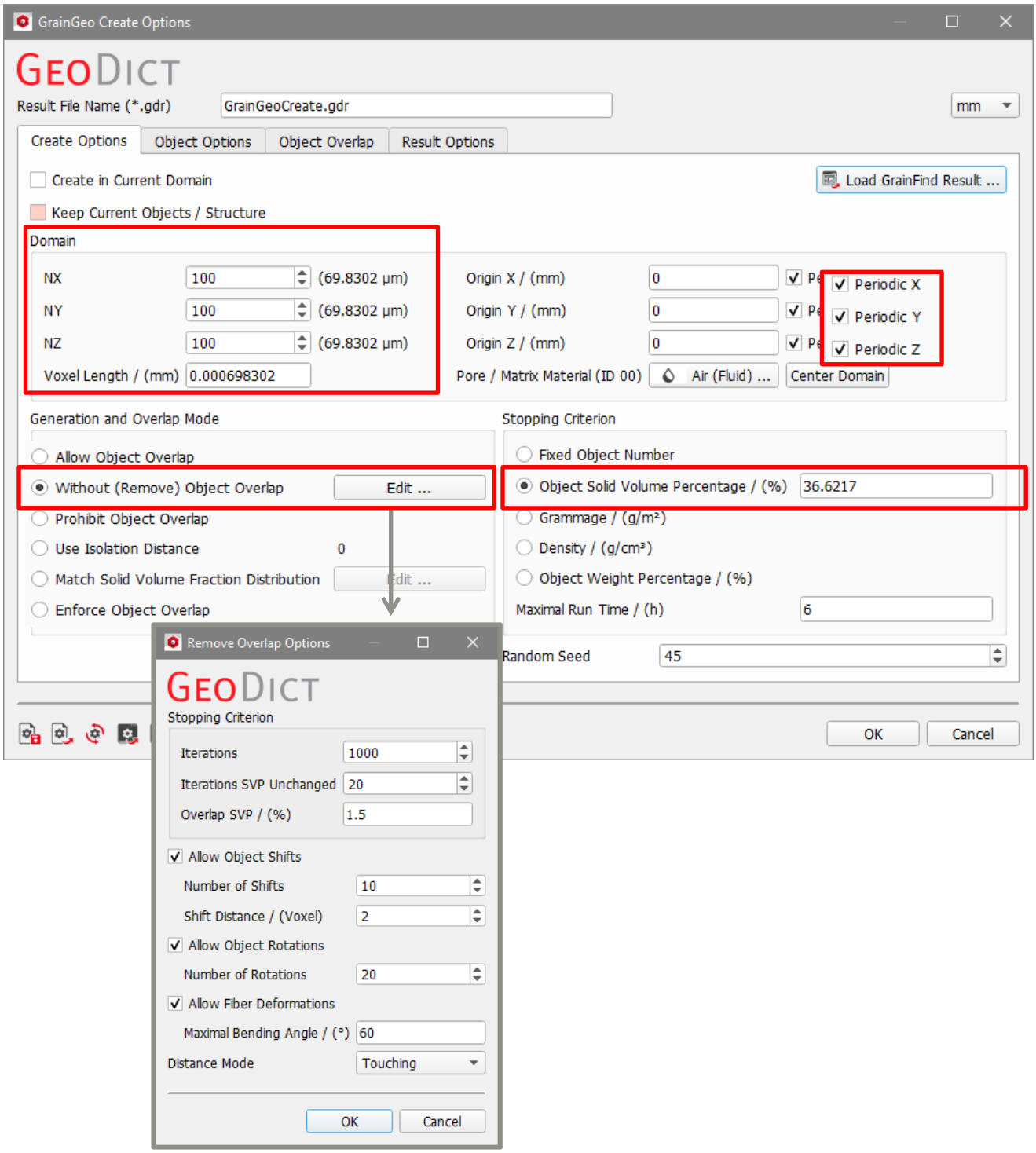
The results of a GrainFind run can be used to generate structures with similar properties in GrainGeo – a "digital twin" of the material can be created. Here, this procedure is shown with the structure used for the examples above.

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.

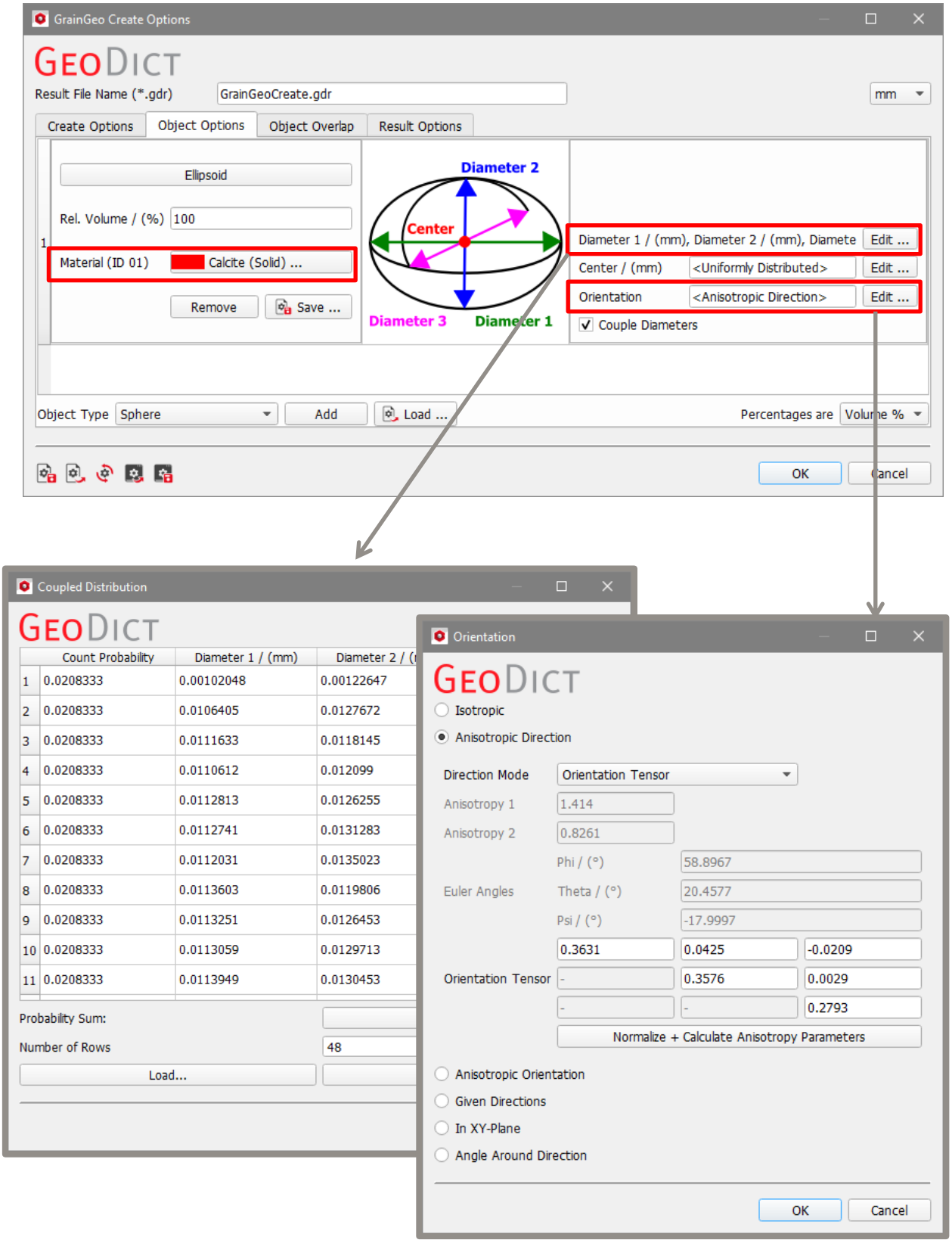
The data from the *.gdr file is now directly loaded into GrainGeo.

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.



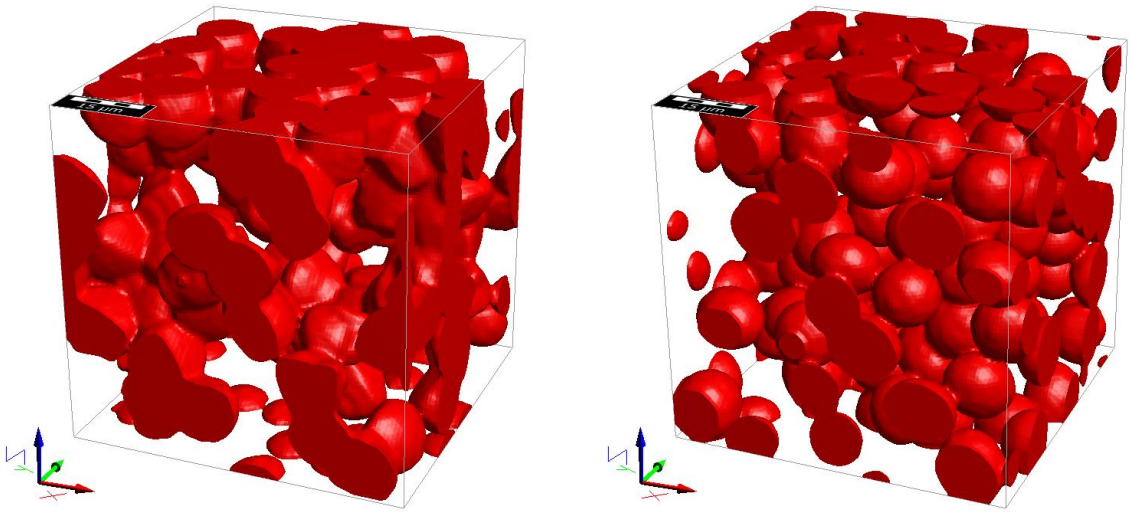
The identification analysis also automatically delivers the **Material** of the identified objects (for example, Calcite), the **Diameter** size and the **Orientation** parameters of the grains under the Object Options tab.



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. For further information about this topic, check out the tutorial Building a Digital Twin of a cathode material with GrainFind and GrainGeo.

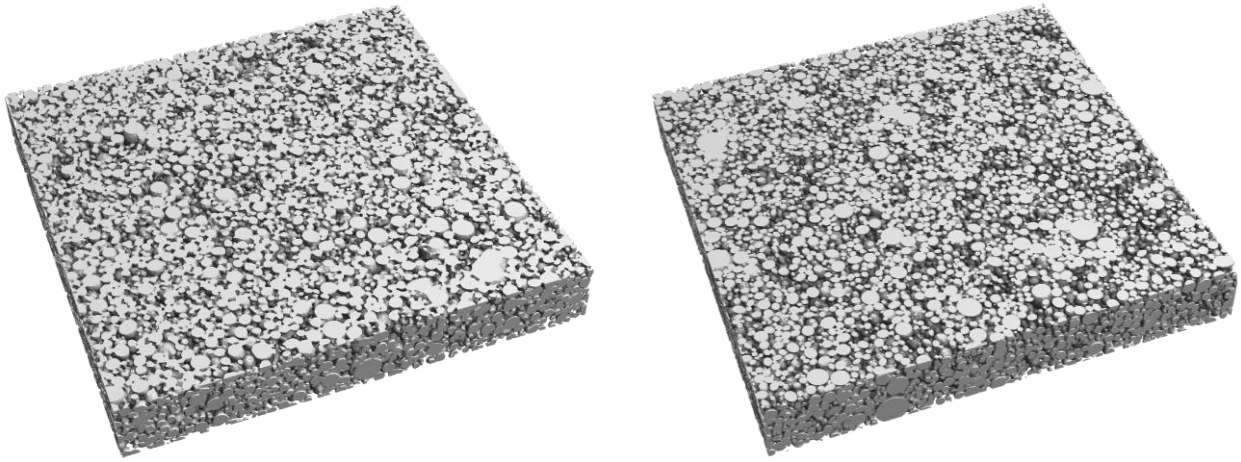
Original structure

Structure created with GrainGeo and "Load GrainFind results"



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 Digital Twin of a cathode material with GrainFind and GrainGeo".



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.

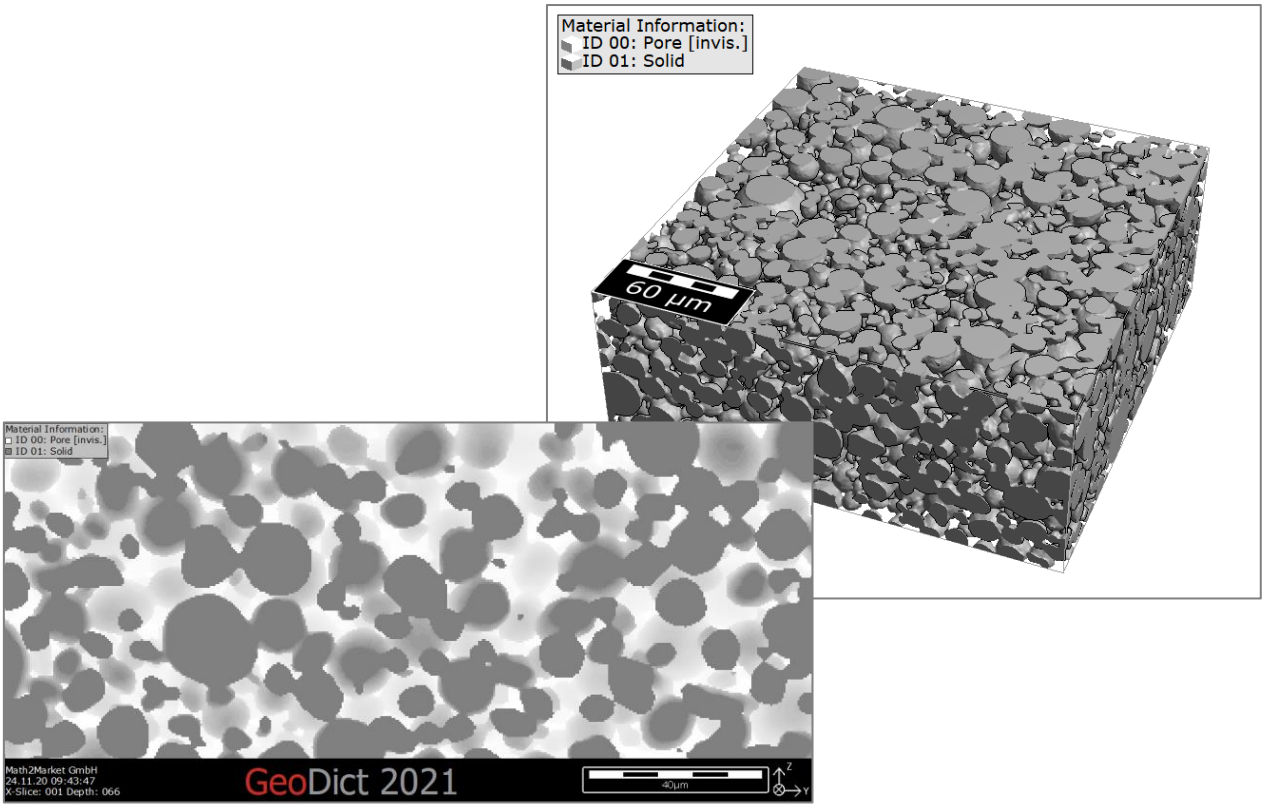
Structure created with GrainGeo and "Load GrainFind Results"

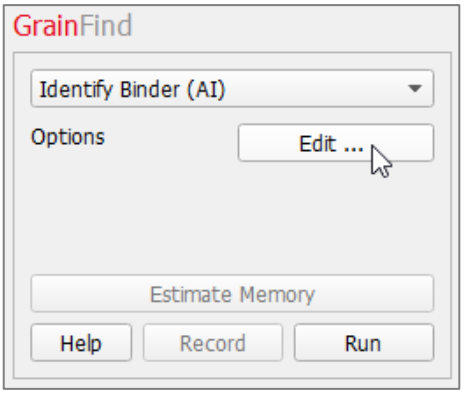
For more information, check the "Building a Digital Twin of a cathode material with GrainFind and GrainGeo" tutorial

IDENTIFY BINDER (AI)

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 this 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 segment of sample of a NMC cathode structure from the Laboratory for Nanoelectronics, ETH Zurich (See page 29 for reference).

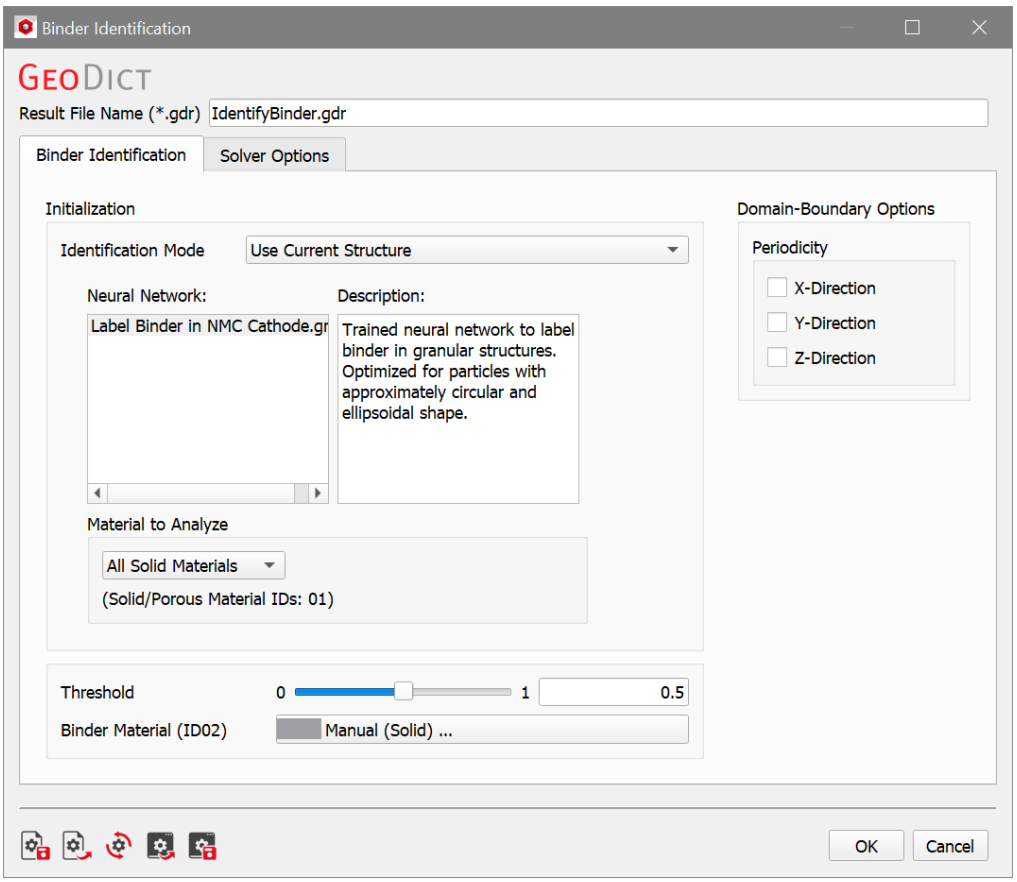




To start, select **Analyze** → **GrainFind** from the menu bar and, in the **GrainFind** section, select **Identify Binder (AI)** from the pull-down menu. Click the **Options**' **Edit...** button.

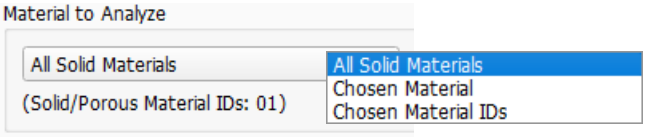
The **Binder Identification** dialog that opens includes the **Binder Identification** and the **Solver Options** tabs.

In the **Binder Identification** tab, select the neural network available under **Neural Network**. In future versions of GeoDict, more than one neural network (.gnn stands for **G**eoDict **n**eural **n**etwork parameter file) will be provided, making it possible to select the best suitable one for the structure under consideration.

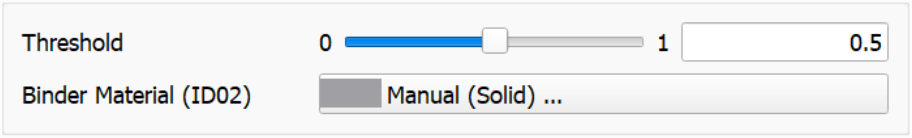


In the **Description**, the current constraints for the application of the neural network are listed, like the fiber cross-section or diameter for that the neural network was trained.

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

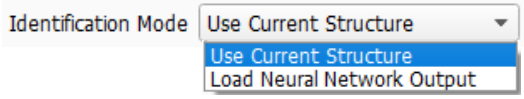


The **Threshold** is an expert parameter that is mostly applied by proficient users at Math2Market. The neural network provides probabilities that a solid voxel is binder or not. The **Threshold** defines the limit for labelling a voxel as binder. It is recommended to keep the default value of 0.5, since this reflects the computed probabilities correctly.

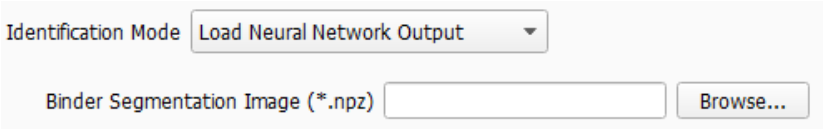


In the lower left of the **Binder Identification** dialog, the **Binder Material ID** specifies the color to label the binder. The first unused material ID is used for the Binder Material. In the example below, the structure contains only material ID 00 and 01, thus the **Binder Material ID** is 02. To be able to distinguish the binder properly from the other materials, the color for this ID should be chosen different from the color of any solid or pore material present in the original structure.

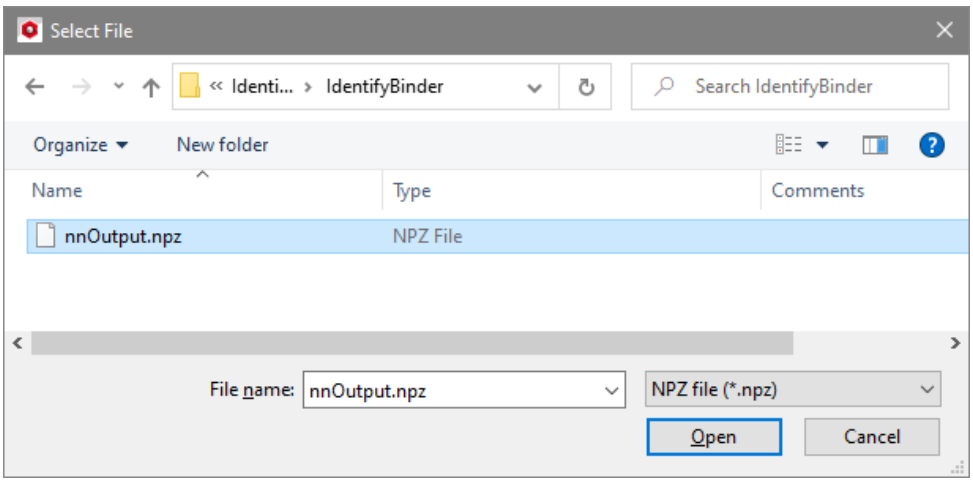
Two choices are available as **Identification Mode**: **Use Current Structure** and **Load Neural Network Output**.



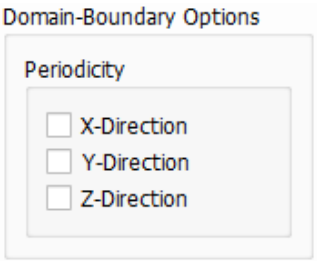
The default **Use Current Structure** applies the binder identification to the structure currently available in GeoDict memory. This is the common use case for Identify Binder. If the evaluation of the output of the neural network should be run again, with a different threshold and without having to re-run the neural network inference step, **Load Neural Network Output** may be chosen.



For the Identification Mode **Load Neural Network Output**, browse to a .npz file from the result folder of a previous run of BinderFind-AI. Since already the output of the neural network is used in that case, no selection of **Neural Network** or **Material to Analyze** is possible and the loaded structure needs to be the same.

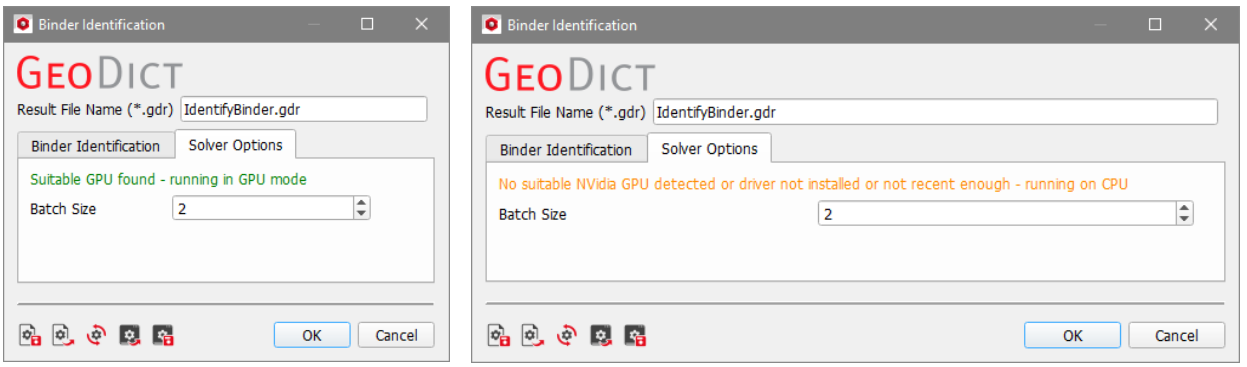


Select one or several boxes on the **Domain-Boundary Options** panel if the underlying structure for the binder identification is periodic in one or several directions. However, periodicity is unusual for most 3-D scans and this setting is rarely changed.



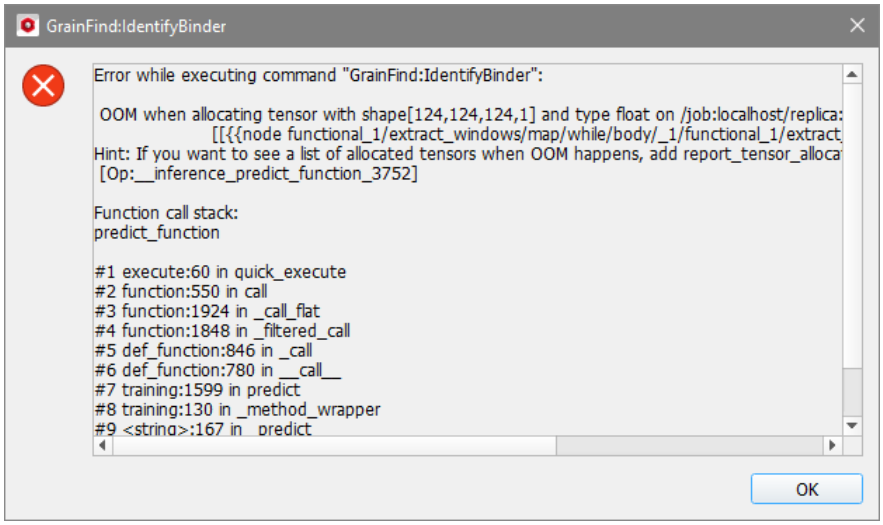
Solver Options

If a suitable graphics card is detected during installation of GeoDict, the GPU mode is used for running FiberFind-AI, otherwise it is running in CPU mode. The version used is displayed on the **Solver Options** tab.



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.

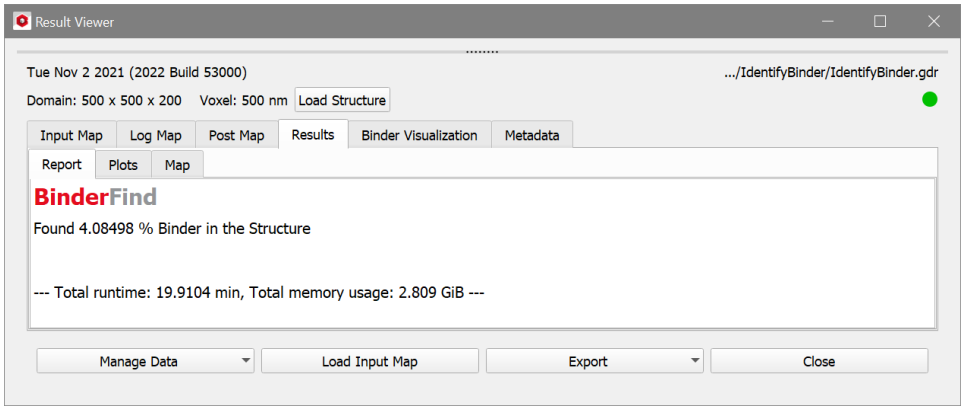


In this case, the number of batches needs to be reduced. Note that for CPU-based computation, the choice of batch size is not critical and can be left at the default.

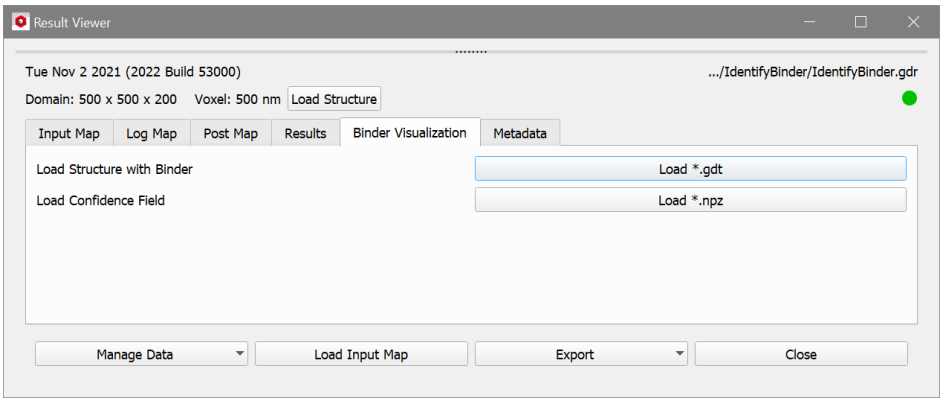
The default setting in GrainFind-Identify Binder for the **Batch Size** is 2, and it is recommended to keep this setting.

RESULTS

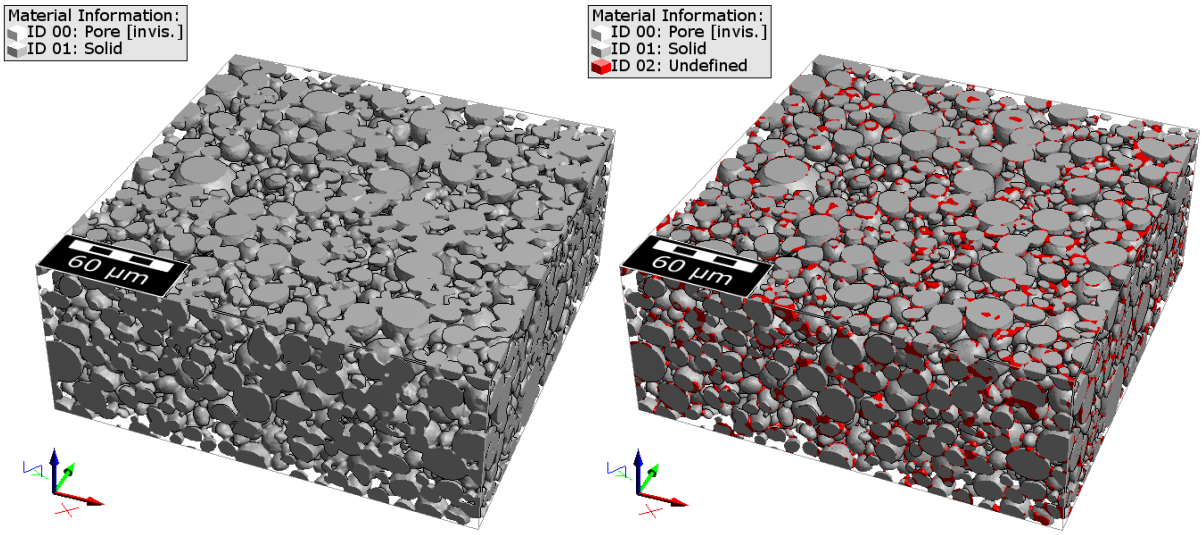
After the successful binder identification, the GeoDict Result Viewer opens for the result file (.gdr). Under the **Results - Report** tab, the percentage of solid voxels identified as binder is shown.



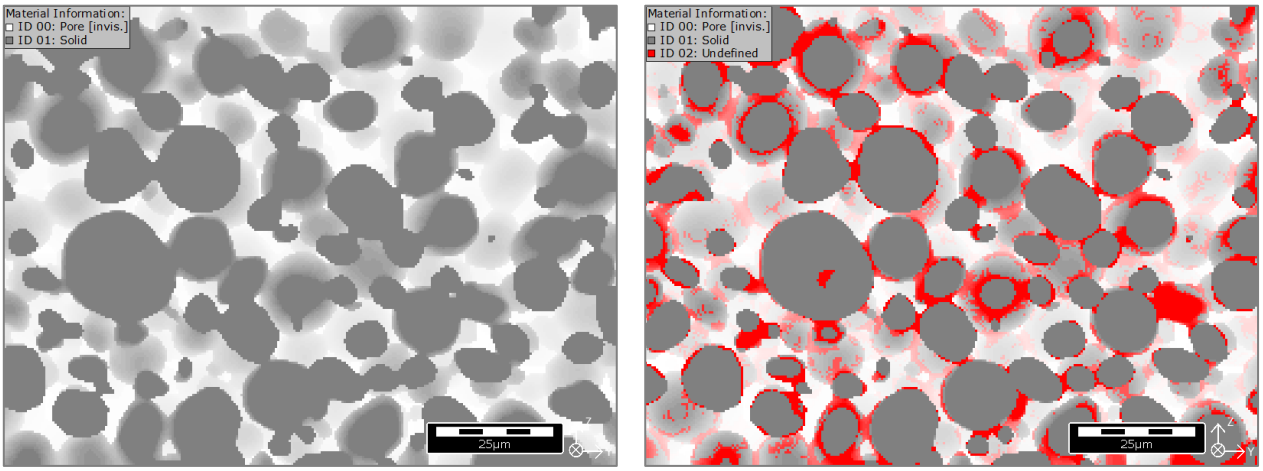
To load the structure with identified binder, by clicking **Load *.gdt** under the **Binder Visualization** tab.



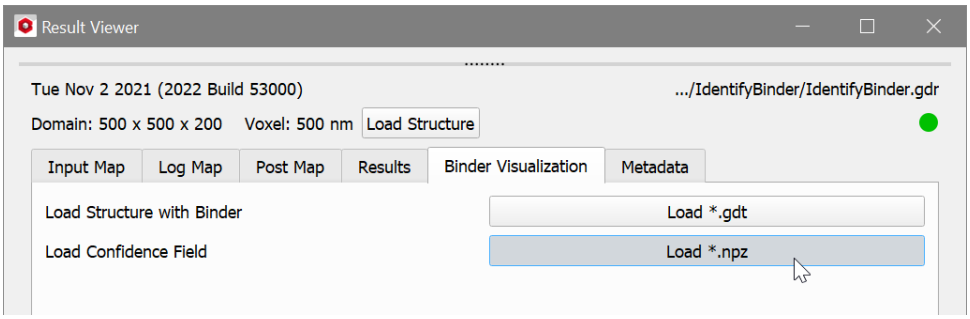
In the 3D visualization, the distribution of binder between the grains is visible for the whole domain.



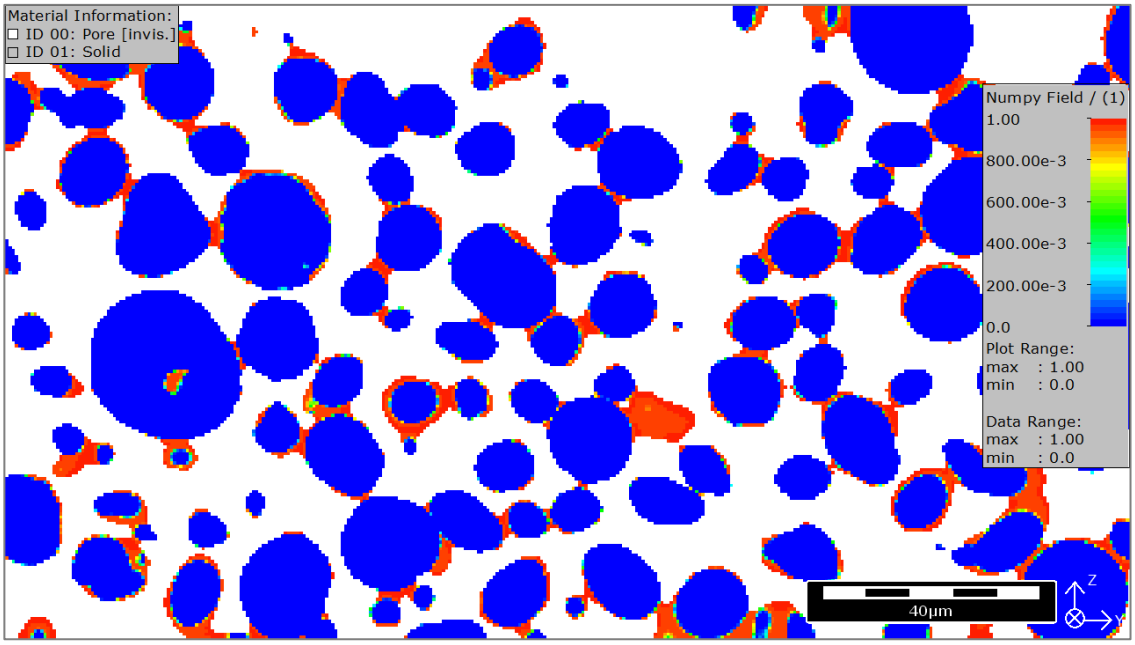
The 2D view is useful to evaluate the result of the binder identification, as seen in the example below (left: without binder identification, right: with binder identification).



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



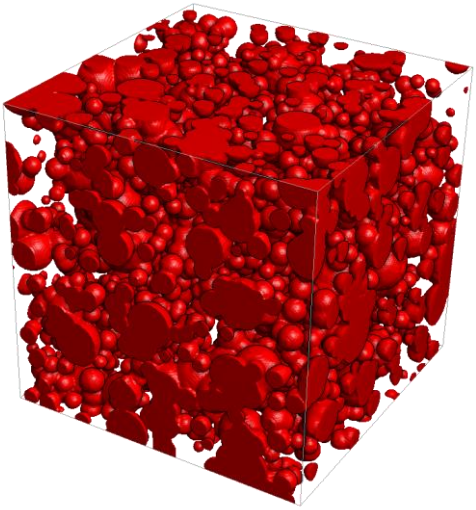
The confidence field contains the probability for each voxel to be binder. In the figure below, it is well visible where the neural network is confident of the choice and where it is uncertain: The dark blue areas are clearly marked as grain, the red areas are clearly marked as binder, and the values 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.

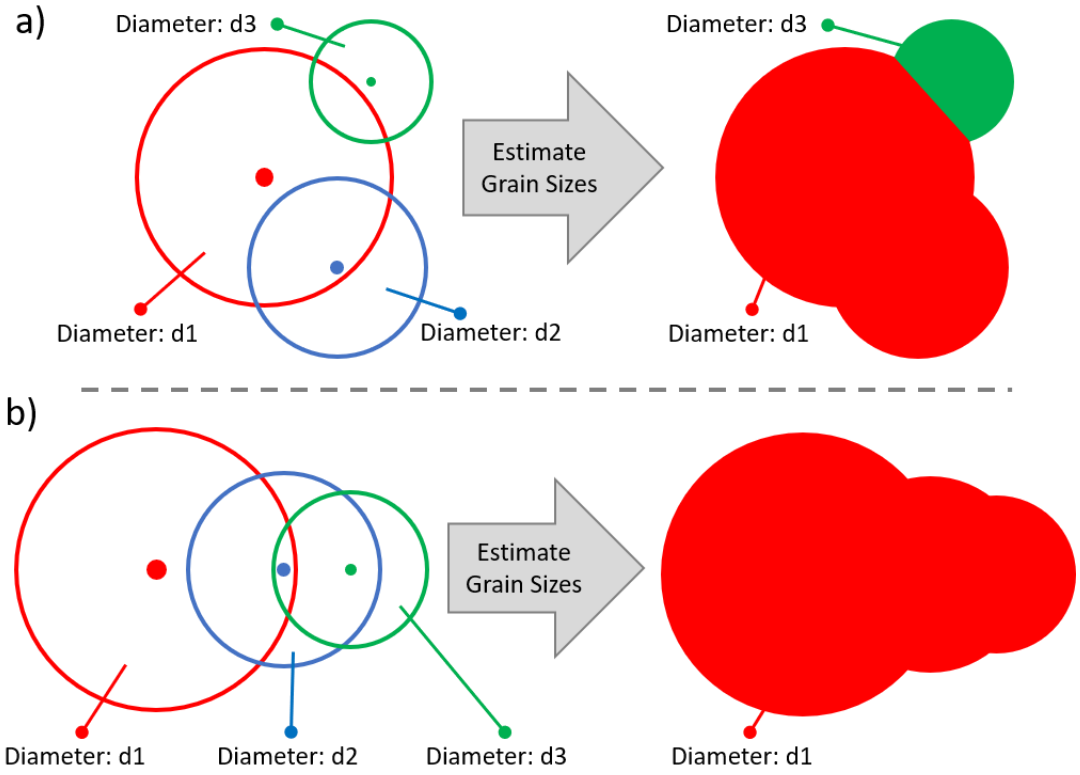
For this part of the User Guide, an example structure created with GrainGeo is used and shown here.



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.

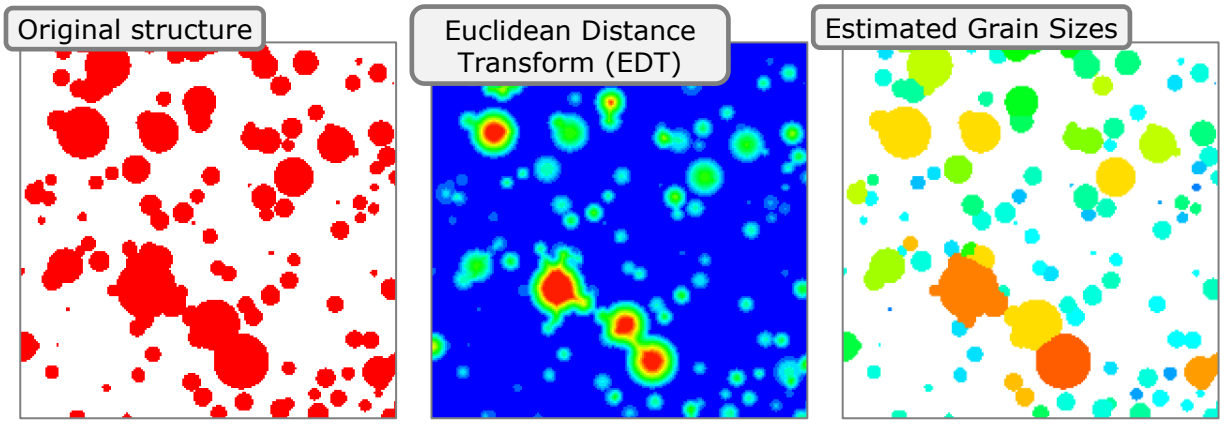
If a voxel is contained in multiple spheres, there are two options:

1. The center of the smaller sphere lays inside the 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 the smaller sphere does not lay inside the 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.

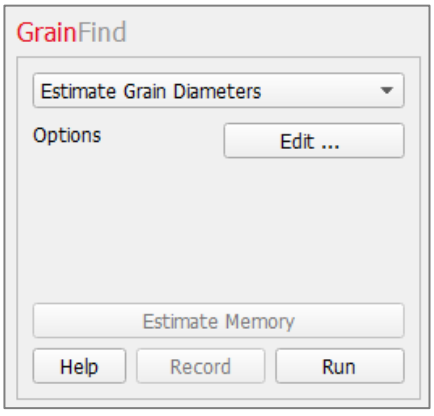
In the figure below, the process of estimating the grain size is illustrated on the example structure shown above. On the left, the original structure (the material which is selected to be analyzed) is shown. In the next step (middle), the EDT (see page *3*) is calculated to find the maximal fitting sphere at every point. On the right, the result of **Estimate Grain Diameters** is displayed.



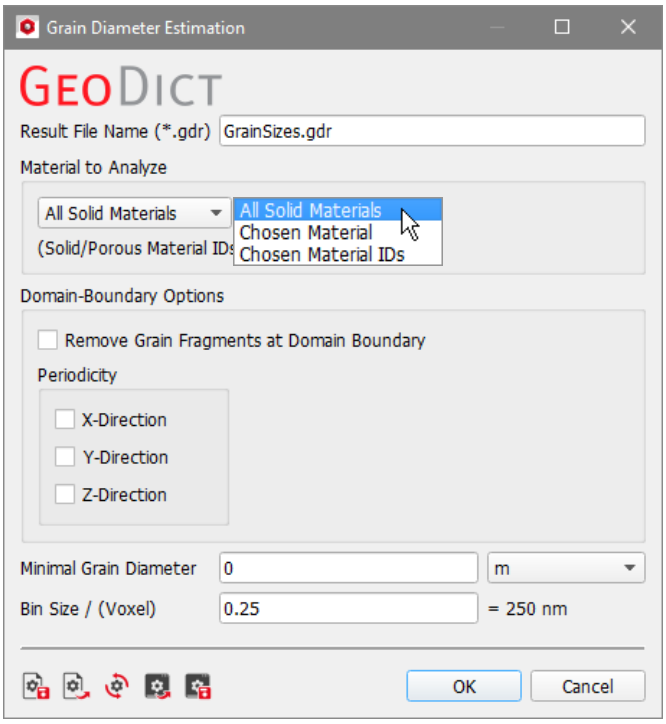
Estimate Grain Diameters

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.

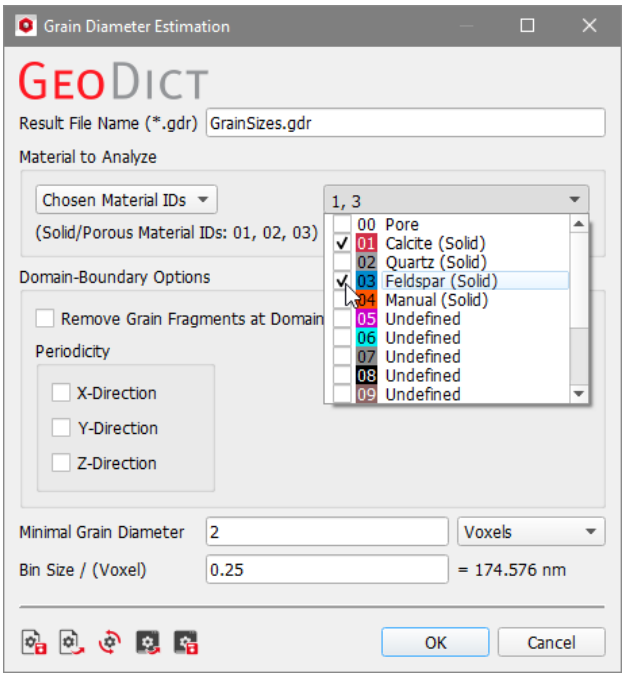


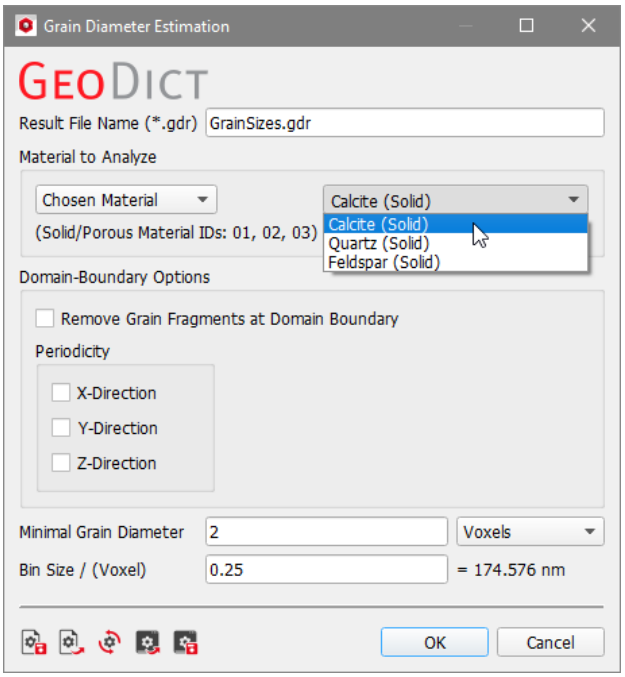
Under **Material to Analyze**, the materials for which the grain size is estimated are chosen.



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.

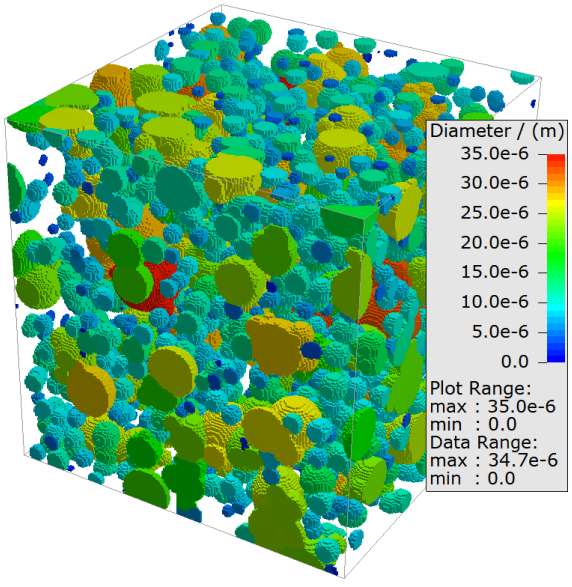


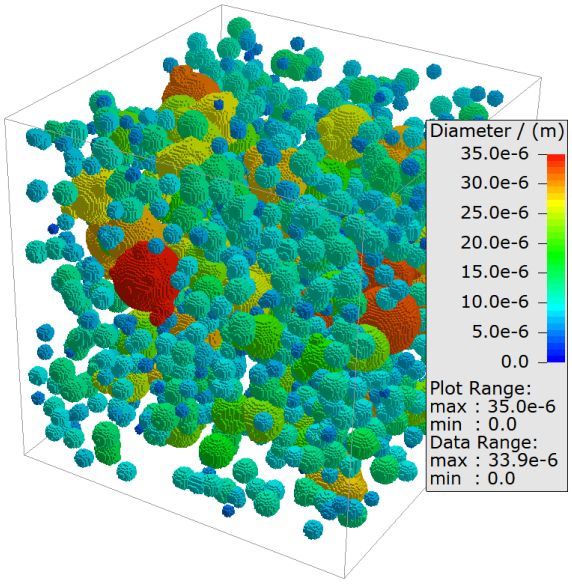


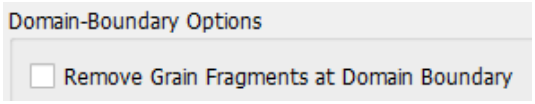
In the Domain-Boundary Options panel, the first option is to **Remove Grain Fragments at Domain Boundary**. A grain fragment in this context is a connected area with the same assigned diameter value.

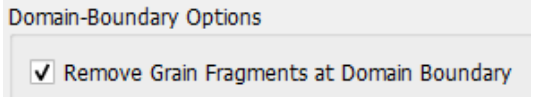
- Grain fragments at the boundary might corrupt the grain diameter estimation, since it cannot be known if the grains at the boundary lie completely in the domain or if they are cut at the domain boundary (compare the images below).
- Nevertheless, removing the boundary grains also influences the diameter 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 Fragments at Domain Boundary** should be used or not.







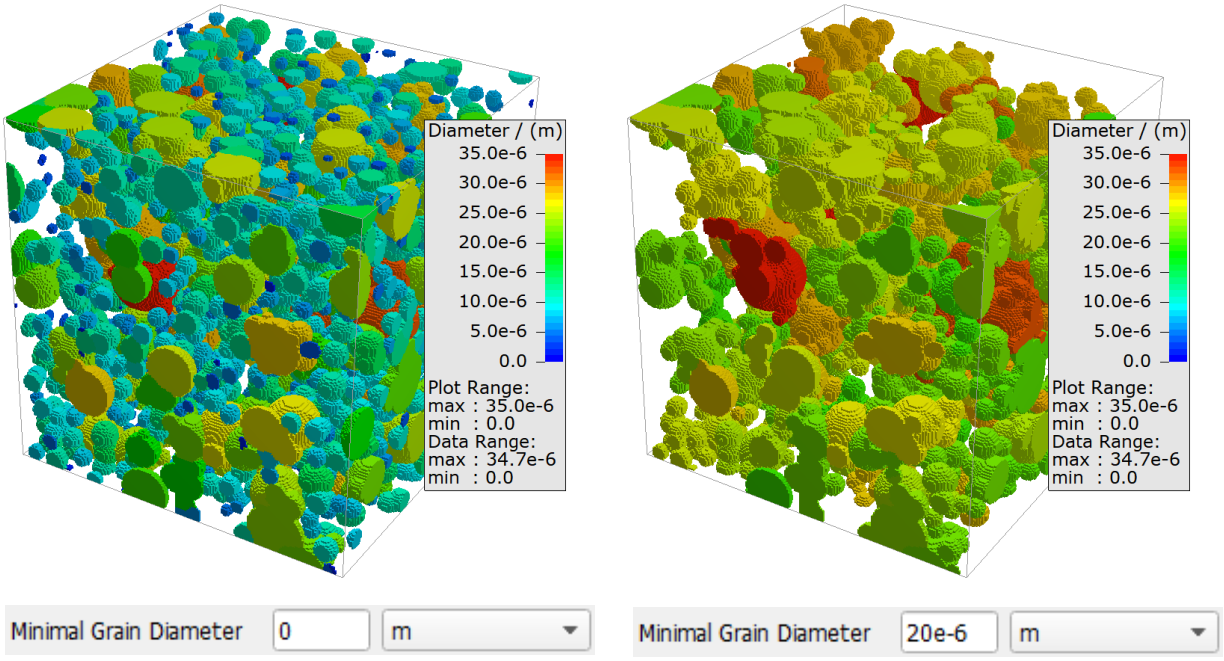


With the **Periodicity** option, the handling of the structure at the domain boundary can be defined. If a direction is chosen, periodic boundary conditions are applied in this direction. Otherwise, symmetric boundary conditions are applied. **Periodicity** should only be chosen if the corresponding 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 valuer 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 (here: green to yellow) are either neglected or merged to larger grain fragments.



Since GeoDict 2020, the units of the **Minimal Grain Diameter** are meters or voxels. The latter is new since GeoDict 2020 and allowed us to set a better built-in default value for the **Minimal Grain Diameter**.

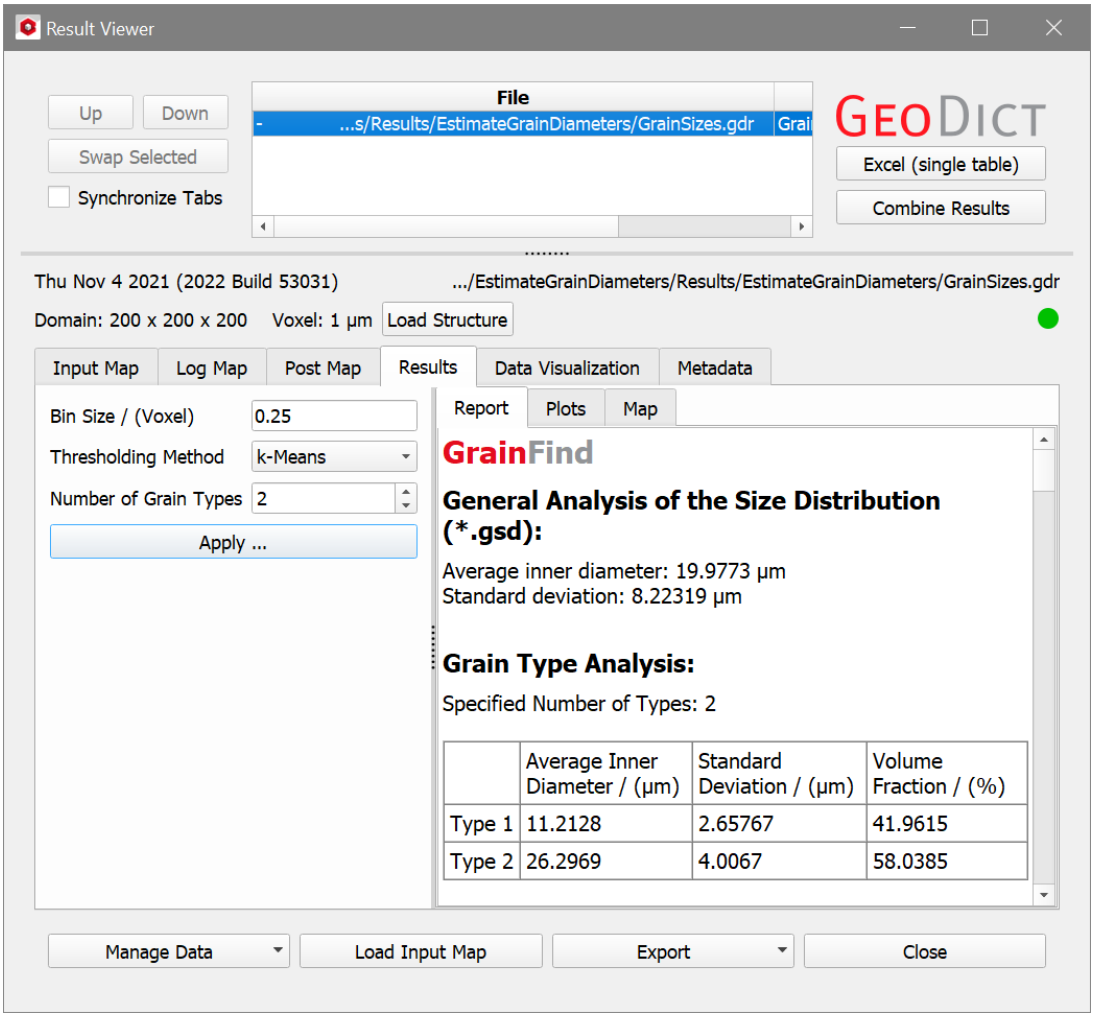
The **Bin Size** is the step size between following sphere diameters, which are fitted in the structure. The choice of the Bin Size is important in post processing. It affects the results in the *.gdr file, e.g. the Inner Grain Diameter Histogram (see page *44*). If it was not chosen as desired, the 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

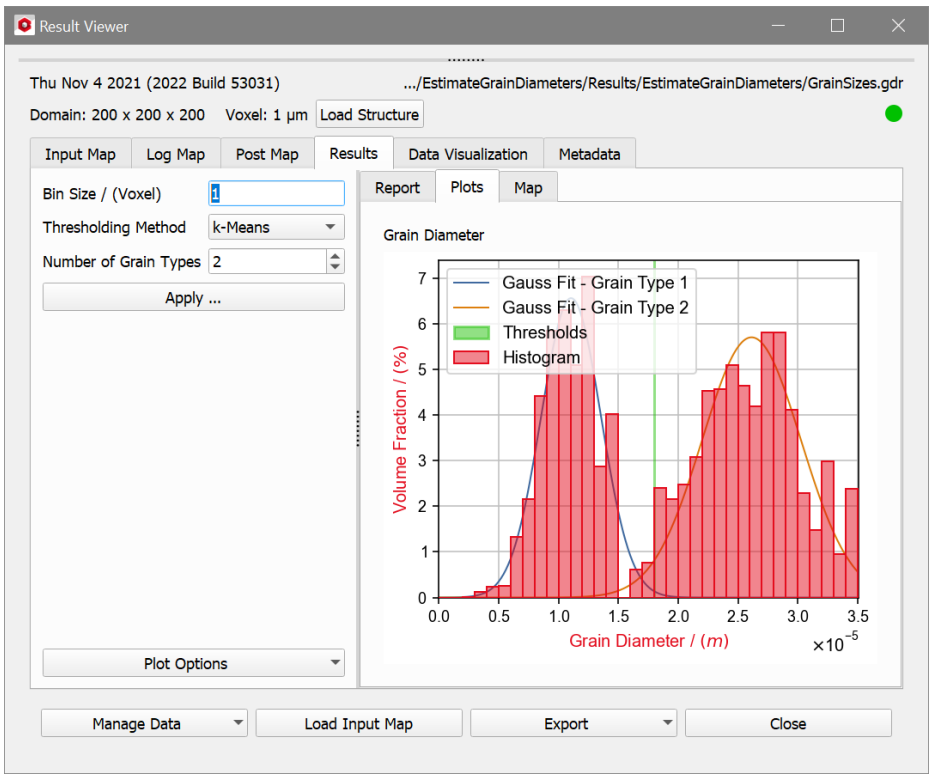
At the end of the estimations of grain diameter, the results are shown in the Result Viewer. Alternatively, they can be loaded at any time by opening the corresponding *.gdr-file in the project folder (File → Open Results (*.gdr)…).

The Result Viewer shows several tabs, but only the **Results** and **Result Visualization** tabs are explained here in detail. The others contain results similar refer to those explained above for **Identify Grains** (page 17).

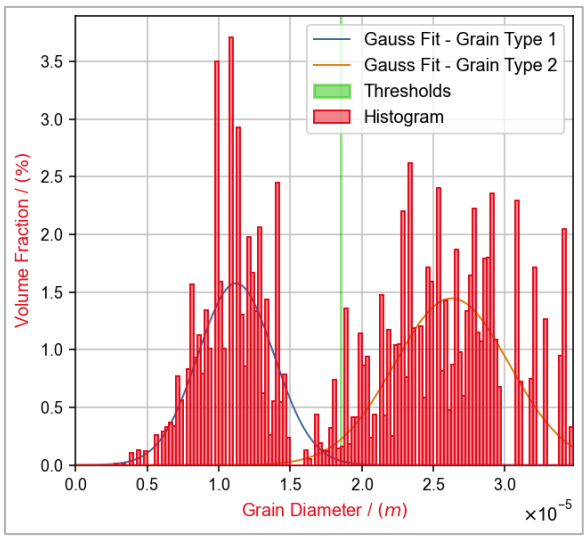
The **Results** tab contains the **Report**, **Plots** and **Map** subtabs, which are strongly interconnected. The **Report** subtab shows the results from the grain type analysis and a table with the bins for the histogram. The **Plots** subtab shows a histogram of the estimated grain diameters. The **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.

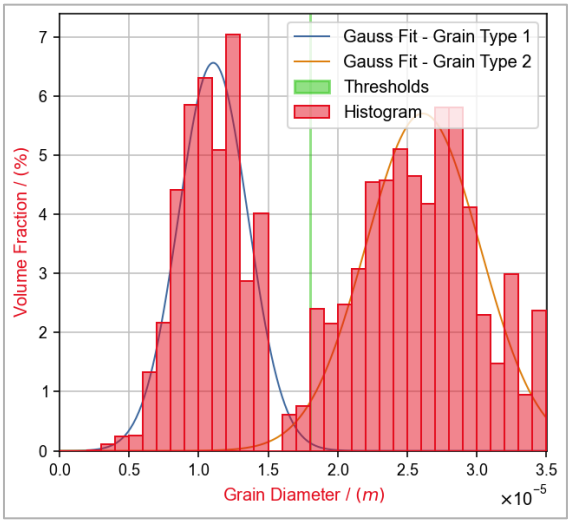


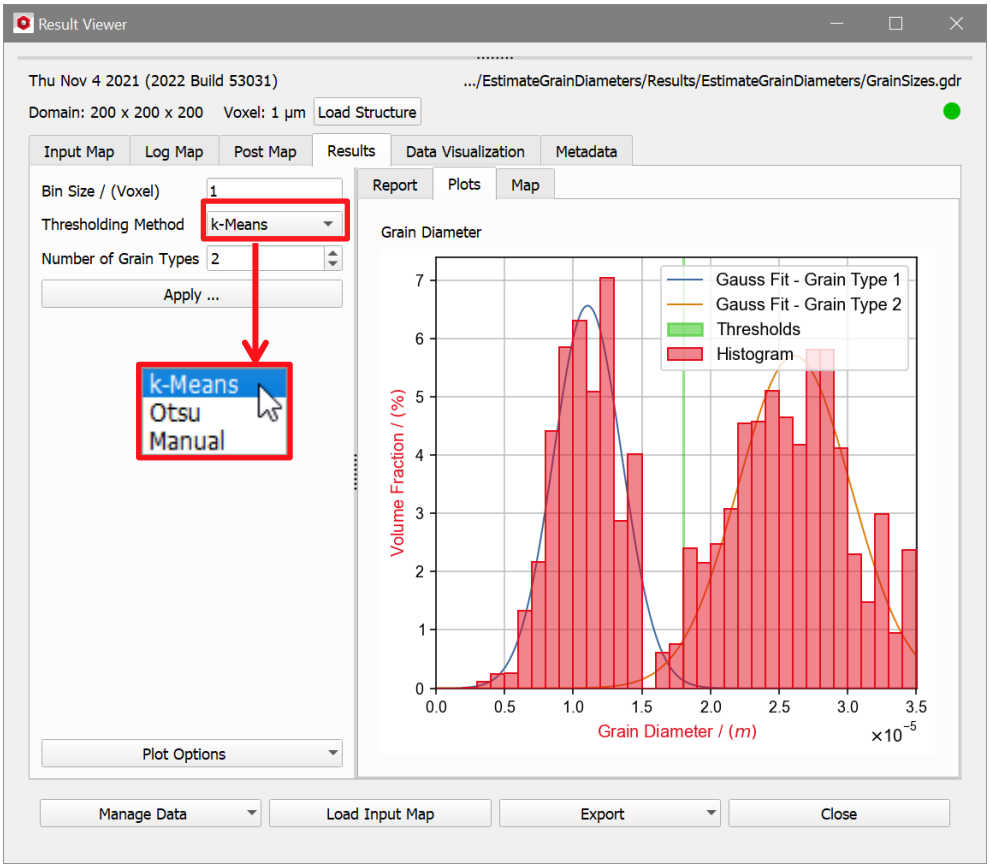
The three subtabs share the (collapsible and expandable) settings panel on the left, where the **Bin Size**, the **Thresholding Method**, and the **Number of Grain Types** can be chosen. Changing a value and clicking **Apply** immediately changes the results in the **Map** subtab, and therefore the tables in the **Report** subtab and the histogram in the **Plots** subtab.



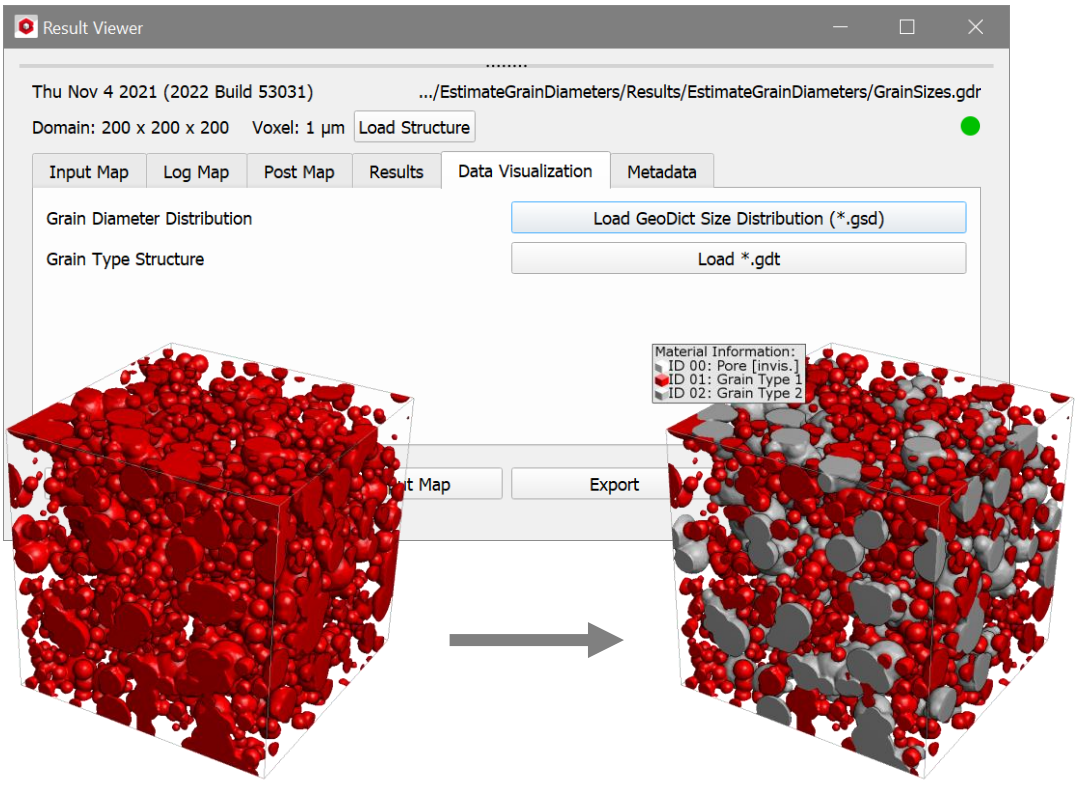
Changing the **Bin Size** mainly effects the resolution of the histogram in the **Plots** tab. A too large **Bin Size** leads to a "blocky" histogram, while a too small **Bin Size** leads to a volatile and noisy histogram. The **Bin Size** should be chosen so that the histogram is smooth and detailed. The effect of the Bin Size on the histogram is illustrated in the three images below.





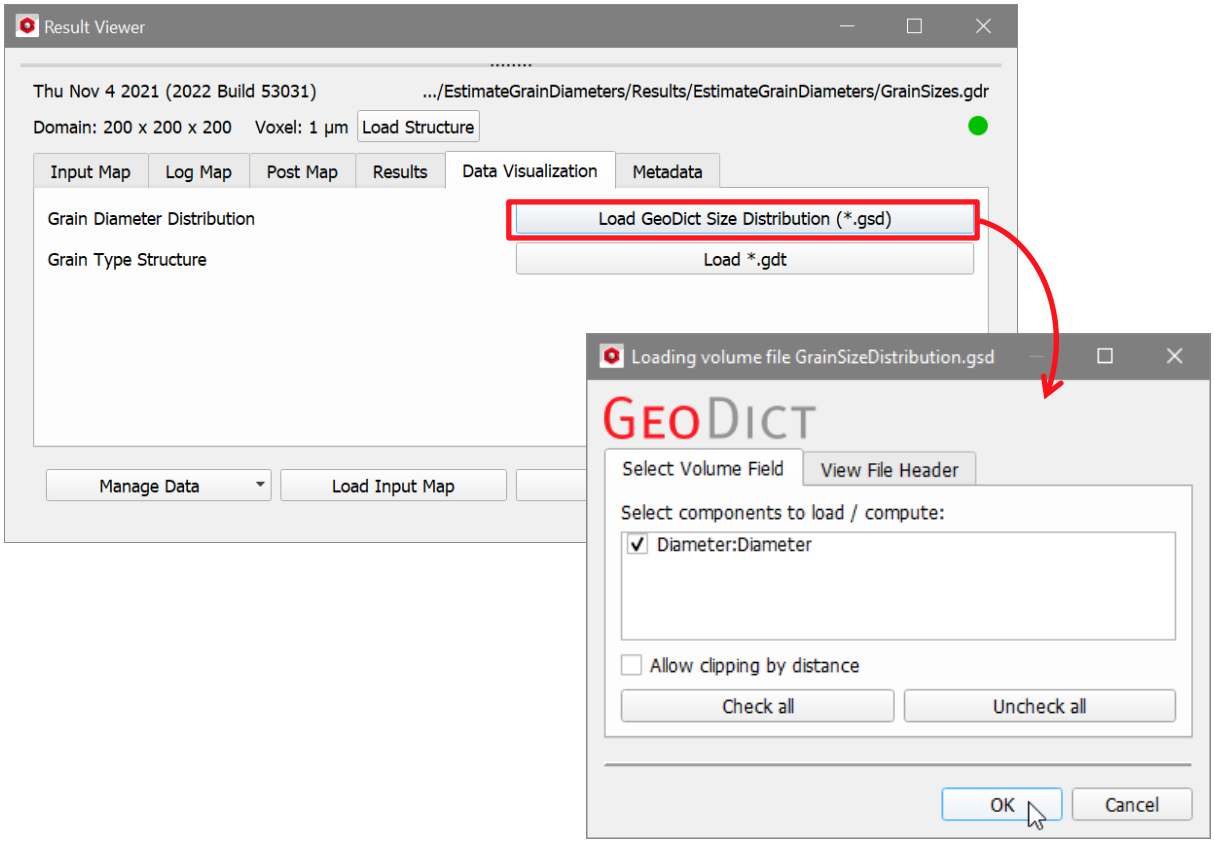


If the **Number of Grain Types** is 2 or higher, the estimated grain diameters are assigned to different diameter classes based on the selected **Thresholding Method**., The **K-Means** method, **Otsu**'s method, and a **Manual** input are available as thresholding methods. Based on these diameter classes, the structure can be segmented by clicking **Grain Type Structure** → **Load *.gdt** in the **Result Visualization** tab, as seen below.

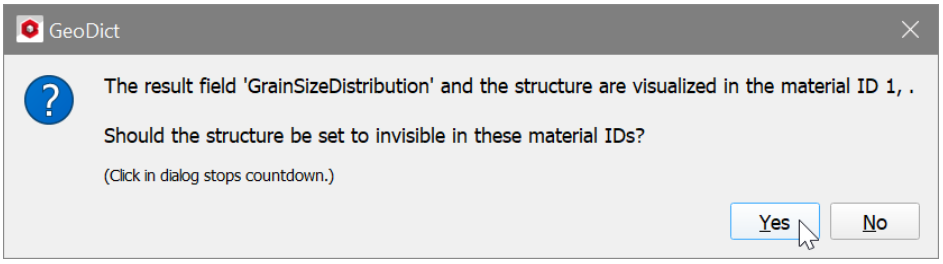


Under the **Result Visualization** tab, the **Grain Diameter Distribution** and the **Grain Type Structure** can be loaded (as explained above). Load the **Grain Diameter Distribution** to visualize and examine in detail the estimated grain diameters in the Visualization area of the GeoDict GUI.

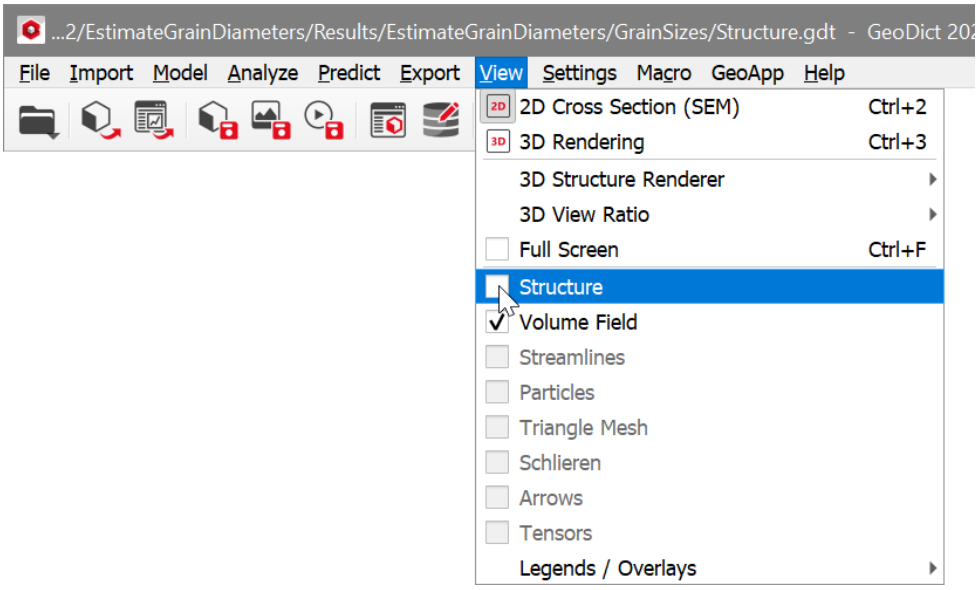
The workflow is as follows: To create images similar to those used for the illustration of the **Domain-Boundary Options** and for the **Minimal Grain Diameter** (see page *41*), open the results file and click **Result Visualization** → **Load GeoDict Size Distribution** (*.gsd). Click **OK** in the pop-up window.



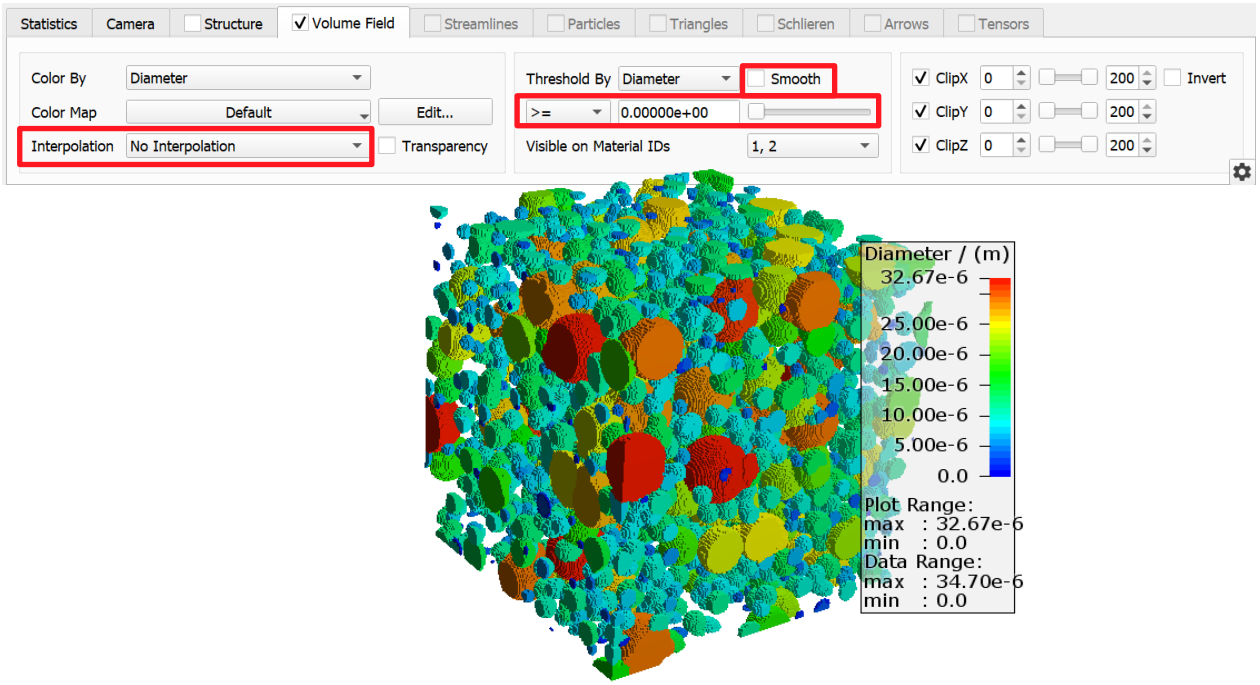
The structure is shown in the Visualization area of the GeoDict GUI with the default visualization settings and a message appears indicating that the visibility of the structure will be turned off (unless the user clicks No). Click **Yes**.



The visualization of the structure can also be turned off by unchecking **View** → **Structure** in the menu bar.



Next, in the Visualization panel, above the Visualization area, 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 **>=**.



https://doi.org/10.30423/userguide.geodict2022-grainfind

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