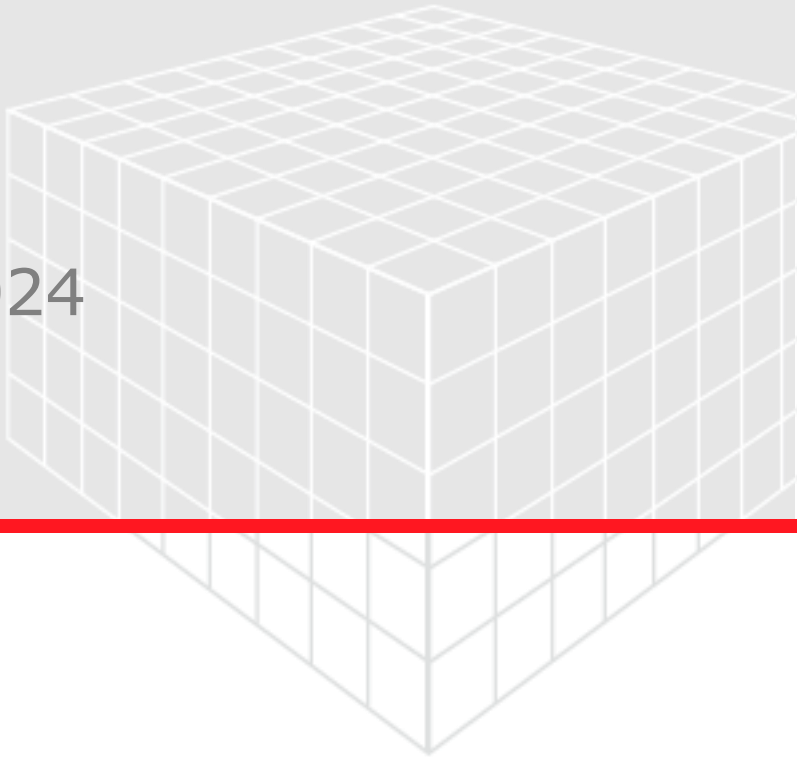
MatDict



User Guide

GeoDict release 2024

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GeoDict

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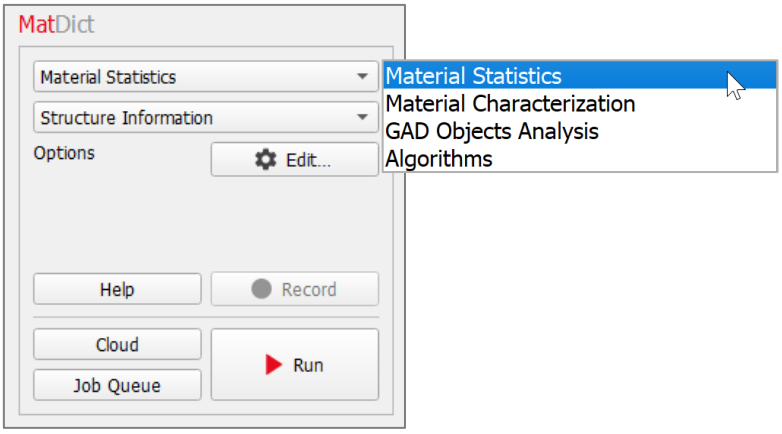
ANALYSIS OF SOLID MATERIAL IN POROUS MEDIA WITH MATDICT

For three-dimensional models of porous media obtained from a tomography image or from a digital model generated with GeoDict, the MatDict module analyzes the characteristics of materials. There is no fixed assignment of a material ID (identification) to solid or pore space. Instead, it depends on the definitions made for the constituent materials.



MatDict's commands are grouped by four topics: Material Statistics, Material Characterization, GAD Objects Analysis and Algorithms.

MATERIAL STATISTICS

- **Structure Information**: The algorithms determine porosity, solid volume fraction, number of GAD objects, density, mass and grammage in all three spatial directions. Values represent average values for the entire material(s) inside the bounding box. Additionally, the individual solid volume fraction of all materials is given as well.
- **Thickness Estimation (1D Statistics)**: The methods determine the solid volume fraction (SVF) of the material in the different spatial directions and measures the material thickness. The SVF is computed in the plane normal to the direction of interest and the average value for each of those planes is reported.
- **2D Density Map**: The algorithms calculate the distribution of grammage, solid volume fraction, and number of objects in the direction of interest. Each pixel in the density map is calculated by averaging the respective property in the direction of interest.
- **3D Inhomogeneity**: The algorithms compute the solid volume fraction, solid density (distribution) and porosity of specified sub-volumes.

MATERIAL CHARACTERIZATION

- The **Solid Size Distribution (Granulometry)** is determined by fitting spheres into the solid objects. To be more precise, a point belongs to a solid object of a diameter larger or equal than *d*, if it is inside any sphere of diameter *d*, which can be fitted into the solid objects.

- For the **Percolation Paths** calculation, the method determines the maximal diameters of spherical particles that can move through the medium. In addition, the shortest paths of the largest particles are calculated and displayed. Also, the shortest path of a given sphere size through the medium may be computed.
- **Connected Components**: The solid fraction of a porous medium is not necessarily a homogeneous medium but can be composed of individual components that (all together) form the solid. Neighborhood relations between voxels inside a component differ from those among different components and between component and pore. The method analyzes the voxel-to-voxel relations of the solid material and computes the components that build up the solid fraction. Results of the method include the number of defined components (material and background), mean number of components per 2D slice in each spatial direction, and their size with respect to volume visualized as a histogram.
- **Estimate Surface Area**: The algorithm calculates an approximation of the surface area by statistical methods and not simply by adding up the voxel surfaces. Therefore, the surface of a sphere is approximated correctly. However, the estimation is slightly biased in case of highly anisotropic media. The method originates from statistical image analysis, where the determination of the four Minkowski measures (Volume, Surface Area, Integral of mean curvature, Integral of total curvature) from voxelized images is an essential task. To determine the surface area, the Crofton formula is used, which relates at first the 3D surface area to an integral over 2D boundary lengths of planar cross sections and then second these lengths to an integral over 1D rays. Based on this formula, an analysis of the intersection points of rays in all space directions with the structure allows determining the surface area.
- **Estimate Three-Phase Contact Line**: The algorithm estimates the length of the contact line between the phases in a three-phase system and the number of voxel edges of the contact line in the Cartesian directions. The length of the contact line, which strongly depends on the structure's topology, is often important for the performance of a material (for example for catalysts).
- The four **Minkowski Parameters** (Volume, Surface Area, Integral of mean curvature, Integral of total curvature) are the structures characterizing parameters to analyze mathematical topology and can be computed for a selected Material ID. These parameters can be used e.g. for image processing, estimating root lengths or hysteresis.
- A **Chord Length Distribution** (CLD) is the distribution of the length of a typical chord of a structure. By being characteristic for any given geometry class, it is a highly precise and sensitive measure to compare the geometries of porous media. The calculation of CLD is particularly useful in 2D tomographic cross-sections, for which the pore size distribution cannot be determined by granulometry or by porosimetry. See the PoroDict handbook for further information about granulometry or porosimetry.
- The **Geodesic Tortuosity** command computes the tortuosity of paths crossing the material, either through pore space or through solid materials. For every voxel on the outflow plane, the algorithm finds the shortest path through the selected material.
- The **2-Point Correlation** computes the probability for two voxels having a certain distance to be similar or equal. For each distance, several voxels are compared if they belong to the same type and a probability is computed based on this information. If two voxels are correlated, the probability is 1, if they are not correlated, for example in a completely random structure, the probability is 0. Then an average probability for each distance is given as result.

GAD Objects Analysis

- **Analyze Objects**. The algorithms analyze GeoDict Analytic Data (GAD) for the total number of GAD objects, number of overlap objects (i.e. the overlaps between different objects), number of objects, overlap solid volume percentage, total number of contacts, mean coordination number, and the individual volume of each component. It provides histograms for object volume and contact area.
- The **GAD Objects Orientation** analysis provides the direction tensor and anisotropy for individual classes of GAD objects.

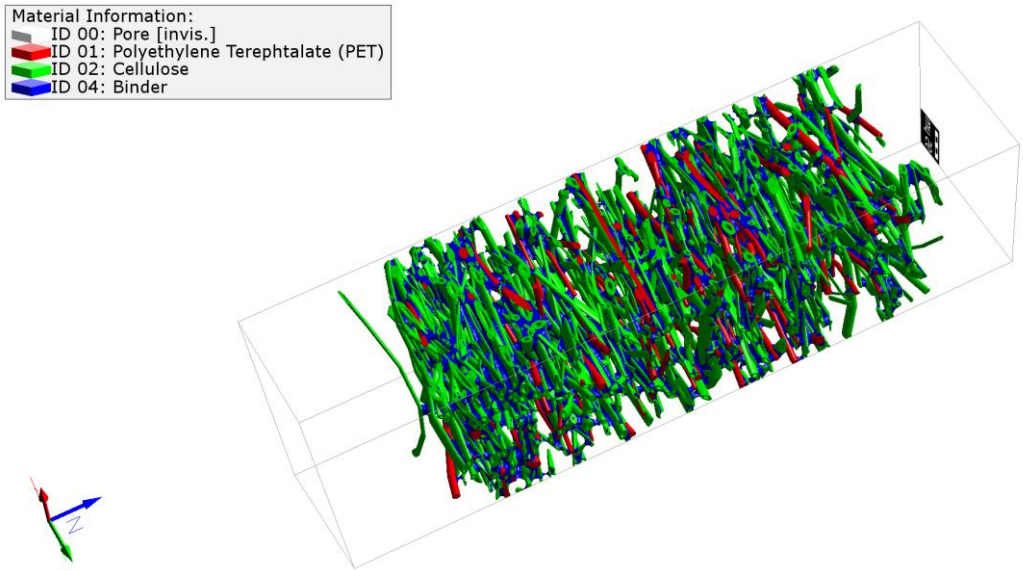
Algorithms

- In the **Euclidean Distance Transform** (EDT), the algorithm calculates the distance from any point (voxel) inside a pore to the nearest pore/solid boundary. This is useful when characterizing the structure's pore morphology.
- The **Skeletonizer** reduces any given structure to its center lines.

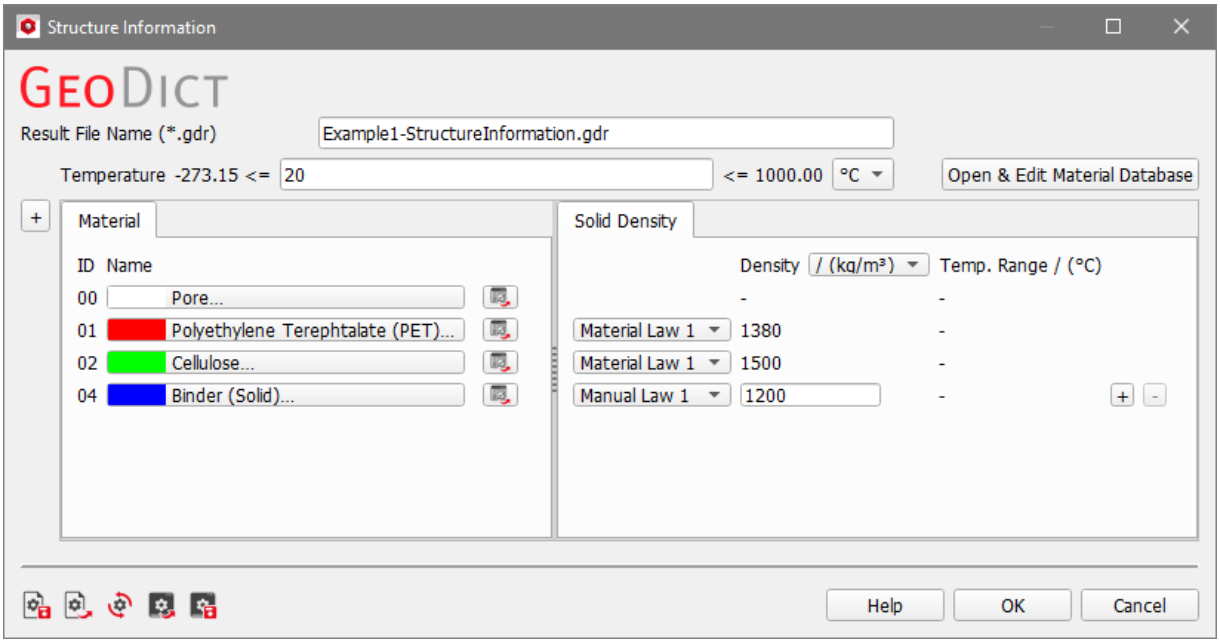
MATERIAL STATISTICS

STRUCTURE INFORMATION

The **Structure Information** command determines porosity, solid volume fraction (SVF), density, mass, and grammage in all three spatial directions for the volume inside the bounding box. For these calculations, the algorithm requires the density of all solid materials as input data.



After selecting **Structure Information** from the pull-down menu and clicking the **Options' Edit...** button, the **Structure Information** dialog opens.



At the top of the dialog, replace the default **Result File Name** by a name according to your current project. The result files are saved in the chosen project folder (**File** → **Choose Project Folder** in the menu bar).

Underneath, the **Material** panel contains the material IDs of the constituent materials present in the current structure, and the **Solid Density** tab contains the density information for each of the present material IDs.

By default, material IDs that are not present in the structure are not displayed under the **Material** tab, but they can be displayed by clicking on the "+" symbol to the left of the **Material** tab.

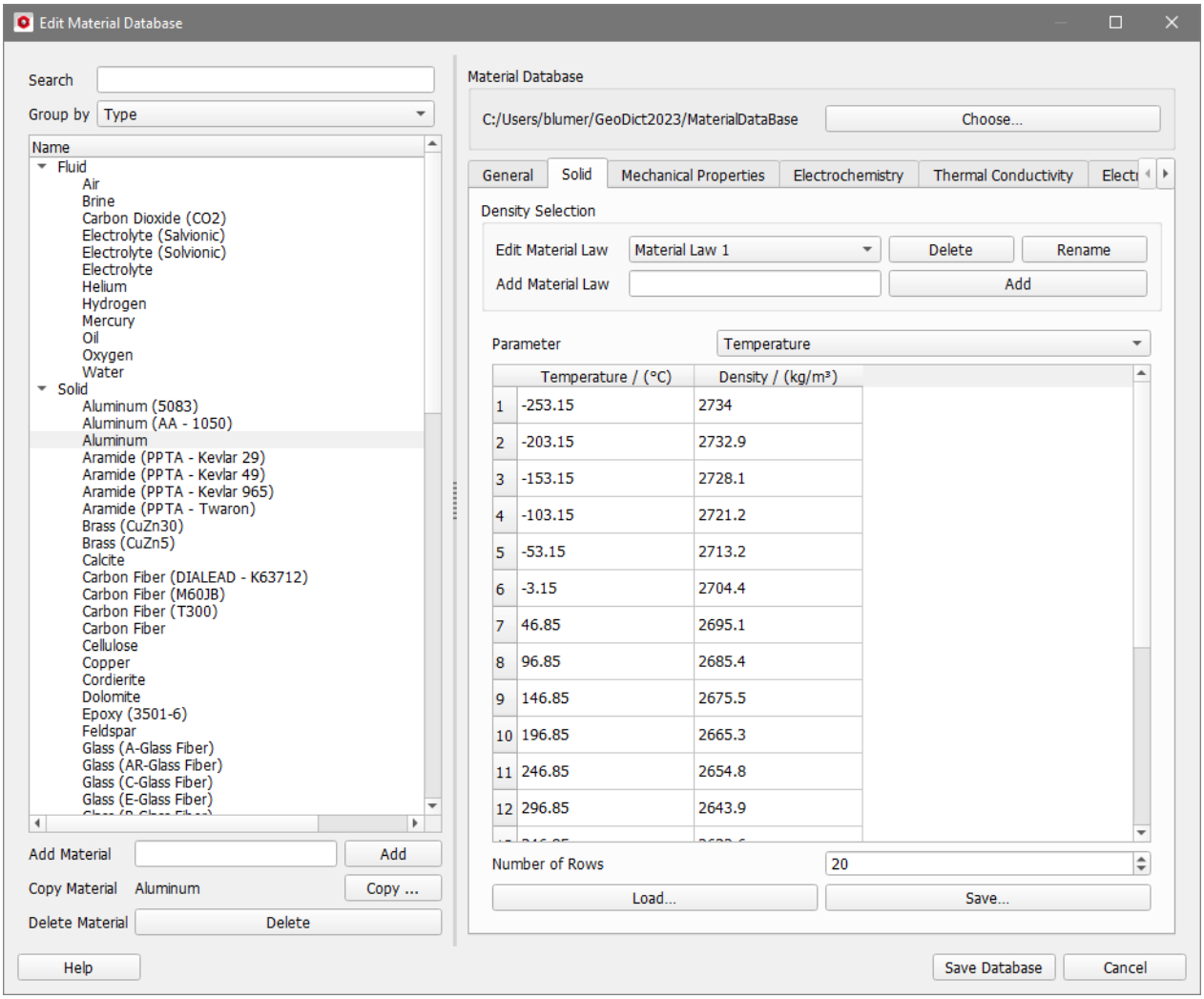
For materials that are defined in GeoDict's Material Database, the density of the material is directly inserted under the **Solid Density** tab for that material ID. If multiple Material Laws are defined the desired one can be selected or a new one can be added by clicking on the name and then **Open & Edit Material Database**.

If a material is not present in the GeoDict Material Database, it can be added in the Material Database and its properties are defined there. Alternatively, a material can be set to **Manual**, and its density can be entered under the **Solid Density** tab. Manual Laws are Material Laws for manual materials and can be added or deleted by clicking the "+" or "-" button in the right column of the manual material. The corresponding values can be directly entered.

The density of the solid materials can be given in kg/m^3 or g/cm^3 for all materials.

The given **Temperature** value and the **Temp. Range** are only of importance if the solid density is defined as a temperature-dependent quantity in the GeoDict Material Database. For example, if Aluminum would be chosen as material, the solid density would be temperature dependent.

More information on materials can be found in the Material Database handbook.

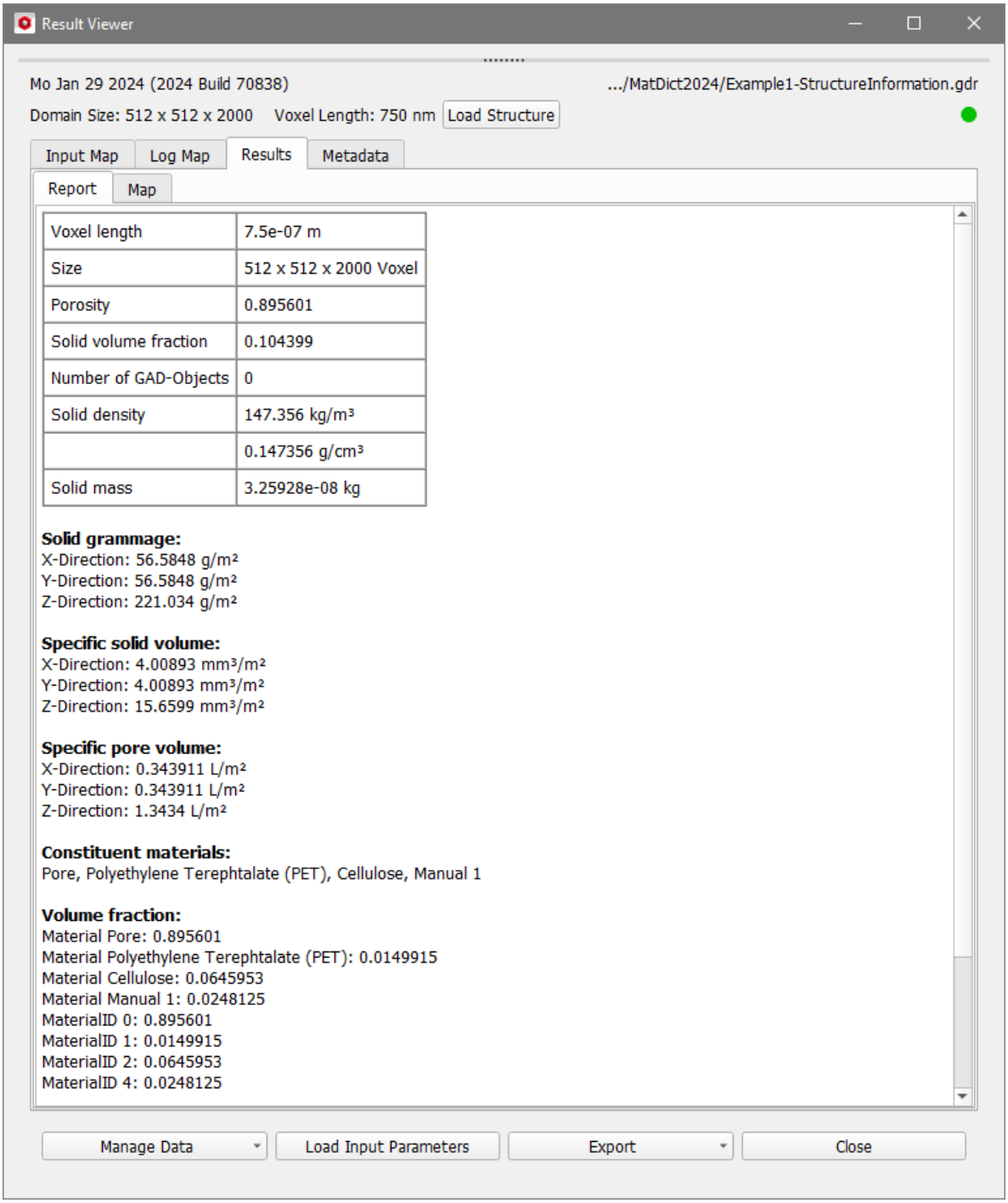


In the above example, the densities of the PET and cellulose fibers are not set to be temperature dependent.

RESULTS

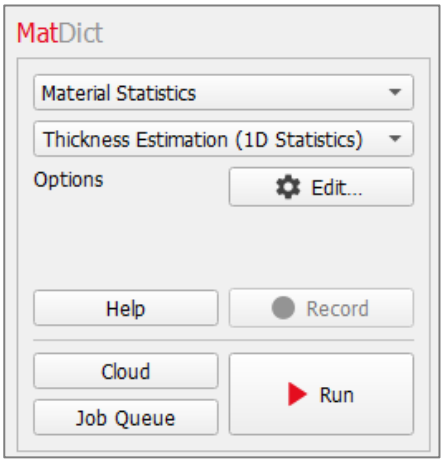
Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is opened in the **Result Viewer** after the computation is finished.

Be aware, that the reported **Solid Grammage** values are only meaningful if the whole thickness of the media is included in the domain. In the example on page 4, this is only true for the value in Z-direction.



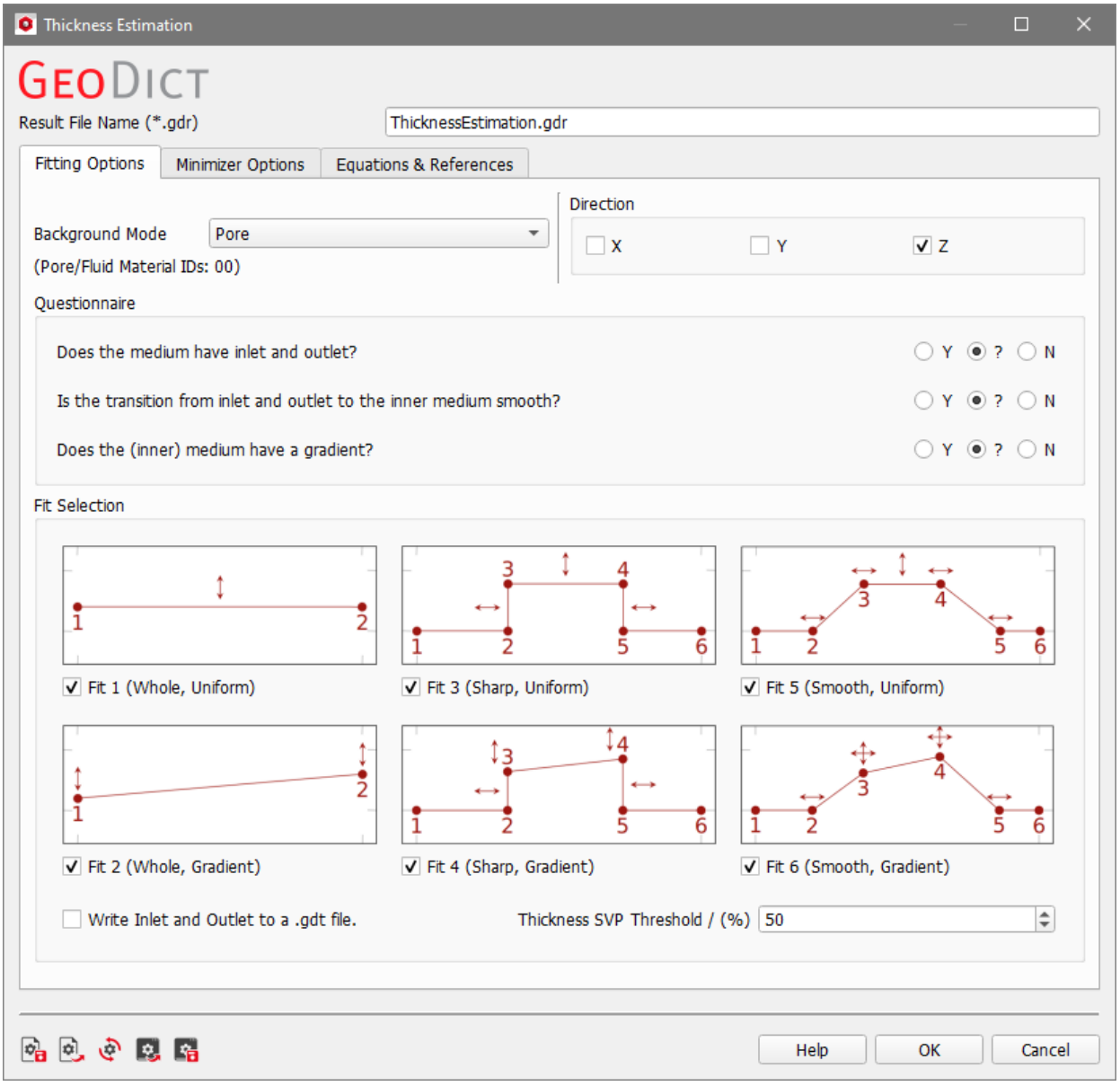
Thickness Estimation (1D Statistics)

The **Thickness Estimation** (called **1D Statistics** up to GeoDict 2023) command calculates the **solid volume percentage** (**SVP**) for each voxel layer perpendicular to the given direction ("through direction").



The user can select various types of fitting functions, Fit 1 to Fit 6, consisting of piecewise linear segments that best describe the type of porous media. For each selected fitting type, GeoDict solves an optimization problem to identify the best-fitting function. The thickness of the solid medium, of the inlet/outlet, and of the medium's surfaces is then derived from this function. Furthermore, the SVP of these regions is computed.

After clicking the **Edit...** button in the **Options** section, the **Thickness Estimation** dialog opens.



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

The parameters are organized into the **Fitting Options** and **Minimizer Options** tabs. The **Equations & References** tab, provides further information about the underlying algorithm.

In the **Background Mode** pull-down menu, choose **Pore** to assign the material ID corresponding to pore space ("background") and exclude it from the calculations. Alternatively, choose **GivenID** to assign one or multiple material IDs to the pore space (only for the calculations within **Thickness Estimation**) and select the material IDs from the **Background MaterialID** pull-down menu.

In the **Direction** panel, one or more through directions for the thickness estimation can be chosen from the three principal directions.

In the **Fit Selection** panel, one or multiple fitting types (Fit 1 to Fit 6) can be selected. In the **Result Viewer**, the selection can be change for post-processing calculations. This feature is particularly useful for comparing results across various fitting types. Additionally, to facilitate an easier selection, users can employ the **Questionnaire**, which automatically chooses fitting types based on the provided responses.

More precisely, a distinction is made between media with a homogeneous density distribution (**"Uniform"**) and media with a density gradient (**"Gradient"**). Furthermore, either the absence (**"Whole"**) or presence of an inlet area and outlet area is considered. In the latter case, these areas can be non-empty, allowing for solids such as fibers to stick out of the medium. The transition between inlet and medium (and medium and outlet) can be approximated either by a sharp transition zone (**"Sharp"**) or by a smooth transition zone, which results in a non-zero surface length (**"Smooth"**).

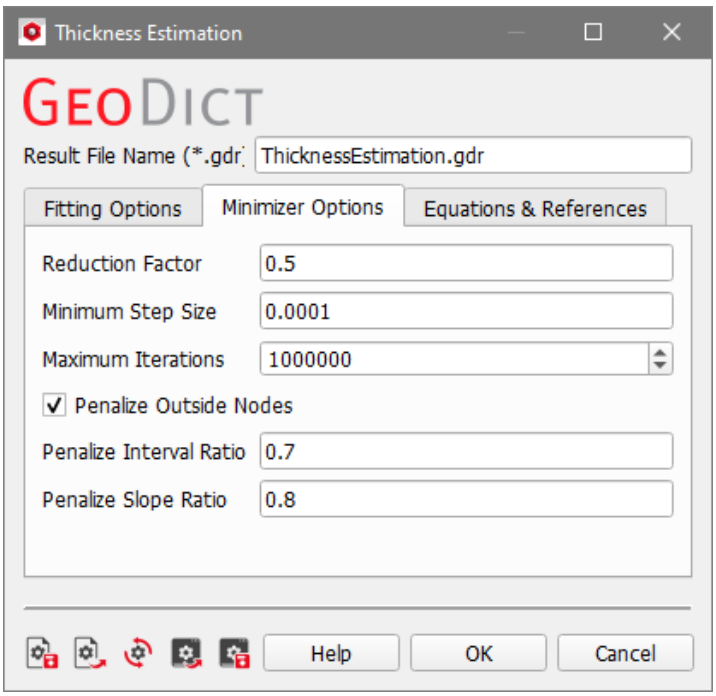
Fits 3 to 6 take an inlet/outlet area into consideration. If **Write Inlet and Outlet to a .gdt-File** is checked, the structure of the detected inlet and outlet is written to a file to a .gdt file in the project folder.

Fits 5 and 6 assume that the medium begins at the center of the inlet area and ends at the center of the outlet area. This definition is modified by adjusting the **Thickness SVP Threshold** value, the technical specifics of which can be found in the tooltip.

The following table gives an overview if and how the fits available in GeoDict 2023 correspond to the new fits in GeoDict 2024.

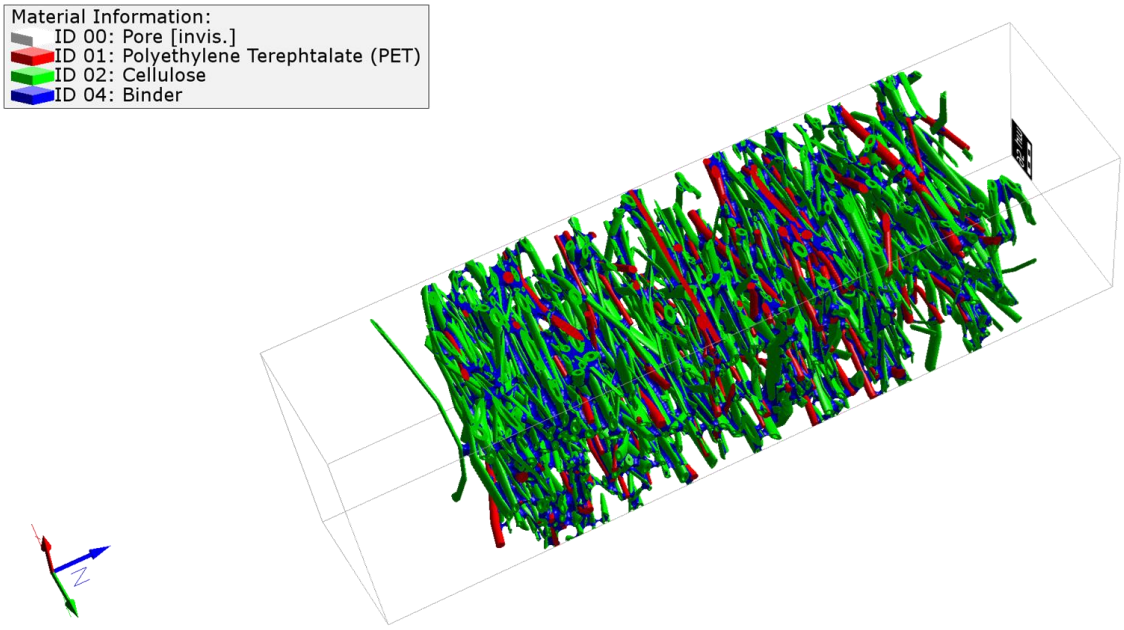
Fit in GeoDict 2023	Fit in GeoDict 2024
Homogeneous media	Fit 1 (Whole, Uniform)
Gradient media	Fit 2 (Whole, Gradient)
-	Fit 3 (Sharp, Uniform)
-	Fit 4 (Sharp, Gradient)
Homogeneous media with non-empty inlet/outlet	Fit 5 (Smooth, Uniform)
Gradient media with non-empty inlet/outlet	Fit 6 (Smooth, Gradient)
Homogeneous media with inlet/outlet	-
Gradient media with inlet/outlet	-

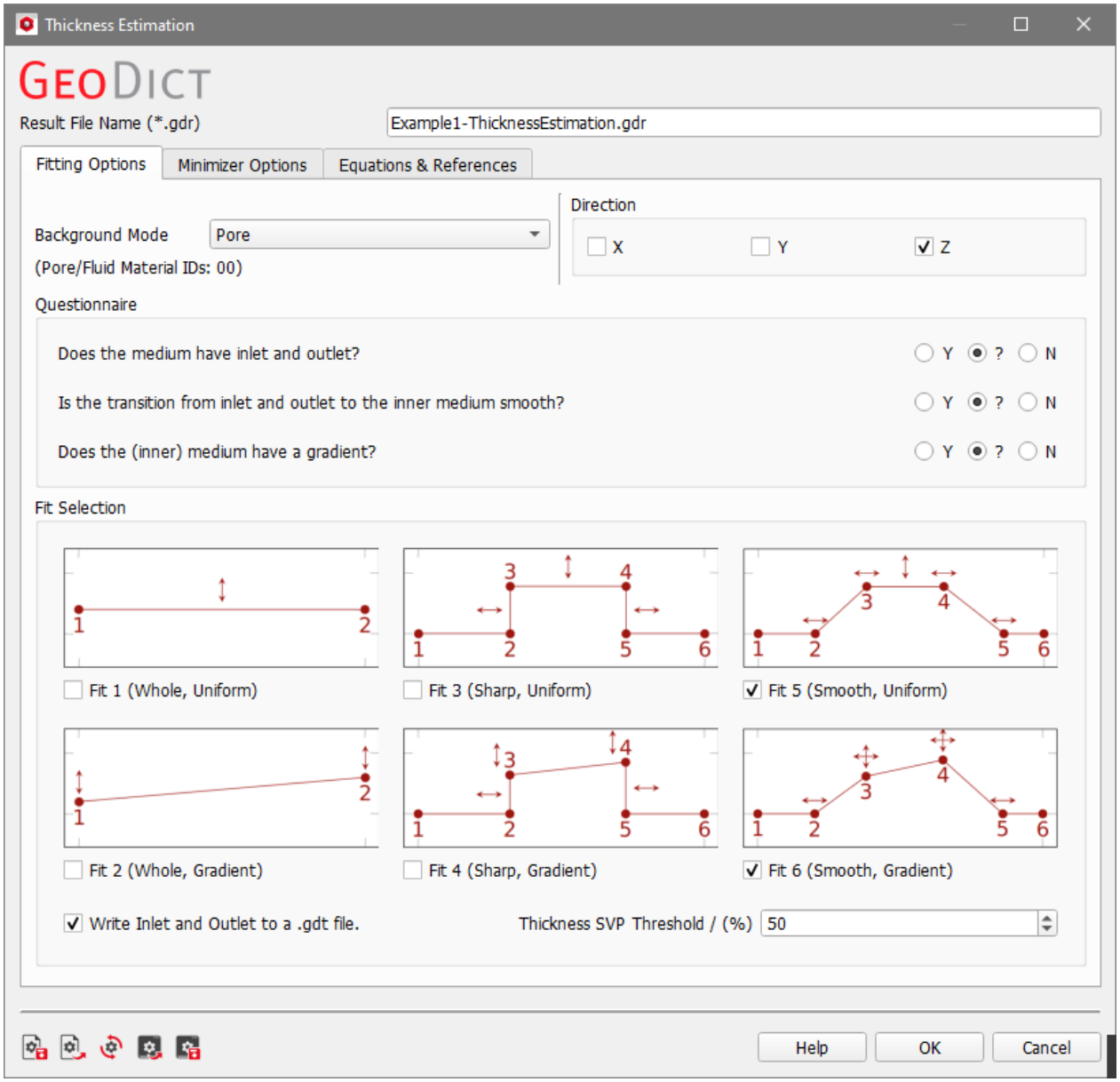
Note that, in GeoDict 2023, the fits for media with inlet/outlet layers with only background material are considered as inlet or outlet. This option is not available anymore in GeoDict 2024, instead you can specify in detail if the transition between media and inlet/outlet is sharp or not.



The minimization method includes several numerical parameters that can be fine-tuned under the **Minimizer Options** tab. Detailed information about these parameters is available in the tooltips and can also be found in the published document (see [1]). These options are intended for experts; the default values are generally suitable for common porous media.

As an example, we analyze a 3D model of a structure with a side length of 1500 µm (1.5 mm) in Z-direction (2000 voxels · voxel length of 0.75 µm/voxel).To analyze the structure, we use the settings shown below. The results are shown in the next section where we explain the content of the result viewer.



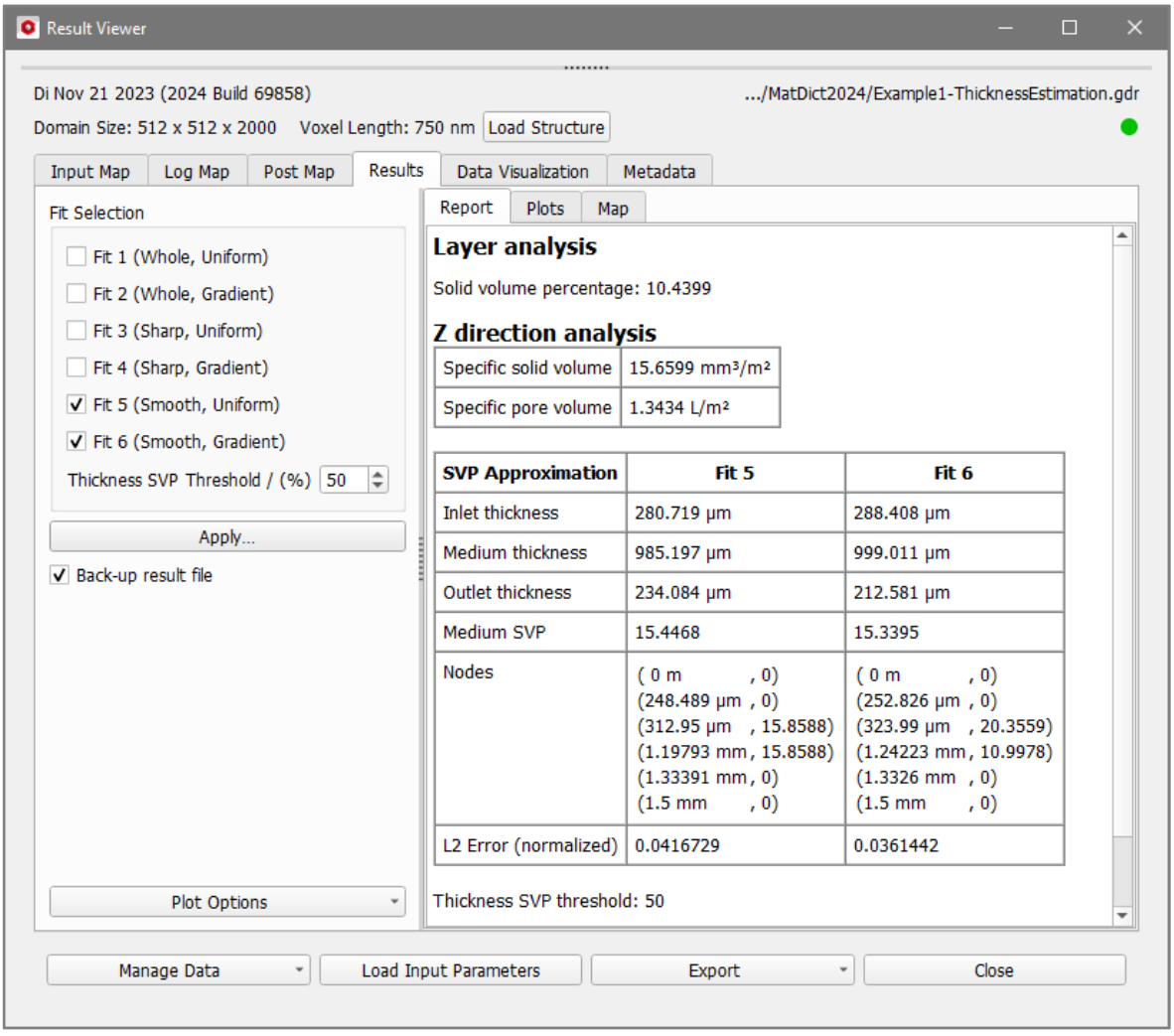

Thickness Estimation
GeoDict
Result File Name (*.gdr)
Example1-ThicknessEstimation.gdr
Fitting Options
Minimizer Options
Equations & References
Background Mode
Pore
(Pore/Fluid Material IDs: 00)
Direction
X
Y
Z
Questionnaire
Does the medium have inlet and outlet?
Y ? N
Is the transition from inlet and outlet to the inner medium smooth?
Y ? N
Does the (inner) medium have a gradient?
Y ? N
Fit Selection
Fit 1 (Whole, Uniform)
Fit 3 (Sharp, Uniform)
Fit 5 (Smooth, Uniform)
Fit 2 (Whole, Gradient)
Fit 4 (Sharp, Gradient)
Fit 6 (Smooth, Gradient)
Write Inlet and Outlet to a .gdt file.
Thickness SVP Threshold / (%)
50
Help
OK
Cancel

RESULTS

Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is opened in the **Result Viewer** after the computation is finished.

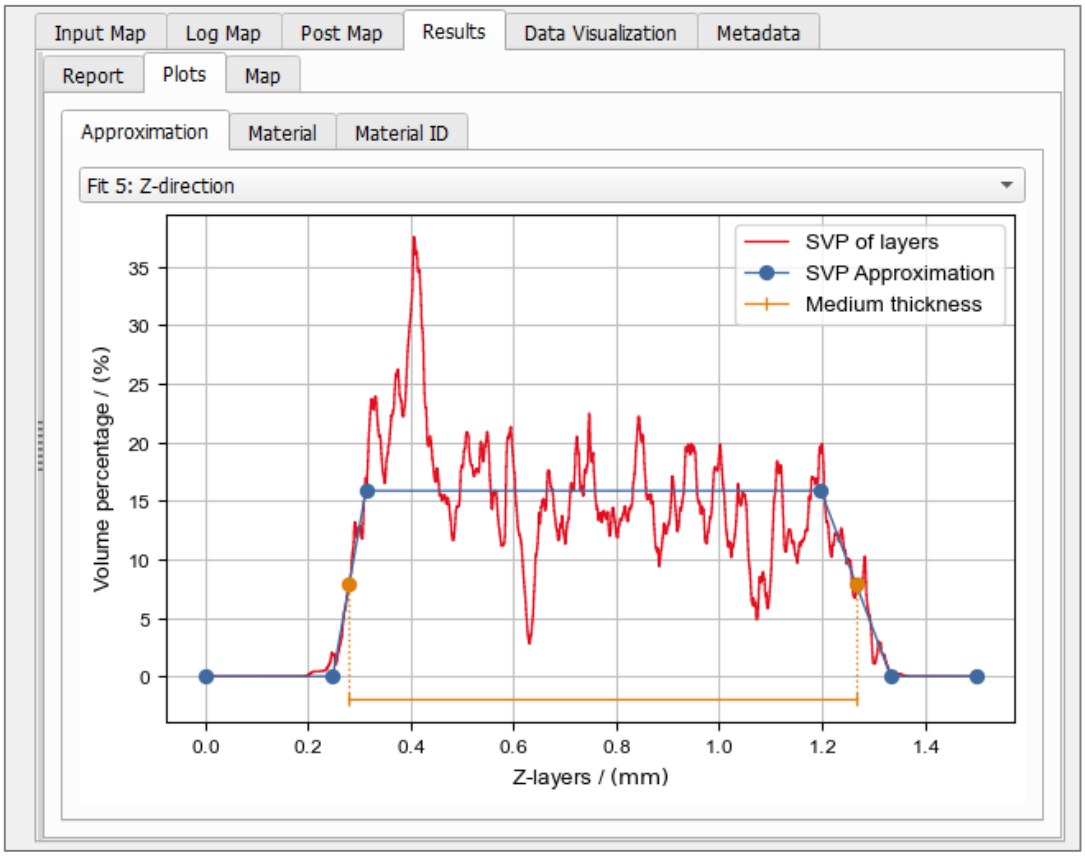
In the **Layer analysis** section, the SVP of the entire structure is reported. In this example, the Z-direction was selected as through direction. Therefore, a **Z direction analysis** section is contained in the report. Initially, the **specific solid volume** and the **specific pore volume** are reported.

Following this, a table displays computed values from the thickness estimation algorithm for the selected fits. The first three rows showcase the thickness of the identified inlet, medium, and outlet, with their cumulative sum equating to the domain size in the Z-direction. The fourth row provides the SVP of the identified medium. The nodes correspond to the piecewise linear approximations that are illustrated in the thickness estimation input dialog, which indicate the coordinate in the through direction and the corresponding SVP. The final row shows the error of the SVP approximation in the L^2 norm. Below the table, the chosen thickness SVP threshold is reported.



In the context menu shown on the left, the **Fit Selection** can be modified and executed as a post-processing step. Additionally, computations can be repeated with a different **Thickness SVP Threshold** value. Click **Apply...** to update the **Report**, the **Plots**, and the corresponding results **Map**.

In the **Plots** tab, the SVP distribution corresponding to the layers of the through direction, their piecewise linear approximation, and the estimated medium thickness are visualized under the **Approximation** subtab for each selected fit. If exactly two fits are selected, two stacked plots will be displayed for comparison purposes. Otherwise, if three or more fits are chosen, you can select the plot you wish to view from the pull-down menu.

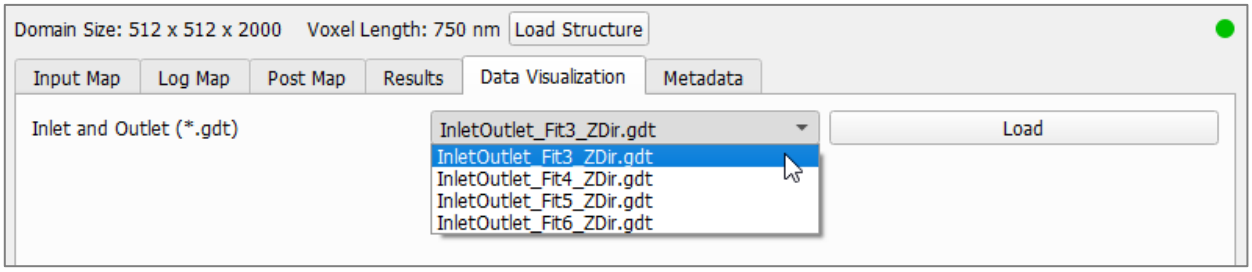


Furthermore, under the **Material** subtab, plots of the SVP of all existing materials are shown:

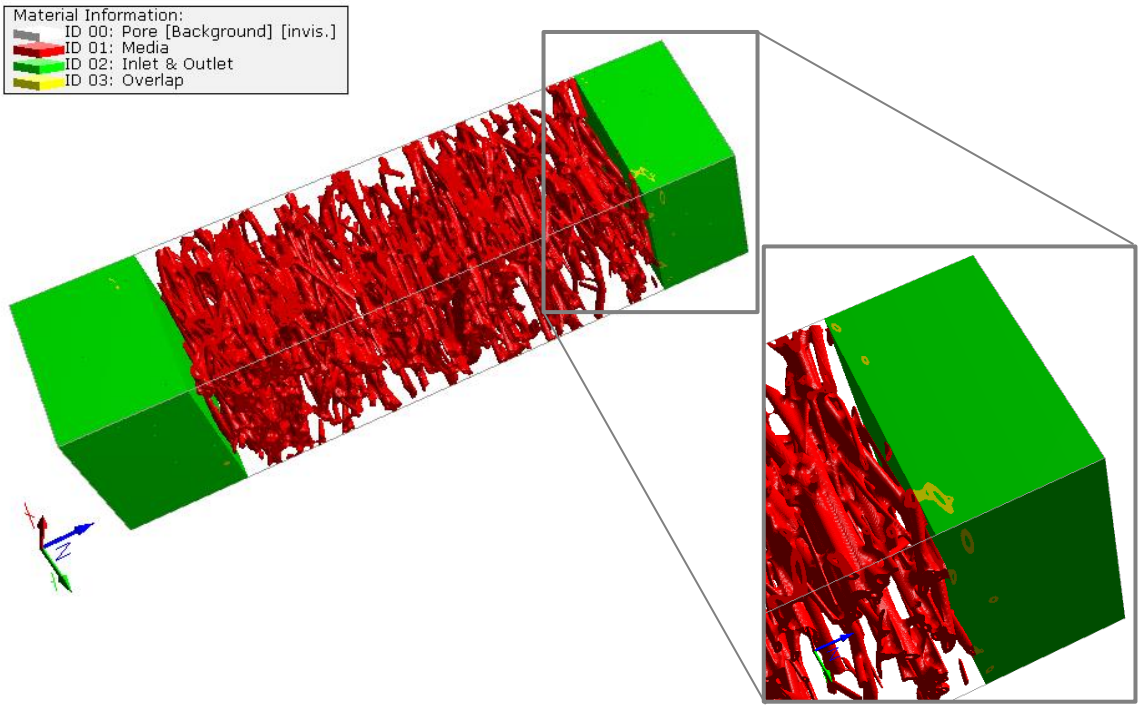
Under the **Material ID** subtab, plots of the SVP of the different materials IDs are shown. The plots differ only from those in the **Material** subtab if several material IDs are assigned to the same material.

Data Visualization

Under the **Data Visualization** tab, a structure showing the identified inlet/outlet regions can be loaded. The inlet and outlet areas are calculated based on the measured SVP and the selected methods. If multiple methods with inlet/outlet are selected, a structure is saved for each of those methods.

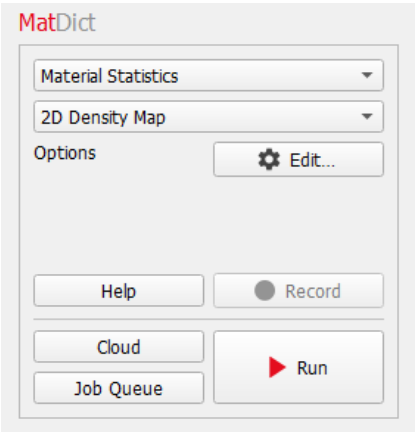


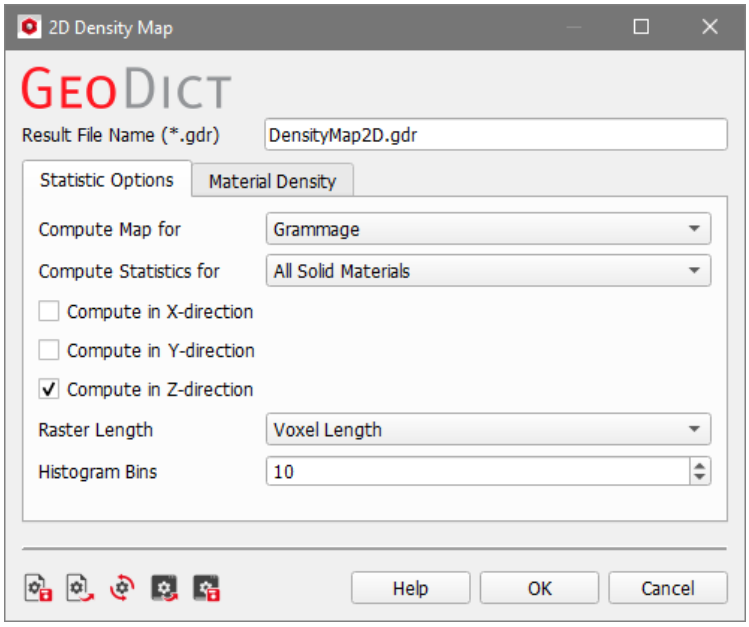
The inlet/outlet volume is assigned to Material ID 02 (here green) and the entire solid structure is assigned to Material ID 01 (here red). Intersections ("overlap") of the structure's fibers and the identified inlet/outlet volume are assigned to Material ID 03 (here yellow).


Material Information:
ID 00: Pore [Background] [invis.]
ID 01: Media
ID 02: Inlet & Outlet
ID 03: Overlap

2D Density Map

The **2D Density Map** command calculates the distribution of **Grammage**, **Solid Volume Fraction** (**SVF**) or the **Number of Objects** in a plane normal to the chosen direction. Each pixel in this plane is calculated by averaging the respective property in the direction of interest at this position.





The **2D Density Map** dialog opens when clicking the **Options**' **Edit...** button. It contains two tabs: **Statistic Options** and **Material Density**.

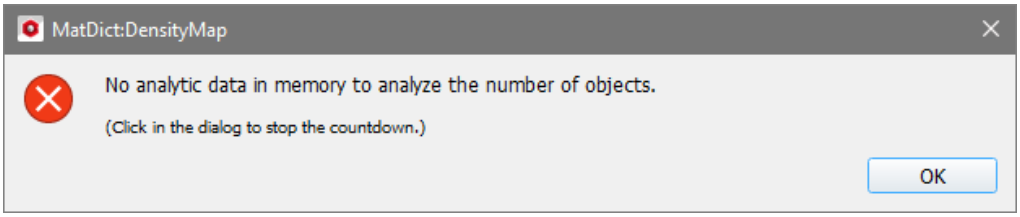
At the top of the dialog, enter the **Result File Name**. The result files are saved in the chosen project folder (**File** → **Choose Project Folder** in the menu bar).

Statistic Options

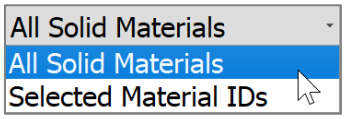
Under the **Statistic Options** tab, choose the property to be computed from the **Compute Map for** pull-down menu.

Only when choosing **Grammage**, the **Material Density** tab is selectable and the density values for the individual Material IDs can be defined. For **Solid Volume Fraction** or **Number of Objects**, the density of the material IDs is not considered in the calculations and the Material Density tab therefore not needed.

When choosing **Number of Objects**, analytic information about the objects in the current structure must be available. Otherwise, a warning message appears, and the density map cannot be computed.



The choice in the **Compute Statistics for** pull-down menu controls whether the property is computed for **All Solid Materials** or only for **Selected Material IDs**.



For **Selected Material IDs**, those can then be chosen from the materials present in the structure in the **Choose Material IDs** pull-down menu.

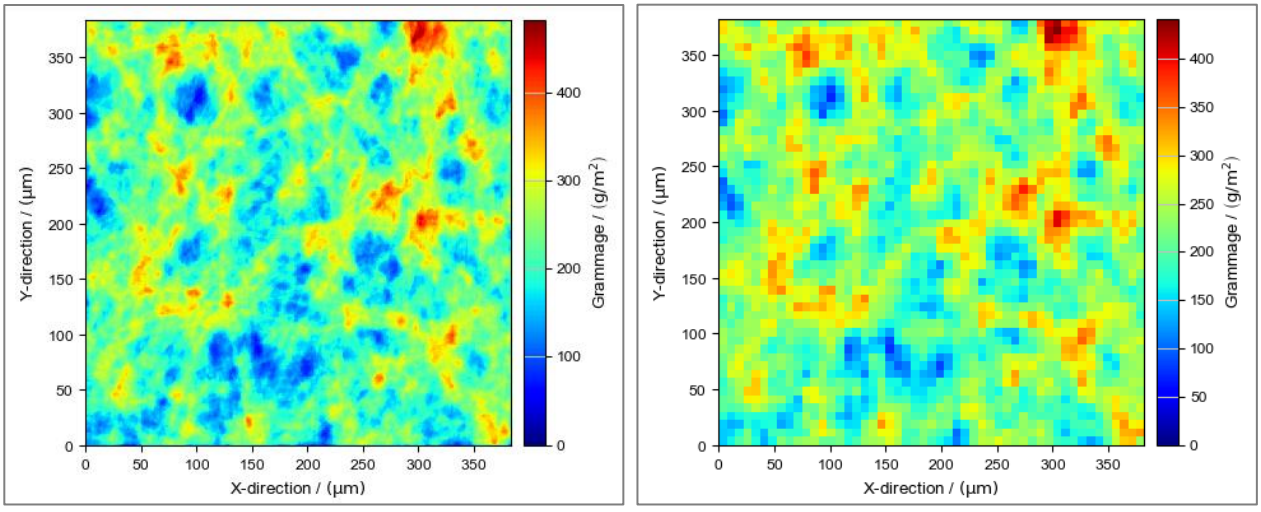
Check **Compute in X-direction**, **Compute in Y-direction**, and/or **Compute in Z-direction** to calculate the chosen properties in these directions.

From the **Raster Length** pull-down menu, choose **Voxel Length** or **Given Length**. This defines the side length of square areas in which Grammage, Solid Volume Fraction, or Number of Objects are computed.

Voxel Length sets the raster length equal to the voxel size and, thus, the 2D density map is computed in the chosen directions for each voxel. If **Given Length** is chosen, the **Length** in units of voxel must be entered to define the resolution for the calculations.

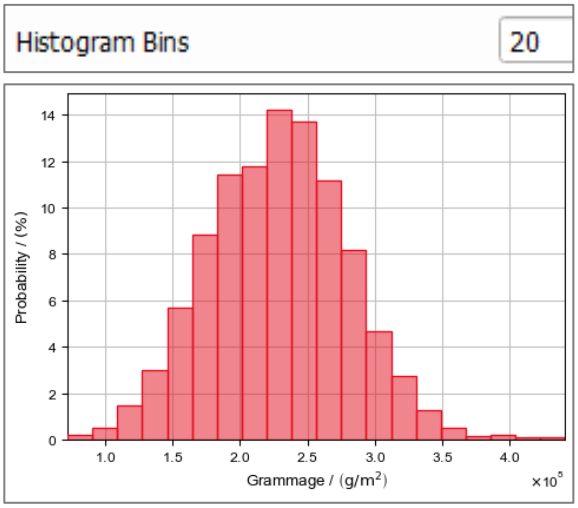
The following figures show the effect of the **Raster Length** on the results:

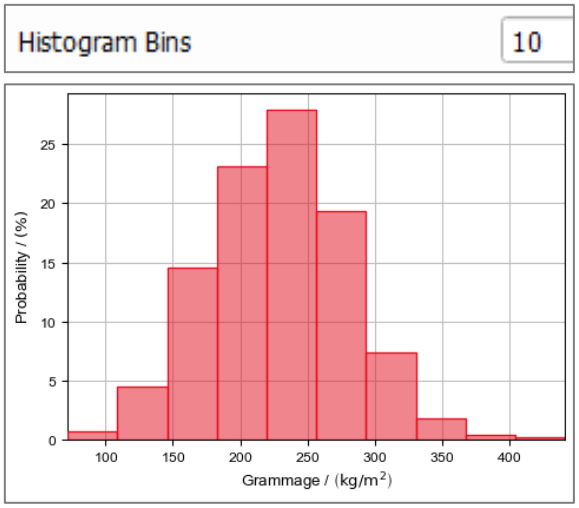
The left picture shows the result for **Voxel Length**, the right picture the result for a **Given Length** of 10 voxels.



Histogram Bins refers to the number of bins used to divide the range of density values (Grammage, Solid Volume Fraction, or Object Number) into a series of equally sized intervals. In the result file, the number of histogram bins is used to create tables and plots with the frequency (probability) of values that fall into each interval.

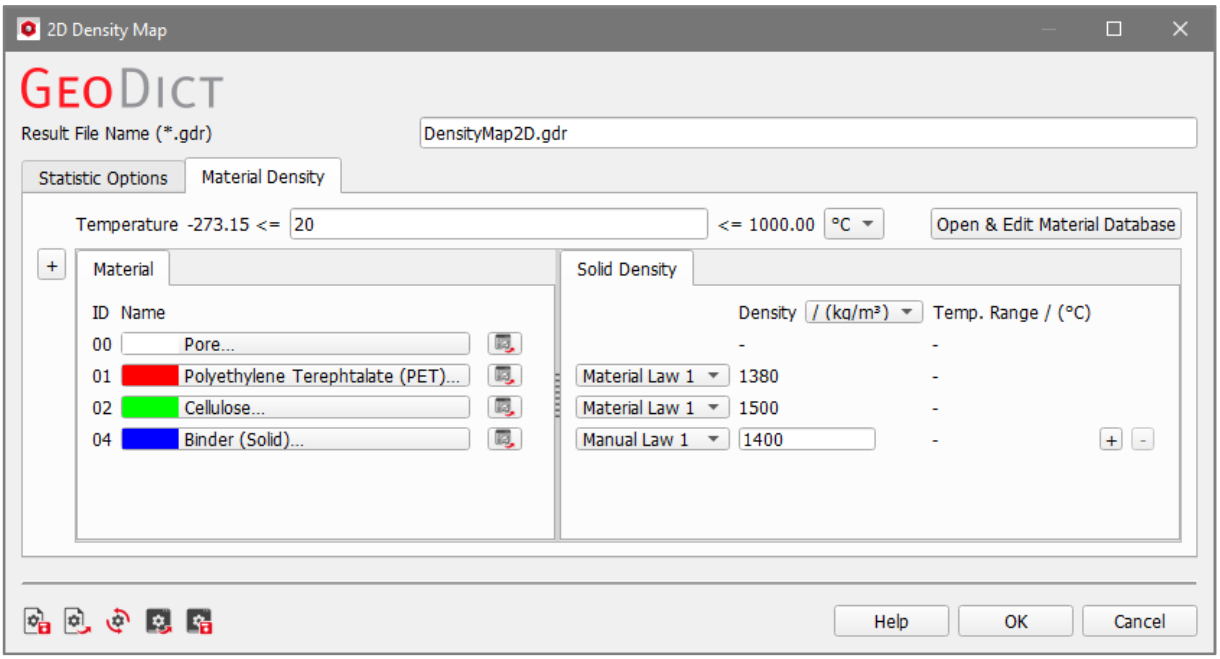
For example, the following plots are taken from result files for the same structure. In the left figure, the histogram is shown with 20 bins, and in the right figure with 10 bins.





Material Density

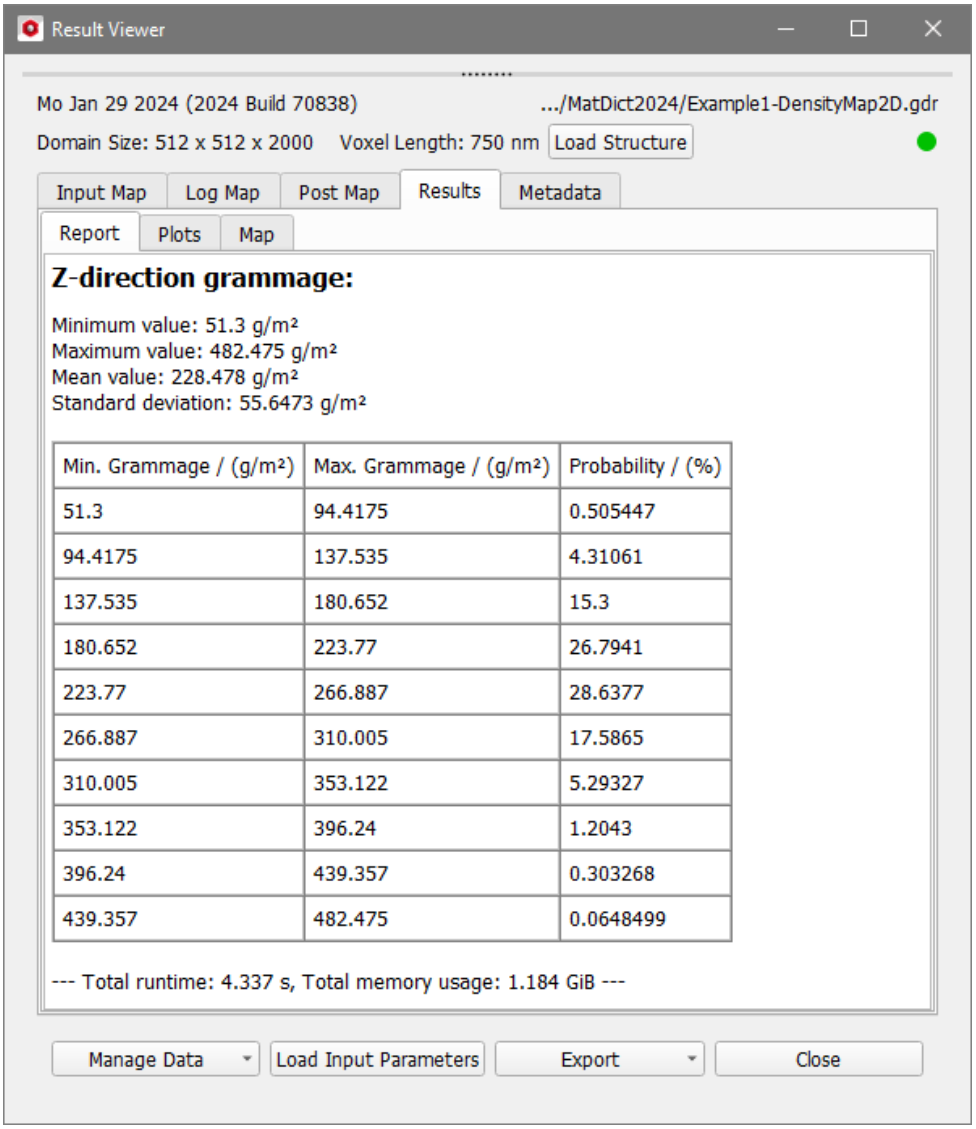
If Grammage is chosen as the computed material property, the density of every material in the structure must be specified under the **Material Density** tab. For materials from the GeoDict Material Database, the density value is entered automatically. If not, manual data can be entered as described on page 5.



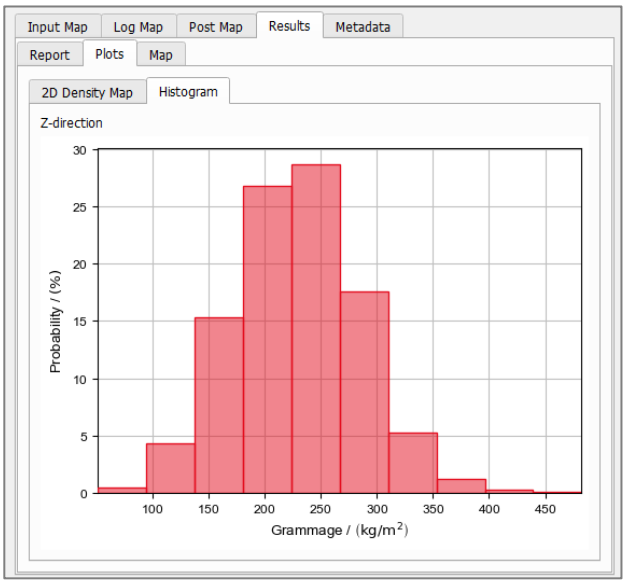
Results

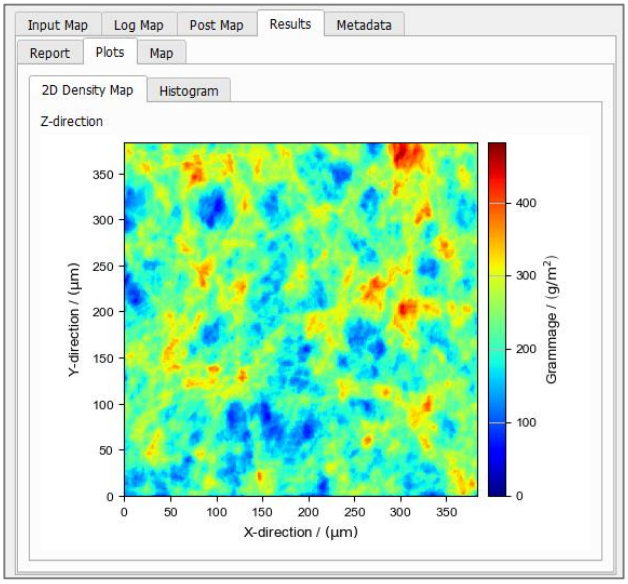
Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is opened in the **Result Viewer** after the computation is finished.

In the **Results - Report** tab, a table shows the computed density distribution. The report table also states the minimal, maximal, and mean values of the computed parameter (here: Grammage) and the standard deviation.



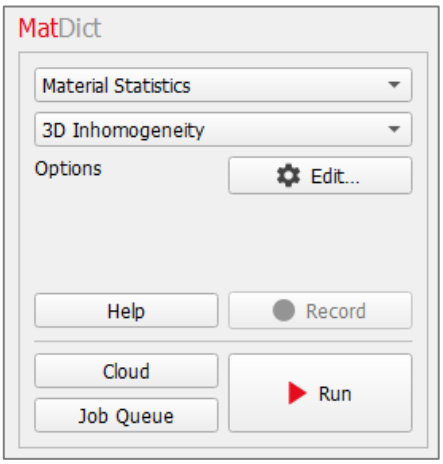
In the **Results – Plots** tab, the table entries are additionally available as a **Histogram** plot. The **2D Density Map** subtab shows the computed result.

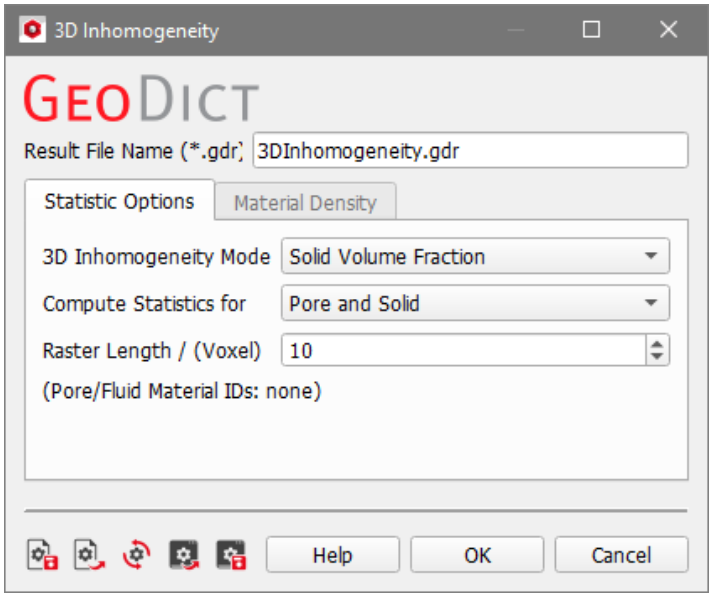




3D INHOMOGENEITY

The **3D Inhomogeneity** command calculates the distribution of the **Solid Volume Fraction, Solid Density** or **Porosity** in specified sub-volumes. Each sub-volume is a cube with a side length that can be specified by the user.



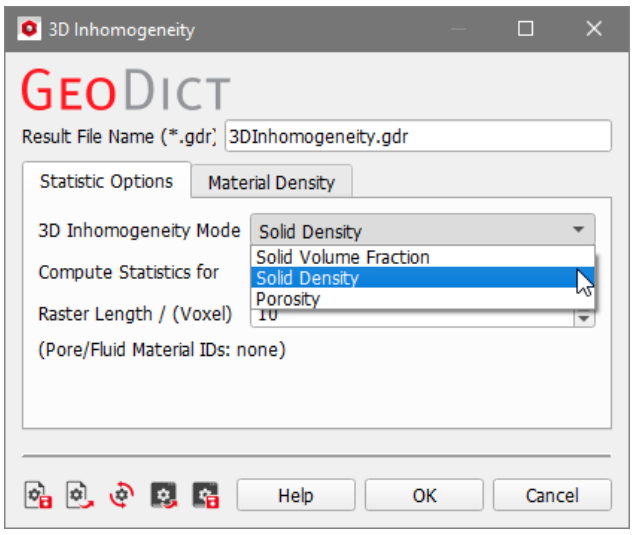


The **3D Inhomogeneity** dialog opens when clicking the **Options' Edit...** button and includes the **Statistic Options** and **Material Density** tabs.

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

STATISTIC OPTIONS

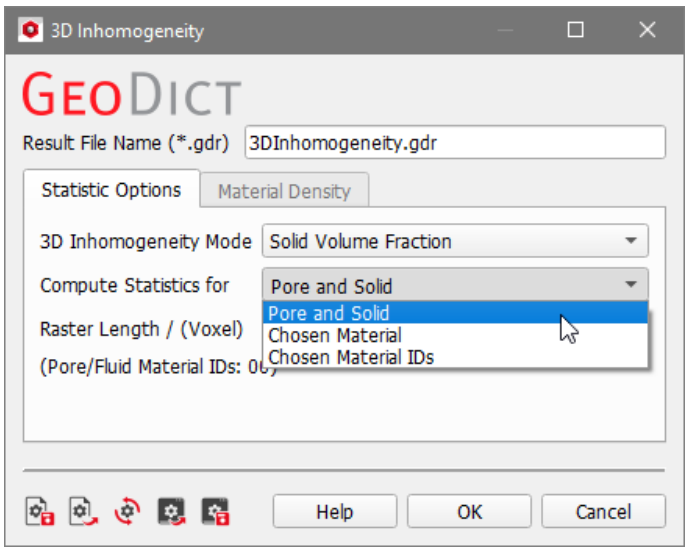
Under the **Statistic Options** tab, choose the property to be computed from the **3D Inhomogeneity Mode** pull-down menu.



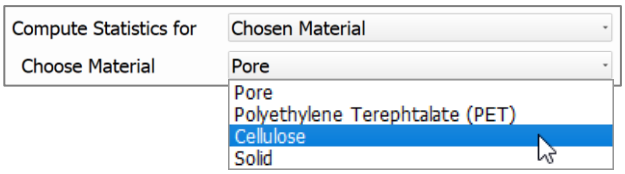
Only when choosing **Solid Density**, the **Material Density** tab is selectable afterwards and the density values for the individual Material IDs can be defined.

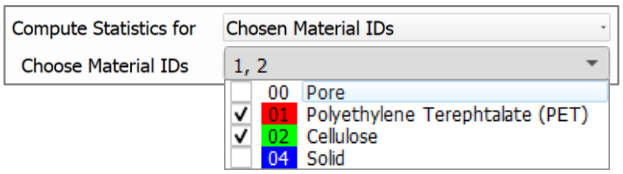
For **Solid Volume Fraction** or **Porosity**, the density of the material IDs is not considered in the calculations and the Material Density tab therefore not needed.

The choice in the **Compute Statistics for** pull-down menu controls whether the property is computed for all materials (**Pore and Solid**) or only for specified materials (**Chosen Material**) or for **Chosen Material IDs**.



After the selection of **Chosen Material IDs**, the IDs can be chosen from the materials present in the structure, which appear under the **Choose Material IDs** pull-down menu.

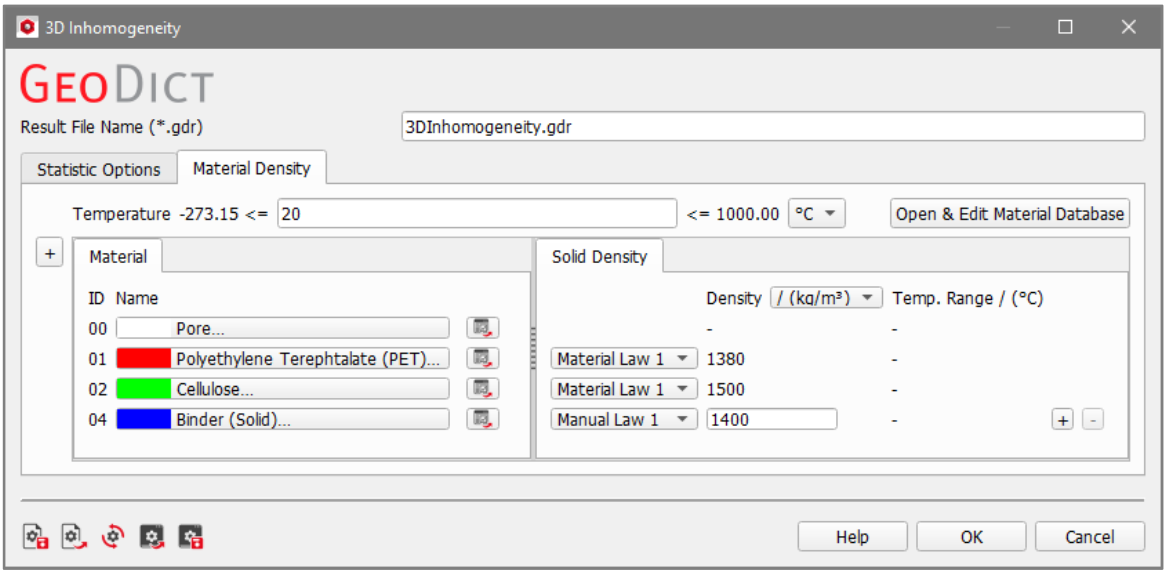




The **Raster Length** determines the side length of the cubic sub-volume in voxels. If **Raster Length** is not a common divisor of the side lengths **NX, NY, NZ** of the current structure, some boundary layers of the current structure will not be contained in any sub-volume. In this case, a warning will be plotted in the result viewer.

Material Density

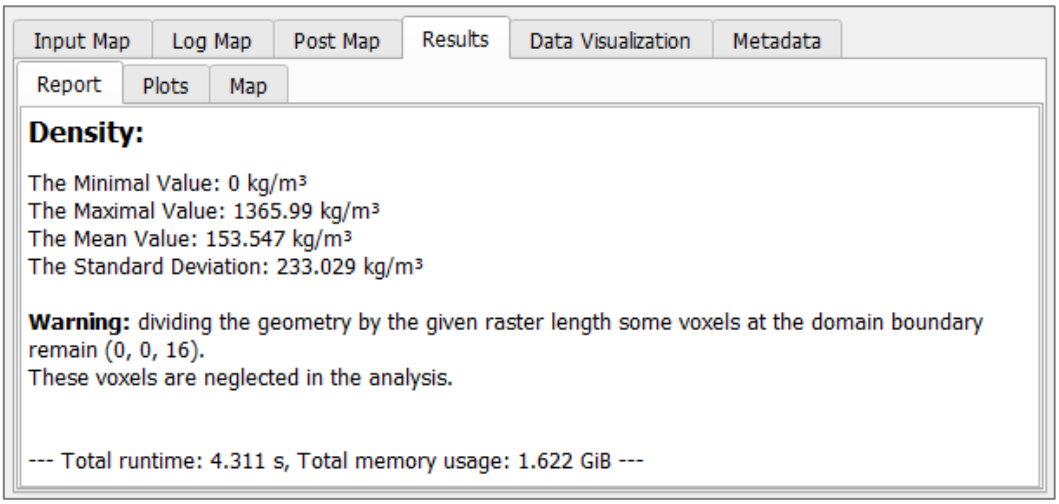
If **Solid Density** is chosen as the material property to be computed, the density of every material in the structure must be specified under the **Material Density** tab.



For materials from the GeoDict Material Database, the density value is entered automatically. Otherwise, see page 5 how to edit the density.

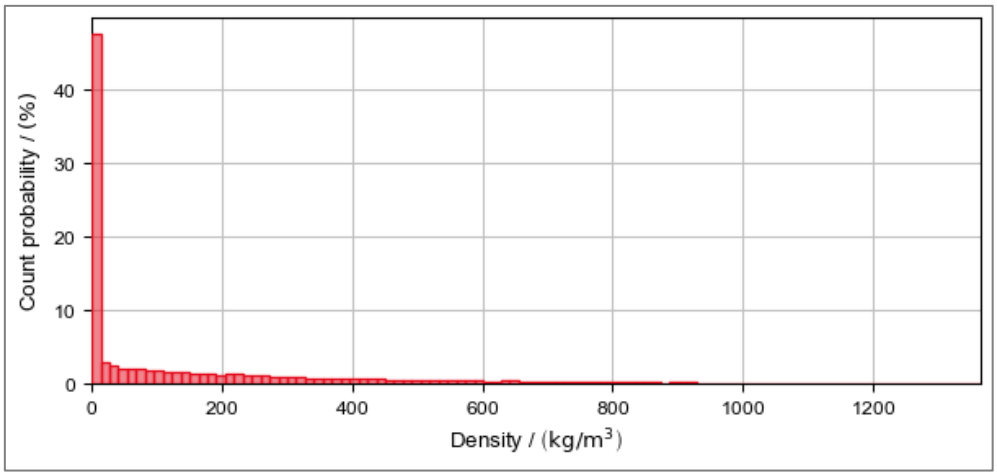
RESULTS

Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is shown in the **Result Viewer** after the computation is finished.



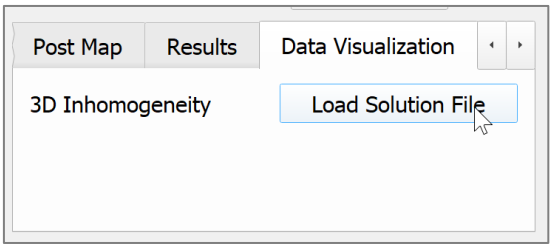
In the **Results - Report** subtab, the minimal and maximal value of the chosen property found in any sub-volume are reported. Additionally, the mean value and the corresponding standard deviation are shown.

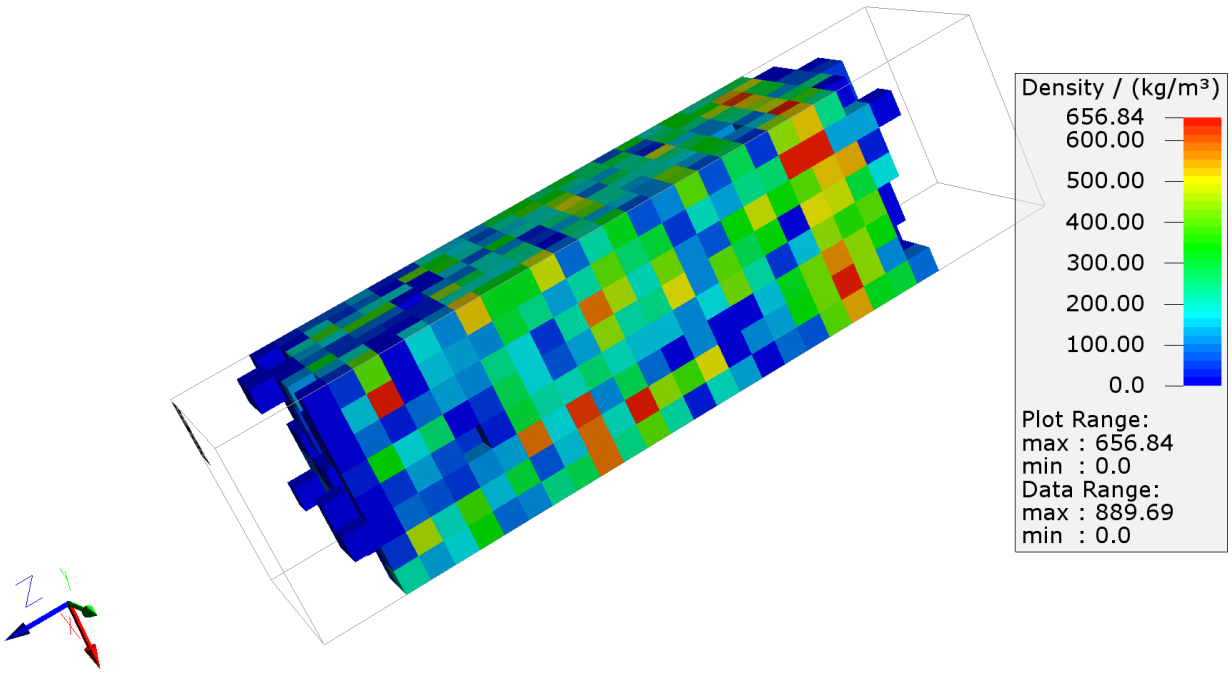
In the **Results – Plots** subtab, a histogram of the Count Probability of the selected property is plotted.



Data Visualization

Under the **Data Visualization** tab, it is possible to visualize the computed densities, porosities, or solid volume fractions of the sub-volumes. Clicking on **Load Solution File** loads the result field.

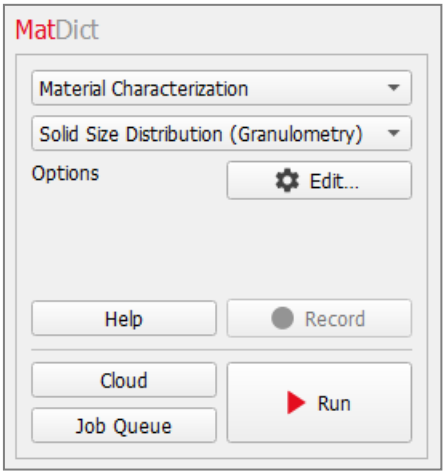




Material Characterization

Solid Size Distribution (Granulometry)

After selecting **Solid Size Distribution (Granulometry)**, the needed parameters can be entered by clicking the **Options' Edit...** button.

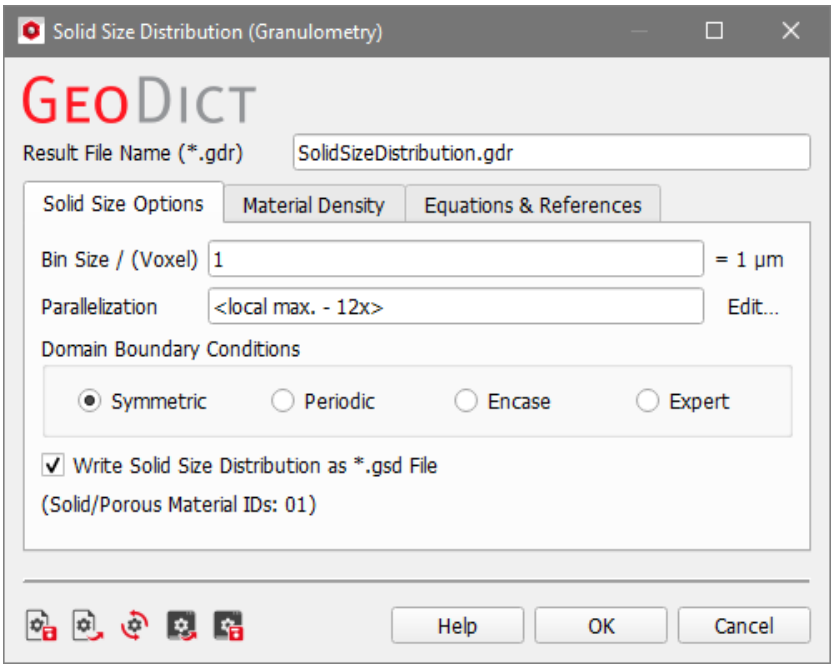


The Solid Size Distribution dialog includes the **Solid Size Options** and the **Material Density** tabs. The last tab, **Equations & References**, provides further information about the underlying algorithm.

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

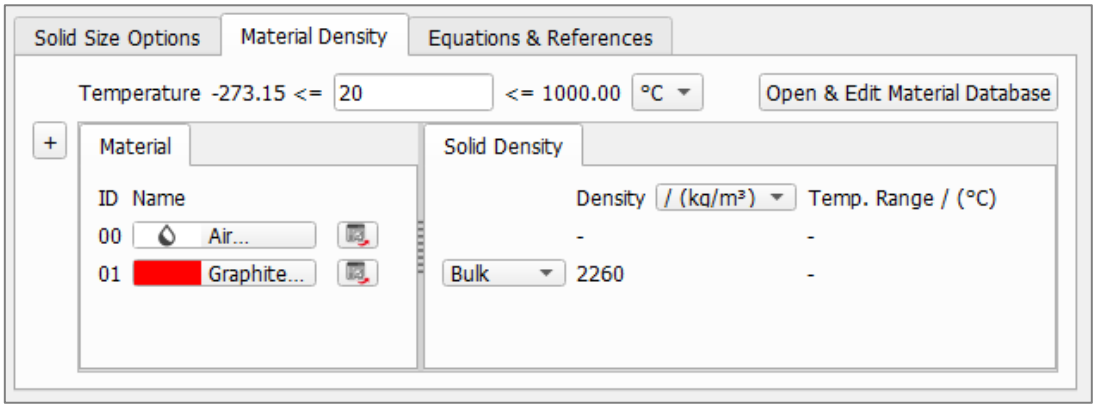
Solid Size Options

The Solid Size Options are similar to those of PoroDict's Pore Size Distribution (Granulometry). For details refer to the PoroDict handbook. Be aware, that *Write Pore Geometries as *.gdt Files* and the settings for fluid in pores is not available here as the material for the solids is already defined.



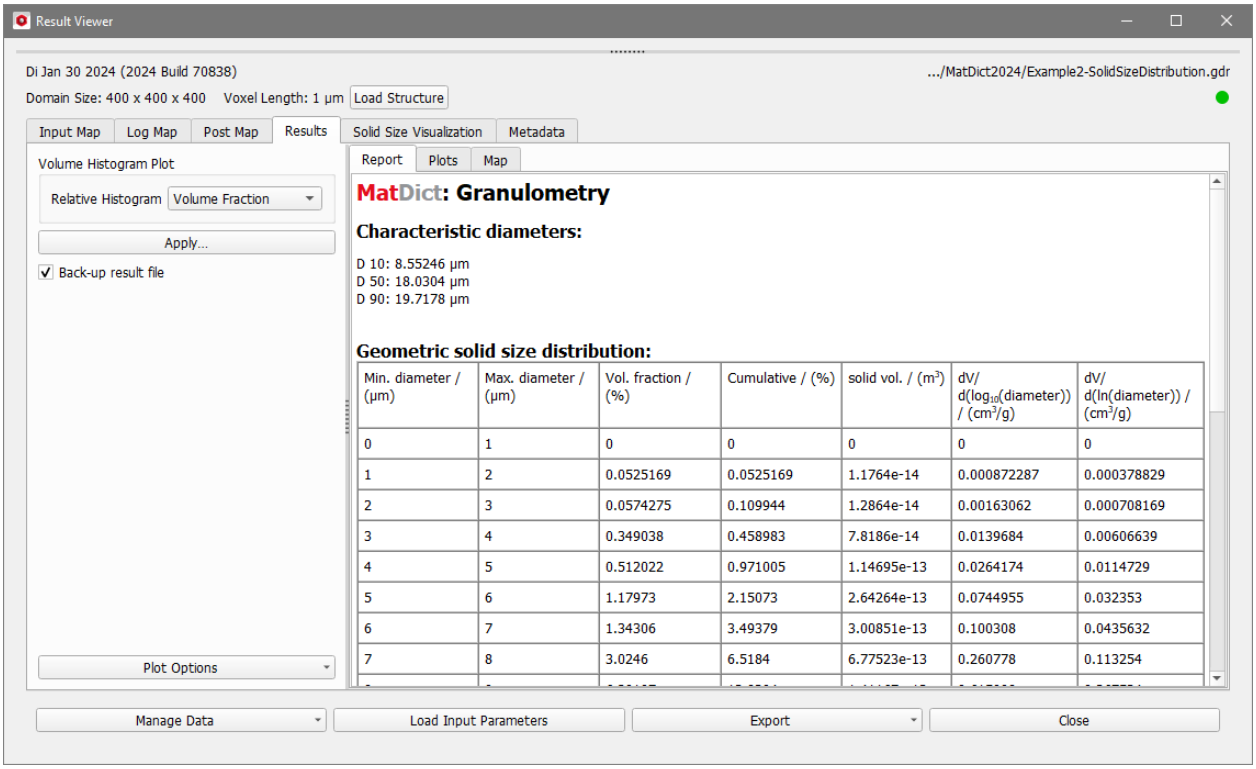
Material Density

Under the **Material Density** tab, the temperature can be edited if the density of a material is temperature dependent. Additionally, the density of every solid material in the structure must be specified in this tab. For materials from the GeoDict Material Database, the density value is entered automatically. Otherwise see page 5 how to edit the density.



Results

Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is opened in the **Result Viewer** after the computation is finished.

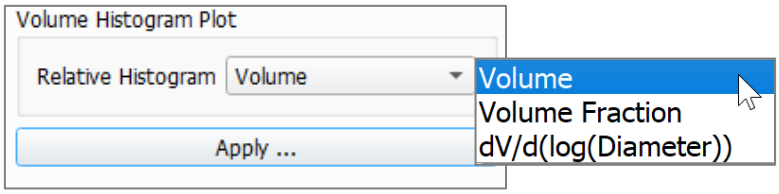


Under the **Results - Report** subtab, the **Characteristic Diameters** are shown. For example, here, the D10 value of 8.55 µm means that 10% of all solids have a smaller diameter than 8.55 µm. The D50 value of 18.03 µm means that 50% of all solids have a diameter smaller than 18.03 µm, and the D90 value of 19.71 µm means that 90% of all solids have a diameter smaller than 19.71 µm.

The discretization error is less than 1 voxel, which means for the presented example, that the D10 is 8.55 µm ± 1.0 µm.

Below the characteristic diameters, a table contains Maximum and Minimum Diameters, Volume Fraction, Cumulative Volume Fraction, the Solid Volume, and the Differential Solid Volume Distribution for every bin. Also, at the bottom of the **Report tab**, the total solid volume percentage of the structure is shown.

Under the **Results – Plots** subtab, different relative and cumulative histograms can be plotted. The histogram of interest, i.e. Volume, Volume Fraction, or dV/d(log(Diameter)) can be chosen in the **Volume Histogram Plot** section.

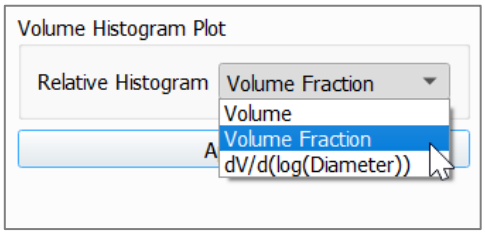


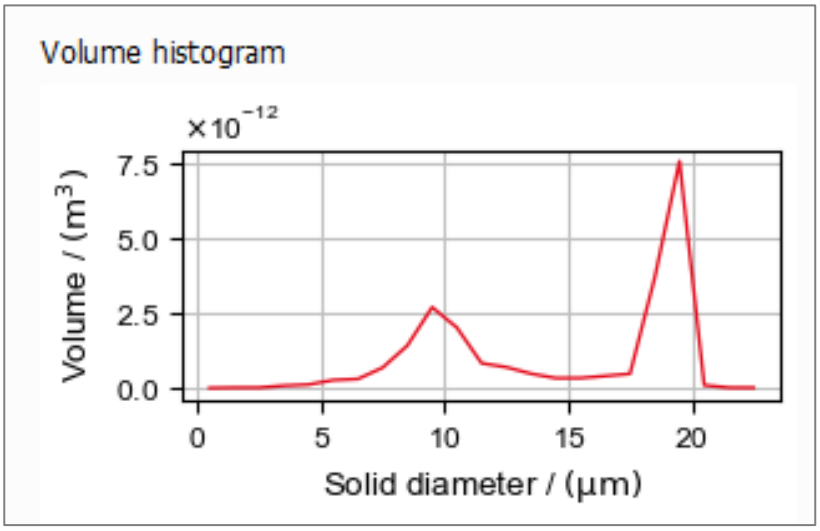
The differential pore volume distribution $dV/d(log(diameter))$ is then computed as

$$\frac{V_{cum}(d_{i+1}) - V_{cum}(d_i)}{(\log(d_{i+1}) - \log(d_i)) \cdot m} \tag{1}$$

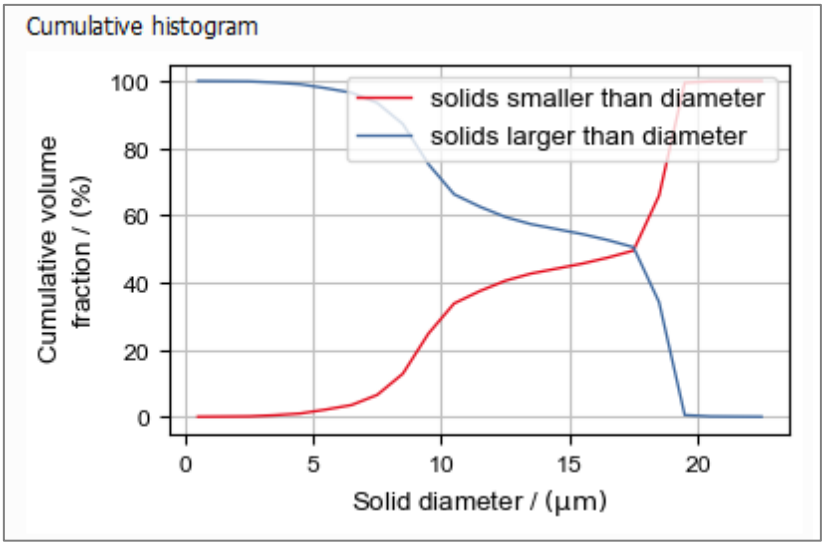
with d_i the pore diameter of the *i*-th bin, V_{cum} the cumulative volume fractions, and m the mass of the structure. The latter is computed using the densities of the solid constituent materials of the sample. This normalization ensures that the value of dV/d(log(Diameter)) is independent of the domain size.

After choosing and clicking **Apply...**, the plots on the right hand-side change accordingly.

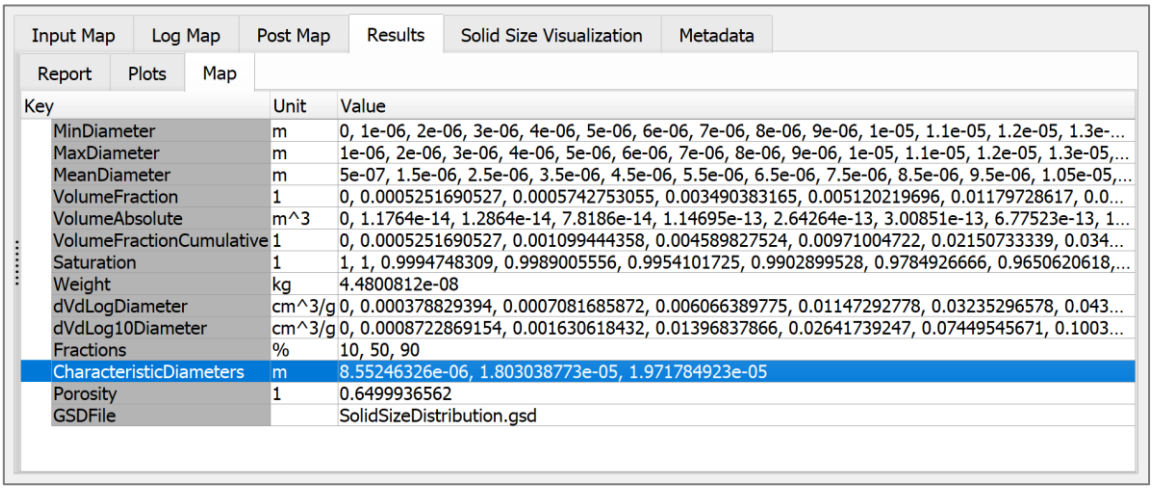




In the **Cumulative Histogram** plot, the red curve shows the volume fraction of solids smaller than a given diameter and the blue curve shows the solids larger than or equal to a given diameter. Both curves sum up to 100% for any given diameter.

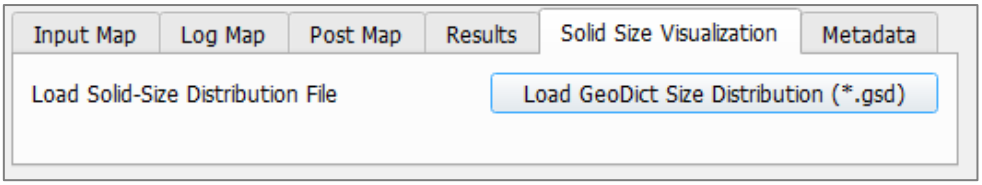


Finally, the **Results - Map** subtab gives access to the values of the computed parameters.



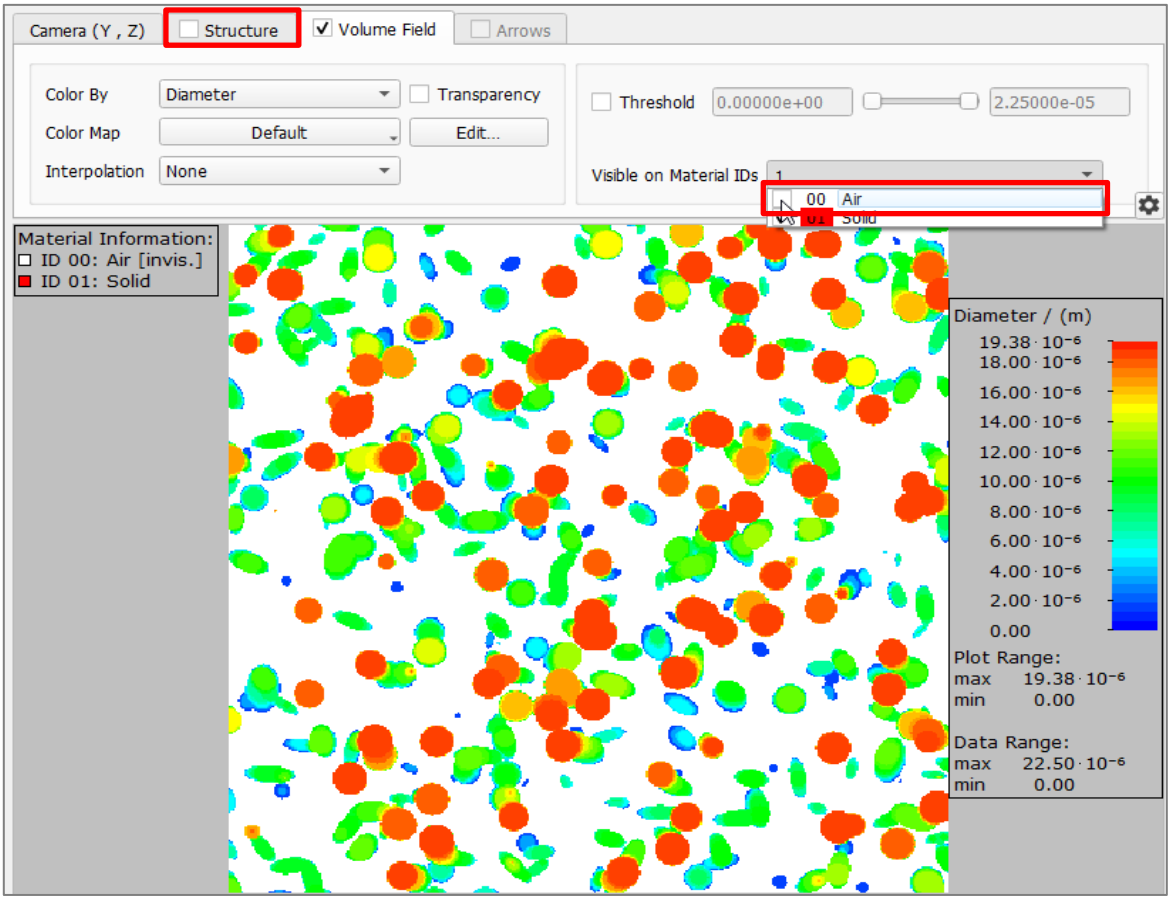
Solid Size Visualization

The distribution of solids is observed in the Volume Fraction/Solid Diameter plot but can also be visualized through the **Solid Size Visualization** tab. When **Write Solid Size Distribution as *.gsd File** was checked before running the command, it is possible to visualize the size distribution by clicking **Load GeoDict Size Distribution (*.gsd)**.



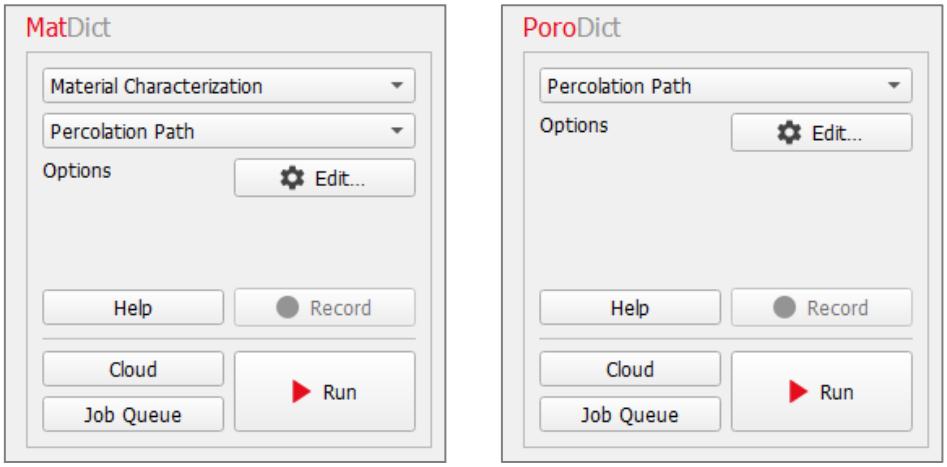
To see the solid size distribution inside of the structure, it is recommended to deactivate the visualization of the structure itself. This can be done by unchecking **Structure** in the tab headers or alternatively in the **View** settings. Additionally, the

visualization of the result field in the pore space (where the value is always zero) can be deactivated by unchecking all pore materials with the option **Visible on Material IDs** under the **Volume Field** tab.



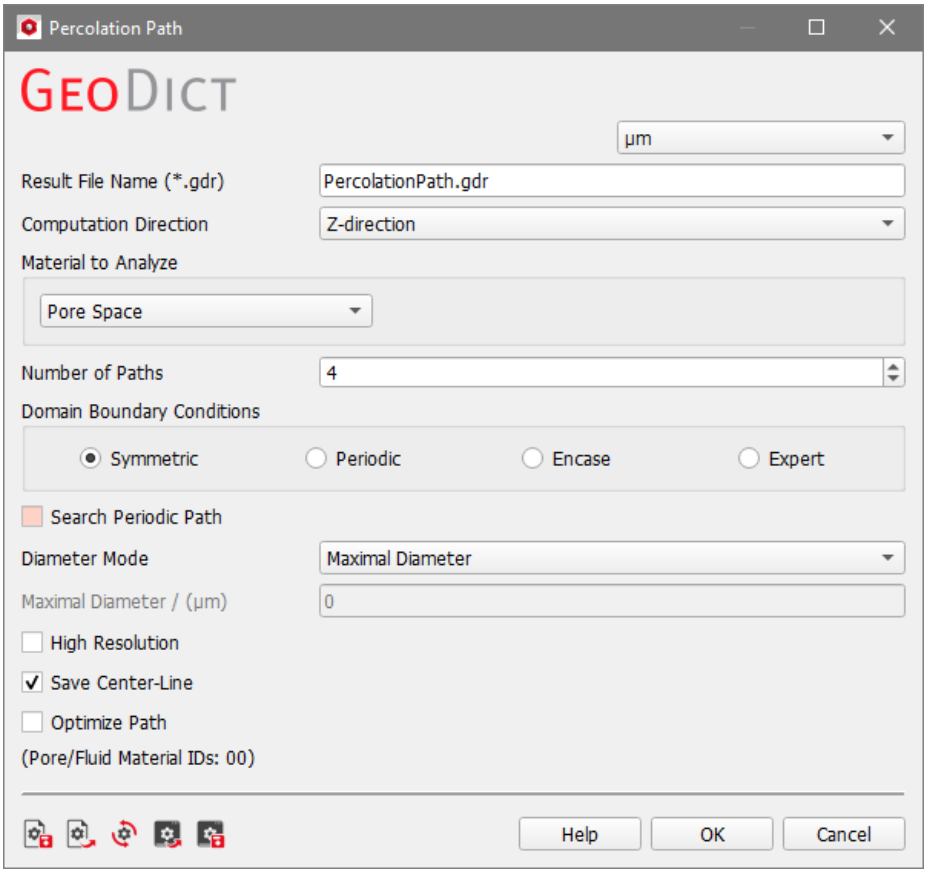
PERCOLATION PATH

The **Percolation Path** command is accessible from MatDict and PoroDict. It can find the shortest percolation paths of maximal diameter in the pore space or through a given material. Two voxels of a percolation path are connected if they share a common face. Thus, the neighborhood mode is always 'Face'.



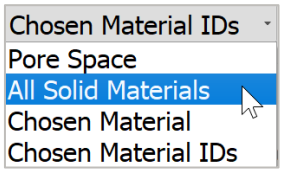
The Percolation Path dialog opens, and the necessary parameters can be entered by clicking the **Options' Edit...** button.

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



The **Computation Direction** defines the direction in which the percolating path should cross the structure.

Material to Analyze defines through which materials the path may run. Four options are available:



Pore Space finds a percolation path through the pores, **All Solid Materials** through the solids. **Chosen Material** allows to choose a single material. The last option, **Chosen Material IDs**, gives the full flexibility to select a list of material IDs where the path may run through.

The number of percolation paths to be detected is set with the **Number of Paths** parameter. Then, the algorithm computes the n best percolation paths.

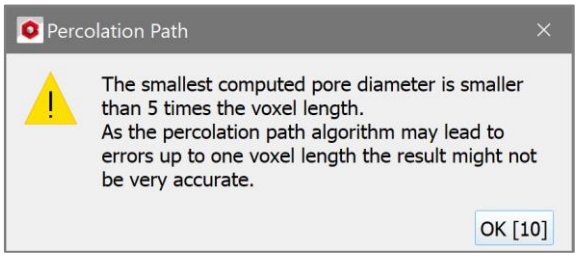
The diameter of pores and solids near the domain boundary is strongly influenced by the selected **Domain Boundary Conditions**. Here, the same boundary conditions as in the granulometry command are available. An example explaining the available options is given in the PoroDict handbook in the section of the Pore Size Distribution (Granulometry) command.

Search Periodic Path is only available for periodic boundary conditions. If checked, the Percolation Path is allowed to cross lateral periodic boundaries. Using this option increases computation time. A periodic percolation path is not necessarily periodic in the computation direction.

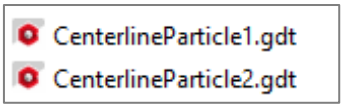
From the **Diameter Mode** pull-down menu, choose to detect percolation paths with the **Maximal Diameter** possible or **Specify Maximal Diameter** and enter a **Maximal Diameter** value below.

To run the calculations in **High Resolution** might be useful when the path space is expected to be narrow. The standard algorithm computes distances directly on the voxel grid, i.e. when determining a pore size, only the distances from the center of a pore voxel to the center of a solid voxel are taken into account. High Resolution also takes the voxel surfaces and edges into account, so the computed distances correspond to the distance to the next surface or edge. The disadvantage of the **High Resolution** mode is that the calculation runtime and memory usage may increase by a factor of eight.

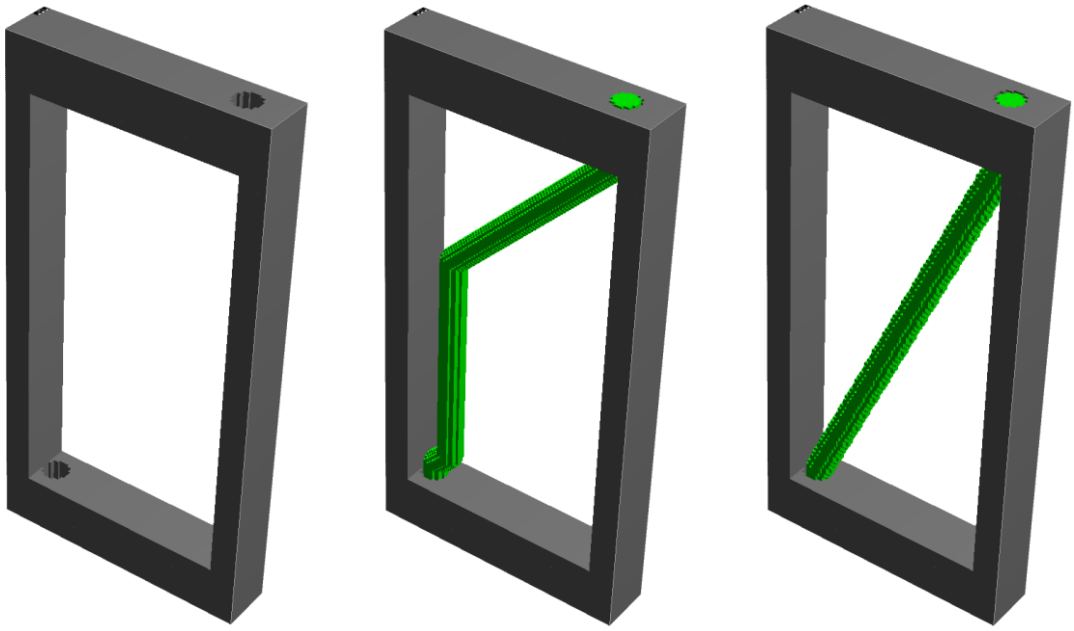
If the largest computed path is smaller than five voxel lengths, and the simulation was run in the standard mode, a warning message is shown. In this case, it is recommended to re-run the simulation in **High Resolution** mode.



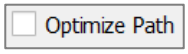
When **Save Center-Line** is checked, the results folder additionally contains *.gdt files with the centerline of the computed percolation paths.

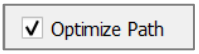


With **Optimize Path**, the length of the percolation path is optimized after the calculation. This shortens the calculated path by removing voxel staircase artifacts: The algorithm for the percolation path works on the voxel structure and can therefore only find paths which run directly through connected voxels. Therefore, the default method might not always find the best path in structures with large open pores. In these cases, it is recommended to select **Optimize Path** (see the examples below).



Structure without a path

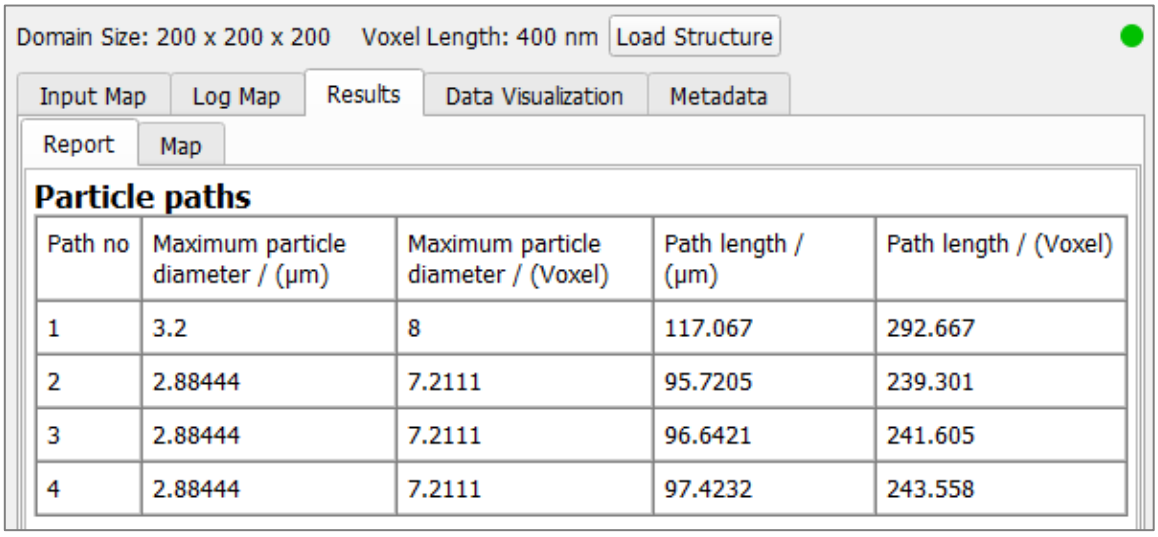




Click **OK** to close the Percolation Path dialog and start the command by clicking **Run**. The Result Viewer automatically opens at the end of the calculations.

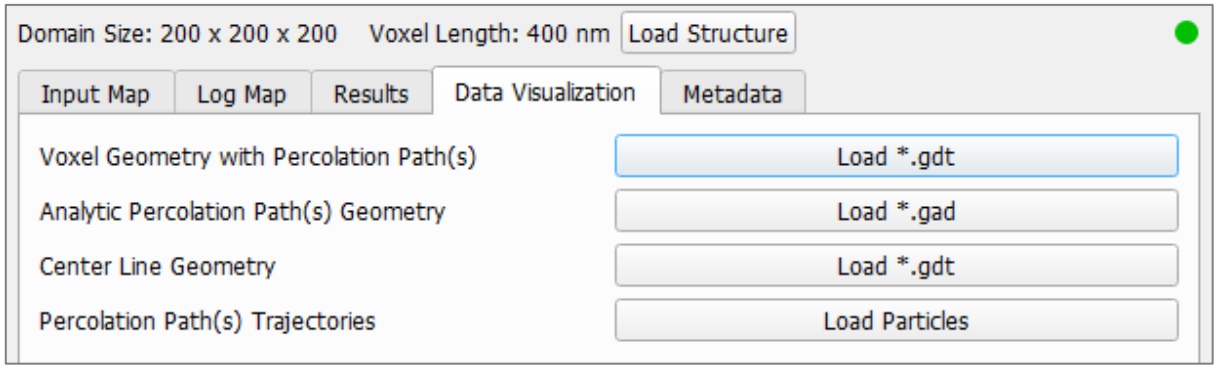
Results

The **Results - Report** subtab includes the **Maximum Particle Diameter** (in µm and voxels) of spherical particles which may pass through the medium, as well as the **Path Length** (in µm and voxels) of the detected percolation path(s).



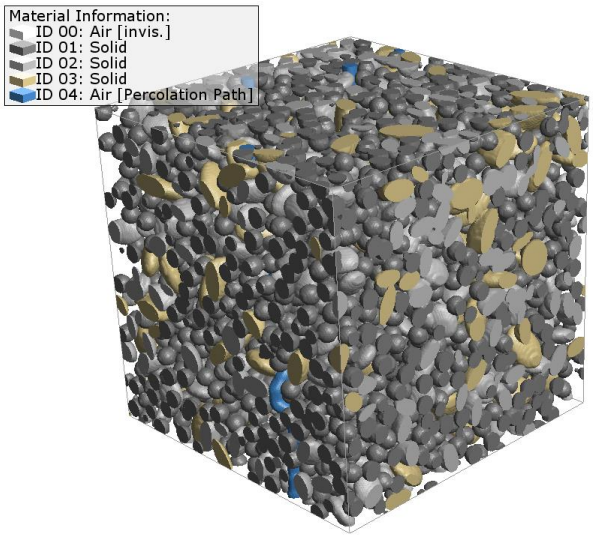
Path no	Maximum particle diameter / (µm)	Maximum particle diameter / (Voxel)	Path length / (µm)	Path length / (Voxel)
1	3.2	8	117.067	292.667
2	2.88444	7.2111	95.7205	239.301
3	2.88444	7.2111	96.6421	241.605
4	2.88444	7.2111	97.4232	243.558

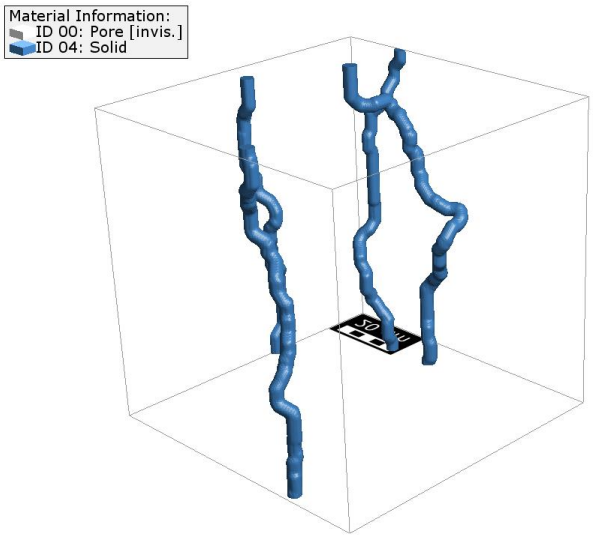
Under the **Data Visualization** tab four options are available.



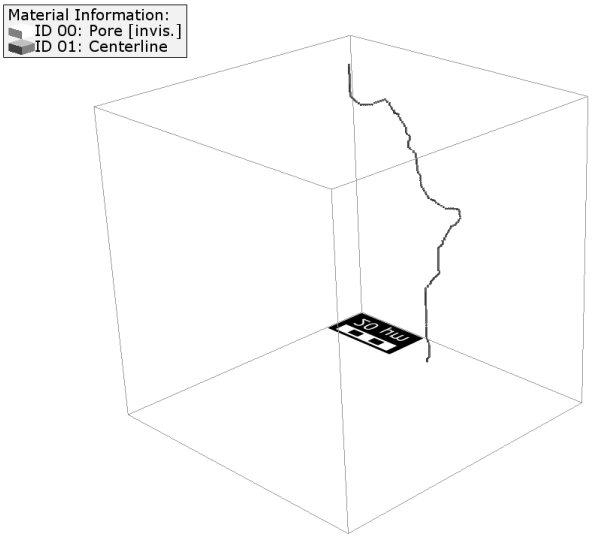
To show the **Voxel Geometry with Percolation Path(s)** click **Load *.gdt**.

The **Analytic Percolation Path(s) Geometry** can be loaded by clicking the **Load *.gad** button and shows only the percolation paths without the structure.





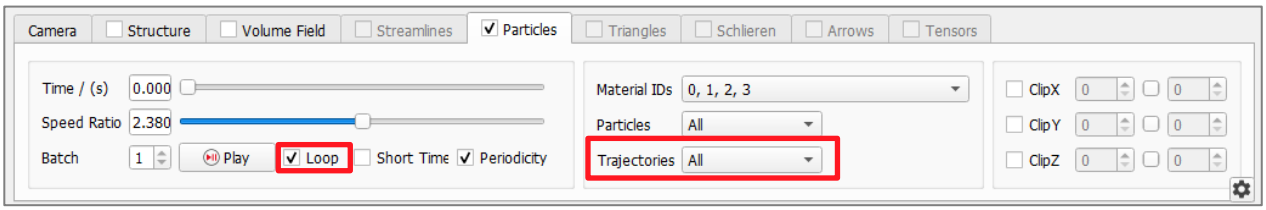
The option **Center Line Geometry** is only available if **Save Center-Line** was activated when running the simulation. It loads a structure file that contains the center line of the path with the maximal diameter.



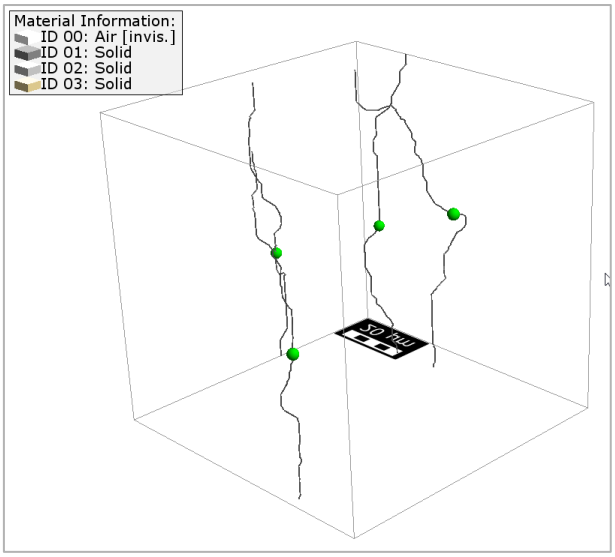
The **Percolation Path(s) Trajectories** can also be visualized with animated spheres moving through the structure. For this, click **Load Particles**. Deactivate the structure

visualization by unchecking the **Structure** tab in the Visualization panel, above the Visualization area.

In the Visualization panel, click **Play** under the **Particles** tab. For convenience, check **Loop** and, for the **Trajectories**, select to show **all**.

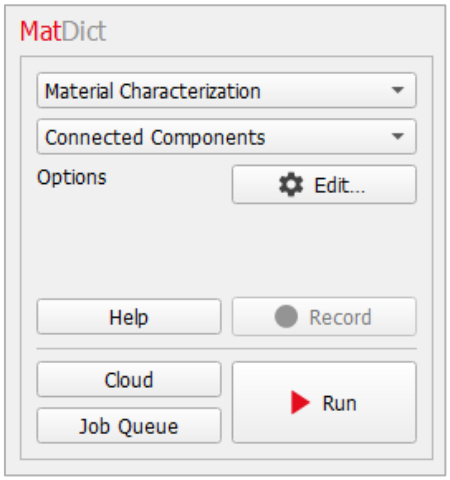


In this example, you can observe four spheres (here green) corresponding to the four percolation paths moving through the volume.

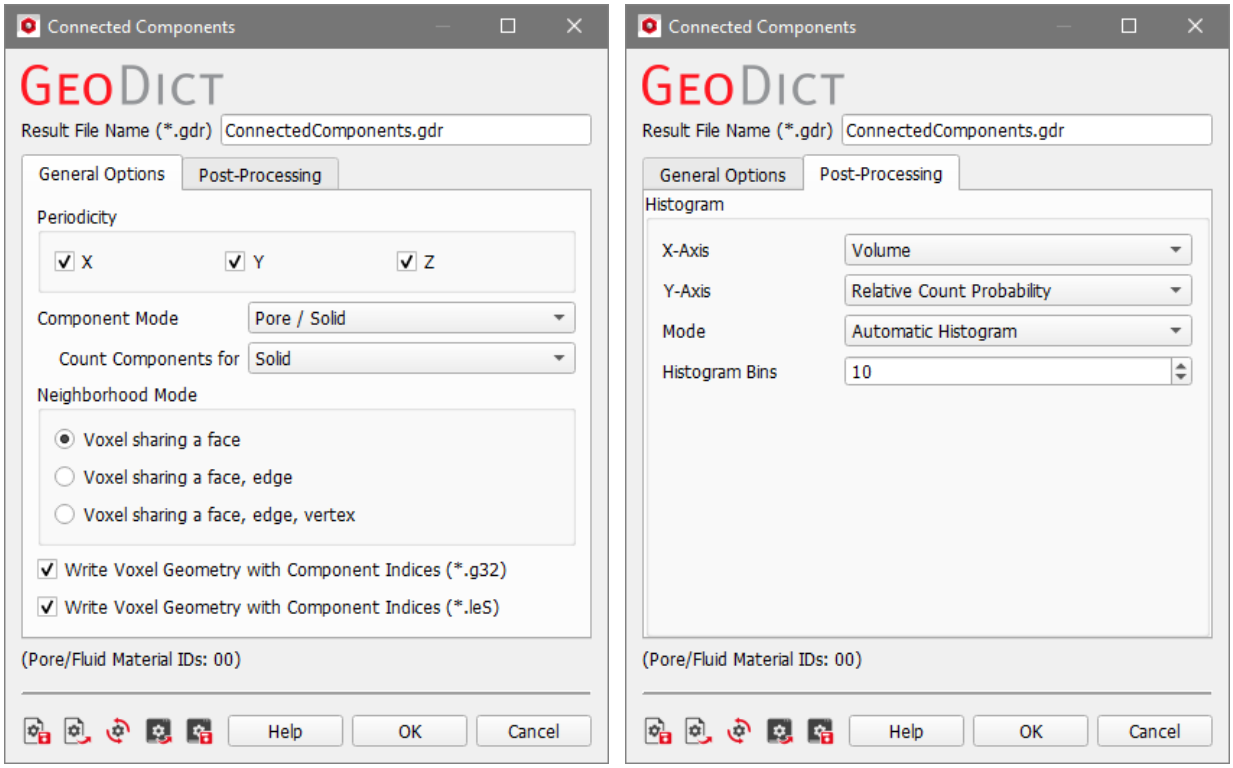


Connected Components

With the **Connected Components** command, it is possible to find and count the number of connected components in the 3D structure. A connected component consists of all voxels that are in contact with each other, and which belong to the same phase, the same material, or the same material ID.



The **Connected Components** dialog opens when clicking the **Options**' **Edit...** button and includes the **General Options** and the **Post-Processing** tabs.



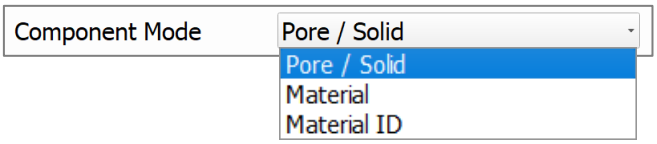
At the top of the dialog, enter the **Result File Name**. The result file is saved in the chosen project folder (**File** → **Choose Project Folder** in the menu bar).

General Options

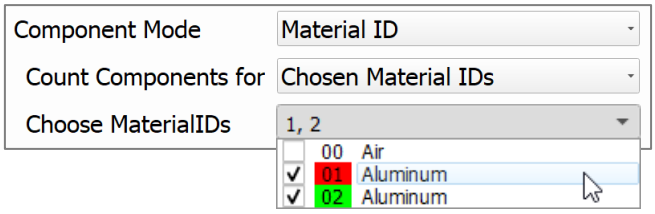
In the **Periodicity** panel, periodic boundaries can be set in the three spatial directions. If the box is checked, every voxel located on the boundary of the domain is connected to a voxel on the opposite side of the domain. Thus, components can be

connected across the domain boundary. If the box is not checked, no connections exist across the domain boundary.

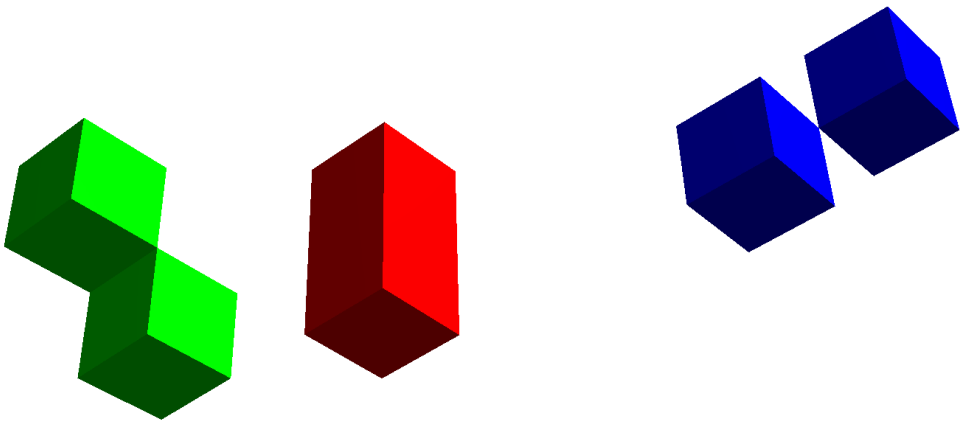
If the **Component Mode** is set to **Material ID**, all voxels belonging to one component must have the same material ID. If it is set to **Material**, all voxels belonging to one component must belong to the same material. If it is set to **Pore / Solid**, the distinction happens only between solid or pore voxels. Thus, in the **Pore / Solid** mode, voxels with different material IDs may form one component. For the user's convenience, all material IDs which denote pore space are shown at the bottom of the dialog.



While the **Component Mode** defines which parts may belong to one component, with **Count Components for** set what is counted and reported. Select if pore and/or solid components are counted. Dependent on the selected **Component Mode**, it is also possible to count components only for a specific material or for specific material IDs.



The meaning of 'connected' is defined in the **Neighborhood Mode** panel. Voxels can be connected through faces, edges, and corners (vertices).



The two red voxels share a face, the green voxels share an edge, and the blue voxels share a vertex. In **Voxels sharing a face** mode, the two red voxels form one component, the green voxels form two components, and the blue voxels form two components. In **Voxels sharing a face, edge** mode, the red voxels form one component, and the green voxels form one component, while the blue voxels still form two components. In **Voxels sharing a face, edge, vertex** mode, the red voxels form one component, the green voxels form one component, and the blue voxels form one component.

When checking **Write Voxel Geometry with Component Indices (*.g32)**, the connected components are saved as objects in a .g32 file. This file can be opened in GeoDict, GeoPy or GeoLab.

When checking **Write Voxel Geometry with Component Indices (*.leS)**, the object indices are stored in an *.leS ASCII file. This file is human readable, but will be considerably larger and slower to read than the *.g32 file. Therefore, it is recommended to use the *.g32 format.

POST-PROCESSING

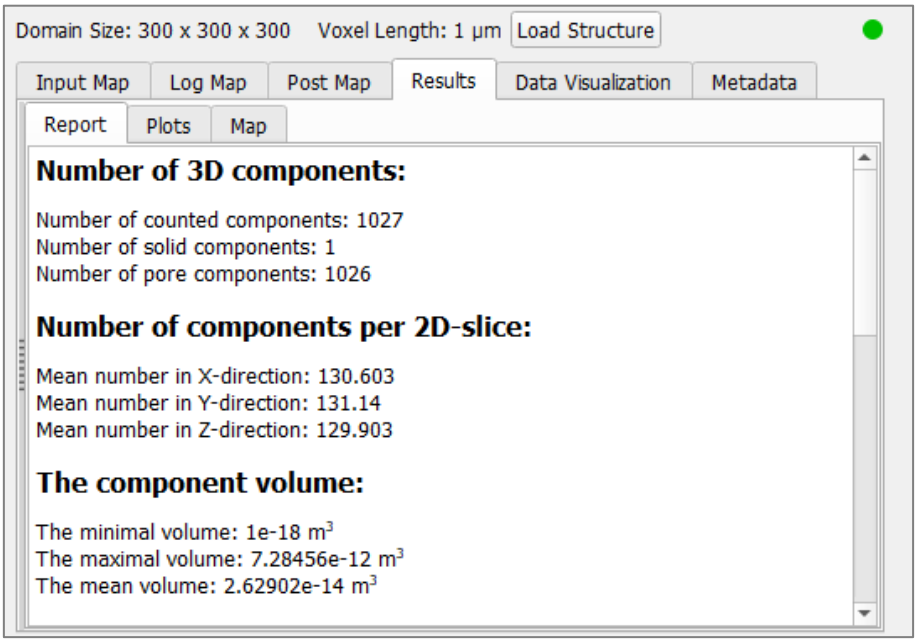
Under the **Post-Processing** tab, the settings used to create the histogram of the analyzed components are defined. It is possible to modify those settings after the computation has been run in the result viewer. The explanation of the input parameters is therefore given in the Results section below.

RESULTS

Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is opened in the **Result Viewer** after the computation is finished.

The left panel of the **Results** tab, can be collapsed (and expanded) by pulling left (or right) the dotted line between the post-processing options and the **Results** – **Report** subtab.

Under the **Results - Report** subtab, the information about the **Number of 3D components**, **Number of components per 2D-slice**, **The component volume** and the **Object volume histogram** is given.



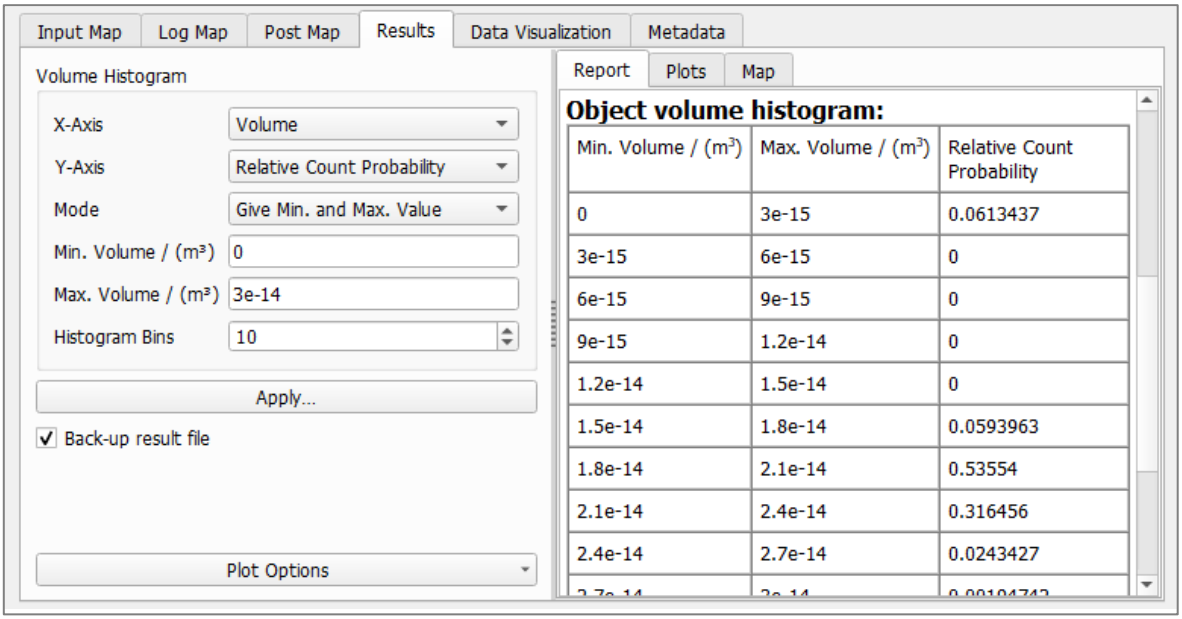
The object volume histogram is also shown under the **Results - Plots** subtab. In the plot, the values for each bin are visualized as bars.

As a post-processing step, the settings of the object volume histogram are adjusted and changed on the left-hand side panel, which can be expanded and collapsed as explained above. Edit the options and click **Apply** to fit values in the **Results** tabs.

The options are the same as the ones available under the **Post-Processing** tab in the Connected Components dialog.

The **X-Axis** pull-down menu allows choosing whether the components should be classified based on volume (**Volume**) or based on volume equivalent sphere diameter (**Equivalent Diameter**).

For the **Y-Axis** pull-down menu, the **Relative Count Probability** provides the number of components in each bin normalized to the total number of components.

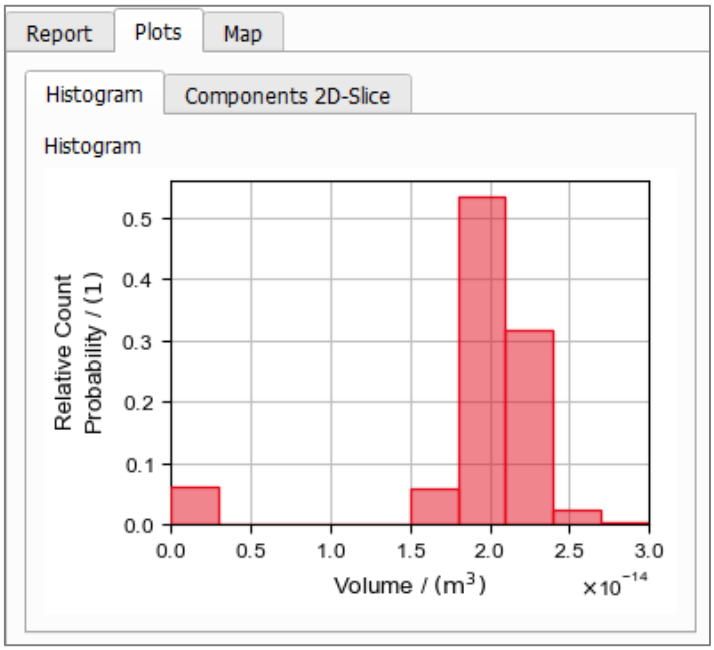


The **Cumulative Count Probability** is the sum of the Relative Count Probability over all bins starting from the smallest bin. **Relative Volume Probability** gives the volume of the components within one bin normalized to the total volume of all components. The **Cumulative Volume Probability** sums up the Relative Volume Probability of each bin of the histogram starting from the smallest one.

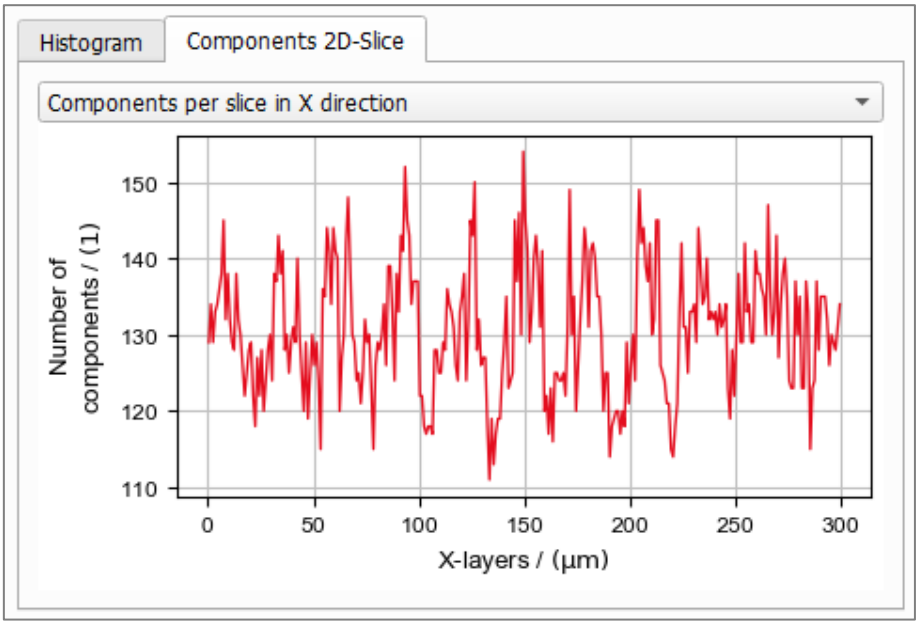
The histogram **Mode** offers the choice between generating an **Automatic Histogram** without further specifications or to **Give Min. and Max Value** for the parameter defined in the X-Axis pull-down menu (Volume or Equivalent Diameter). Either **Min. Volume** and **Max. Volume** or **Min. Diameter** and **Max. Diameter** can be directly entered here.

The number of **Histogram Bins** determines the number of rows in the **Object Volume Histogram** table.

The table and plot are updated when the **Apply...** button is clicked after changing the Volume Histogram input parameters.

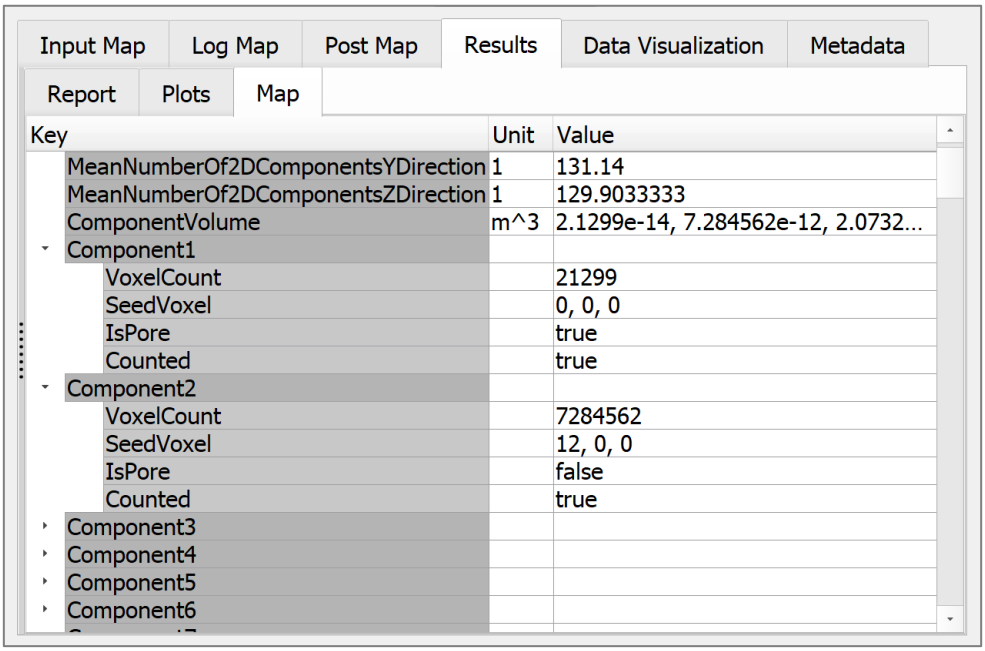


Under the **Plots** tab, also the computed **Number of Components per 2D Slice** is visualized by three graphs, which are selectable in the drop-down menu.



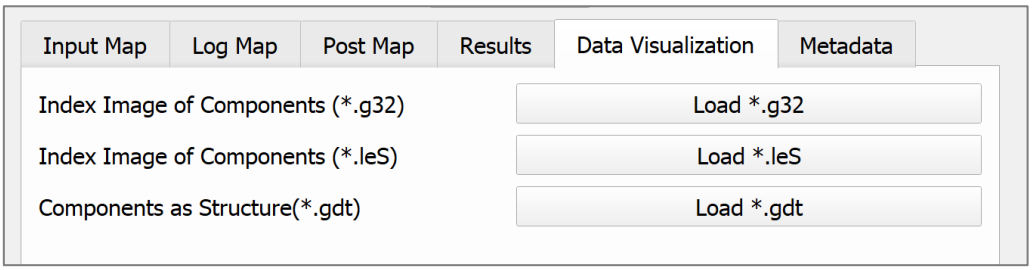
The **Results-Map** subtab additionally contains an overview of the computed parameters, such as component volume, number of 2D components in each direction and mean values of each. Moreover, the details for every found component are given:

- **VoxelCount** states the number of voxels inside of a component.
- **SeedVoxel** is an arbitrary voxel inside of this component.
- **IsPore** states if this component is pore or solid.
- **Counted** states if this component is counted.



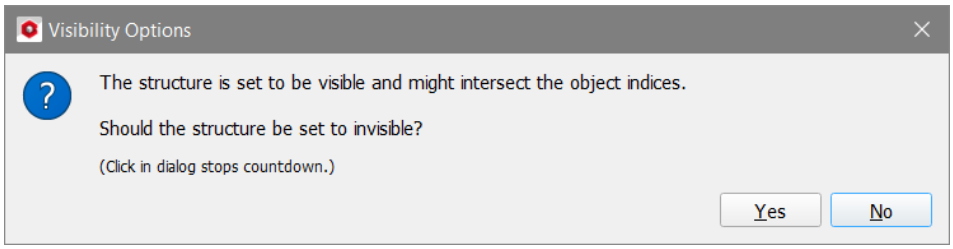
DATA VISUALIZATION

The detected connected components can be visualized in the GeoDict visualization area in two different ways.



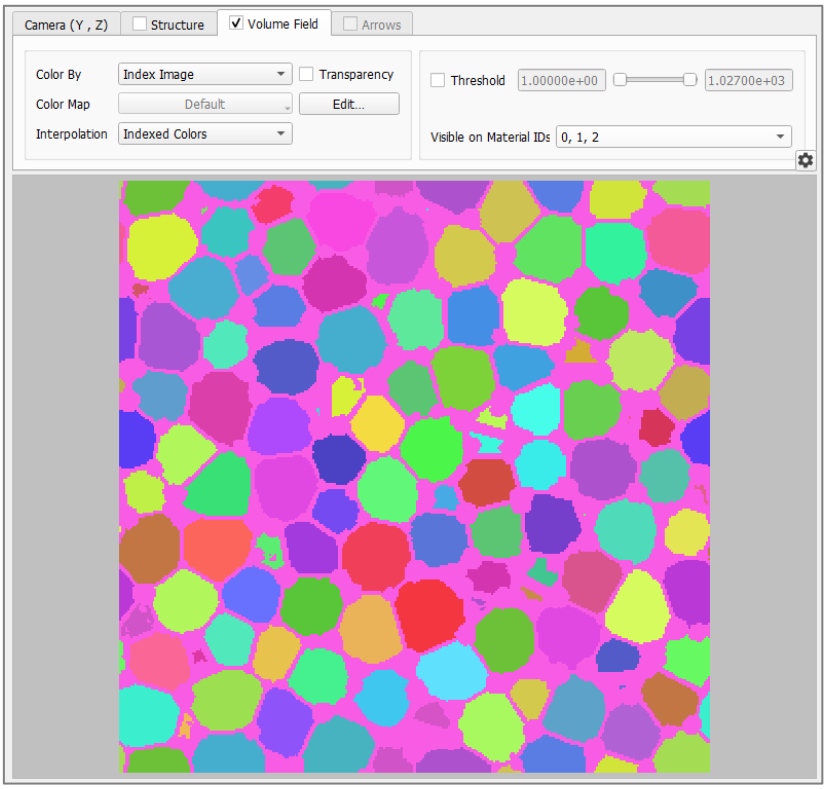
The first two options load the index image in *.g32 or *.leS format. These are 3D images, where for every voxel the index number of the corresponding component is stored. For example, if the structure consists of 1027 components, the file will contain numbers from 1 to 1027. Click **Load *.g32** or **Load *.leS** to load the index image.

After clicking **OK** in the appearing dialog, the **Visibility Options** dialog pops up.

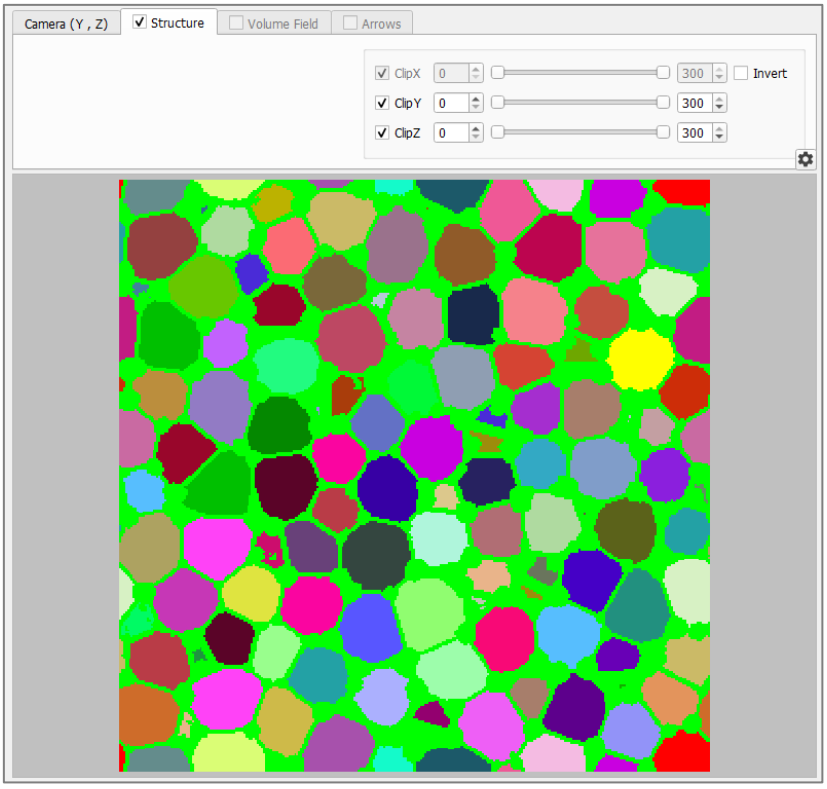


For the visualization of the index image, it is recommended to set the structure visualization to invisible by clicking **Yes**, so that the indices can also be seen in the solid parts of the structure.

In the index image visualization, every index is highlighted with a different color. The example below shows the index image of a closed-cell foam in 2D, where every cell of the foam belongs to another connected component of the pore space.



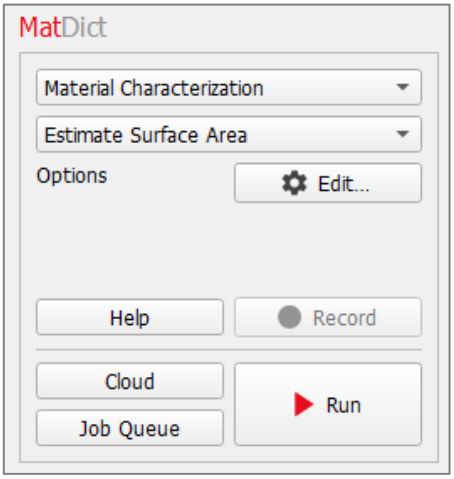
The third option is to load the components as a structure file in GeoDict's *.gdt file format. Every component is assigned a material ID based on the index number as shown in the following picture.

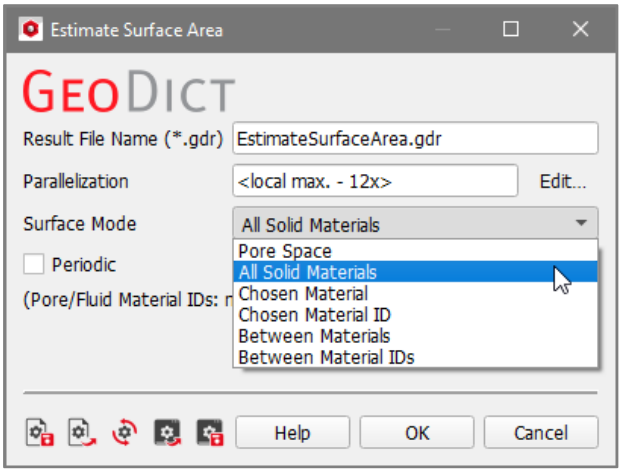


Be aware, that this format supports only 256 different material IDs. This might lead to neighboring components getting assigned to the same ID. In the example, every 255th foam cell gets assigned to the same ID as the cell walls, and therefore disappears in the visualization.

Estimate Surface Area

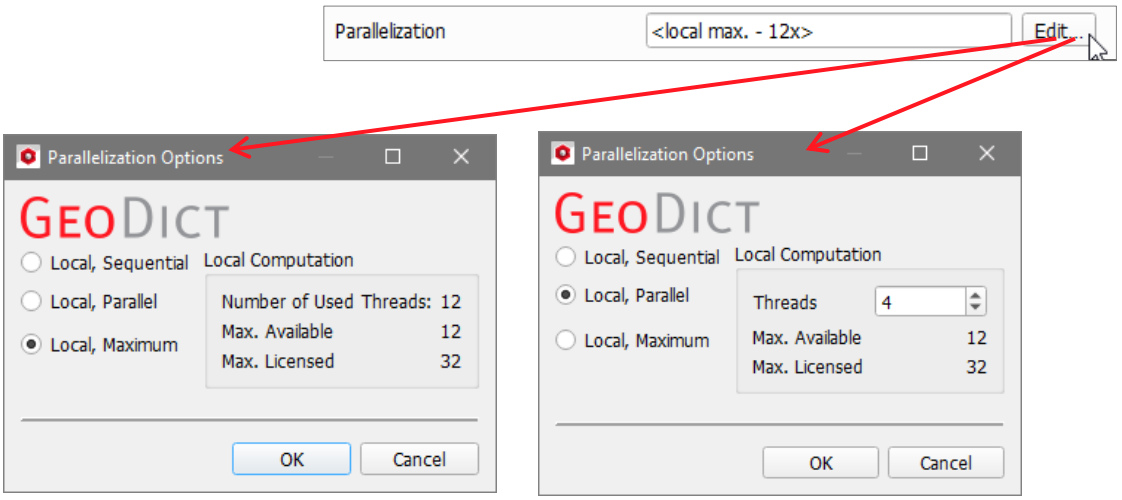
With **Estimate Surface Area**, the surface area of the structure is estimated with a method based on statistical measures. The **Estimate Surface Area** options open when clicking the **Options**' **Edit...** button.





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

Calculations can be parallelized if the user's license and hardware allow it. The **Parallelization Options** dialog opens when clicking the **Edit...** button, to choose between **Local, Sequential**, **Local, Parallel** or **Local, Maximum**.



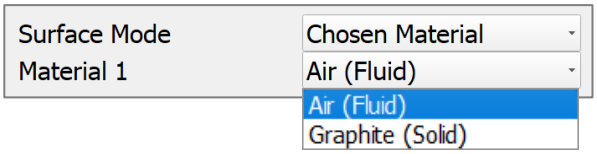
When **Local, Parallel** is selected, the number of **Threads** can be entered. Then the maximum number of available processors and the maximum number of licensed parallel processes is shown in the dialog.

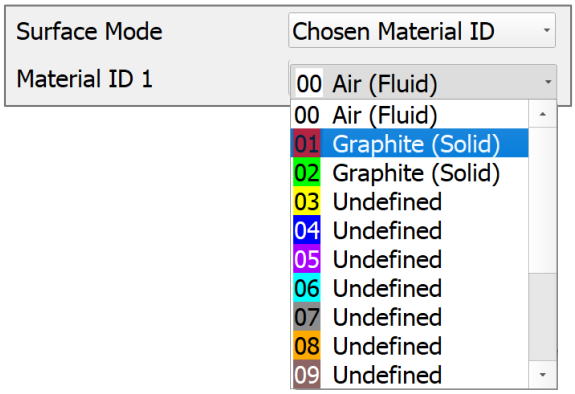
Under **Surface Mode** choose the materials or material IDs for which the surface area should be calculated. The surface is defined as the boundary between the chosen materials (material IDs) and all other materials (material IDs) or between two given materials (material IDs).

Pore Space computes the surface of the pore space, which is the union of *Pore* and all *Fluid* materials. It returns the same result as **All Solid Materials**, which computes the surface of all solid and porous materials combined to one material. Especially, **All**

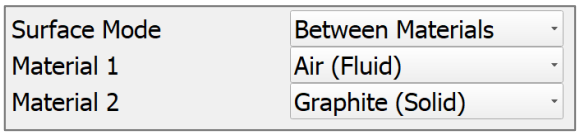
Solid Materials does not include the inner surfaces between different solid materials or material IDs.

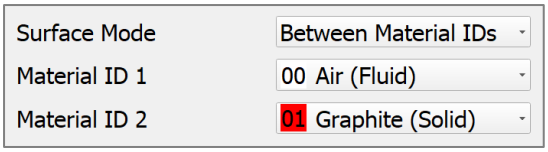
If **Chosen Material** or **Chosen Material ID** is selected, choose the desired material (material ID) from the pull-down menu that appears below.





For the surface modes **Between Materials** and **Between Material IDs** select the two materials (material IDs) to be considered for the surface area.





Selecting **Periodic**, the algorithm estimates the surface area assuming that the structure is periodic, so that the material that ends on one side of the volume reappears on the opposite side.

RESULTS

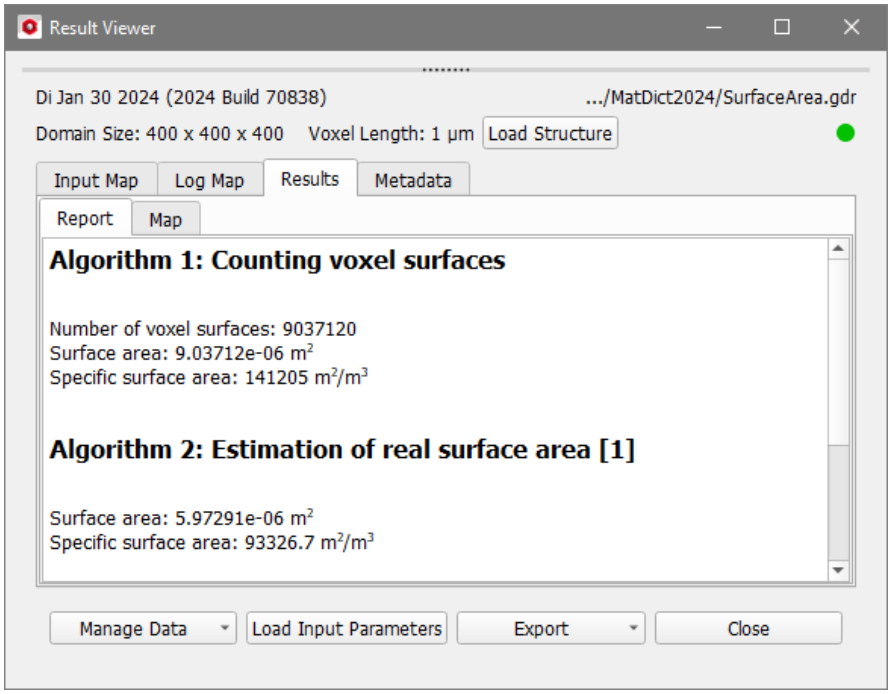
Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is opened in the **Result Viewer** after the computation is finished.

These values include the **Number of voxel surfaces**, the **Surface area**, and the **Specific surface area**, defined as the Surface Area normalized by the total volume of the structure.

Algorithm 1 computes the surface area by adding up the voxel surfaces.

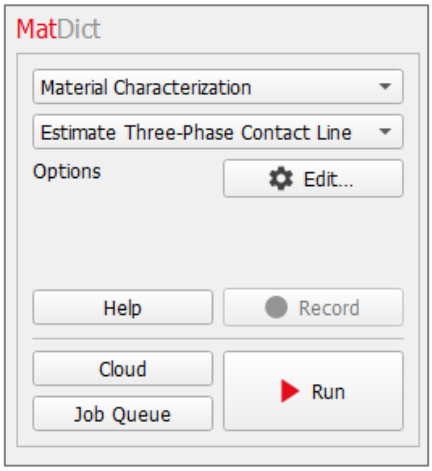
Algorithm 2 estimates the real surface area, originating from statistical image analysis, where the determination of the four Minkowski measures (Volume, Surface Area, Integral of mean curvature, Integral of total curvature, see also [2]) from voxelized images is an essential task.

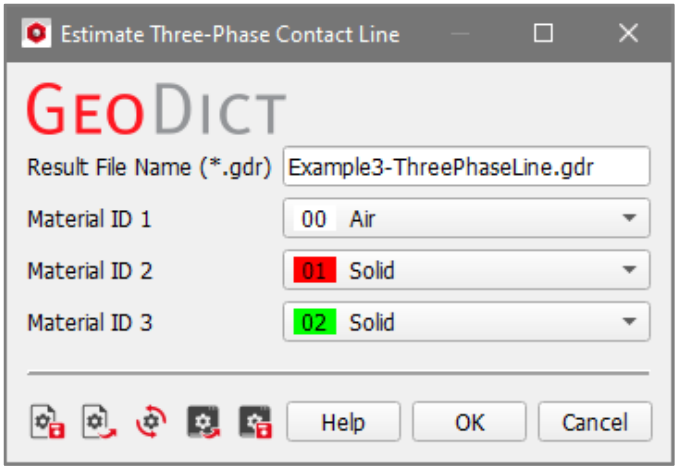
Algorithm 2 uses a staggered grid, which means it uses the voxel centers of the original grid as corners. In this grid, half a voxel cell is left over on each side. When using **Periodic** boundary conditions, those half-cells are completed across the domain boundary again to full grid cells, and this way the whole volume is taken into account. Without periodic boundary conditions, these half-cells are discarded. This means, that without periodic boundary conditions half a voxel is cut away on every side, so a slightly smaller volume is considered when computing the specific surface area.


Result Viewer
Di Jan 30 2024 (2024 Build 70838)
.../MatDict2024/SurfaceArea.gdr
Domain Size: 400 x 400 x 400
Voxel Length: 1 µm
Load Structure
Input Map
Log Map
Results
Metadata
Report
Map
Algorithm 1: Counting voxel surfaces
Number of voxel surfaces: 9037120
Surface area: 9.03712e-06 m²
Specific surface area: 141205 m²/m³
Algorithm 2: Estimation of real surface area [1]
Surface area: 5.97291e-06 m²
Specific surface area: 93326.7 m²/m³
Manage Data
Load Input Parameters
Export
Close

Estimate Three-Phase Contact Line

With **Estimate Three-Phase Contact Line**, the length of the contact line between the phases in a three-phase system and the number of voxel edges of the contact line in the cartesian directions can be computed. The **Estimate Three-Phase Contact Line** options are opened by clicking the **Options' Edit...** button.





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

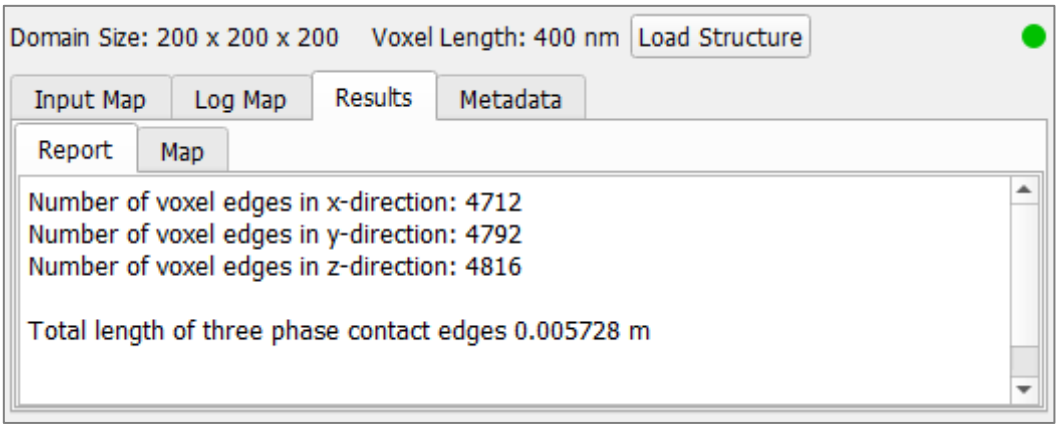
Through the **Material ID 1**, **Material ID 2**, and **Material ID 3** pull-down menus, the three-phase material IDs for which the **Three-Phase Contact Line** length should be computed are selected.

Results

Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is opened in the **Result Viewer** after the computation is finished.

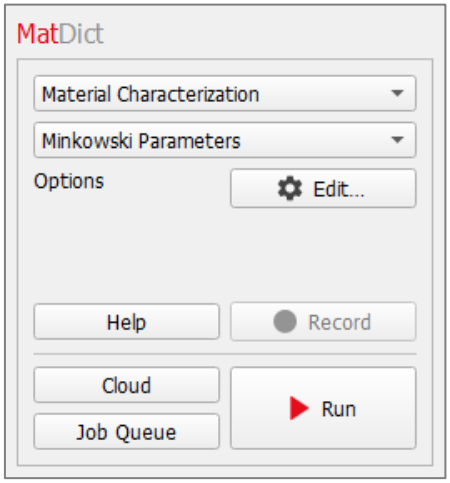
In this algorithm, all voxel edges are found that are adjacent to all three materials.

The report contains the computed values for **Number of voxel edges in x-, y-, and z-direction**, as well as the **Total length of three-phase contact edges**, which is computed by multiplying the sum of the above numbers with the voxel length.

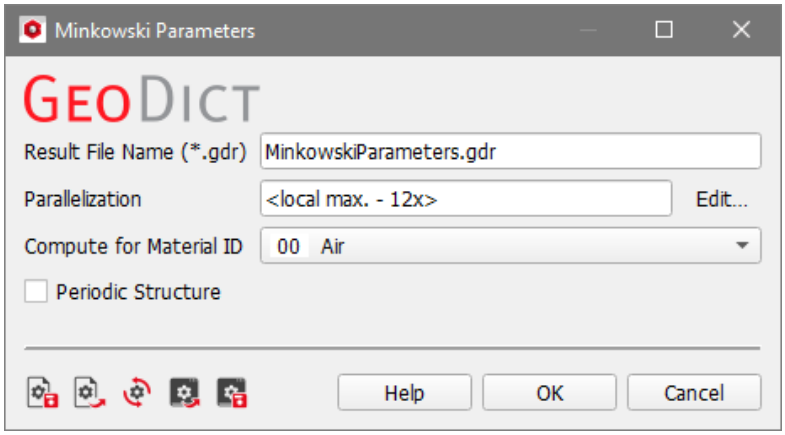


MINKOWSKI PARAMETERS

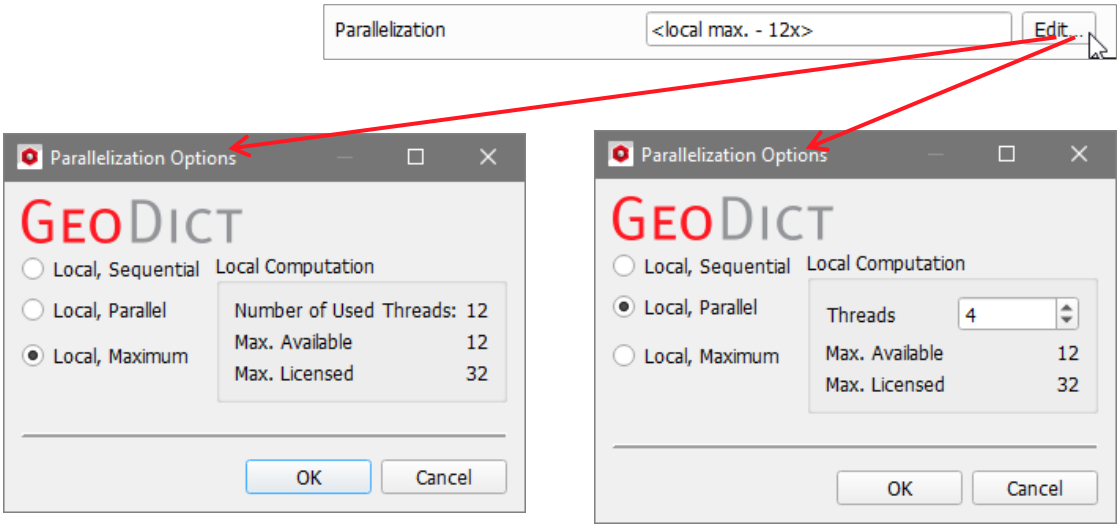
To compute the **Minkowski Parameters** (Volume, Surface Area, Integral of mean curvature, Integral of total curvature), the needed parameters can be entered by clicking the **Options' Edit...** button.



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



Calculations can be parallelized if the user's license and hardware allow it. The **Parallelization Options** dialog opens when clicking the **Edit...** button, to choose between **Local, Sequential**, **Local, Parallel** or **Local, Maximum**.



When **Local, Parallel** is selected, the number of **Threads** can be entered. Then the maximum number of available processors and the maximum number of licensed parallel processes is shown in the dialog.

Compute for Material ID defines the Material ID for which the Minkowski Parameters are computed.

Selecting **Periodic**, the structure is assumed to be periodic, so that the material that ends on one side of the volume reappears on the opposite side. Otherwise, symmetric boundary conditions are used.

RESULTS

Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is opened in the **Result Viewer** after the computation is finished. Under the **Results-Report** subtab the four **Minkowski Parameters** characterize the mathematical topology of the structure:

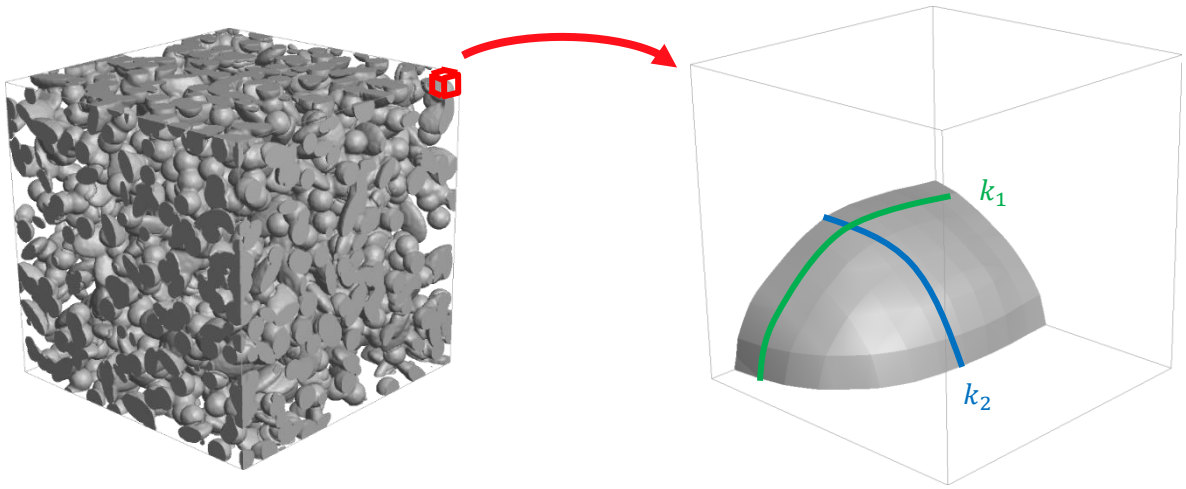
- The parameter **Volume** is the volume occupied of the chosen Material ID. Its percentage is also given by **Volume Fraction**.
- The **Surface area** is the boundary between the chosen Material ID and all other Material IDs. It is computed as in **Algorithm 2** of the **Estimate Surface Area** command (see also [2]).
- The **Integral of mean curvature** describes the mean curvature of the selected Material ID, given by the following formula:

$$C_M(X) = \frac{1}{2}\int_{\delta X} k_1 + k_2 \, \mathrm{d}s = \frac{1}{2}\int_{\delta X} \frac{1}{r_1(s)} + \frac{1}{r_2(s)} \, \mathrm{d}s \tag{2}$$

- And the **Integral of total curvature** describes the total curvature of the selected Material ID:

$$C_T(X) = \int_{\delta X} k_1 \, k_2 \, \mathrm{d}s = \int_{\delta X} \frac{1}{r_1(s) r_2(s)} \, \mathrm{d}s \tag{3}$$

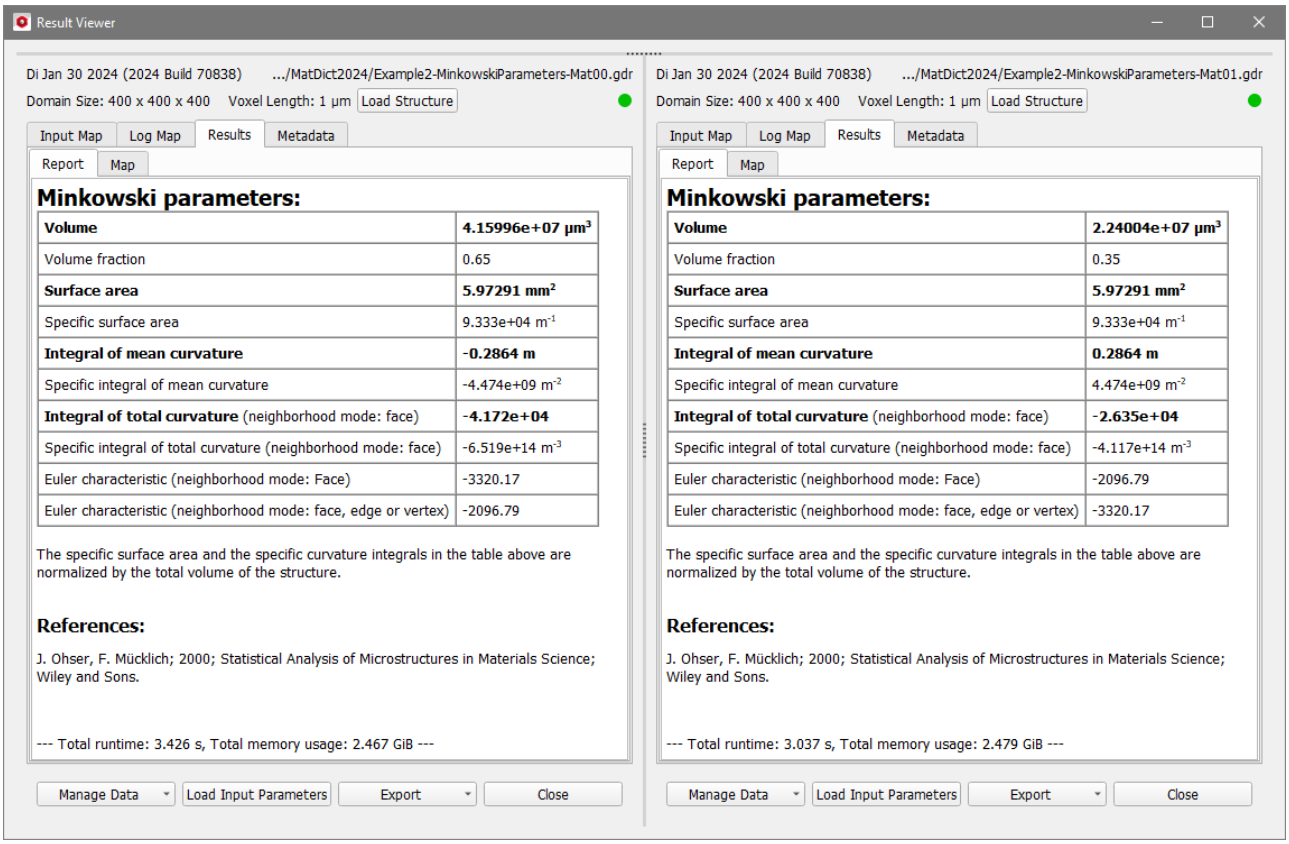
where X is the chosen material ID, s is a surface element of the chosen Material ID and the parameters $r_1(s)$ and $r_2(s)$ are defined as the radii of the two principal curvatures k_1 and k_2 from the respective surface element.



surface element s

The surface area and the curvature values are given additionally as specific values, which are normalized by the total volume of the structure.

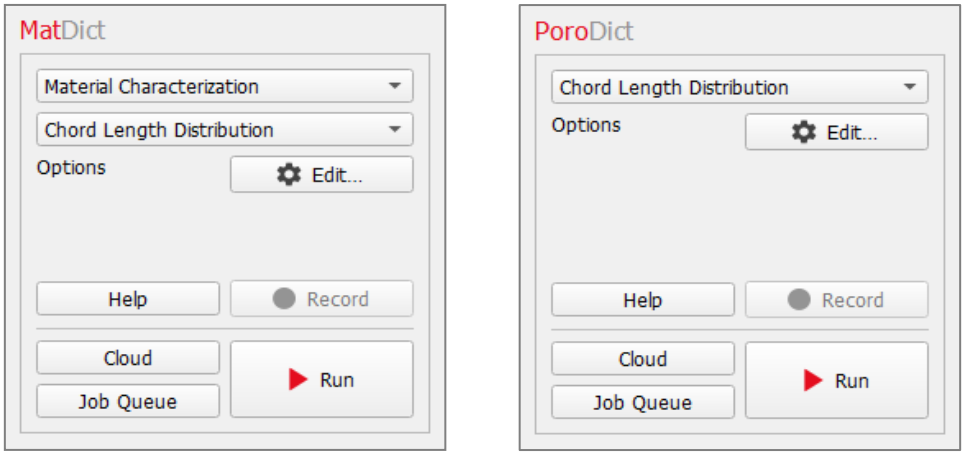
The **Euler characteristic** (E) is a topological number, that describes to what extent the structure is connected. It equals $\frac{1}{4\pi}$ times the integral of total curvature. This results in $E = N - L + C$, where N is the number of objects, L is the number of loops and C is the number of cavities.



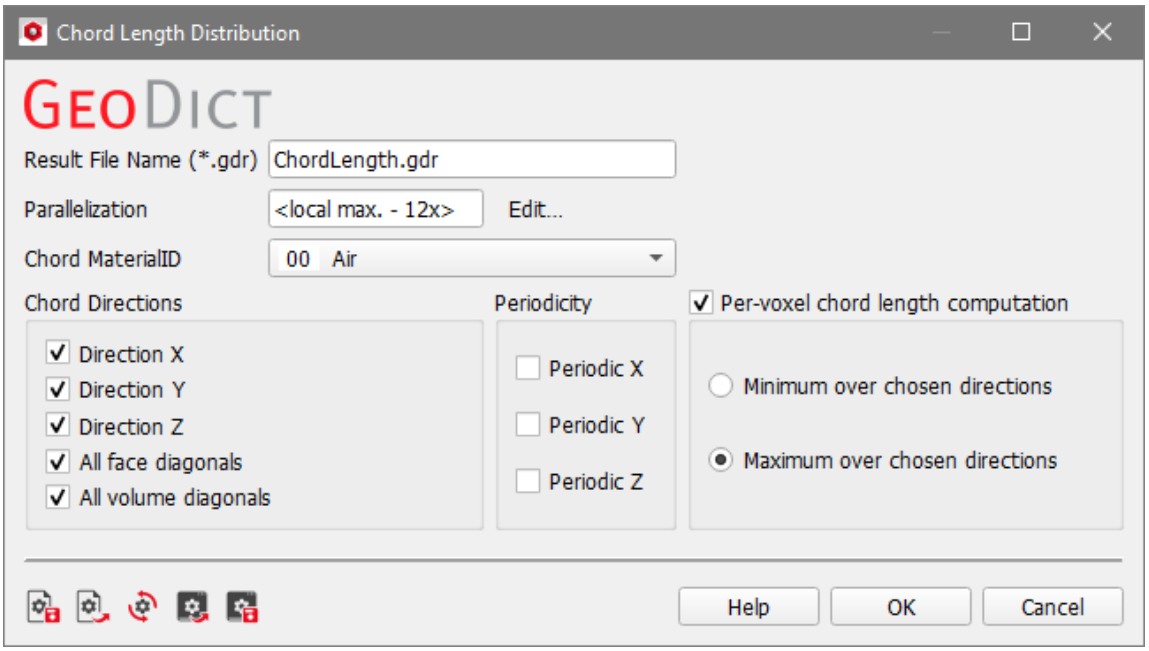
The screenshot shows the computed Minkowski parameters for the pore space (here material ID 00, on the left), and the solid material (ID 01, right) of the structure shown above.

Chord Length Distribution

The **Chord Length Distribution** command is accessible from MatDict and PoroDict. The **Chord Length** is defined as the number of connected voxels along the computational direction. Pseudo-code of the algorithm used for the computation can be found in [2]. After selecting **Chord Length Distribution** from the pull-down menu, the settings for the calculations can be modified through the **Edit...** button.

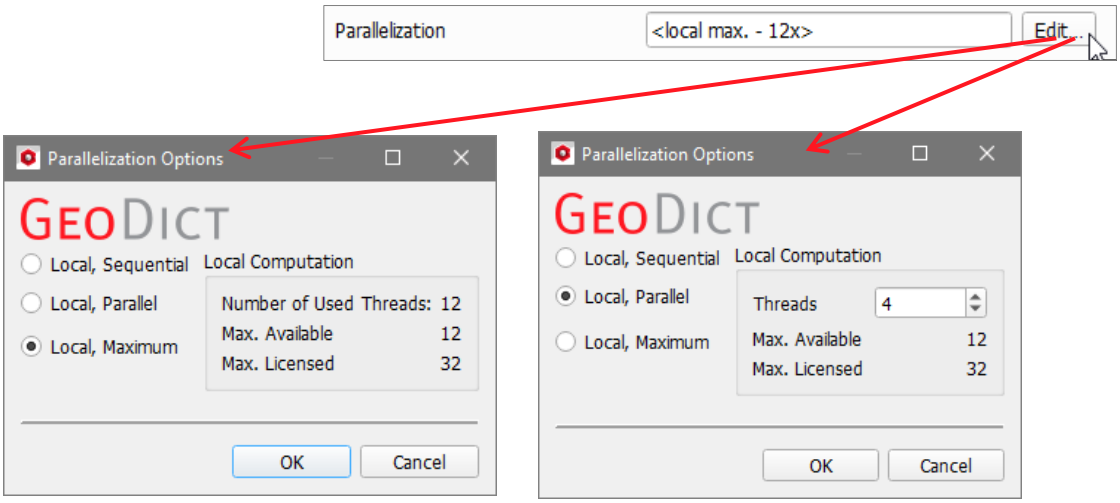


At the top of the dialog, enter the **Result File Name**. The result file is saved in the chosen project folder (**File → Choose Project Folder** in the menu bar).



Calculations can be parallelized if the user's license and hardware allow it. The **Parallelization Options** dialog opens when clicking the **Edit...** button, to choose between **Local, Sequential**, **Local, Parallel** or **Local, Maximum**.

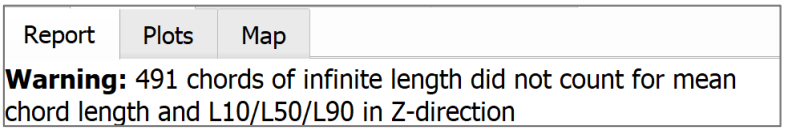
When **Local, Parallel** is selected, the number of **Threads** can be entered. Then the maximum number of available processors and the maximum number of licensed parallel processes is shown in the dialog.



In the **Chord Length Distribution** dialog, choose the material ID of the material (**Chord MaterialID**) for which the chord length distribution is to be calculated. This can be done for pore or solid materials alike.

In the **Chord Directions** section, select the direction(s) in which the chord lengths are determined. This can be done along the axes (**Direction X**, **Direction Y** or **Direction Z**), along the two-dimensional diagonals (**All face diagonals**), or along the three-dimensional diagonals (**All volume diagonals**).

Periodicity can be applied in the X-, Y-, and/or Z-direction for the calculation. Periodicity means, that chords continue on the opposite side of the domain. This can lead to infinitely long chord lengths, if a complete ray along the chosen direction is inside of the selected **Chord Material ID**. Such chords are neglected when computing the distribution results, and a warning is plotted on top of the resulting report if this occurs:



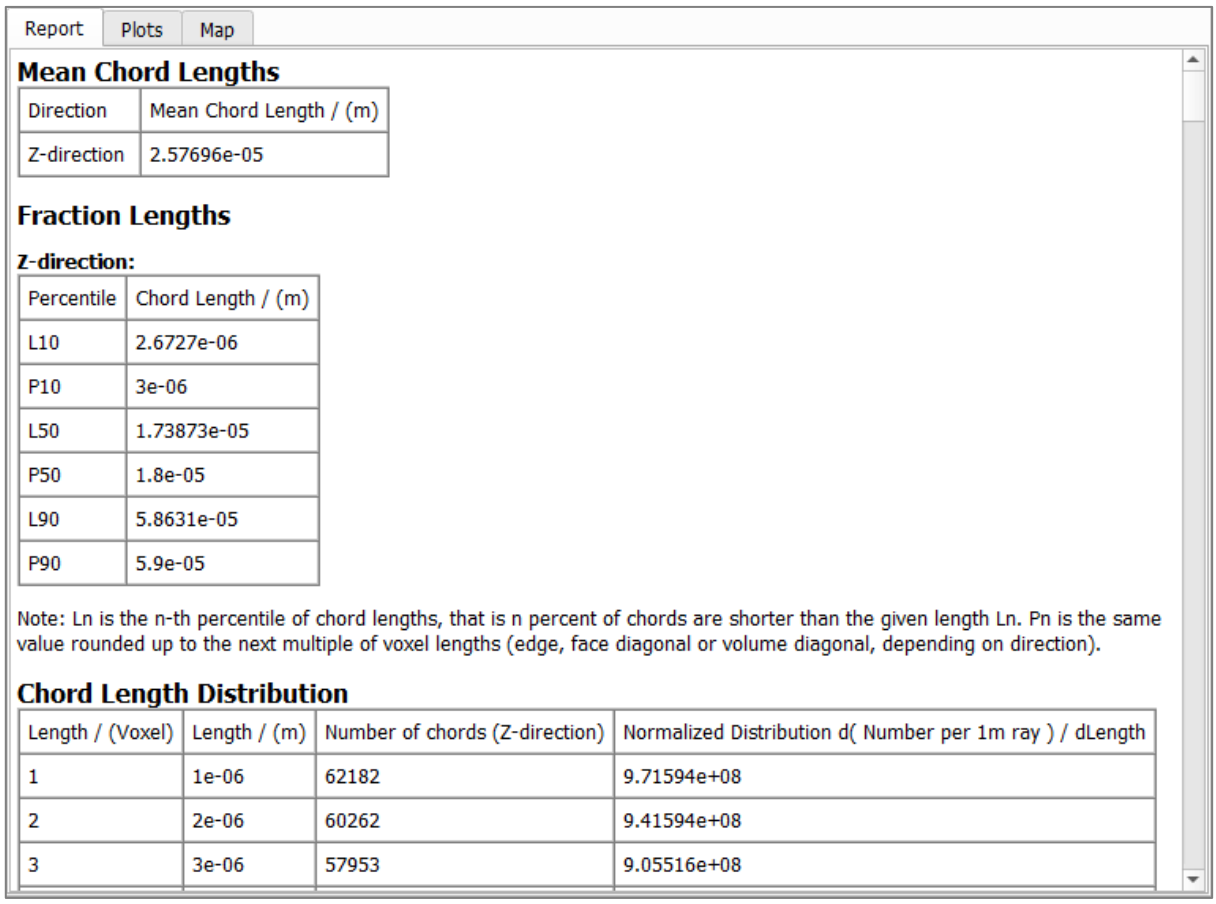
Check **Per-voxel chord length computation** for the output to include a scalar field in which, for each voxel, the length of the minimum or maximum chord through that voxel over all chosen directions is stored. For this, choose between **Minimum over chosen directions** or **Maximum over chosen directions**.

RESULTS

Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The Result Viewer opens at the end of the calculation.

Due to the voxelization, the chord length can only be measured in multiples of the voxel length. A chord length of *d* meters includes all chord lengths with a distance of half the voxel length around *d*. For example, a chord length of 2µm with voxel length 1µm actually means all chords between 1.5µm and 2.5µm.

Under the **Report** tab, the **Mean chord lengths**, the **Fraction lengths** L10, L50, L90 and P10, P50, P90 in the selected chord direction(s), and the complete **Chord length distribution** in the selected direction(s) is shown. The fraction lengths table reports the chord lengths smaller than 10%, 50%, 90% of all chord lengths (L10, L50, L90). The P-values (P10, P50, P90) are the same, but rounded up to the next largest multiple of the voxel length.



Report | Plots | Map

Mean Chord Lengths

Direction	Mean Chord Length / (m)
Z-direction	2.57696e-05

Fraction Lengths

Z-direction:

Percentile	Chord Length / (m)
L10	2.6727e-06
P10	3e-06
L50	1.73873e-05
P50	1.8e-05
L90	5.8631e-05
P90	5.9e-05

Note: Ln is the n-th percentile of chord lengths, that is n percent of chords are shorter than the given length Ln. Pn is the same value rounded up to the next multiple of voxel lengths (edge, face diagonal or volume diagonal, depending on direction).

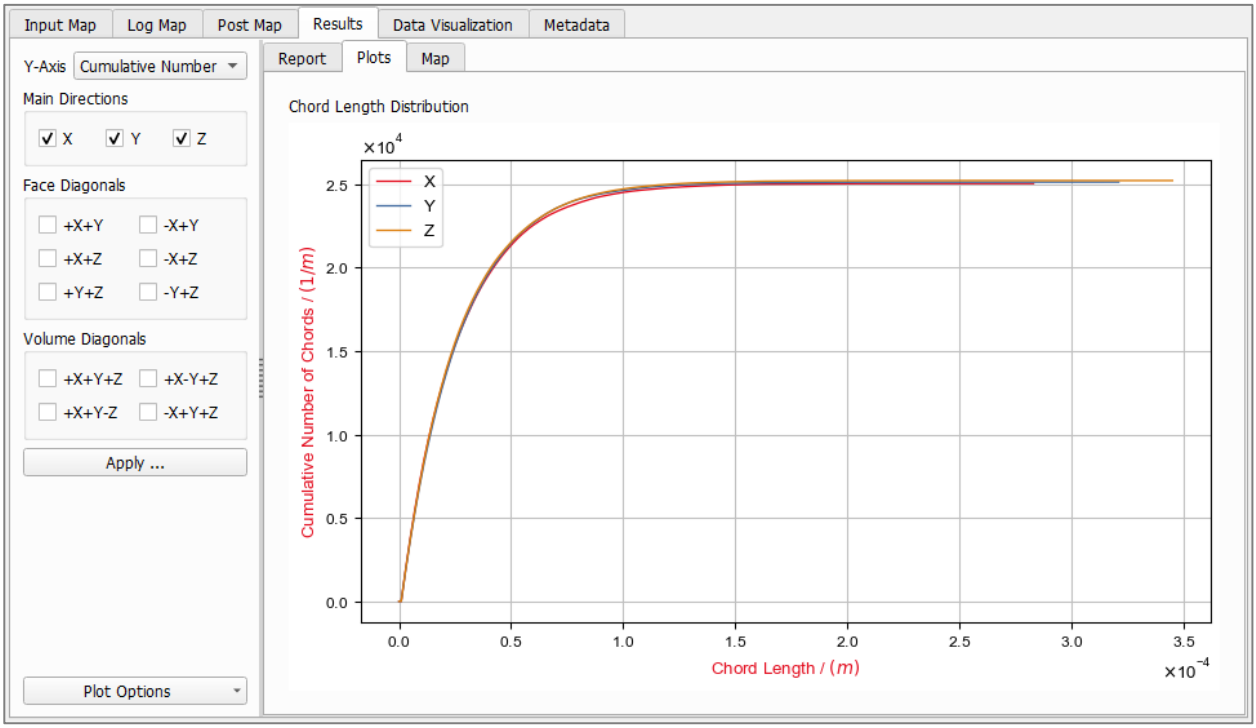
Chord Length Distribution

Length / (Voxel)	Length / (m)	Number of chords (Z-direction)	Normalized Distribution d(Number per 1m ray) / dLength
1	1e-06	62182	9.71594e+08
2	2e-06	60262	9.41594e+08
3	3e-06	57953	9.05516e+08

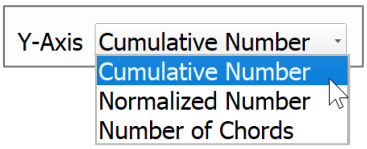
For example, a L10 of 2.6 µm means that 10% of all chords are smaller than this length. A L50 of 17.4 µm means that 50% of all chords are smaller than this length. A L90 of 58.6 µm means that 90% of all chords are smaller than this length.

For P10 the L10 value of 2.6 is rounded up to 3e-6 and means that this length (3 µm) is larger than or equal to the length of 10% of all chords. A P50 of 1.8e-5 means that this length (18 µm) is larger than or equal to the length of 50% of all chords. A P90 of 5.9e-5 means that this length (59 µm) is larger than or equal to the length of 90% of all chords.

The plot of the computed chord length distribution appears under the **Results-Plots** subtab.



In the context menu shown on the left, the chord length distribution plot can be customized. For the **Y-Axis**, the **Cumulative Number**, the **Normalized Number**, or the **Number of Chords** can be selected.



The normalized number of chords is the difference quotient of the cumulative chord length distribution, where the step size is the current voxel length.

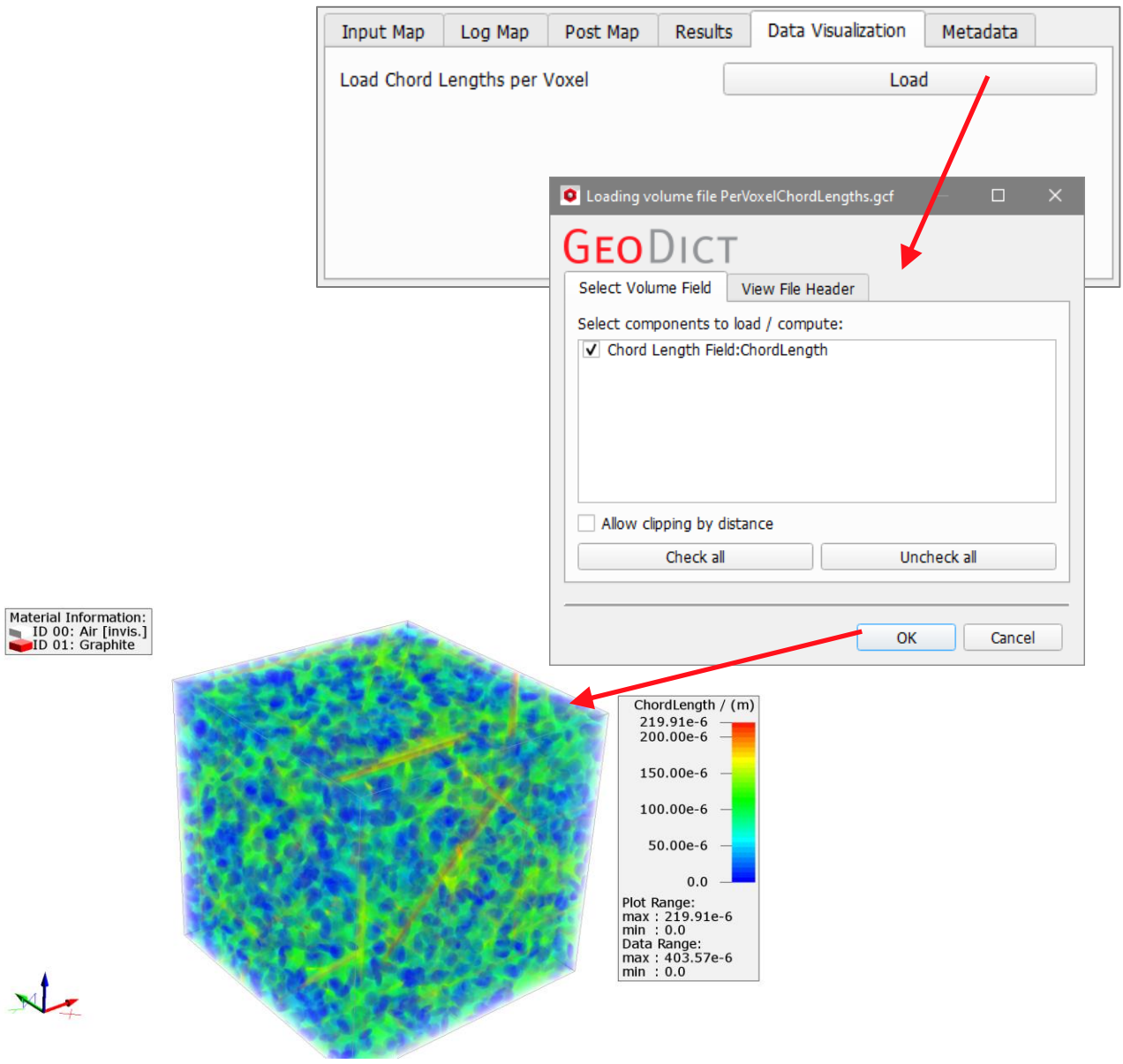
Alternatively, the normalized number of chords can also be obtained from the number of chords histogram. For example, the normalized number of chords in X-direction can be computed as follows: First, the number of chords is divided by NY*NZ, which equals the total number of rays, to obtain the number of chords per ray. Then, this number is normalized by NX*voxel length to obtain the number of chords per meter. As the accuracy of the measurement of the chord length is restricted by the voxel length, the histogram bin size is also given in voxels. To reflect this, the number of chords per meter must again be divided by the voxel length (which equals the bin size) in the last step. This allows to compare results for structures with different voxel lengths.

In addition, if more than one direction was chosen for the computations, it can be chosen for which directions the distribution should be shown (**Main Directions**, **Face Diagonals**, **Volume Diagonals**).

Click **Apply...** to update the shown plot.

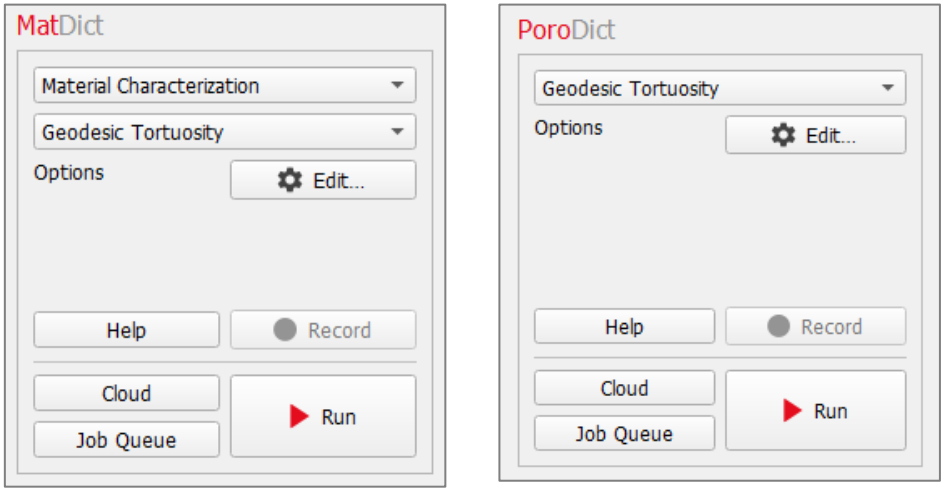
Data Visualization

By clicking the **Load** button under the **Data Visualization** tab, the corresponding per voxel chord length can be loaded and visualized over the structure, if **Per-voxel chord length computation** was previously checked (see page 48).

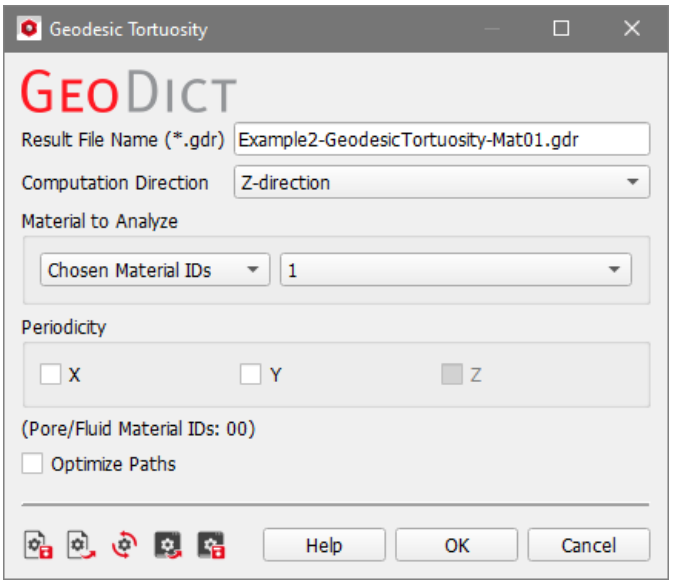

Input Map
Log Map
Post Map
Results
Data Visualization
Metadata
Load Chord Lengths per Voxel
Load
Loading volume file PerVoxelChordLengths.gcf
GEODICT
Select Volume Field
View File Header
Select components to load / compute:
Chord Length Field:ChordLength
Allow clipping by distance
Check all
Uncheck all
OK
Cancel
Material Information:
ID 00: Air [Invis.]
ID 01: Graphite
ChordLength / (m)
219.91e-6
200.00e-6
150.00e-6
100.00e-6
50.00e-6
0.0
Plot Range:
max : 219.91e-6
min : 0.0
Data Range:
max : 403.57e-6
min : 0.0

GEODESIC TORTUOSITY

The **Geodesic Tortuosity** command is accessible from MatDict and PoroDict. It computes the tortuosity of paths crossing the material, either through pore space or through solid materials.



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



Set the direction of the paths by selecting the **Computation Direction**.

The algorithm searches for paths in the selected **Material to Analyze**, either **Pore Space**, **All Solid Materials**, **Chosen Material**, or a list of **Chosen Material IDs**.

Paths might leave the domain and enter again on the opposite side if **Periodicity** is selected for this direction. The chosen computational direction cannot be chosen to be periodic. The option **Optimize Paths** is explained on page 30.

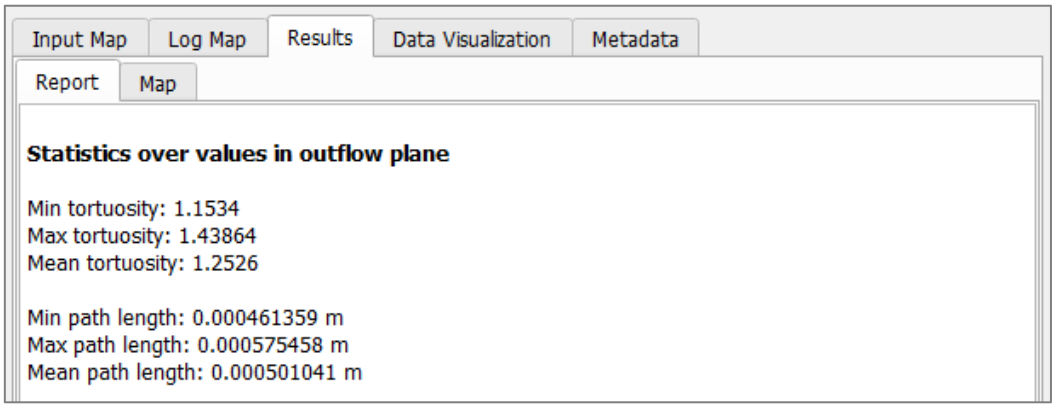
RESULTS

Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The Result Viewer opens at the end of the calculation.

For every voxel on the outflow plane, the algorithm finds the shortest path through the selected **Material to Analyze**. The corresponding geodesic tortuosity is then computed as

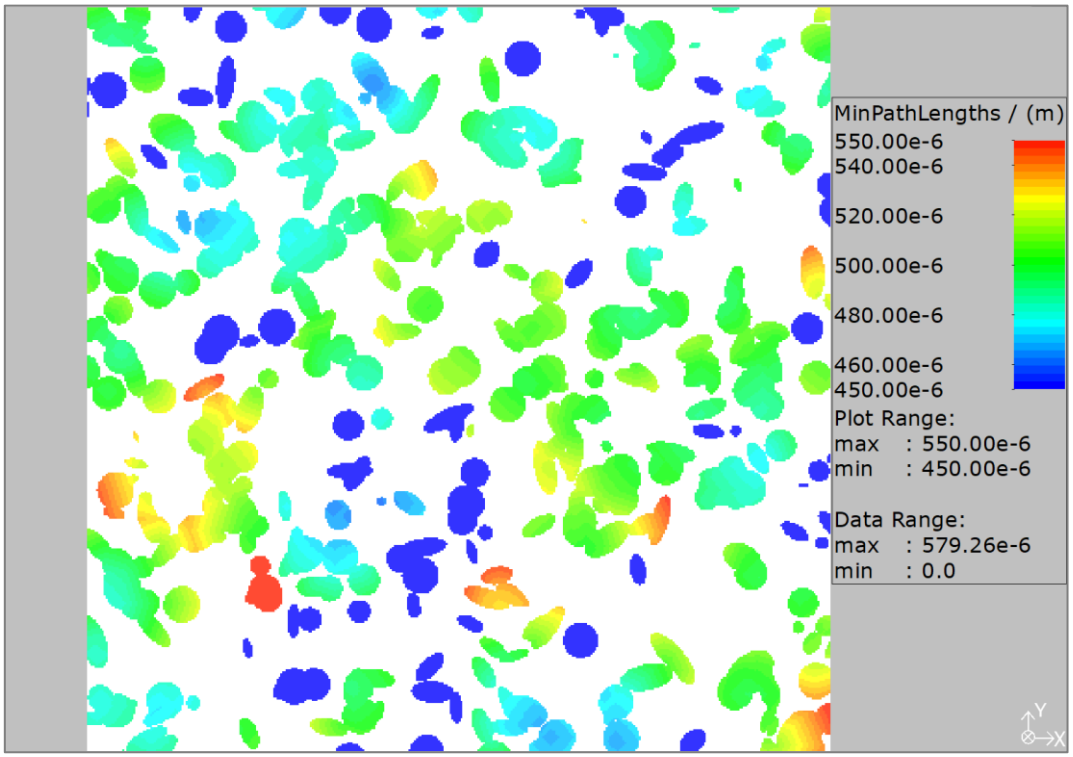
$$\tau = \frac{\text{shortest path to inflow plane}}{\text{distance to inflow plane}} \tag{4}$$

In the **Report** tab, the minimal, maximal, and mean geodesic tortuosity are shown. The corresponding minimal and maximal path lengths and the mean length of all paths are also given.



Data Visualization

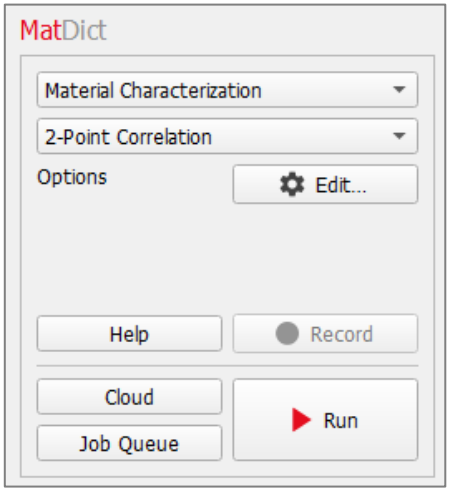
When clicking the **Load** button under the **Data Visualization** tab, the scalar **geodesic tortuosity field** is loaded. It contains for each voxel inside the selected material the shortest path distance between this voxel and the inflow plane. Therefore, on the inflow plane all voxels contain the value 0. Shown below are voxels on the outflow plane, where the voxel values show the computed path lengths as given above. Their local distribution around the mean value of 501 µm can be observed.

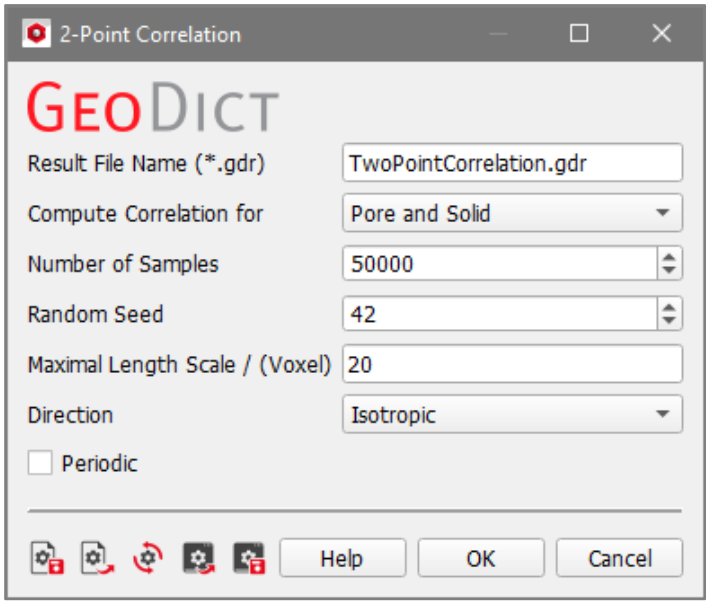


2-Point Correlation

The **2-Point Correlation** command computes the probability for two points having a certain distance to be correlated, which means that they belong to the same type.

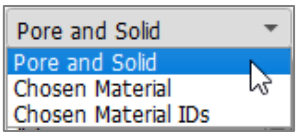
The **2-Point Correlation** dialog opens when clicking the **Options' Edit...** button.





At the top of the **2-Point Correlation** dialog, enter the **Result File Name**. The result file is saved in the chosen project folder (**File** → **Choose Project Folder** in the menu bar).

Next, decide to **Compute Correlation for** either **Pore and Solid**, **Chosen Material** or **Chosen Material ID**.



Using the mode **Pore and Solid**, two points are positively correlated if they both belong to Pore or both belong to Solid. They are negatively correlated if one point belongs to pore and the other to solid.

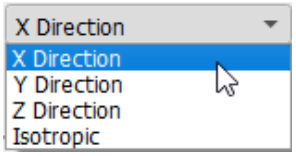
For **Chosen Material** two points are positively correlated if they belong to the same material. They are negatively correlated if the two points belong to different materials.

For **Chosen Material ID** two points are positively correlated if they have the same Material ID. They are negatively correlated if they have different Material IDs.

To find the probability distribution for different distances, several samples of point pairs for each distance are generated. The **Number of Samples** can be entered in the dialog and the **Random Seed** can be specified. For different random seeds different randomly chosen points are compared if they belong to the same type. If yes, the autocorrelation value is 1, otherwise -1. For distance 0, the correlation is always 1, since a voxel has always the same Material ID as itself. Then for each distance an average probability is computed, which is more accurate the more samples are taken.

The **Maximal Length Scale/(Voxel)** defines the largest distance for which the probability is computed.

The distance can be measured either in **X Direction, Y Direction** or **Z Direction** or in all three directions by choosing **Isotropic**.



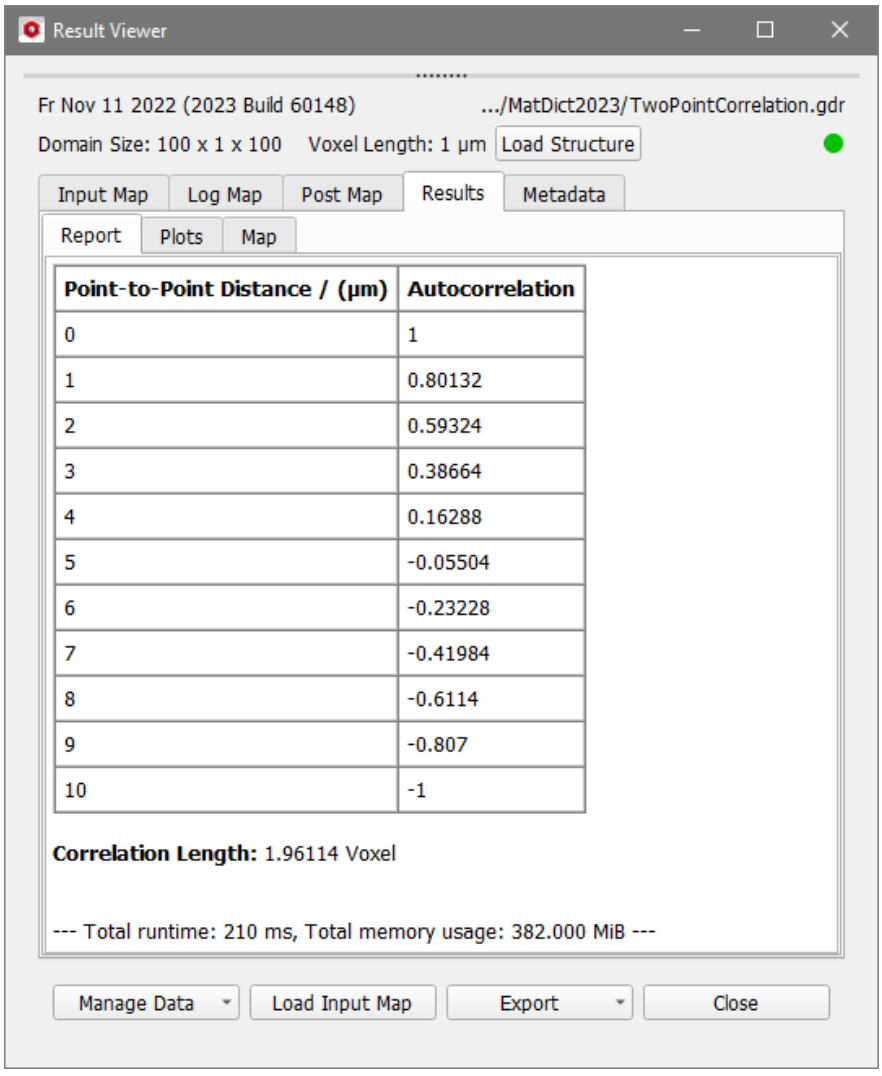
If **Periodic** is chosen, the structure is assumed to be periodic in the chosen computational directions. Thus, the autocorrelation repeats periodically for distances larger than the domain size. If Periodic is not checked, only distances smaller or equal than the domain size in the computational direction are allowed. If Isotropic is chosen as direction, the distance is not allowed to be larger than the smallest domain length.

RESULTS

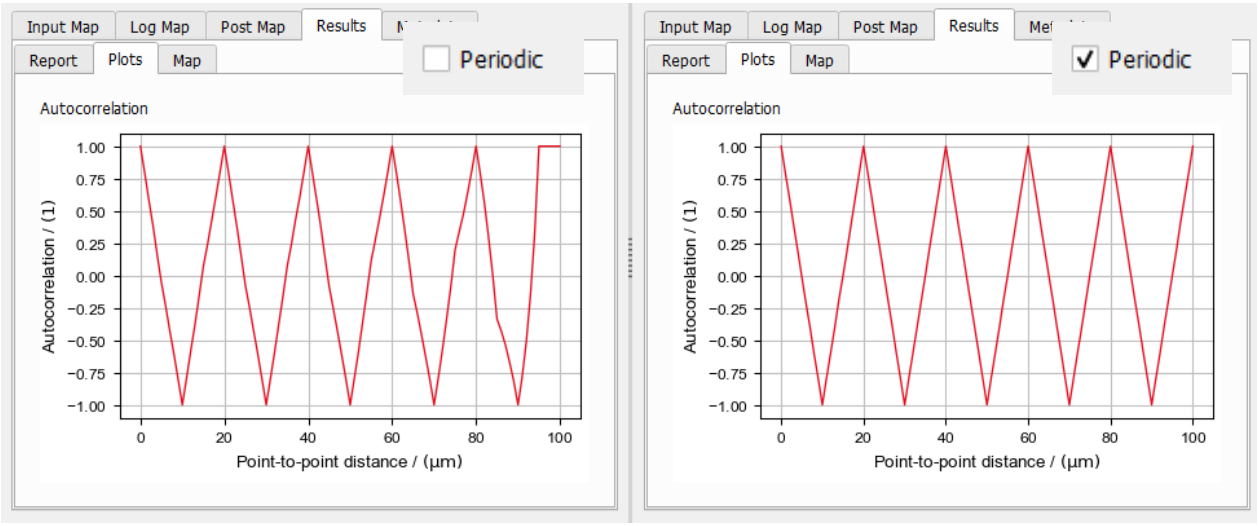
Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The Result Viewer opens at the end of the calculation.

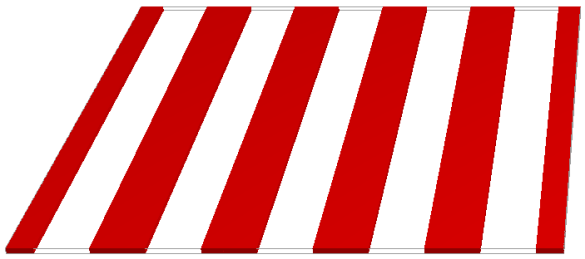
In the Results – Report tab a table shows for each distance the computed autocorrelation of two points having this distance. At the bottom, the **Correlation Length** in voxel is given.

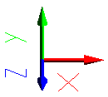
In the **Report – Plots** subtab the values from the table are graphically shown.



In the example below, a structure with bars of width 10µm each and space of 10µm between them is shown. The voxel length is 1µm and the structure has a size of 100x1x100 voxel. The 2-point correlation is computed in X Direction and with a maximal distance of 100 Voxel. Compare the results with and without **Periodic** checked.



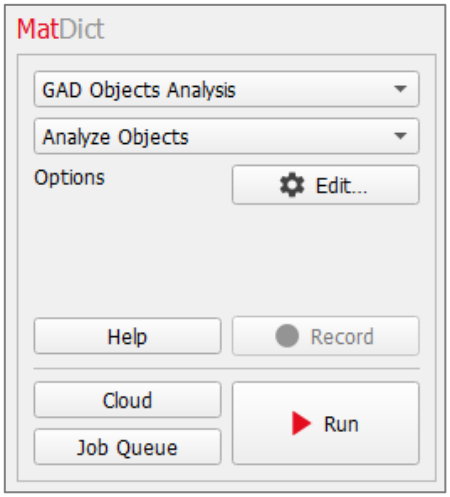


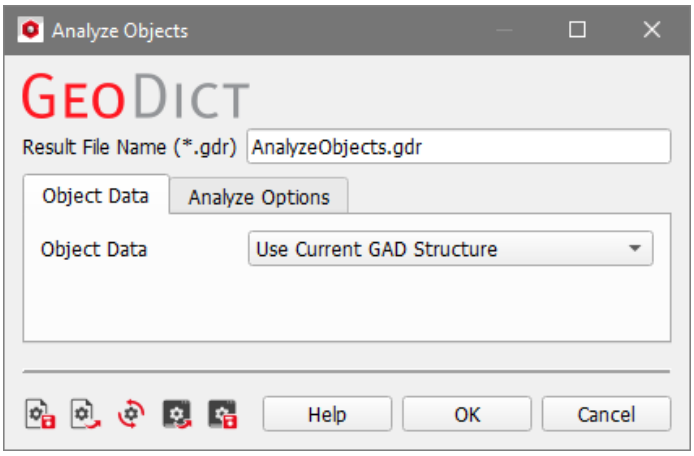


GAD Objects Analysis

Analyze Objects

With the **Analyze Objects** command, it is possible to analyze the geometrical objects forming the 3D micro-structure, e.g. fibers, spheres or ellipsoids, and how they are in contact with each other. Therefore, this command requires that the structure is not only described by a voxel grid, but also that the underlying analytic **Object Data** is available.





The **Analyze Objects** dialog opens when clicking the **Options**' **Edit...** button and includes the **Object Data** and the **Analyze Options** tabs.

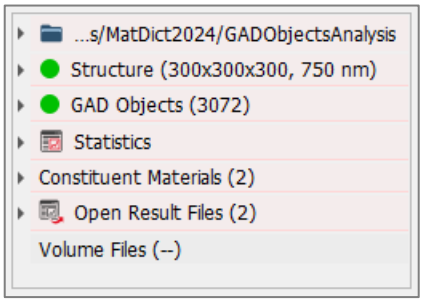
At the top of the dialog, enter a name for the **Result File Name**.

Object Data

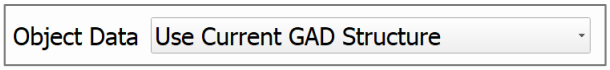
The necessary geometrical information, required by the analysis can be taken from two different sources:

1. The information is already available for the current 3D structure.

   If this is the case, a green dot is displayed in the **GAD Objects** row in the **Project Status** section, at the left of the GUI.



   To use the current object information, set **Object Data** to **Use Current GAD Structure.**

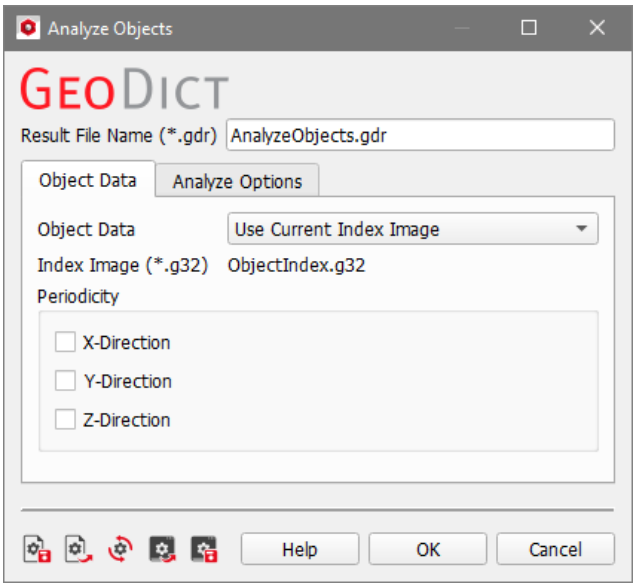


2. The second option is to use an Index Image (*.**g32 File**).

   This file type might be the result of object analysis commands in GeoDict, e.g. MatDict's Connected Components analysis.

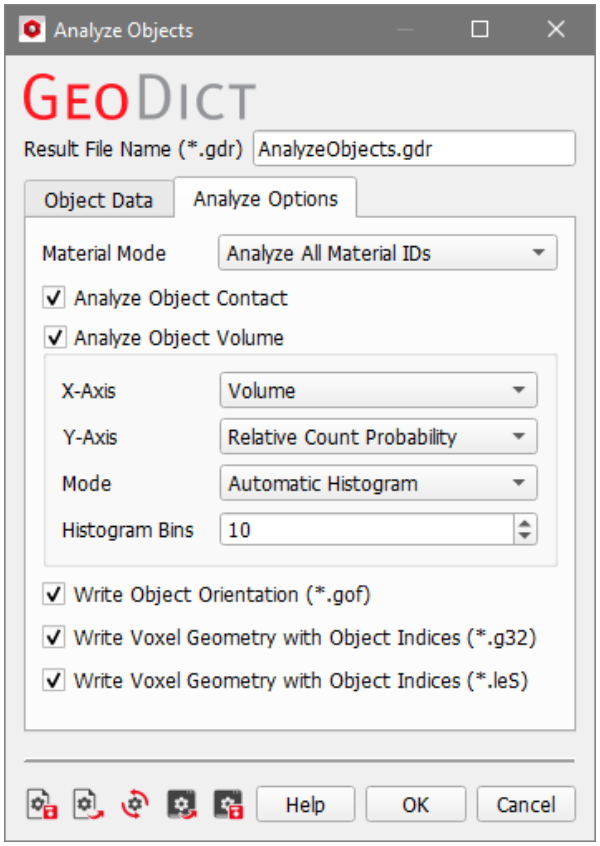
   To use this option, a *.g32 file must be loaded as Volume Field. Then set **Object Data** to **Use Current Index Image**.

   Additionally, the periodicity may be chosen



ANALYZE OPTIONS

In the **Material Mode** pull-down menu, choose **Analyze All Material IDs** to analyze all materials present in the structure, or select **Analyze Selected Material ID** to analyze only one material. This material ID must be chosen from the corresponding pull-down menu.



The number of GAD objects and their overlap percentage are computed. Additionally, a *.gdt file with the objects and their overlaps is written and saved as **ObjectsAndOverlap.gdt** in the result folder.

When **Analyze Object Contact** is checked, the number of contacts, the contact area, and the mean coordination number are computed.

When **Analyze Object Volume** is checked, the volume of each object is computed, and a histogram of all object sizes is created. The parameters in the panel below the checkbox describe the settings for the object volume histogram plot. They can be changed in the post-processing step and are explained in the Results section below.

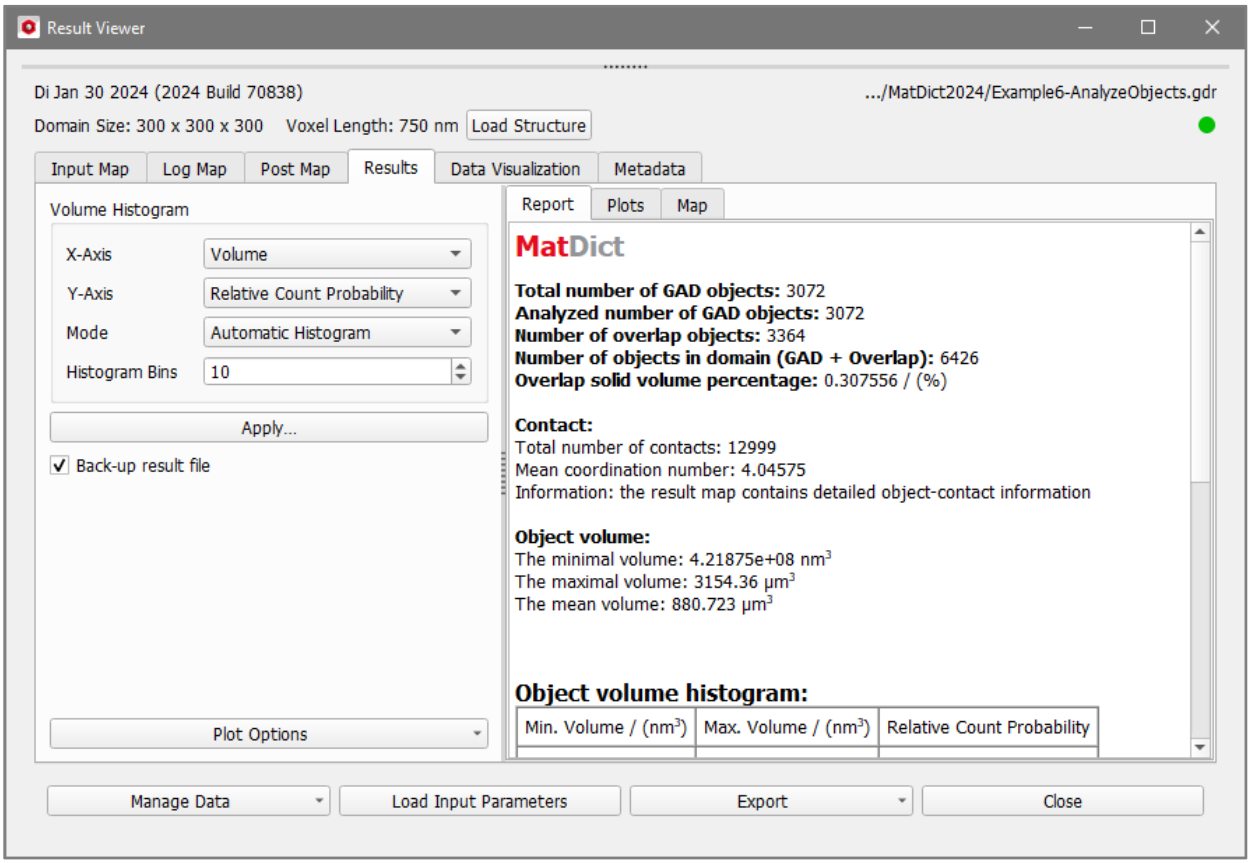
If **Use Current GAD Structure** is selected in the **Object Data** tab, the following options are available under the **Analyze Options** tab:

When checking **Write Object Orientation (*.gof)**, the data on the orientation of the objects is saved as **ObjectOrientation.gof** in the project folder.

When checking **Write Voxel Geometry with Object Indices (*.g32)** or **Write Voxel Geometry with Object Indices (*.leS)**, the objects are saved into a 3D image file in which the object ID corresponding to each voxel is stored. Choosing these options generates one file in GeoDict's format in binary format (*.g32) and one file in ASCII (*.leS).

RESULTS

Click **OK** to input the entered parameters (here, **Use Current GAD Structure** was used), and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is opened in the **Result Viewer** after the computation is finished.

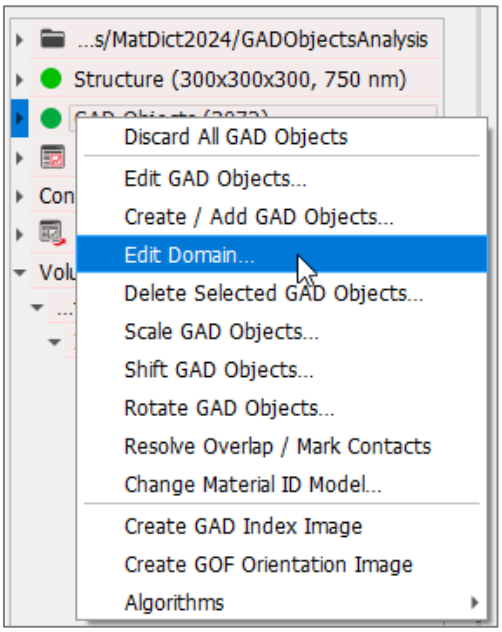


In the **Results - Report** subtab, the following values are reported:

- **Total number of GAD objects** is the number of all objects present in the 3D structure.
- **Analyzed number of GAD objects** is the number of objects considered in the analysis. This number is different from the above number if **Analyze Selected Material ID** was chosen. In this case only the number of GAD objects of the selected material ID is reported here.
- The **Number of overlap objects** shows how many overlap objects are present in the structure.
- The **Number of objects in domain (GAD + Overlap)** is the sum of the total number of GAD objects and the number of overlap objects inside the current domain. It is possible that some objects lie completely outside of the domain, and in this case, they are not counted here.
- **Overlap solid volume percentage** is the volume fraction of the overlap objects.

The resulting numbers depend on the way overlapping objects are treated. How overlap is handled is typically defined at the creation of the structure but can also be modified later using the **Edit Domain** command from the **Objects**' context menu.

See the GadGeo handbook for a more detailed description of this command.

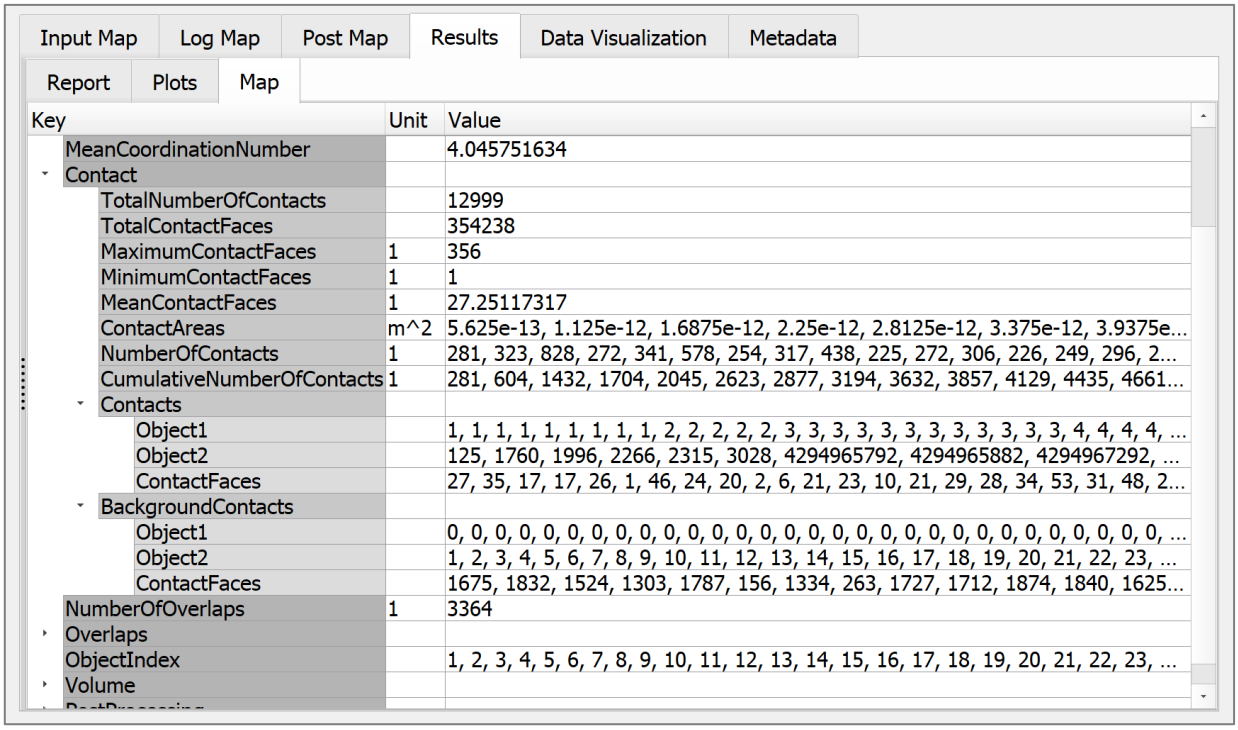


If **Analyze Object Contact** was checked (see page 59), the total number of contacts and the mean coordination number are reported in the **Contact** section of the report.

Here, the **Mean Coordination Number** is defined as

2 * Total Number of Contacts / Number of Objects in Domain (GAD + Overlap)

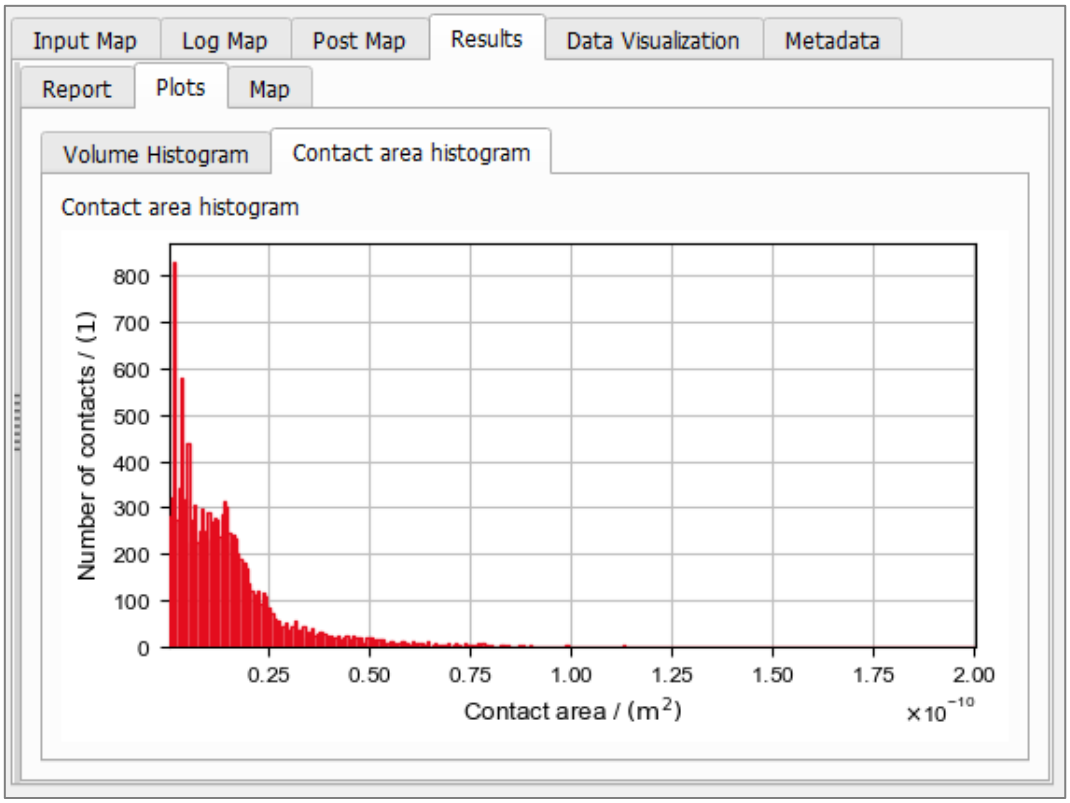
More detailed results for all contacts are available under the **Results - Map** subtab:



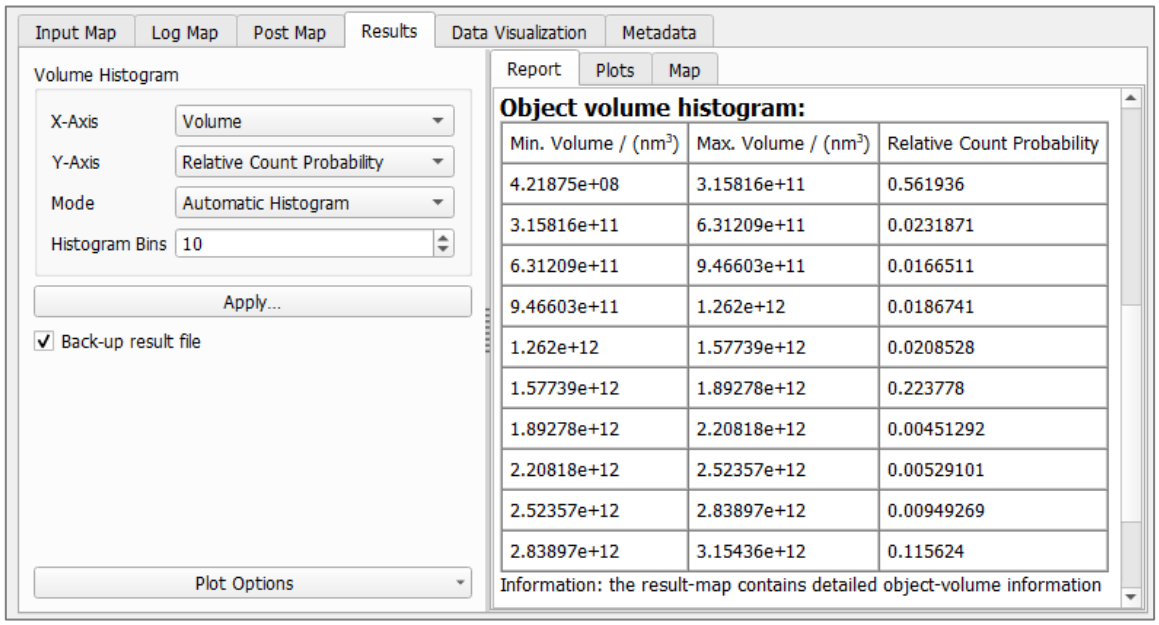
Key	Unit	Value
MeanCoordinationNumber		4.045751634
Contact		
TotalNumberOfContacts		12999
TotalContactFaces		354238
MaximumContactFaces	1	356
MinimumContactFaces	1	1
MeanContactFaces	1	27.25117317
ContactAreas	m^2	5.625e-13, 1.125e-12, 1.6875e-12, 2.25e-12, 2.8125e-12, 3.375e-12, 3.9375e...
NumberOfContacts	1	281, 323, 828, 272, 341, 578, 254, 317, 438, 225, 272, 306, 226, 249, 296, 2...
CumulativeNumberOfContacts	1	281, 604, 1432, 1704, 2045, 2623, 2877, 3194, 3632, 3857, 4129, 4435, 4661...
Contacts		
Object1		1, 1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 3, 3, 3, 3, 3, 3, 3, 3, 3, 3, 3, 4, 4, 4, 4, ...
Object2		125, 1760, 1996, 2266, 2315, 3028, 4294965792, 4294965882, 4294967292, ...
ContactFaces		27, 35, 17, 17, 26, 1, 46, 24, 20, 2, 6, 21, 23, 10, 21, 29, 28, 34, 53, 31, 48, 2...
BackgroundContacts		
Object1		0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, ...
Object2		1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, ...
ContactFaces		1675, 1832, 1524, 1303, 1787, 156, 1334, 263, 1727, 1712, 1874, 1840, 1625...
NumberOfOverlaps	1	3364
Overlaps		
ObjectIndex		1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21, 22, 23, ...
Volume		

Under the **Contacts** key, for each contact the index numbers of both objects and the number of contact faces are given. In the above example, the first contact is between object number 1 and object number 125 and has a size of 27 voxel faces. The second contact is between object number 1 and object number 1760 and has a size of 35 voxel faces.

Under the **Results - Plots** subtab, the **Contact Area Histogram** visualizes the size distribution of the contact areas:



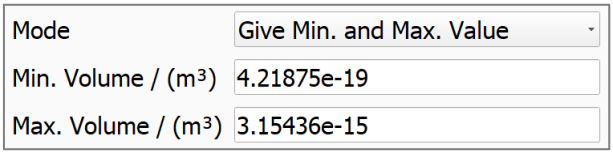
If **Analyze Object Volume** was checked (see page 59), the minimal, maximal, and mean volume are stated in the **Object Volume** section. Furthermore, an **Object volume histogram** table is plotted based on the **Volume Histogram** settings defined in the post-processing panel on the left-hand side of the **Report** tab.



The **X-Axis** pull-down menu allows choosing whether the components should be classified based on volume (**Volume**) or based on volume equivalent sphere diameter (**Equivalent Diameter**).

For the **Y-Axis** pull-down menu, the **Relative Count Probability** provides the number of components in each bin normalized to the total number of components. The **Cumulative Count Probability** is the sum of the Relative Count Probability over all bins starting from the smallest bin. **Relative Volume Probability** gives the volume of the components within one bin normalized to the total volume of all components. The **Cumulative Volume Probability** sums up the Relative Volume Probability of each bin of the histogram starting from the smallest one.

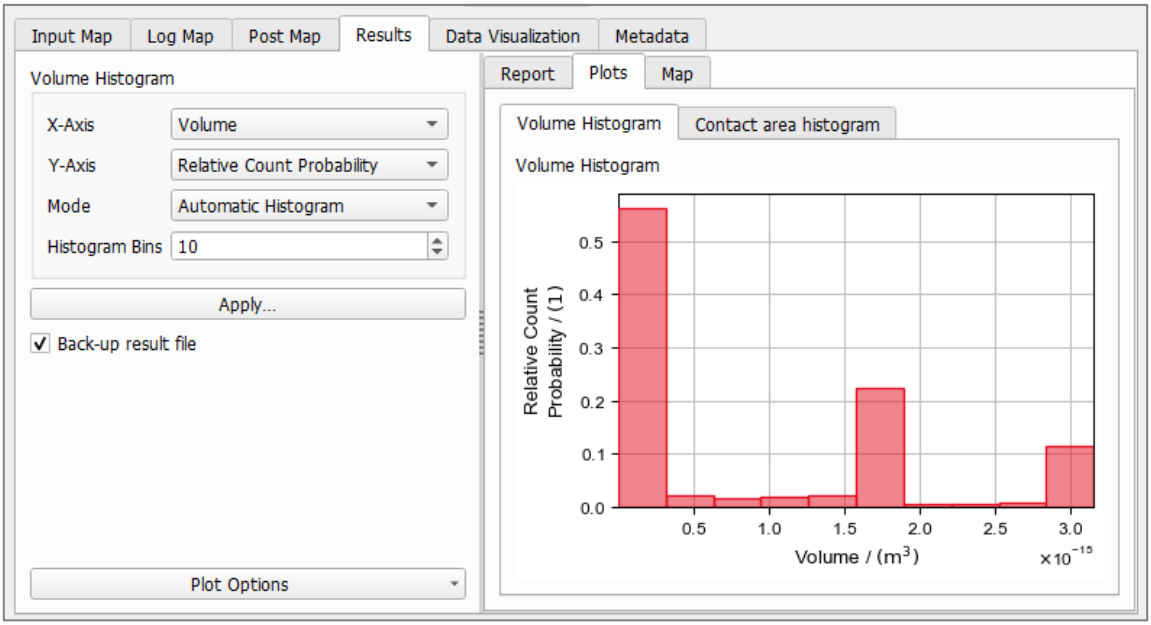
The histogram **Mode** offers the choice between generating an **Automatic Histogram** without further specifications or to **Give Min. and Max Value** for the parameter defined in the X-Axis pull-down menu (Volume or Equivalent Diameter). Either **Min. Volume** and **Max. Volume** or **Min. Diameter** and **Max. Diameter** can be directly entered here.



The number of **Histogram Bins** determines the number of rows in the **Object Volume Histogram** table.

The object volume histogram is graphically shown under the **Result - Plots** subtab. In the plot, the values for each bin are visualized as bars.

The table and plot update when the **Apply...** button is clicked after changing the Volume Histogram input parameters.

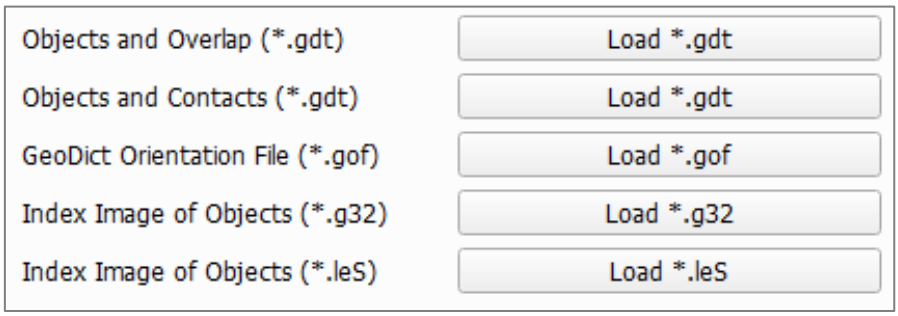


More parameters can be defined by clicking **Plot Options** at the bottom of the panel and choose **Edit Axis Settings** or **Edit Graph Styles** for the desired plot.

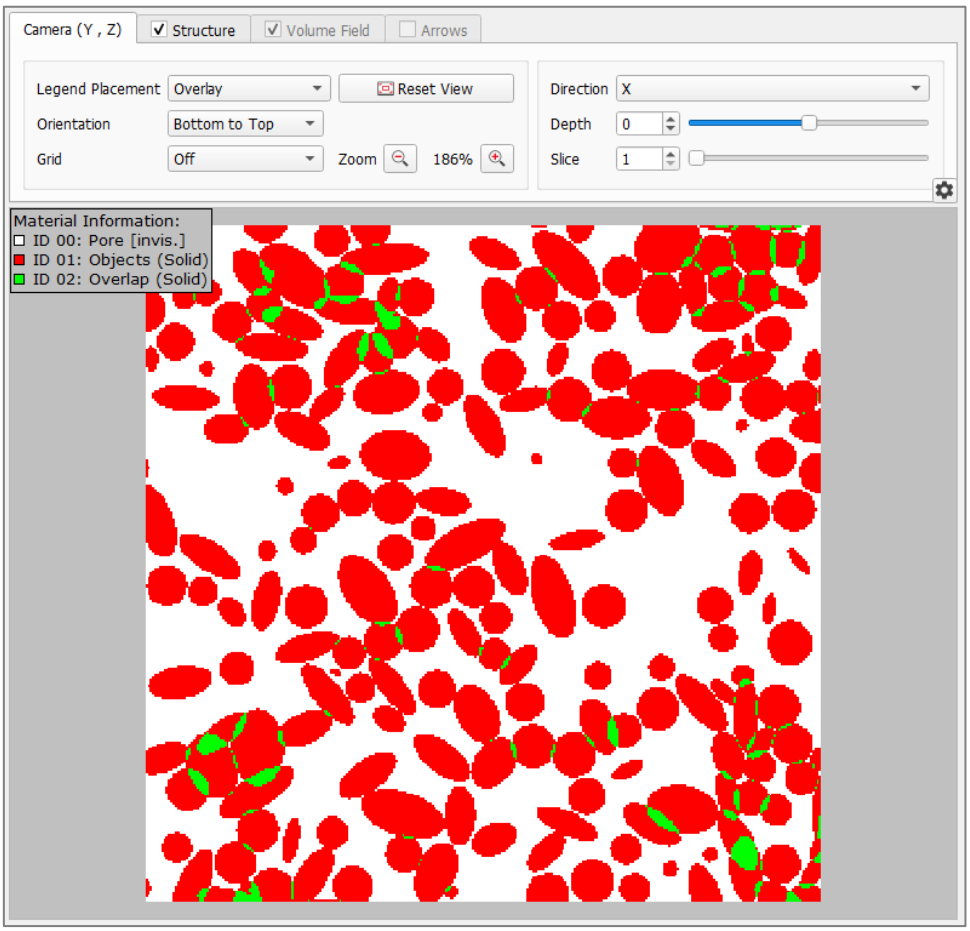
DATA VISUALIZATION

Depending on the input data file type and the options chosen in the input dialog, the **Data Visualization** tab allows different visualization options.

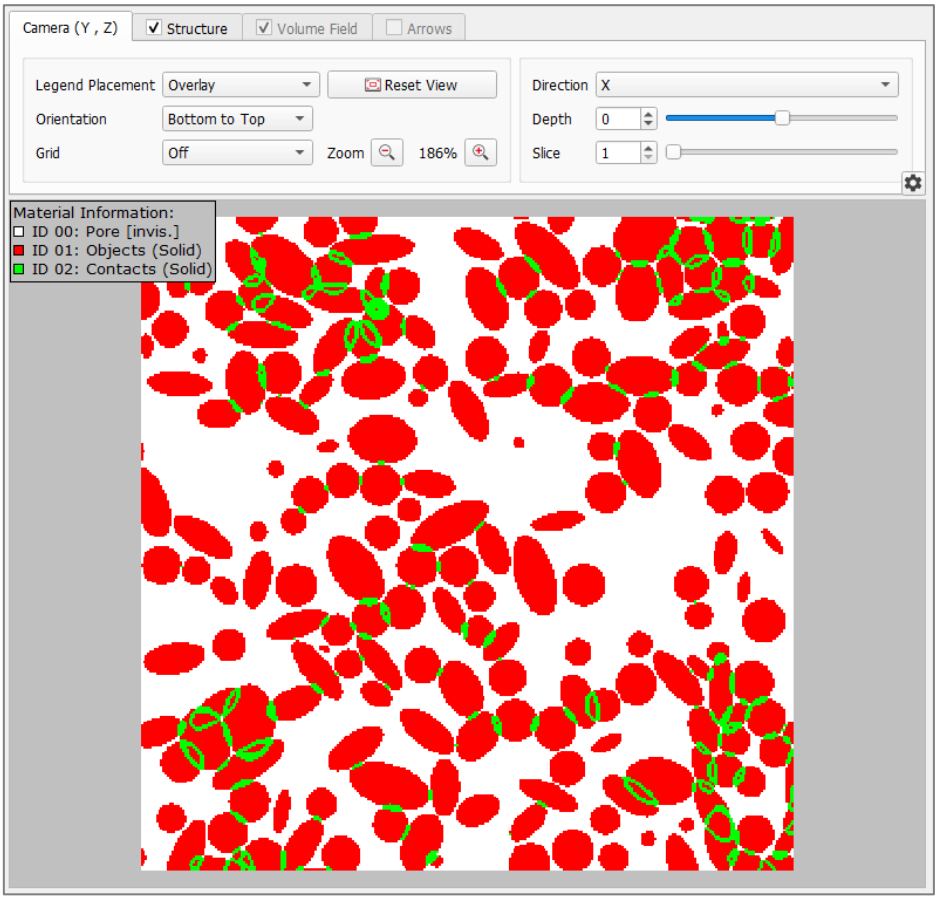
If **Use Current GAD Structure** was used as **Object Data** input, the Data Visualization tab offers visualization of object overlap and object orientation.



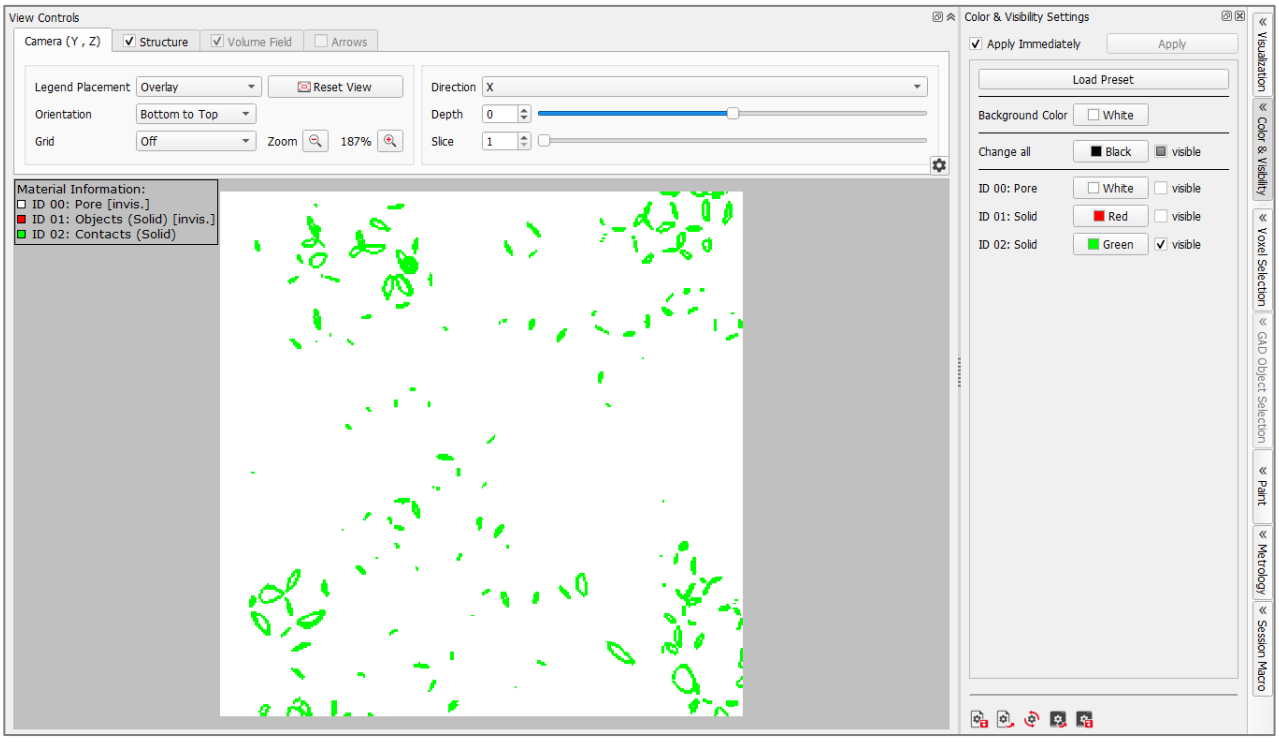
By clicking the **Objects and Overlap (*.gdt)**'s **Load *.gdt** button, the overlap between objects is displayed. All objects are assigned to Material ID 01 and the overlap is assigned to Material ID 02.



It is possible to visualize the contact voxels by clicking on the **Objects and Contacts (*.gdt)**'s **Load *.gdt** button. All contact voxels will be marked with material ID 02:

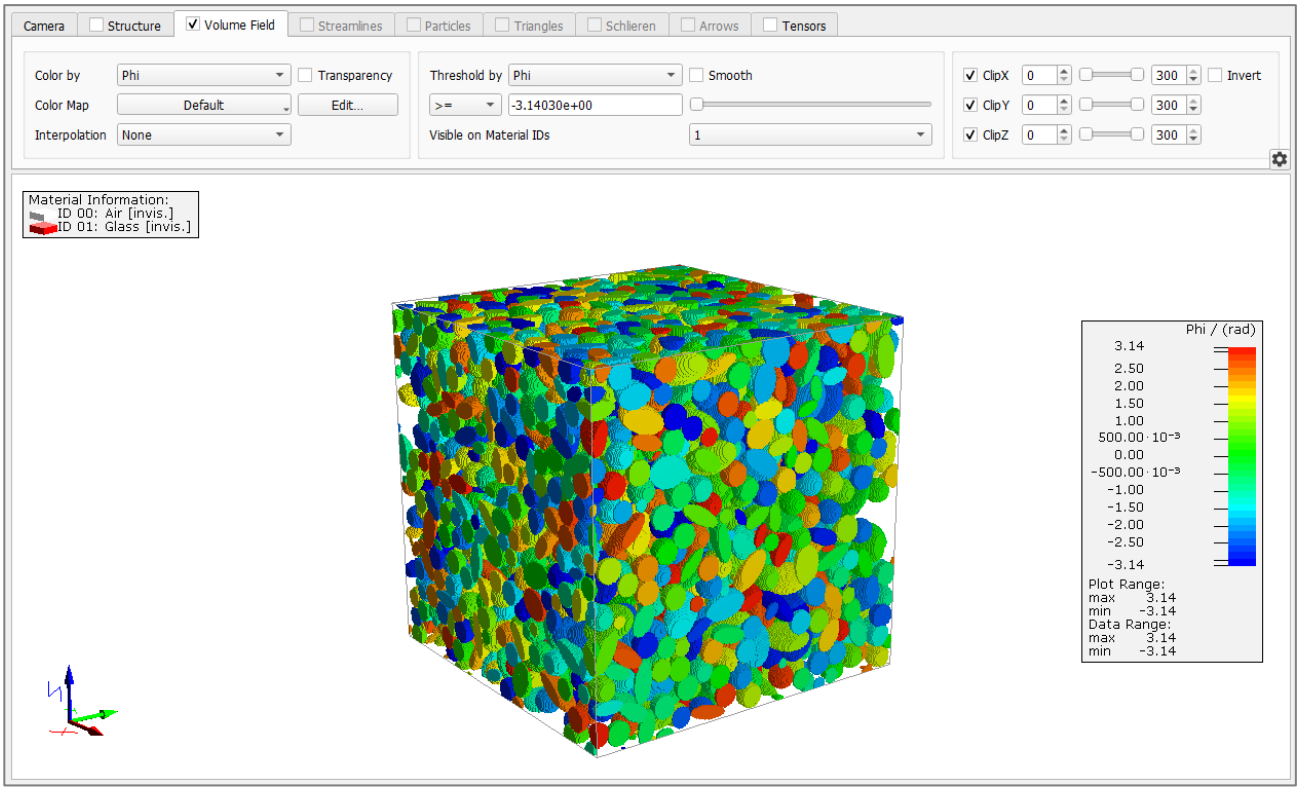


For the visualization of the labeled contacts only, select **Settings → Color & Visibility Settings** in the menu bar. Uncheck the visibility of all the material IDs in the structure model and check only the visibility of the Material ID 02.



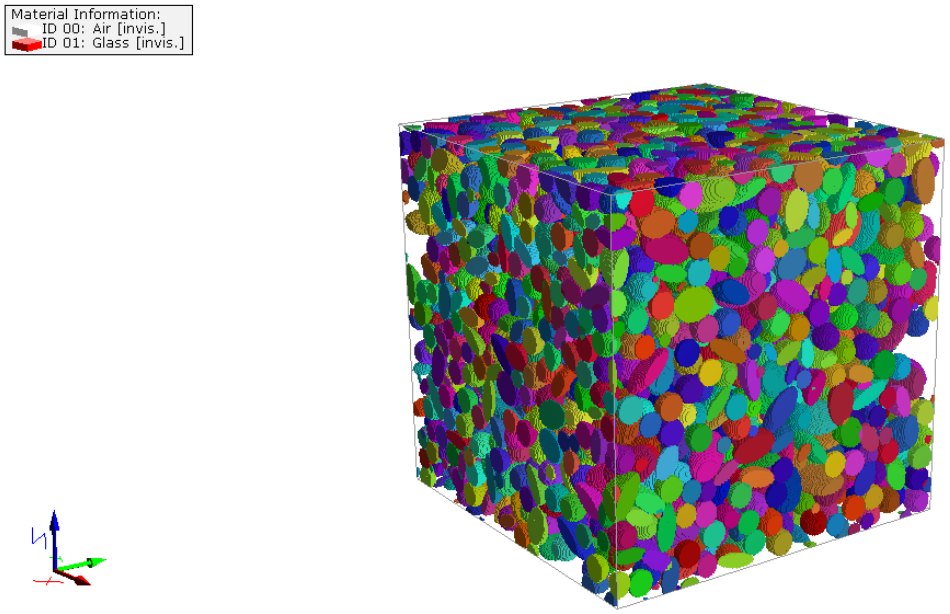
If **Write Object Orientation (*.gof)** was checked (see page 59), the orientation of the objects can be displayed by clicking the **Load *.gof** button for **GeoDict Orientation file (*.gof)**.

To properly see the orientation data of each object, uncheck **View → Structure** in the Visualization Settings, uncheck the Pore material in the **Material** selector under the **Visible on Material IDs** menu under the **Volume Field** tab as shown below.



If **Write Voxel Geometry with Object Indices (*.g32)** or **Write Voxel Geometry with Object Indices and (*.leS)** was checked (see page 59), the index image of the identified objects is loaded by clicking on the **Load *.g32** or **Load *.leS** button.

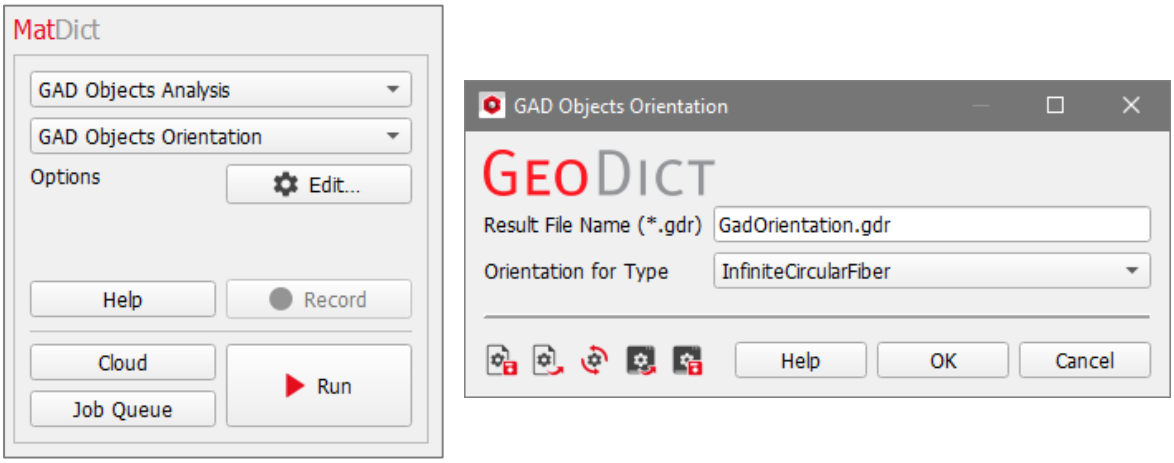
In this image, every object is visualized with a different color. Again, to visualize the results, it is important to uncheck **View → Structure** in the main menu.



GAD Objects Orientation

The **GAD Objects Orientation** command computes the orientation of GAD objects.

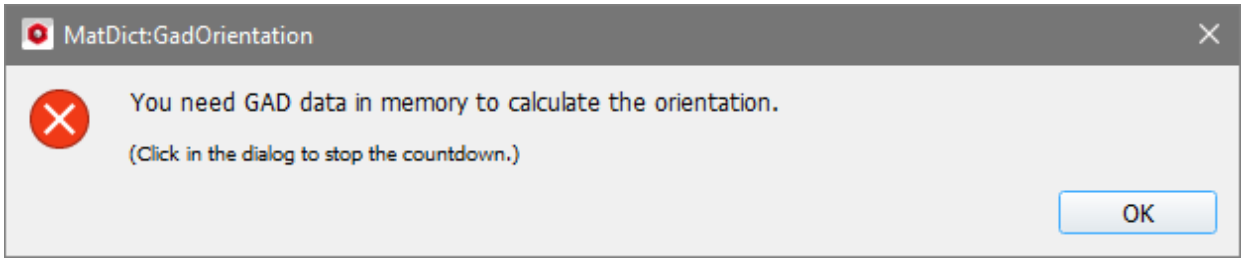
The **GAD Objects Orientation** dialog opens when clicking the **Options**' **Edit...** button.



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

From the **Orientation for Type** pull-down menu, select the object type that should be analyzed. All object types present in the current structure are identified automatically and are listed in the pull-down menu.

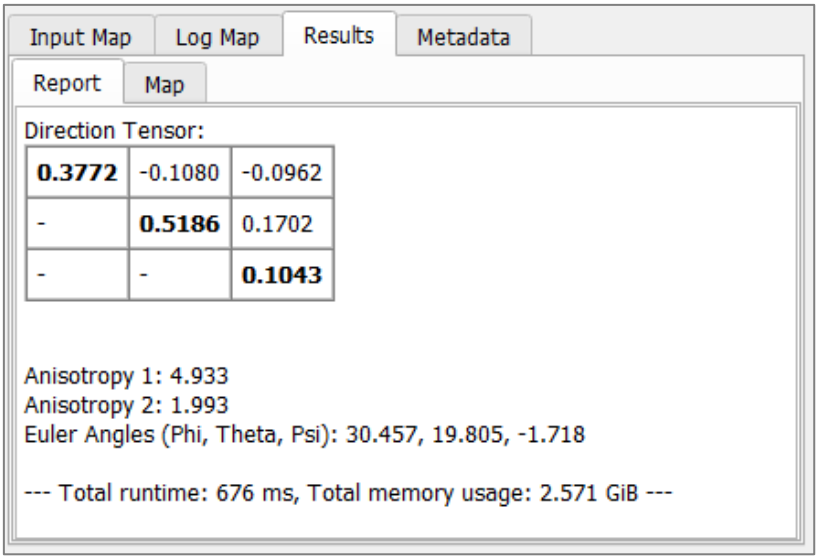
If no analytic data is available for the current structure, the object orientation analysis is not carried out after clicking **Run** in the MatDict section, and a warning message appears.



Not all object types are suitable for an orientation analysis. If this is the case an error message appears.

Results

Click **OK** to input the entered settings, and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is opened in the **Result Viewer** after the computation is finished.



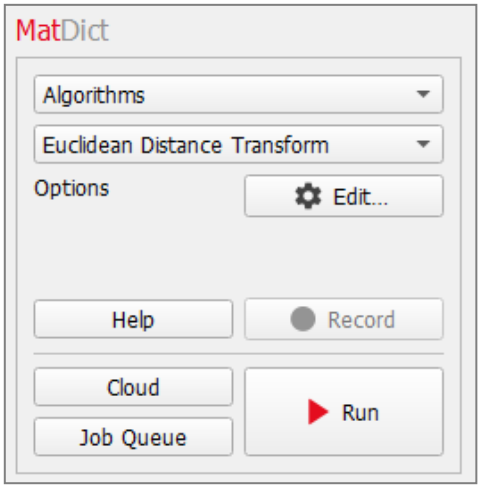
The definition of these parameters is the same as in the FiberGeo module. See the FiberGeo handbook for a more detailed description of these parameters.

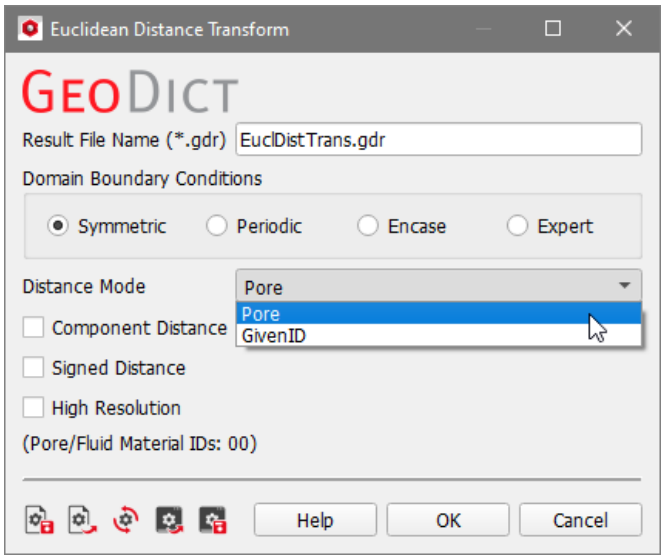
In FiberGeo, the parameters are used to describe the orientation of the randomly created fibers. That means, MatDict **GAD Objects Orientation** can be used to generate a 3D structure with FiberGeo that has a similar orientation.

ALGORITHMS

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). After selecting **Euclidean Distance Transform** (EDT) from the pull-down menu, the settings for the calculations can be modified through the **Edit...** button.

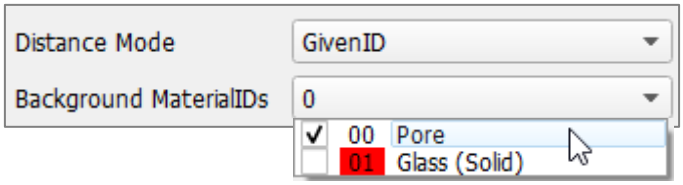




In the **Euclidean Distance Transform** dialog, choose the **Result File Name**.

Decide which **Domain Boundary Conditions** should be used during the calculations. More detailed information about this feature is given in the PoroDict handbook in the section of the Pore Size Distribution (Granulometry) command.

The **Distance Mode** defines the material IDs that are considered. From any point (voxel) inside these material IDs the distance to the nearest boundary to all other material IDs is calculated. The default is to analyze the pore space. However, if switching the Distance Mode to **GivenID**, all material IDs present in the structure can be selected.



If **Component Distance** is selected, for each point of the domain the distance to the next boundary is computed. In this case all boundaries between the materials are considered, including the pore space. When **Component Distance** is checked, the selection of Distance Mode is disabled, as the EDT is used for all structure components at once.

If **Signed Distance** is checked, a modified version of the EDT is used. In the pore space or background materials, the signed EDT will be the same as in the original version, but the signed EDT will also compute a negative distance inside of the solid or foreground material.

To run the calculations with **High Resolution** might be useful when the pore space is expected to be especially narrow. The calculation run time and memory usage are increased. See page 29 for more explanations.

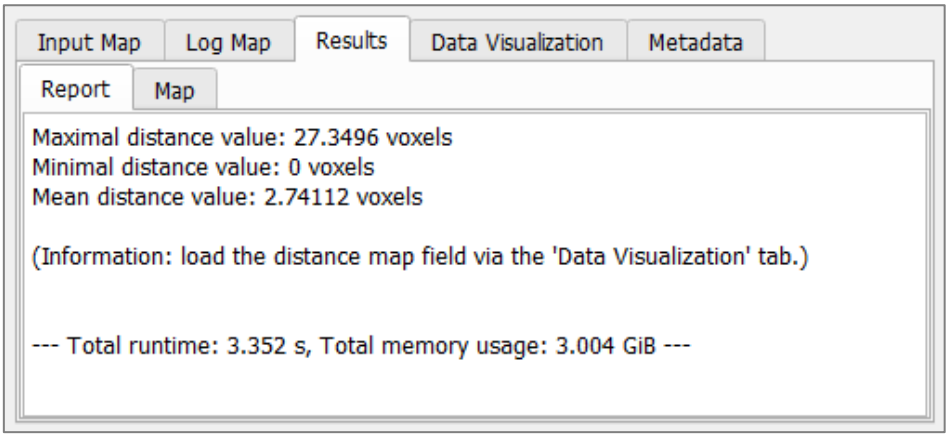
Results

Click **OK** to input the entered parameters and then click **Run** in the MatDict section to start the structure analysis. The **Result Viewer** opens at the end of the computation and the result file is automatically saved in the project folder. In the **Results – Report** tab three values can be found.

The **Maximal distance value** is the maximal value found in the computed Euclidean distance map. It corresponds to the maximal distance a point within the selected Material IDs can have to the next boundary.

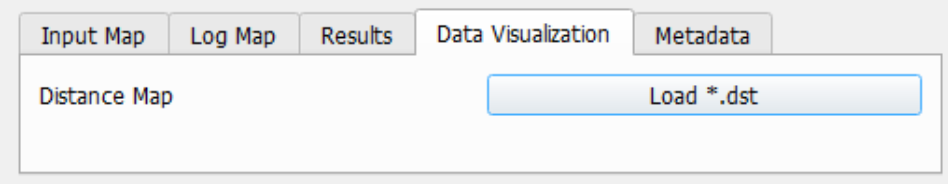
The **Minimal distance value** is the minimal value found in the computed Euclidean distance map. Be aware, that this is in general not the minimal distance a point within the selected Material IDs can have to the next boundary, because also the values inside of the solid materials are taken into account. In the standard case, the Minimal distance value will be 0. For signed distance maps, the result corresponds to the maximal (negative) distance a point within the solid material can have to the boundary.

The **Mean distance value** is the average of all values in the computed Euclidean distance map. All materials (foreground and background) are taken into account when the average distance is determined.



Data Visualization

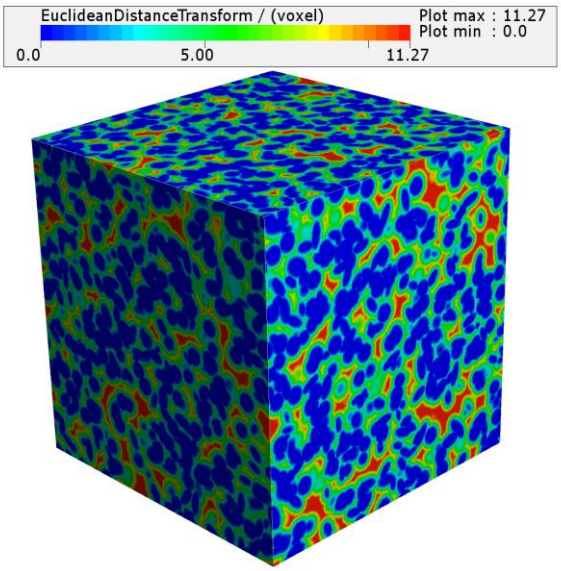
The **Euclidean Distance Transform** result can be visualized in 2D-Cross section view or 3D-Rendering when selecting the **Data Visualization** tab of the result file.

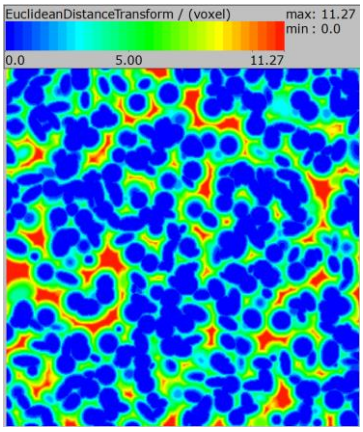


By clicking **Load *.dst**, the computed **Distance Map** is loaded into GeoDict.

The **Volume Field** tab (in 2D Cross section view and in 3D Rendering) becomes selectable in the Visualization Panel above the Visualization Area to fine-tune the visualization settings.

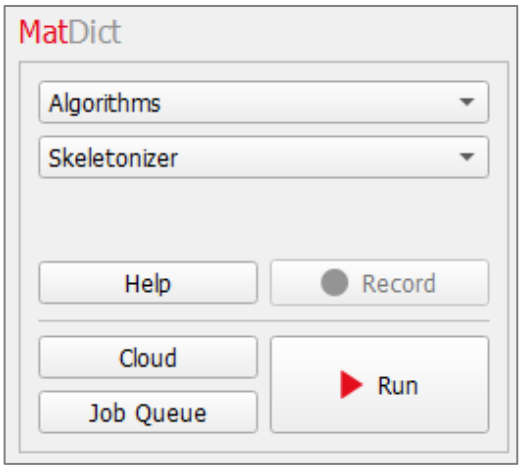
To see only the volume field, turn off the visualization of the structure (uncheck **Structure** in the tab header).

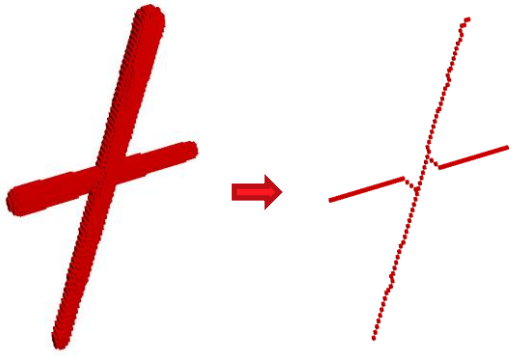




SKELETONIZER

The **Skeletonizer** reduces a structure to its center lines. This command might be useful as an intermediate step in some workflows creating or analyzing certain structure types.

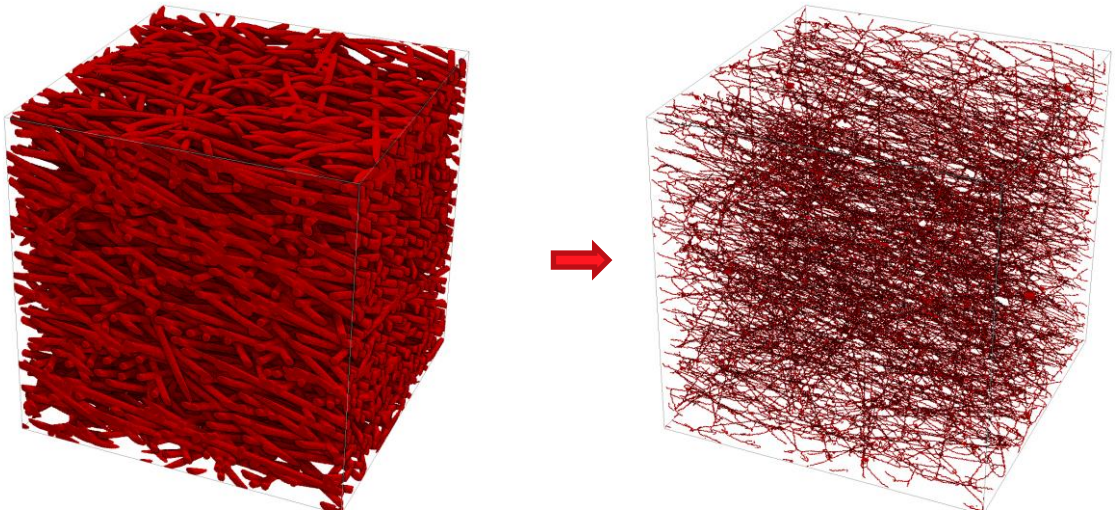




The command requires no parameters. It can directly be started by clicking **Run** in the MatDict section.

RESULTS

In contrast to all other commands in MatDict, the Skeletonizer command does not create a result file. Rather, it directly modifies the current structure and creates a new voxel structure which consists only of the center lines.



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