MatDict

User Guide

GeoDict release 2022

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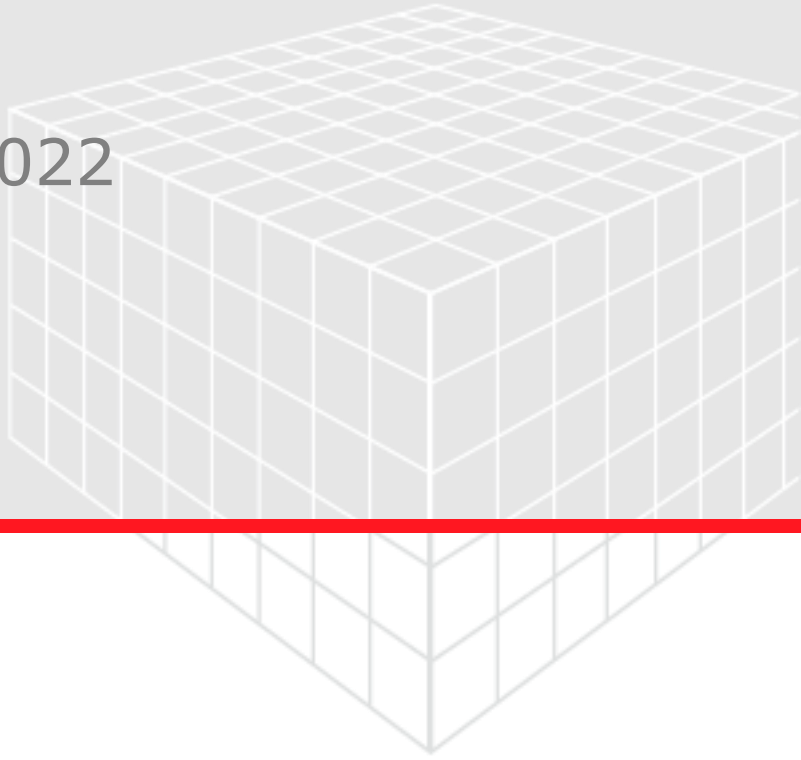
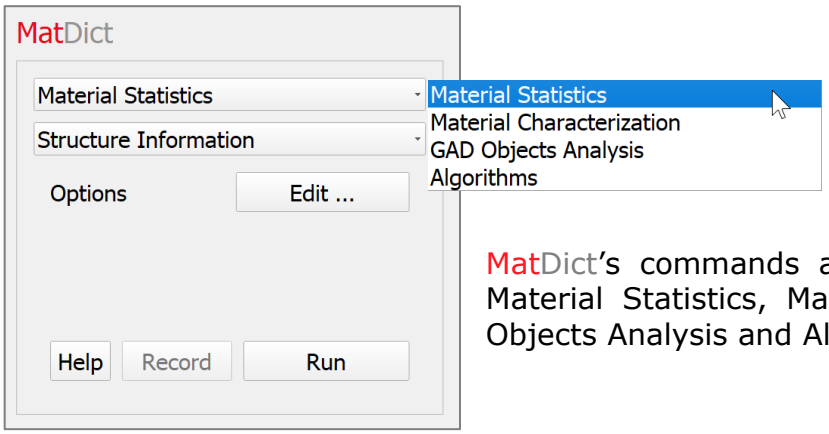


GeoDict

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

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 fix 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 algorithm determines 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.
- **1D Statistics**: The method determines 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 in the 1D Statistics.
- **2D Density Map**: The algorithm calculates 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 algorithm computes the solid volume fraction and density (distribution) of specified subvolumes.

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 than *d*, if it is inside any sphere of diameter *d*, which can be fitted into the solid objects.

- For the calculation of **Percolation Paths**, 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. Furthermore, one can compute the shortest path of a given sphere size through the medium.

- **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. 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 PoroDict 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.

GAD Objects Analysis

- **Analyze Objects**. The algorithm analyzes 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

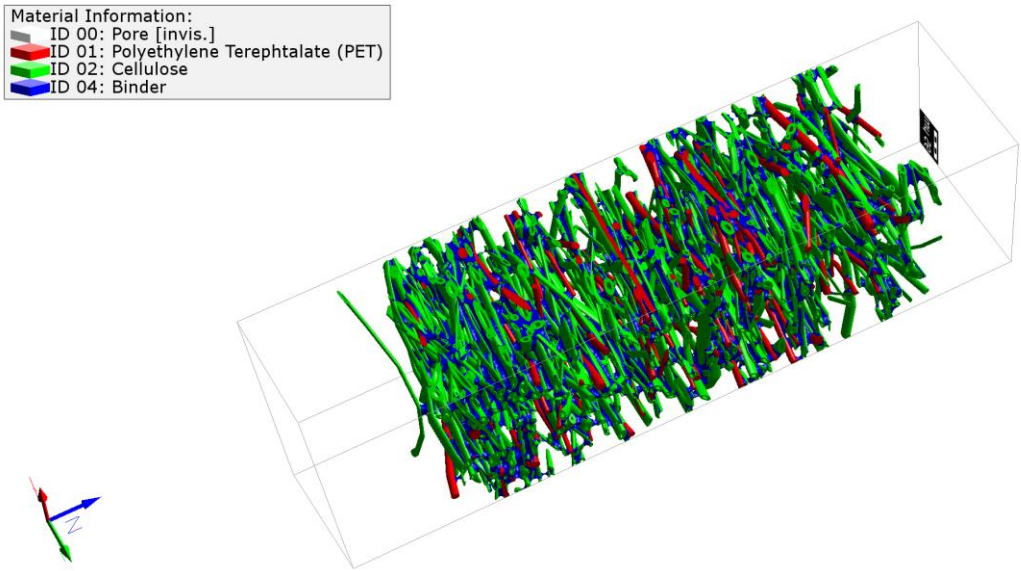
- In the **Euclidean Distance Transform** (EDT), the algorithm calculates the distance from any point (voxel) inside a pore to the nearest pore/solid boundary. This is useful when characterizing the structure's pore morphology.
- The **Skeletonizer** reduces any given structure to its center lines.

During the simulations, the results from all MatDict computations are saved as ***.gdr** files in the project folder. In addition, the results can be opened, analyzed, and plotted using the GeoDexcel spreadsheet.

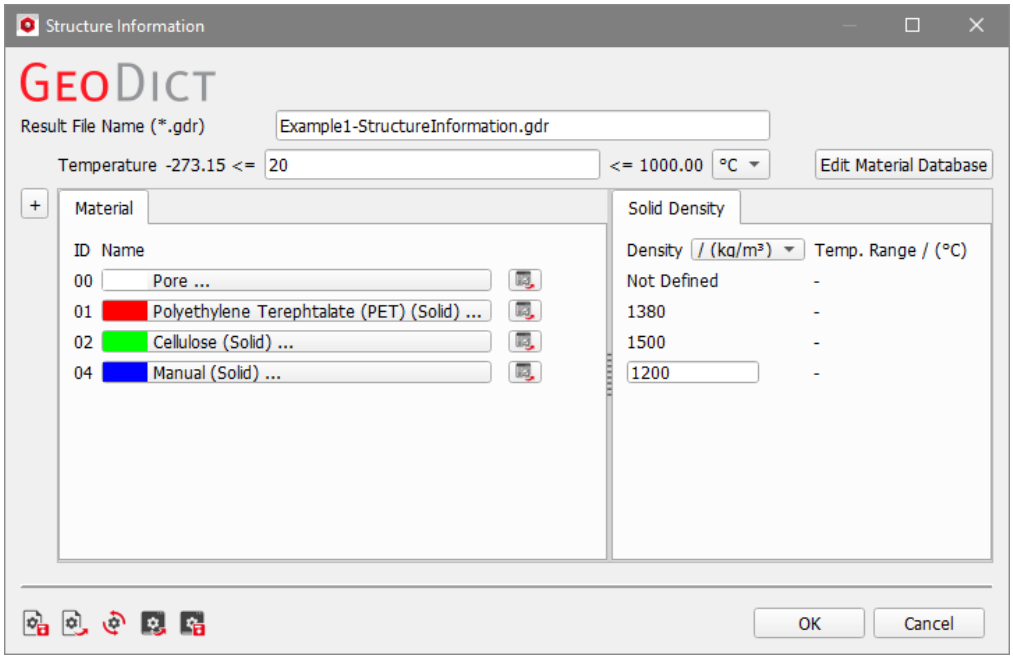
MATERIAL STATISTICS

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 box opens.



At the top of the dialog box, 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.

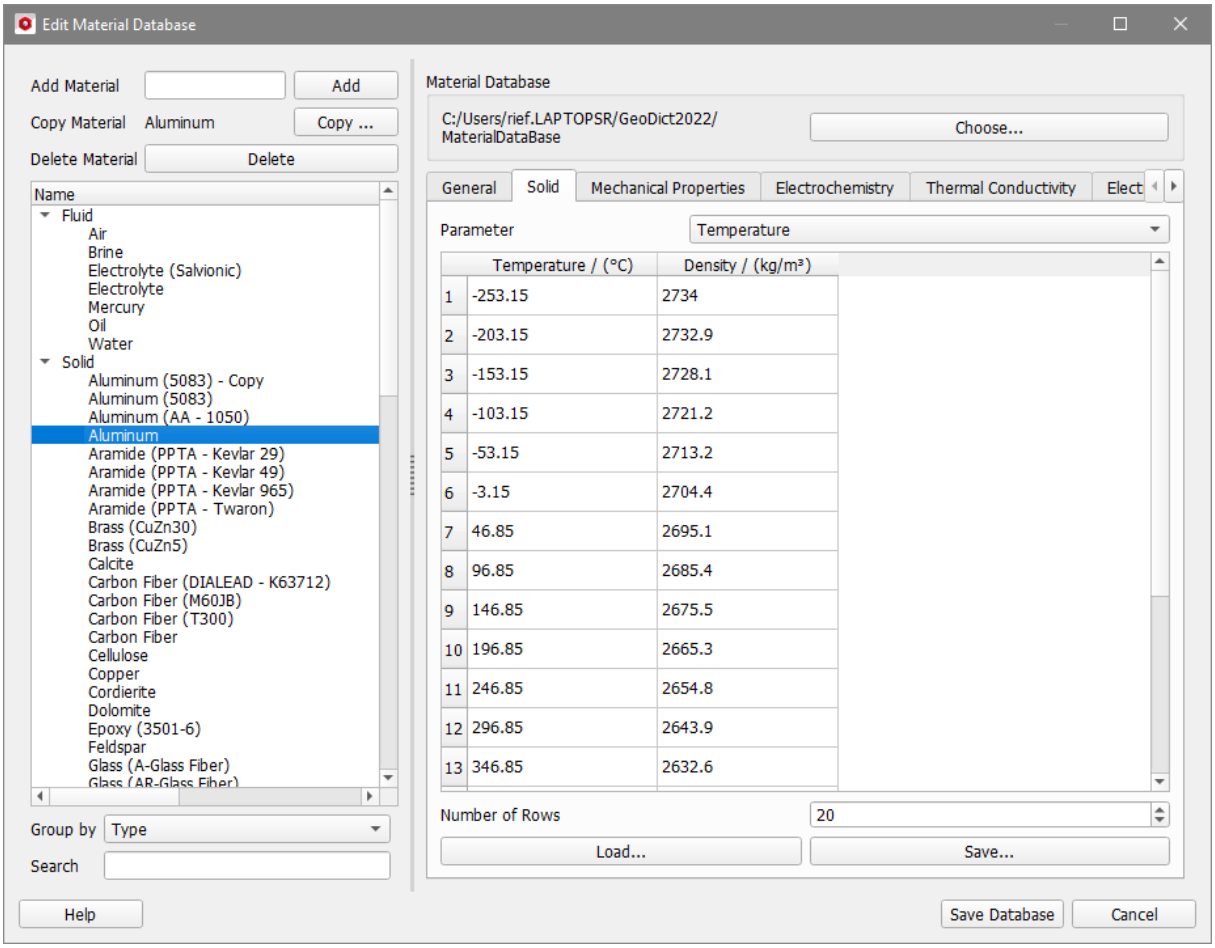
By default, material IDs that are not present in the structure are not displayed under the **Material** tab, but they can be displayed by clicking on the "+" symbol to the left of the **Material** tab.

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 a material is not present in the GeoDict Material Database, it can be added by clicking **Edit Material Database** and defining its properties. Alternatively, a material can be set to **Manual**, and its density can be entered under the **Solid Density** tab.

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:

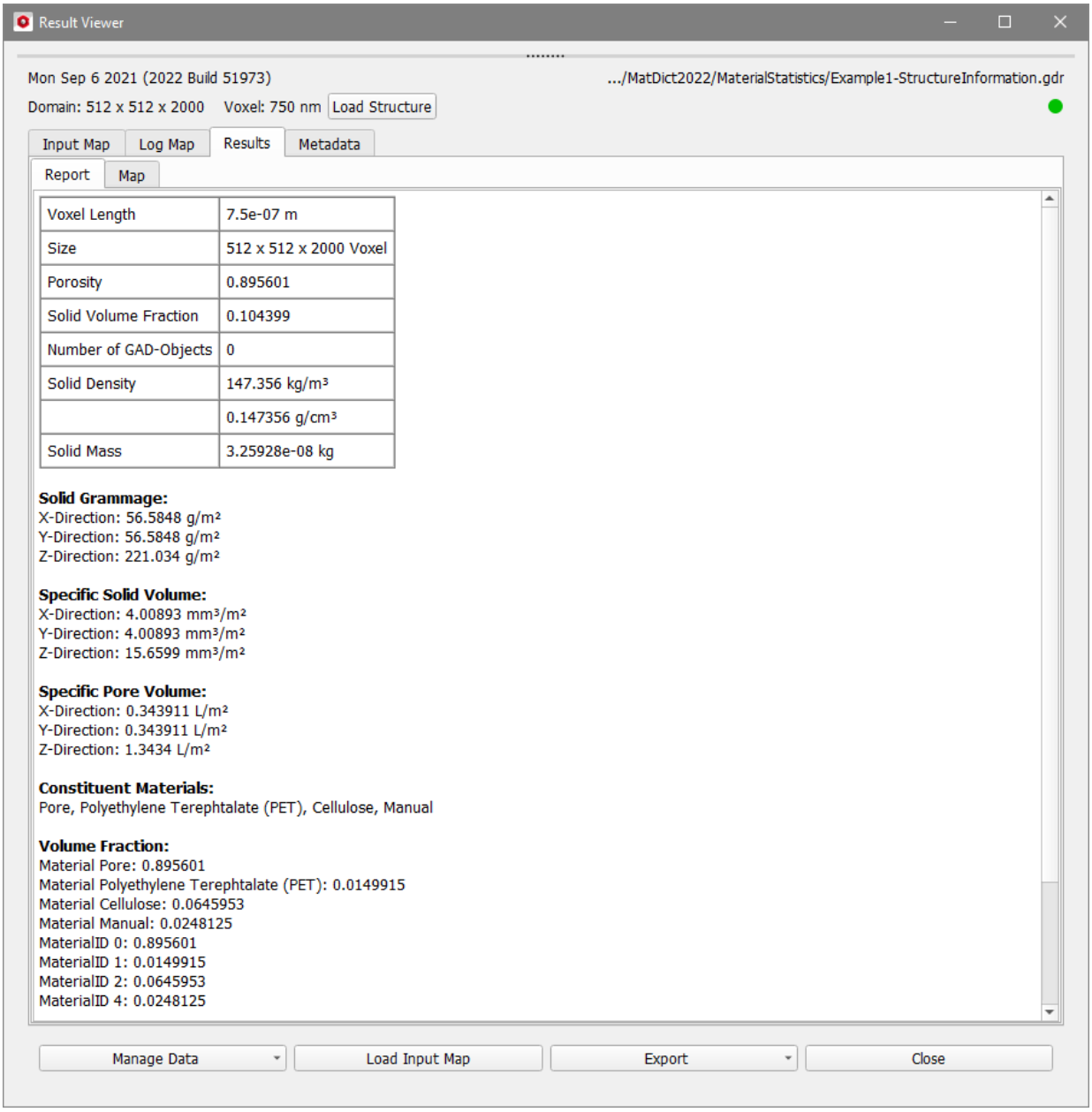


In the above example, the densities of the PET and cellulose fibers are not set to be temperature dependent.

RESULTS

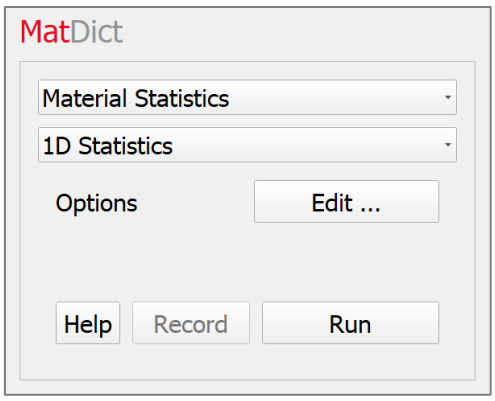
Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is opened in the **Result Viewer** after the computation is finished.

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.

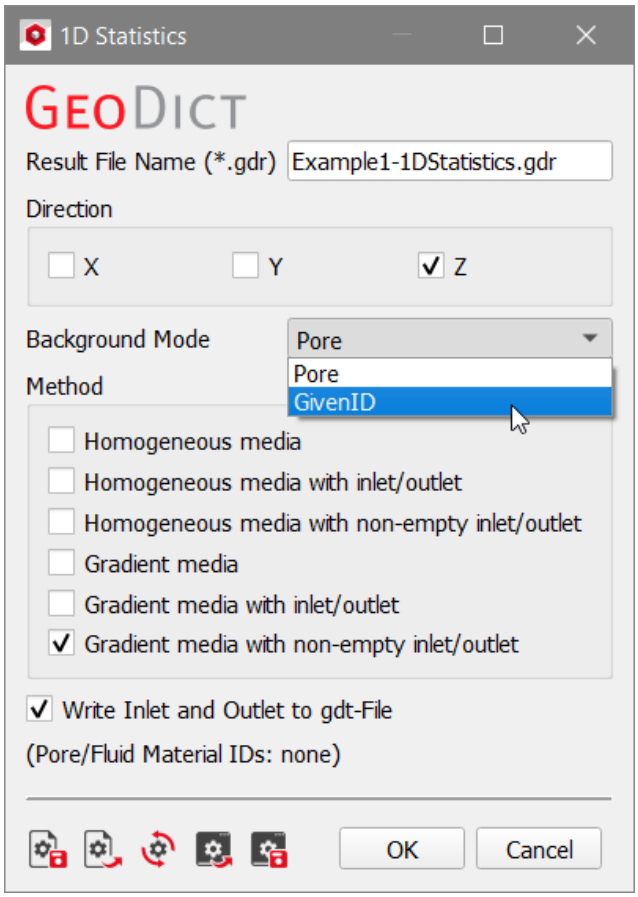


1D Statistics

The **1D Statistics** command calculates the **solid volume fraction** (**SVF**) and the **thickness** of the solid material in the given direction. The SVF is computed on the plane (layer) normal to the direction of interest and the average value for each of those layers is reported in the 1D Statistics.



After clicking the **Options' Edit...** button, the **1D Statistics** dialog box opens.



At the top of the dialog box, 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).

In the **Direction** panel, the direction(s) for the 1D analysis can be chosen from the three spatial directions.

In the **Background Mode** pull-down menu, choose **Pore** to assign the material ID corresponding to pore space (background) and exclude it from the 1D statistics calculations. Alternatively, choose **GivenID** to assign one or multiple material IDs to the pore space (only for the calculations within the 1D Statistics) and select the material IDs from the **Background MaterialID** pull-down menu.

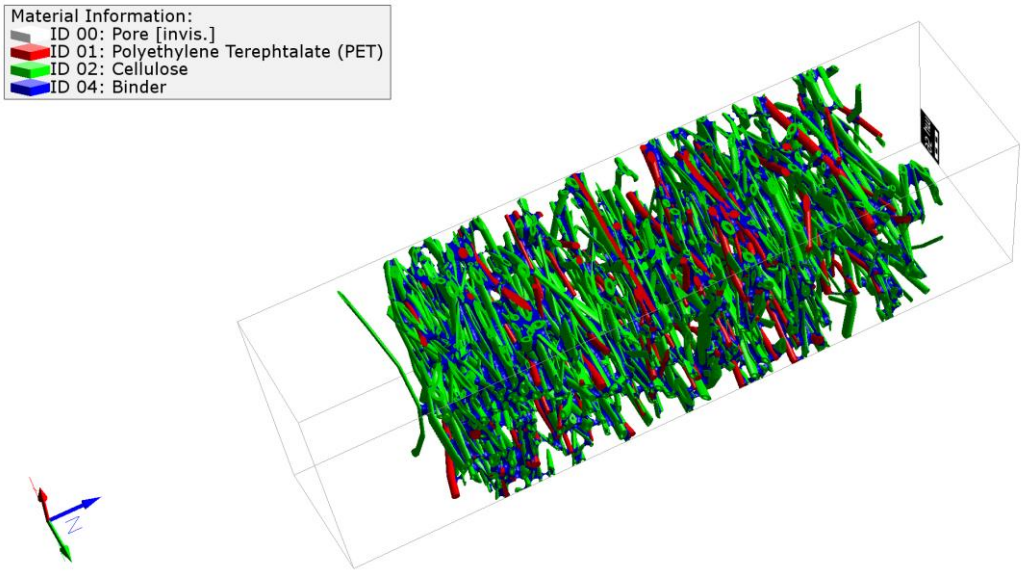
Besides the measured SVF, the algorithm computes an estimated SVF of the structure to determine the thickness of the media. The estimated SVF is computed based on a least squares fit on the measured SVF. For this, choose one or multiple types of fit in the **Method** panel. Multiple methods can be selected, and the results for all selected methods are computed. Additionally, all these methods can be calculated in the post-processing in the **Result Viewer**. This is especially convenient if one wants to compare the results between different methods.

A distinction is made between media with a homogeneous density distribution (**Homogeneous media**) and media with a density gradient (**Gradient media**).

With **Homogeneous media with inlet/outlet** or **Gradient media with inlet/outlet**, layers that contain only background material are considered as inlet/outlet regions. These are excluded from the calculation of the estimated SVF.

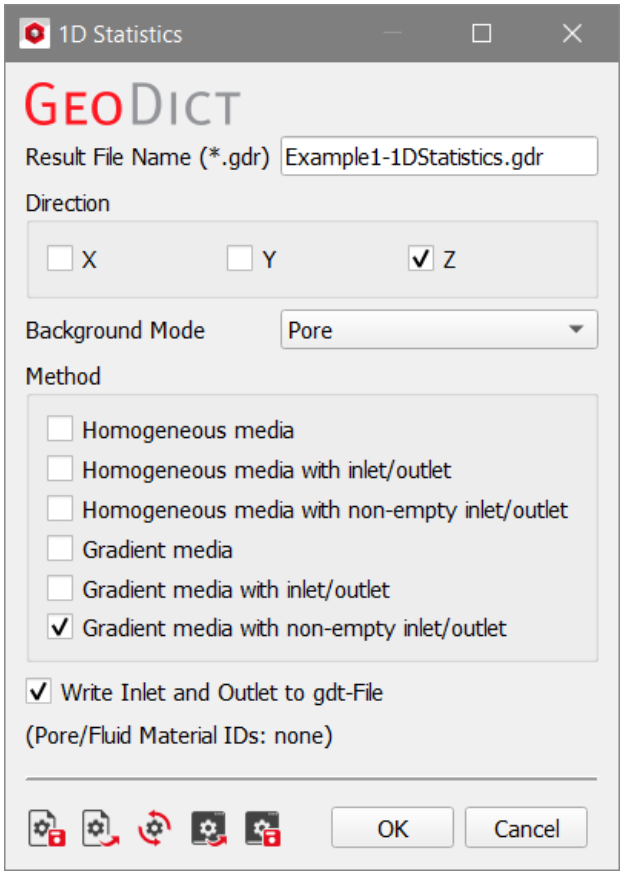
For structures that include a non-empty inlet/outlet region due to e.g. a few fibers that stick out from the media, choose **Homogeneous media with non-empty inlet/outlet** or **Gradient media with non-empty inlet/outlet**.

As example, we analyze a 3D model of a structure with a side length of 1500 µm (1.5 mm) in Z-direction (2000 voxels **x** voxel length of 0.75 µm/voxel).



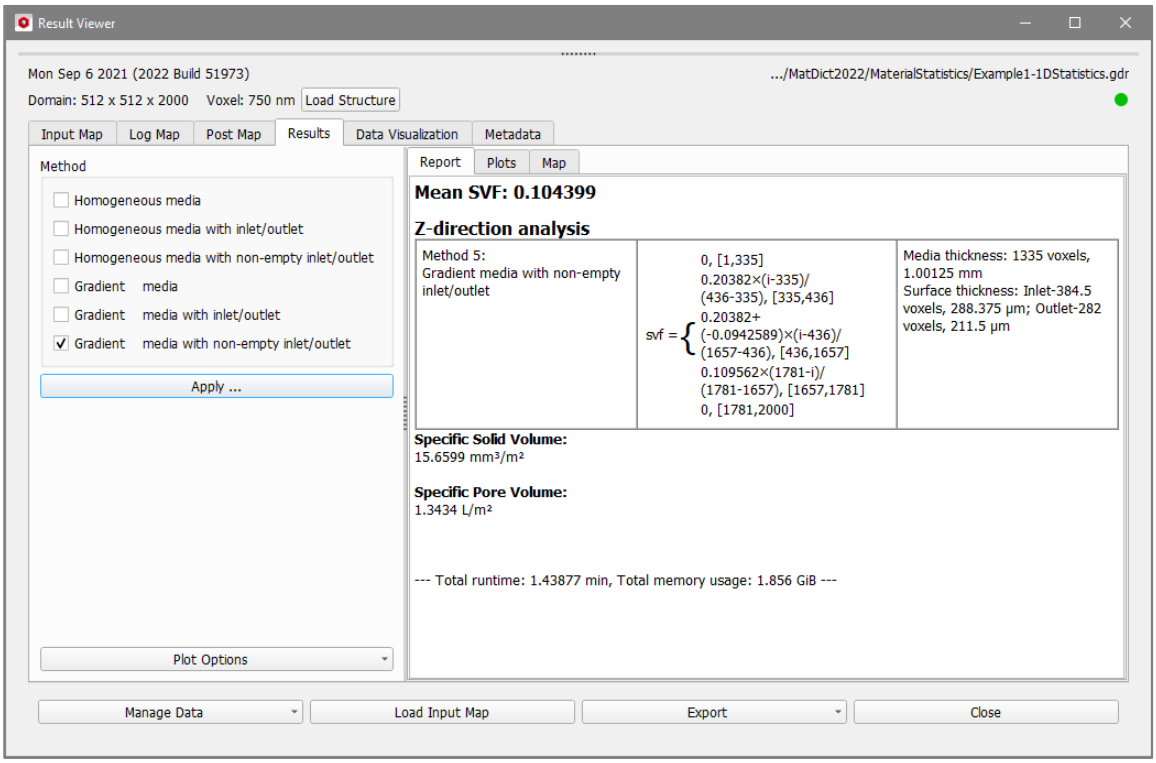
To analyze the structure, we use the settings shown on the right.

For inlet / outlet methods, check **Write Inlet and Outlet to gdt-File** to save the geometry of the detected inlet and outlet to a file called **InletOutlet.gdt**.



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.



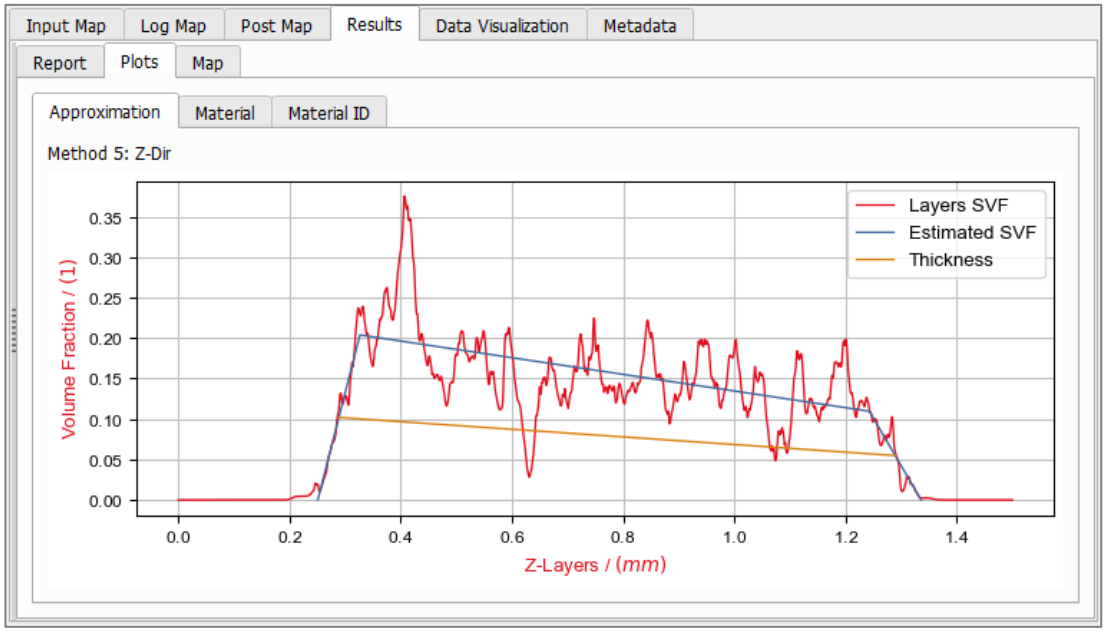
The reported **Mean SVF** is the solid volume fraction of the whole sample.

In this example, the Z-axis was selected for analysis. Therefore, the **Z-direction analysis** is contained in the report. It shows the computed least squares fit for the solid volume fraction distribution as a piecewise linear function that consists of up to five intervals describing

a. Inlet
b. Upstream media surface
c. Porous media
d. Downstream media surface
e. Outlet

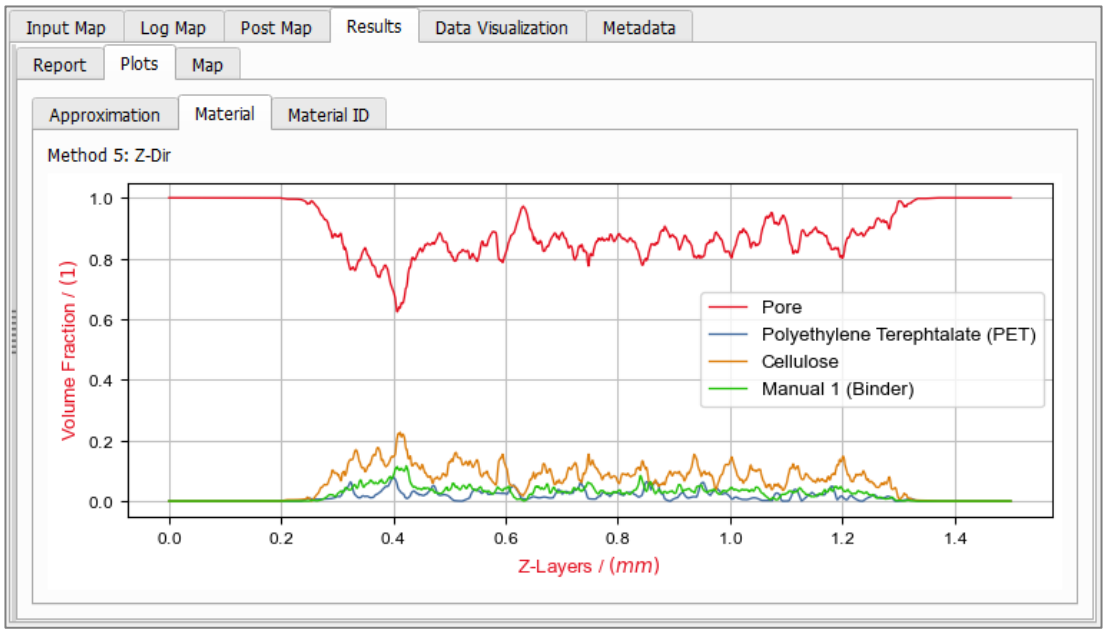
The reported **Media thickness** is computed as the distance between the center of the upstream media surface interval and the center of the downstream media surface interval.

The solid volume fraction distribution, the least squares fit, and the estimated thickness are visualized under the **Approximation** subtab:

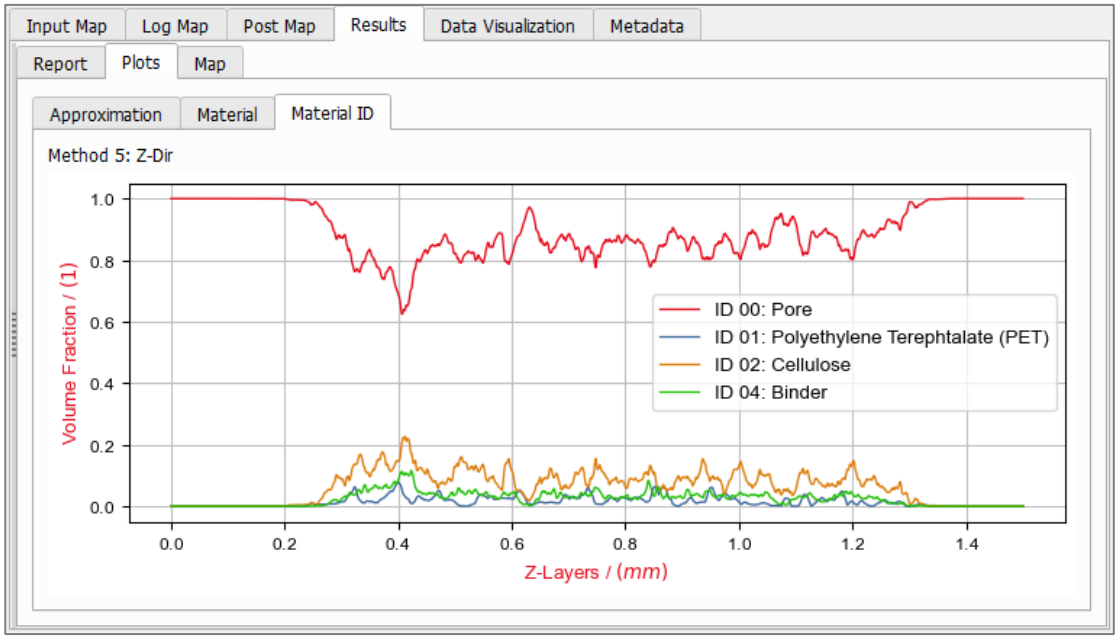


The **Layers SVF** plots the mean solid volume fraction of each individual layer, the **Estimated SVF** plots the computed least squares fit of the mean solid volume fractions, and the **Thickness** bar visualizes the computed media thickness.

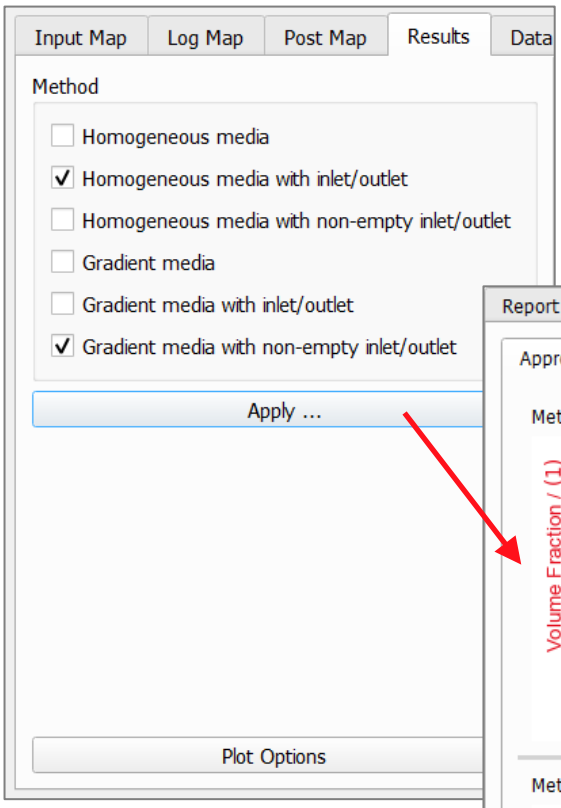
Furthermore, under the **Material** subtab, plots of the solid volume fraction of the different materials are shown:



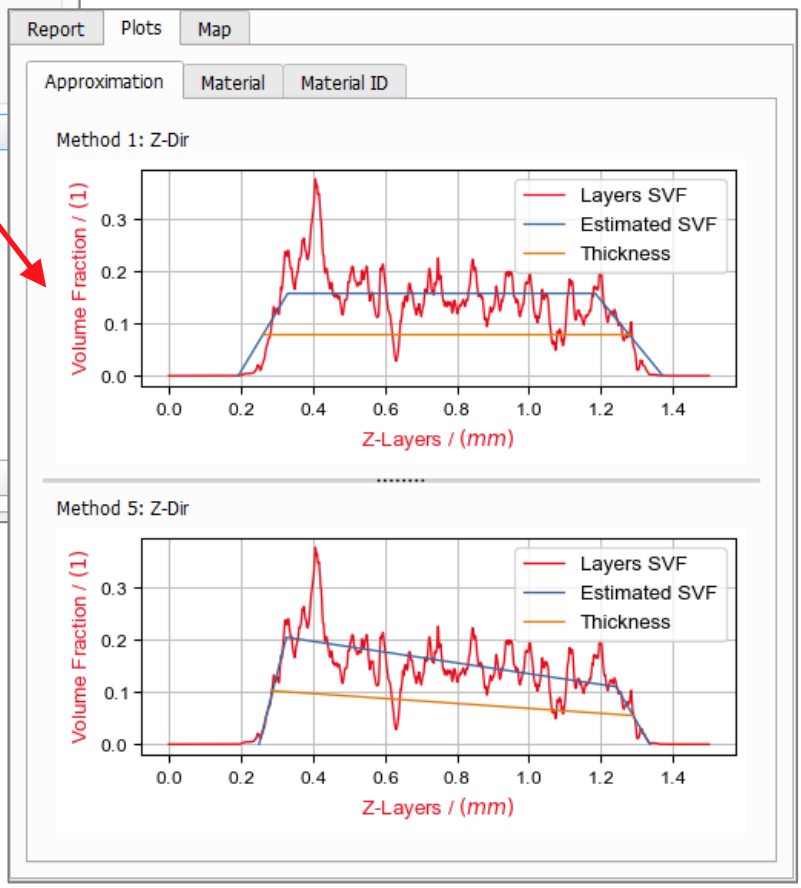
Under the **Material ID** subtab plots of the solid volume fraction of the different materials IDs are shown. The plots differ only from those in the **Material** subtab, if several material IDs are assigned to the same material.



Depending on the number of chosen directions (X, Y, Z) for the 1D Statistics analysis, the Results – Plots subtab contains 1, 2, or 3 entries in the pull-down menu for the analyzed directions (X-Dir, Y-Dir, Z-Dir).

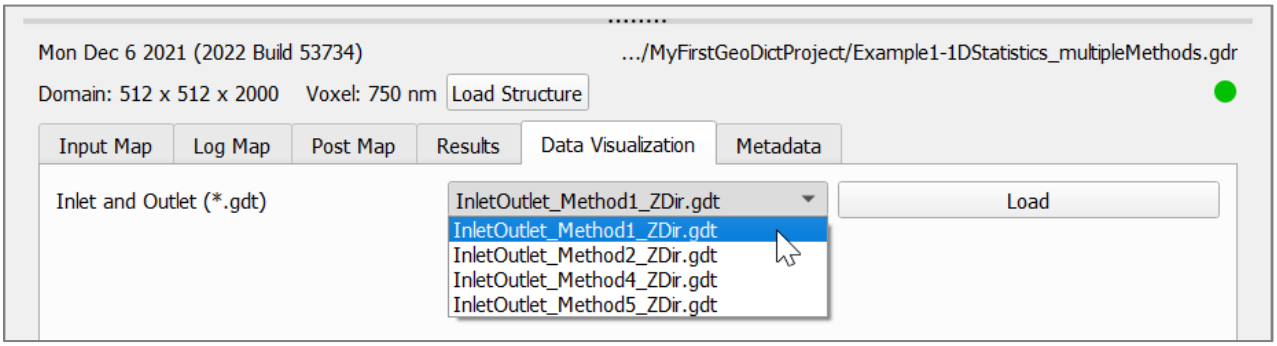


The methods for the analysis can be selected in the result viewer. Click Apply to update the **Report** and the **Plots** and the corresponding results **Map**. If multiple methods are selected, all of them are shown in the report and in the plots.



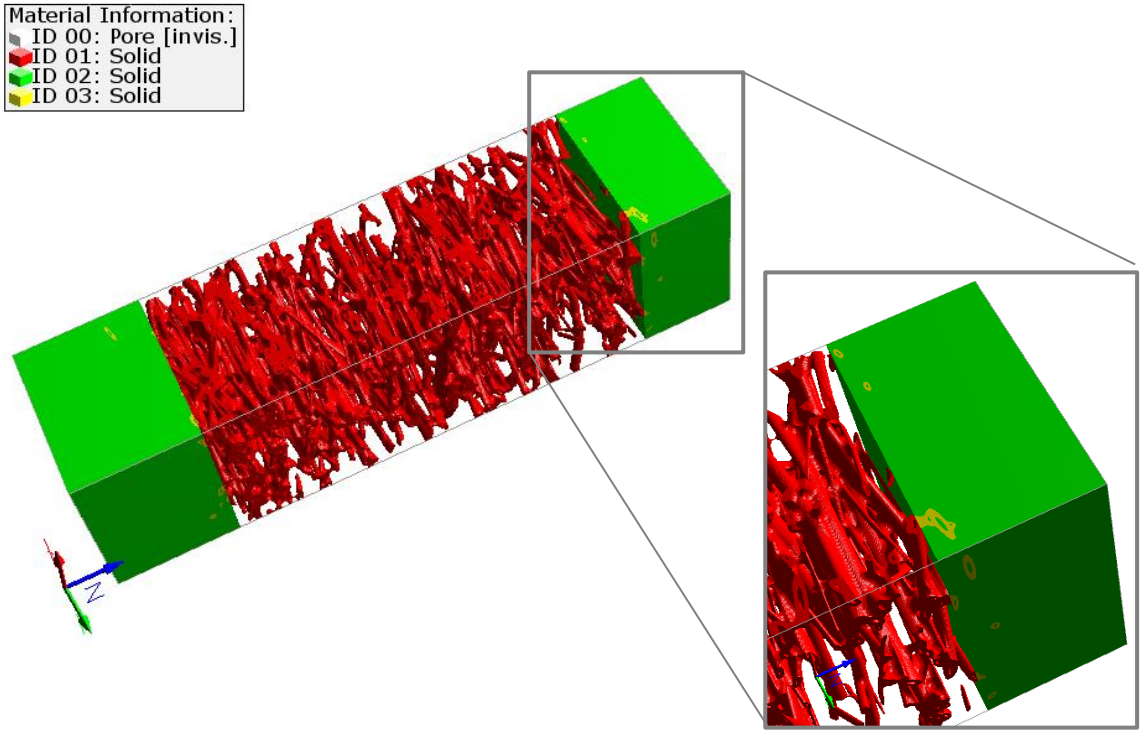
DATA VISUALIZATION

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 SVF 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).

Where the structure's fibers overlap with the identified inlet/outlet volume, they are assigned to Material ID 03 (here yellow).

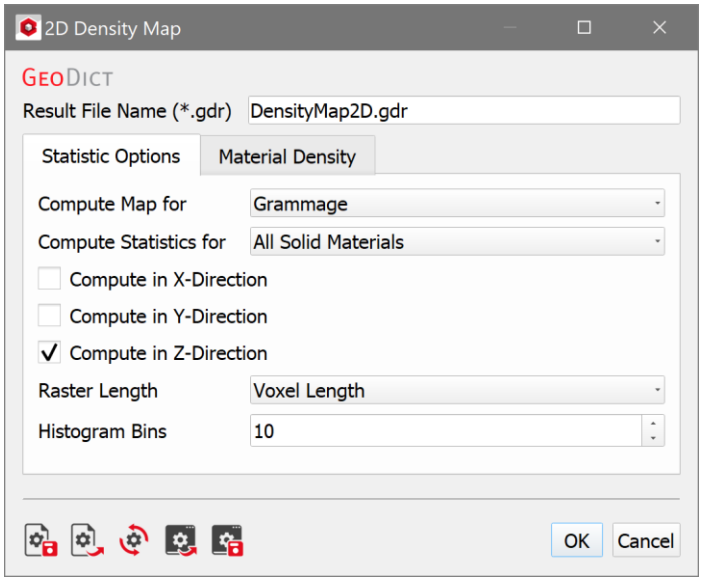


2D Density Map

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 box opens when clicking the **Options' Edit...** button. It contains two tabs: **Statistic Options** and **Material Density**.

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

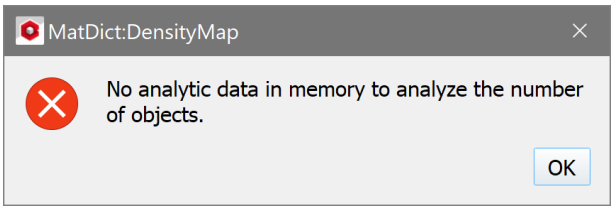


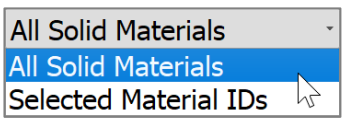
Statistic Options

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.





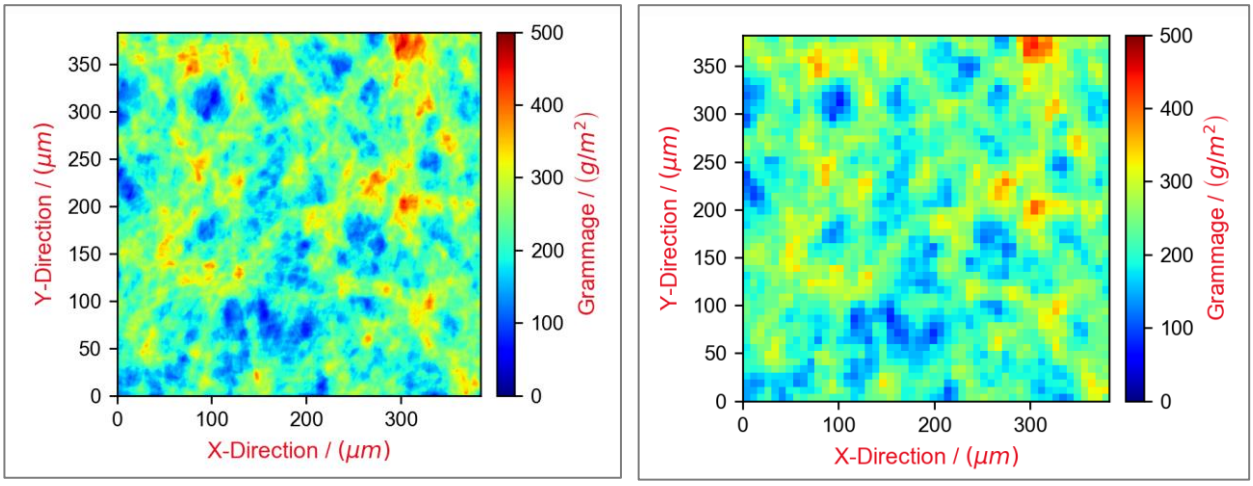
The choice in the **Compute Statistics for** pull-down menu controls whether the property is computed for **All Solid Materials** or only for **Selected Material IDs**.

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.

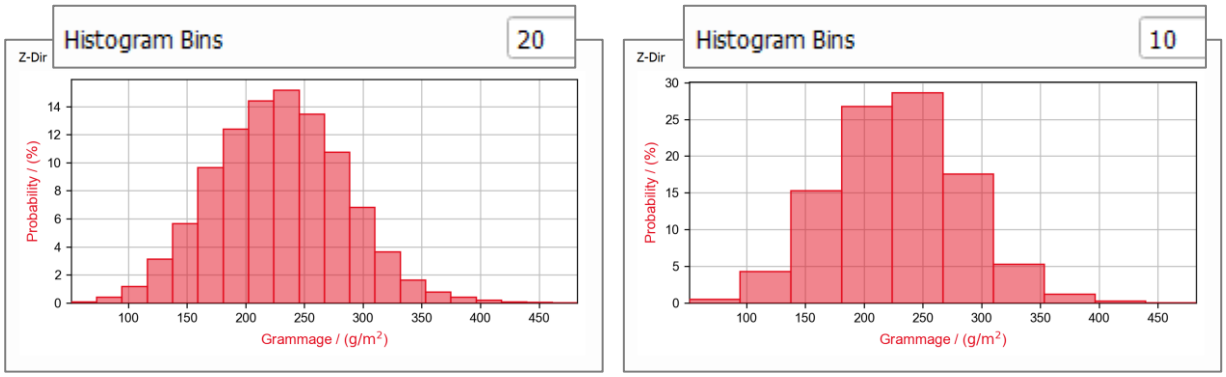
From the **Raster Length** pull-down menu, choose **Voxel Length** or **Given Length** to define the resolution at which Grammage, Solid Volume Fraction, or Number of Objects are computed.

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** 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.



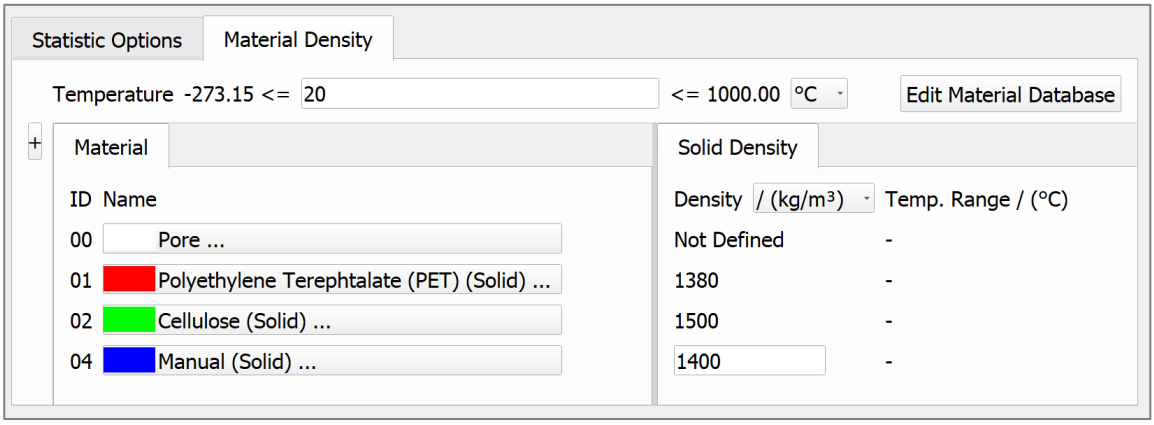
Histogram Bins refers to the number of bins used to divide the range of density values (Grammage, Solid Volume Fraction, or Object Number) into a series of equally sized intervals. In the result file, the number of histogram bins is used to create tables and plots with the frequency (probability) of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



Material Density

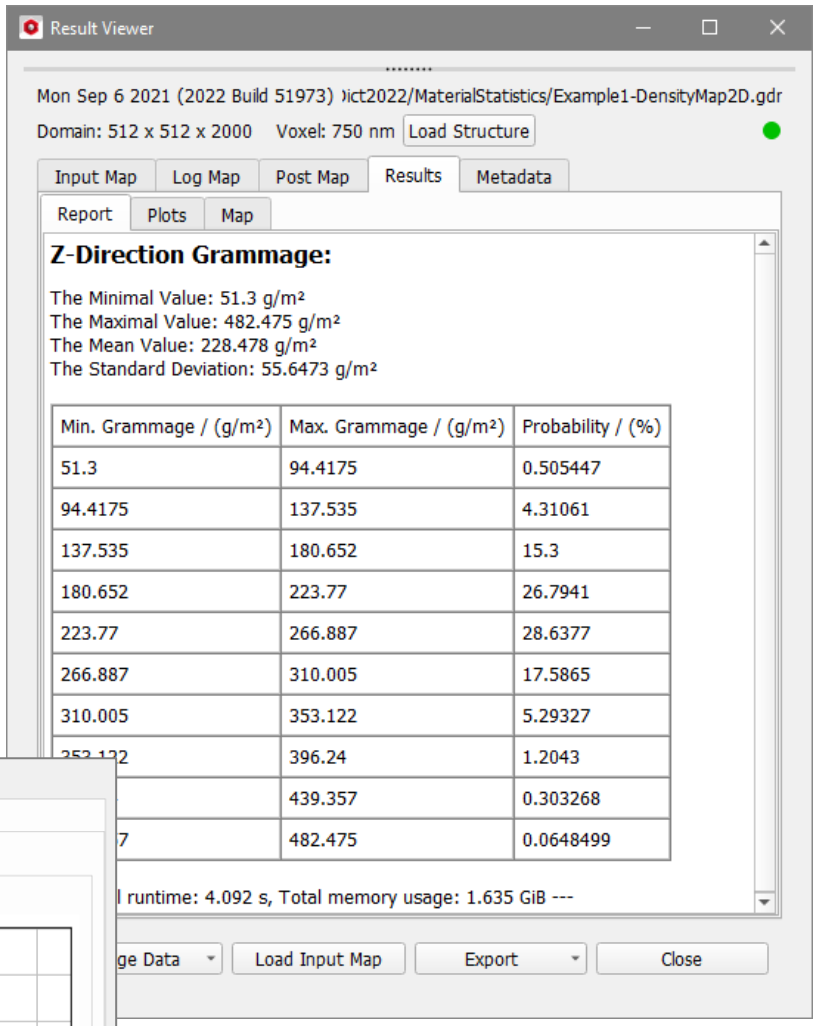
If grammage is chosen as the computed material property, the density of every material in the structure must be specified under the **Material Density** tab. For materials from the GeoDict Material Database, the density value is entered automatically.

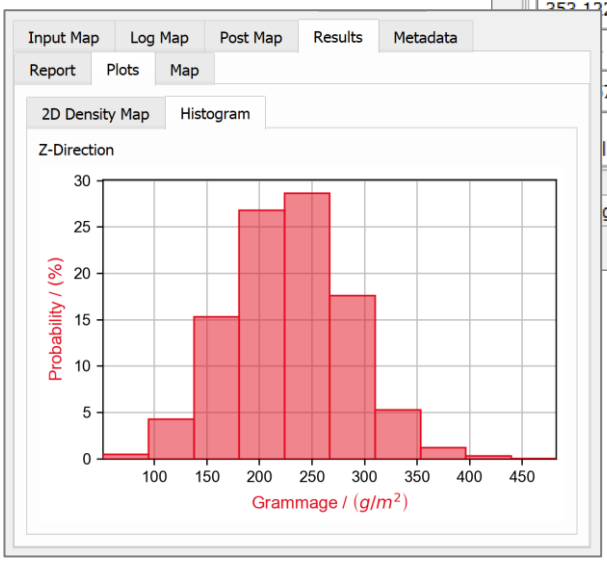


RESULTS

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.

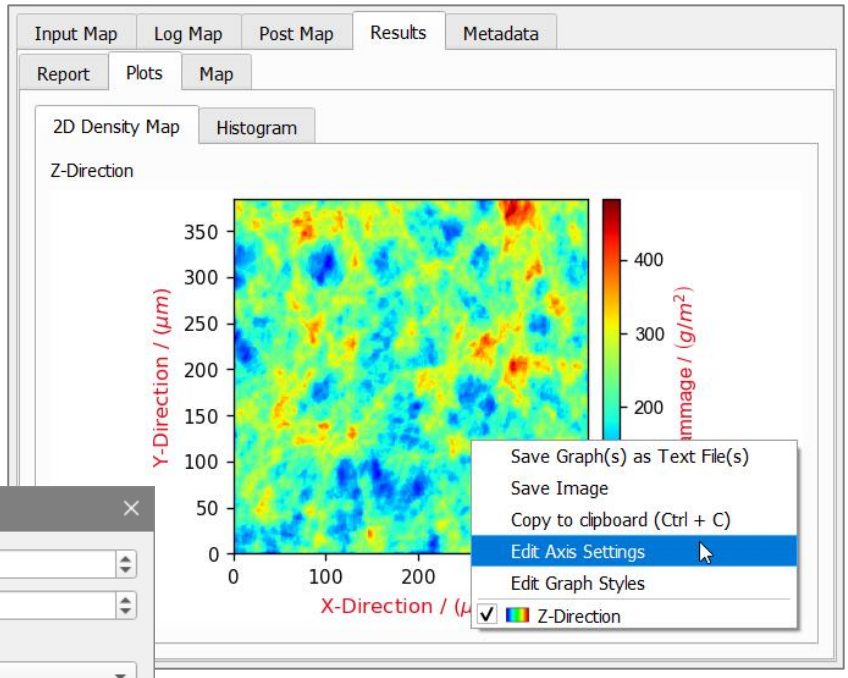
In the **Results - Report** tab, a table shows the computed density distribution. The report table also states minimal, maximal, and mean value of the computed parameter (here: grammage).



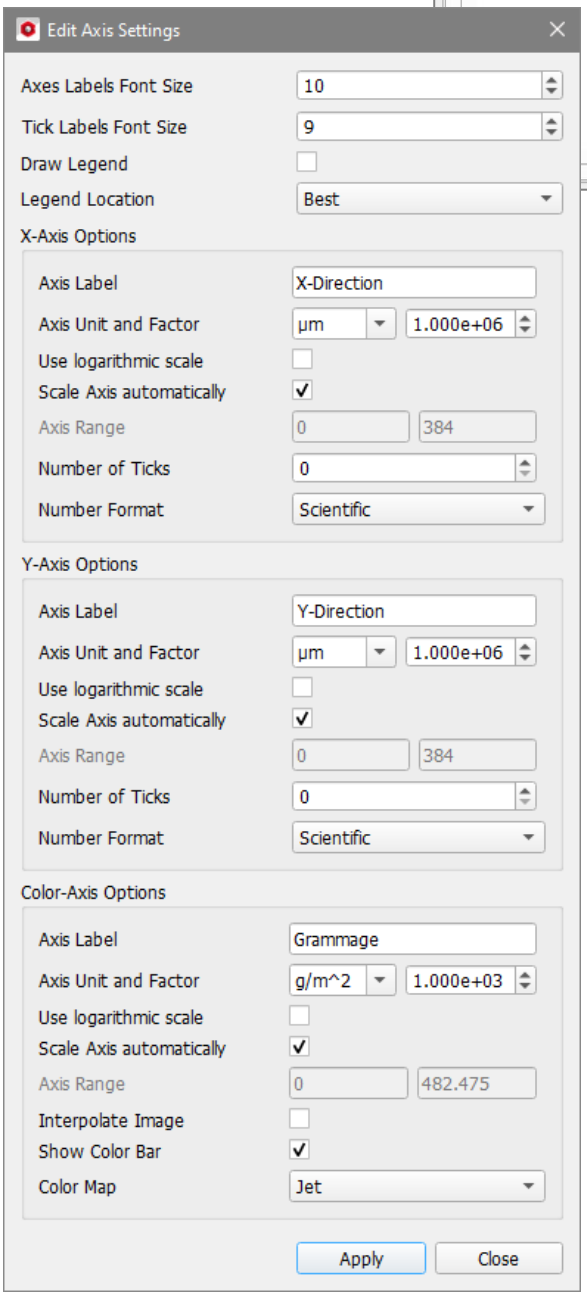


In the **Results – Plots** tab, the table entries are additionally available as a **Histogram** plot.

The **2D Density Map** subtab shows the computed result.



Right-click on the image to get additional options. **Save Image** allows to save the shown picture. **Edit Axis Settings** opens the **Edit Axis Settings** dialog.



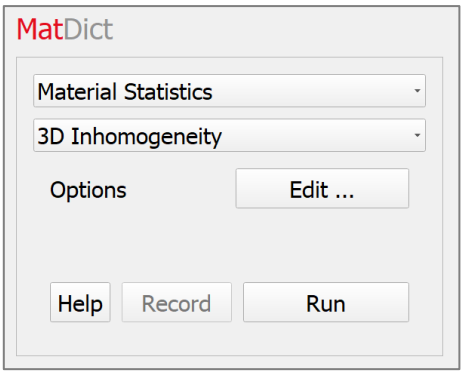
In the dialog, the font sizes of axes and tick labels and the layout of the X and Y axes can be modified.

When 0 is entered as **Number of Ticks**, GeoDict selects the tick number automatically.

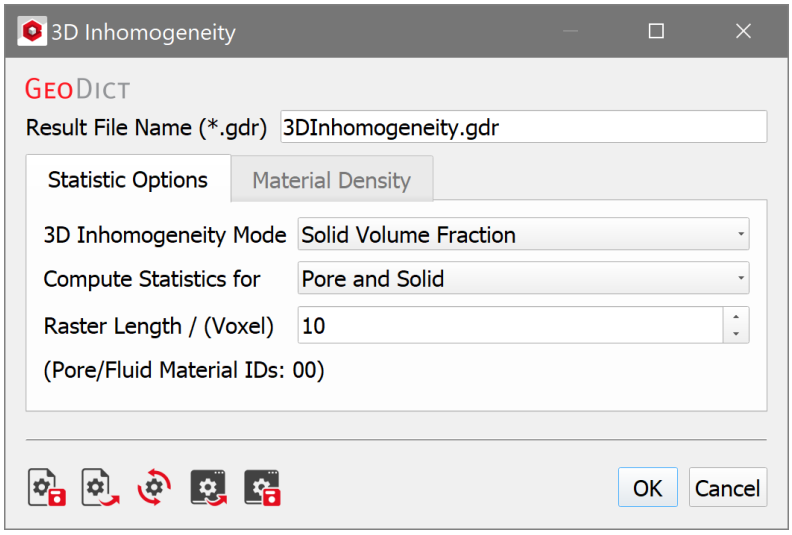
In the **Color-Axis Options**, various color schemes are selectable under **Color Map**. The **Axis Range** sets the lower and upper bound. Values lower than the lower bound are visualized with the color at the lower bound, values higher than the upper bound are visualized with the color at the upper bound.

3D INHOMOGENEITY

The **3D Inhomogeneity** command calculates the distribution of the **solid volume fraction** or **density** 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 box opens when clicking the **Options' Edit...** button and includes the **Statistic Options** and the **Material Density** tabs.

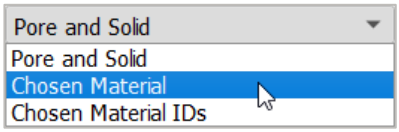


At the top of the dialog box, enter the **Result File Name**. The result file is saved in the chosen project folder (**File → Choose Project Folder**, in the menu bar).

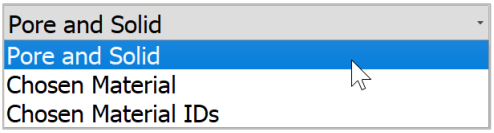
STATISTIC OPTIONS

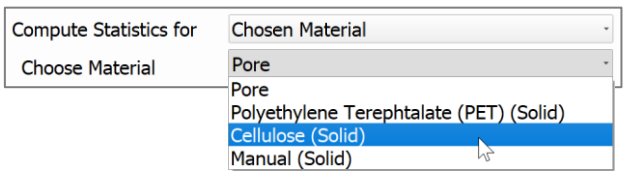
Under the **Statistic Options** tab, choose the property to be computed from the **3D Inhomogeneity Mode** pull-down menu.

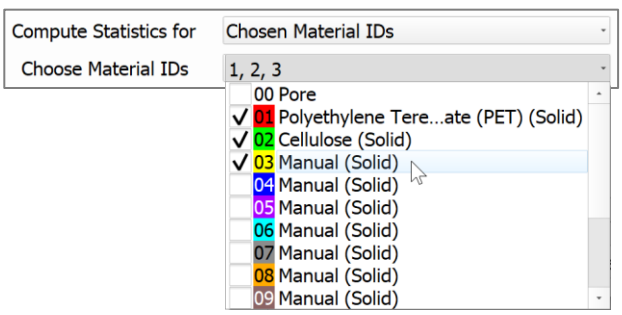
Only when choosing **Solid Density**, the **Material Density** tab is selectable and the density values for the individual Material IDs can be defined. For **Solid Volume Fraction** or **Porosity**, the density of the material IDs is not considered in the calculations and the Material Density tab therefore 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**. For **Chosen Material IDs**, those can then be chosen from the materials present in the structure in the **Choose Material IDs** pull-down menu.



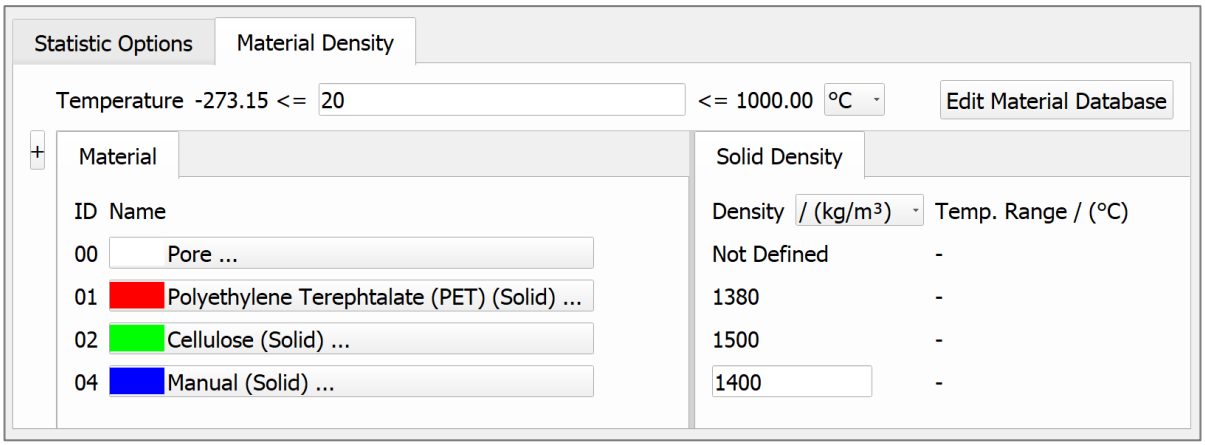




The **Raster Length** determines the side length of the cubic sub-volume in voxels. If **Raster Length** is not a common divisor of the side lengths **NX, NY, NZ** of the current structure, some boundary layers of the current structure will not be contained in any sub-volume. In this case, a warning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

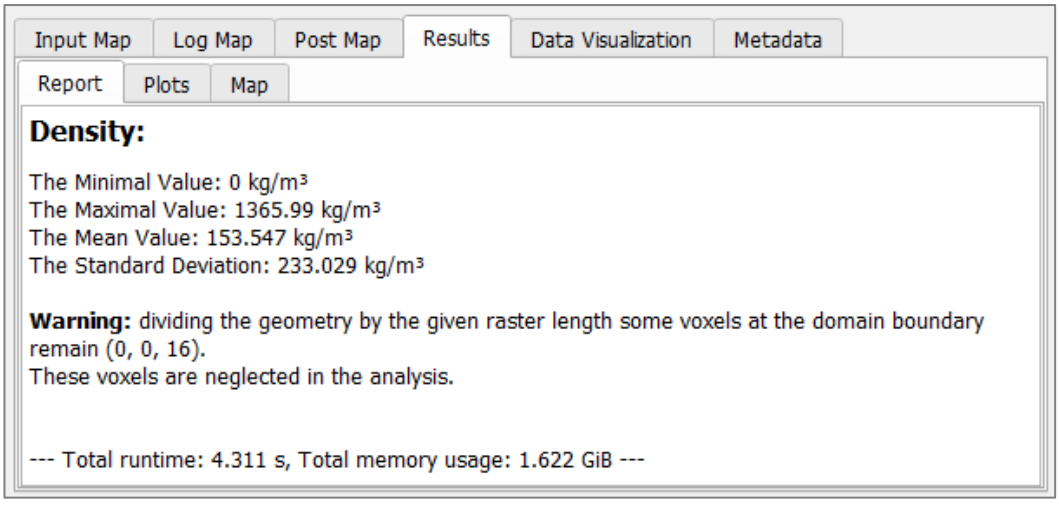
Material Density

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.



Results

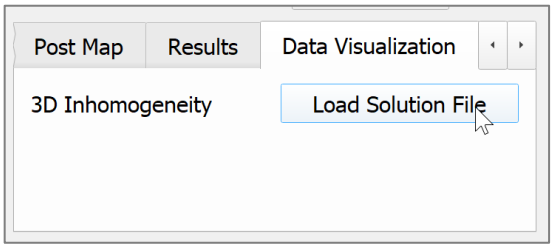
Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is opened in the **Result Viewer** after the computation is finished.

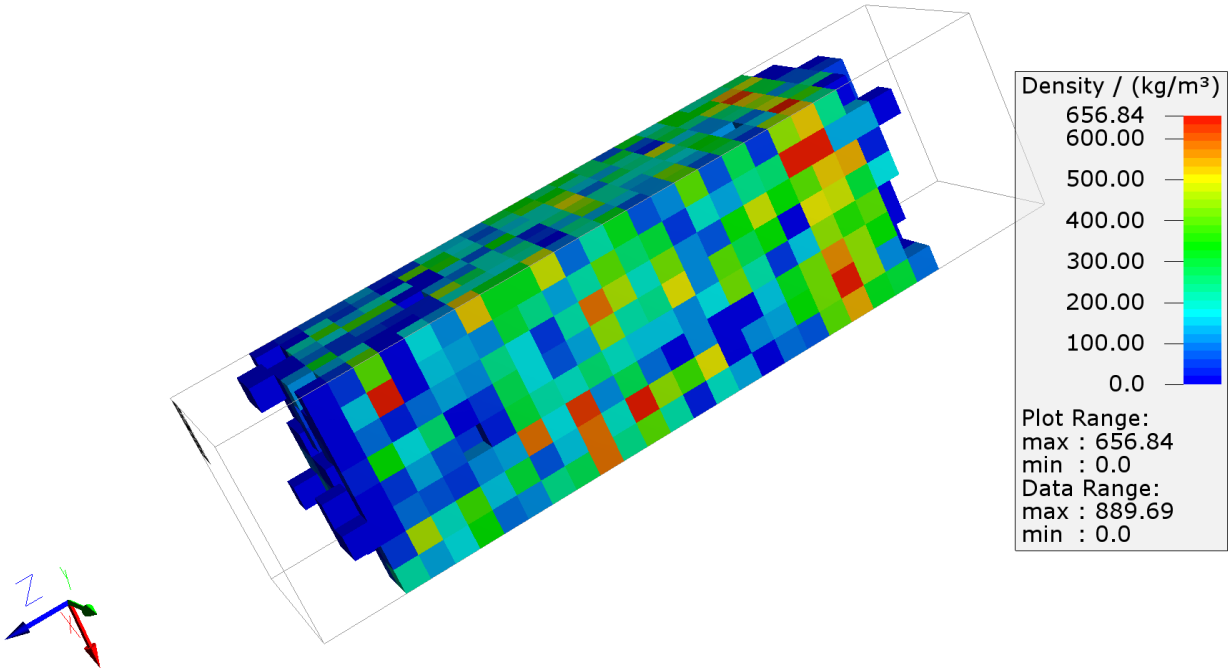


In the **Results - Report** subtab, the minimal and maximal density or solid volume fraction found in any sub-volume are reported. Additionally, the mean value of all densities and the corresponding standard deviation is shown.

Data Visualization

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

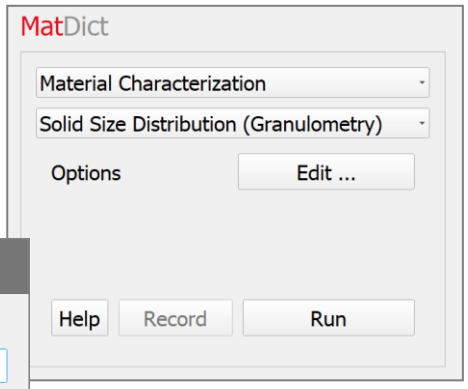


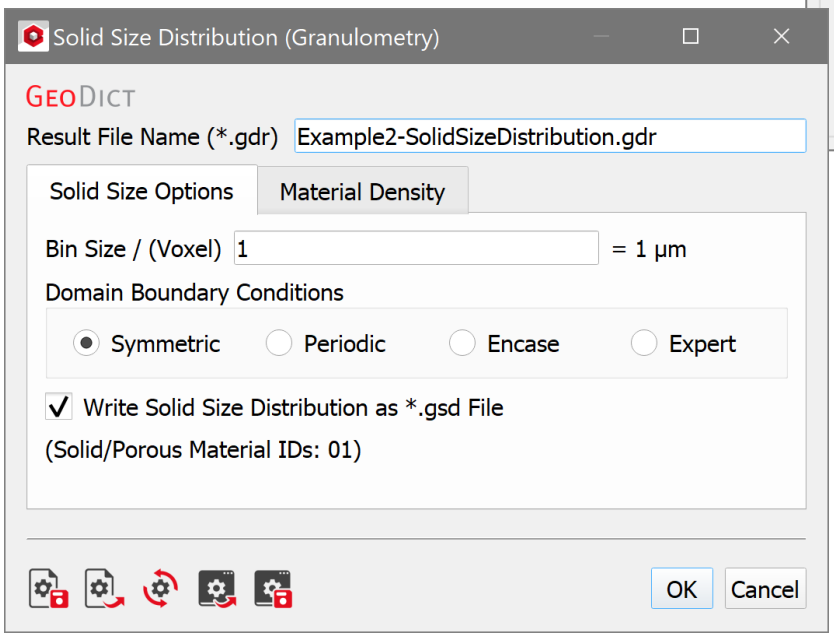


Material Characterization

Solid Size Distribution (Granulometry)

After selecting **Solid Size Distribution (Granulometry)**, the needed parameters can be entered by clicking the **Options' Edit...** button. The Pore Size Distribution dialog includes the **Pore Size Options** and the **Material Density** tabs.





At the top of the dialog box, 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 **Bin Size** can be entered (or modified). The bin size units are voxels and their equivalent in metric length units is shown. The solids are classified by their diameter into bins with given **Bin Size**. All bins are of equal size, and each bin contains objects with a diameter in the range between [(i – 1) x Bin size] and [i x Bin size], being i the bin number.

For example, when analyzing a porous structure with a voxel size of 1 µm, setting the **Bin Size** to 2 or to 4 voxels (i.e. 2 µm or 4 µm) leads to the bins shown in the table below:

Bin number (i)	Object diameter between [(i – 1) x Bin size] - [i x Bin size]	
	Bin Size 2 µm	Bin Size 4 µm
1	0 - 2 µm	0 - 4 µm
2	2 - 4 µm	4 - 8 µm
3	4 - 6 µm	8 - 12 µm
..	...	

When choosing the **Bin Size**, be aware that the underlying algorithm to compute the Euclidean distance operates directly on the voxel grid. Thus, the smallest possible

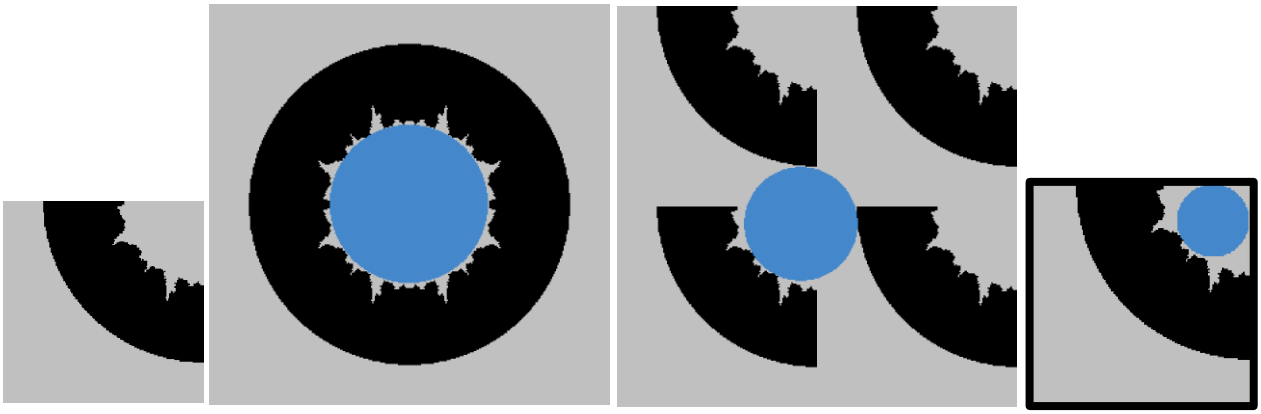
distance between two grid points is 1 Voxel, which corresponds to a radius of 1 Voxel. Thus, the smallest diameter that the algorithm can find is 2 Voxel lengths.

The **Domain Boundary Conditions** can be chosen to be **Symmetric**, **Periodic, Encase**, or any combinations of those boundary conditions in all three directions with the choice of **Expert**.

Choosing the appropriate boundary condition depends on the structure's design.

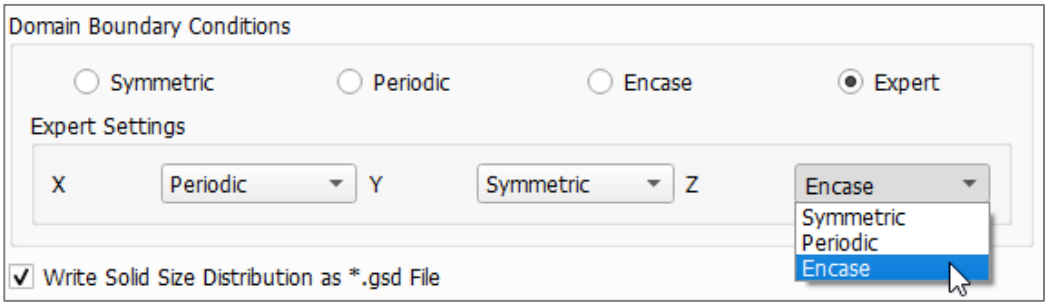
For example, imagine a structure with a cross-section as shown in (a). For the three boundary condition options shown in (b), (c) and (d) the resulting size is visualized in blue.

- If the geometry has mirror symmetry (b), **Symmetric** boundary conditions should be used, which would be a good approximation e.g. for a cut-out from a CT image.
- If instead the expected pattern of the geometry is repeated in all directions (c), **Periodic** boundary conditions should be selected. That has the effect that the structure's objects and pores ending on one side of the structure reappear in the opposite side.
- If the structure is encased in a closed wall (d), the **Encase** boundary conditions should be used.



(a) (b) (c) (d)

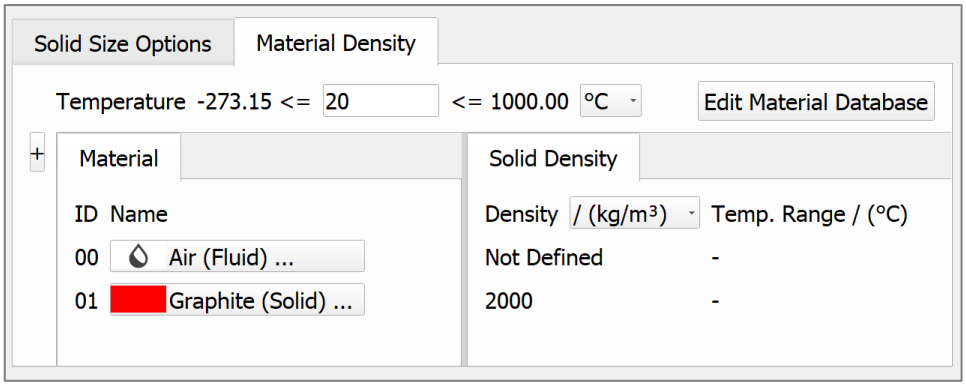
When different boundary conditions need to be specified for the three directions, choose the **Expert** option. Then, the boundary conditions can be set differently for each direction. For example, the boundary conditions could be chosen to be **Encase** in X-direction, **Symmetric** in the Y-direction and **Periodic** in Z-direction.



When **Write Solid Size Distribution as *.gsd File** is checked, a volume field with the name SolidSizeDistribution.gsd (in *.gsd format) is saved in the results folder inside the project folder. The file contains the calculated sphere diameter in each voxel written of the structure.

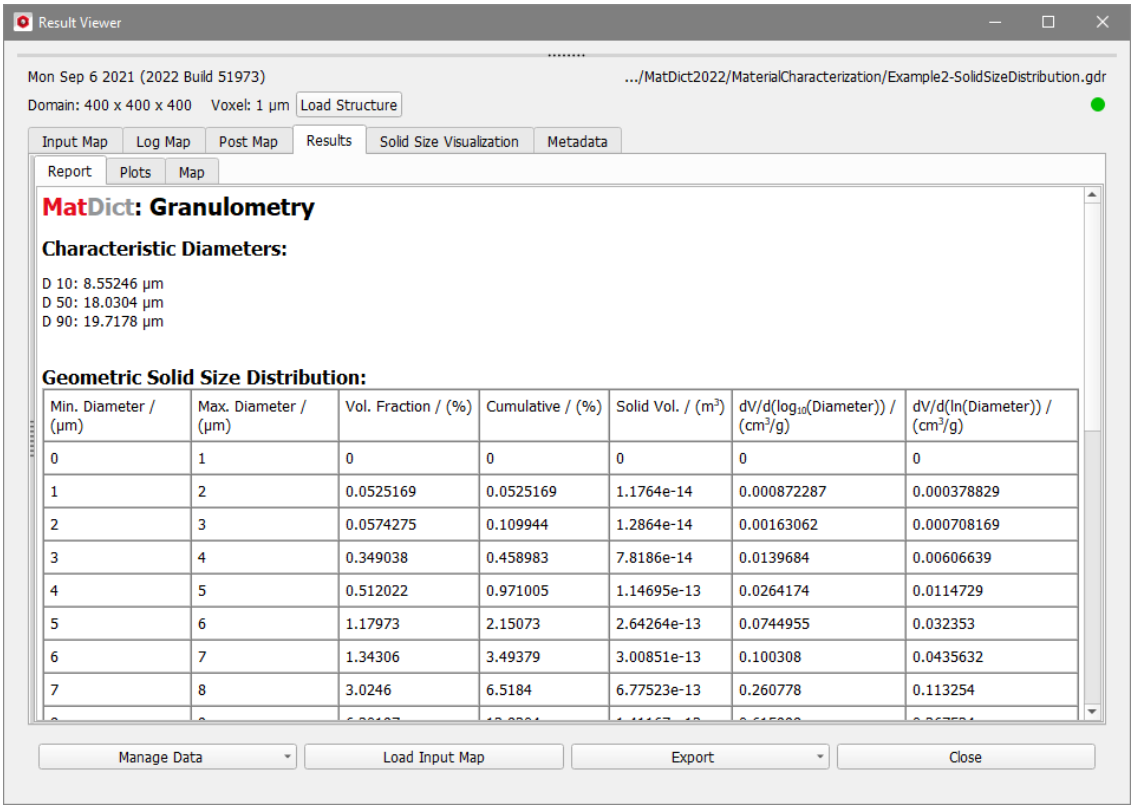
Material Density

Under the **Material Density** tab, the temperature can be edited, and 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.



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.

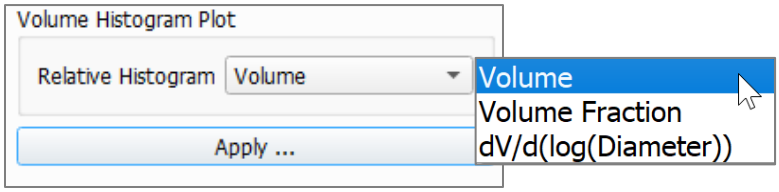


Min. Diameter / (µm)	Max. Diameter / (µm)	Vol. Fraction / (%)	Cumulative / (%)	Solid Vol. / (m^3)	dV/d($\log_{10}$(Diameter)) / (cm^3/g)	dV/d(ln(Diameter)) / (cm^3/g)
0	1	0	0	0	0	0
1	2	0.0525169	0.0525169	1.1764e-14	0.000872287	0.000378829
2	3	0.0574275	0.109944	1.2864e-14	0.00163062	0.000708169
3	4	0.349038	0.458983	7.8186e-14	0.0139684	0.00606639
4	5	0.512022	0.971005	1.14695e-13	0.0264174	0.0114729
5	6	1.17973	2.15073	2.64264e-13	0.0744955	0.032353
6	7	1.34306	3.49379	3.00851e-13	0.100308	0.0435632
7	8	3.0246	6.5184	6.77523e-13	0.260778	0.113254

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 pores have a smaller than 8.55 µm. The D50 value of 18.03 µm means that 50% of all pores have a diameter smaller than 18.03 µm, and the D90 value of 19.71 µm means that 90% of all pores 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 Pore Volume, and the Differential Pore Volume Distribution for every bin size.



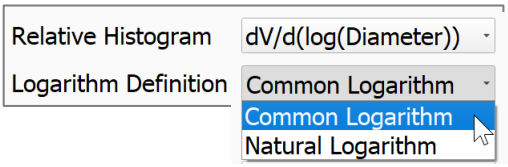
Under the **Results – Plots** subtab, different relative and cumulative histograms can be plotted. The histogram of interest, i.e. Volume, Volume Fraction, or dV/dlog(Diameter) can be chosen in the **Volume Histogram Plot** section.

The differential solid volume distribution dV/dlog(Diameter) is computed as

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

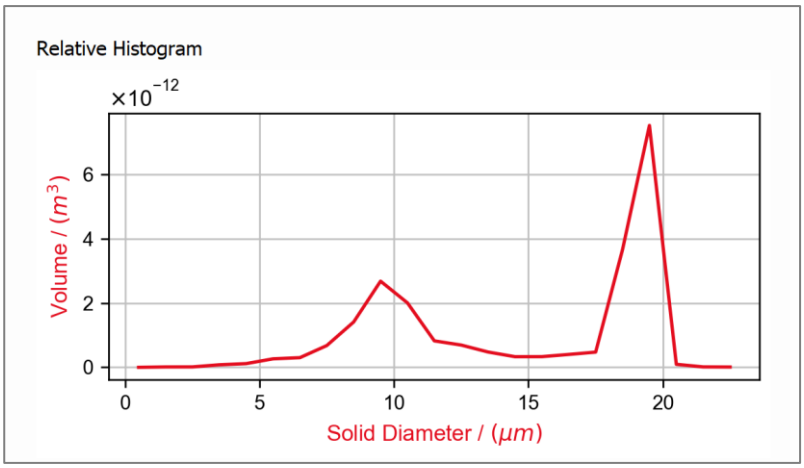
where the d_i are the diameters, V_{cum} the cumulative volume fractions, and m is the mass of the structure. The mass of the structure is computed using the densities of the solid constituent materials of the sample. This normalization ensures that the value of dV/dlog(Diameter) is independent of the size of the domain.

For the option **dV/dlog(Diameter)**, it can be chosen if the natural logarithm $\ln$ or the common logarithm $\log_{10}$ should be used.

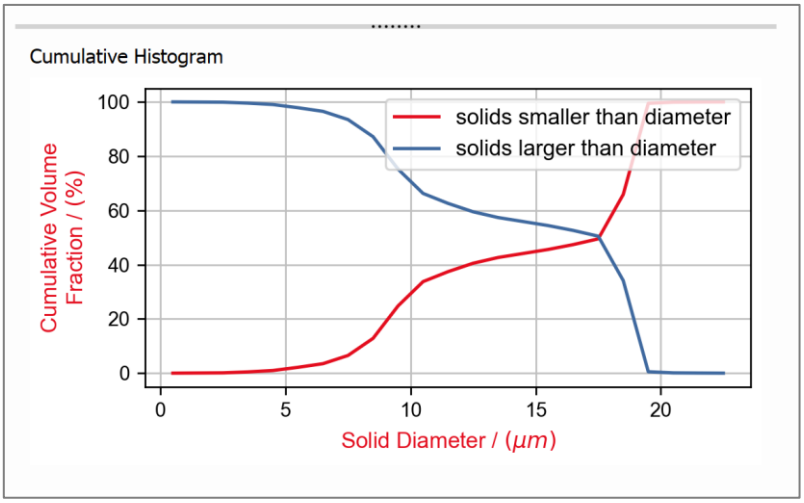


Furthermore, the user can define several visualization options, such as Length Unit, Fraction Unit, Histogram Style, X-Axis Range, Y-Axis Range, and if the X-Axis scaling should be logarithmic.

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

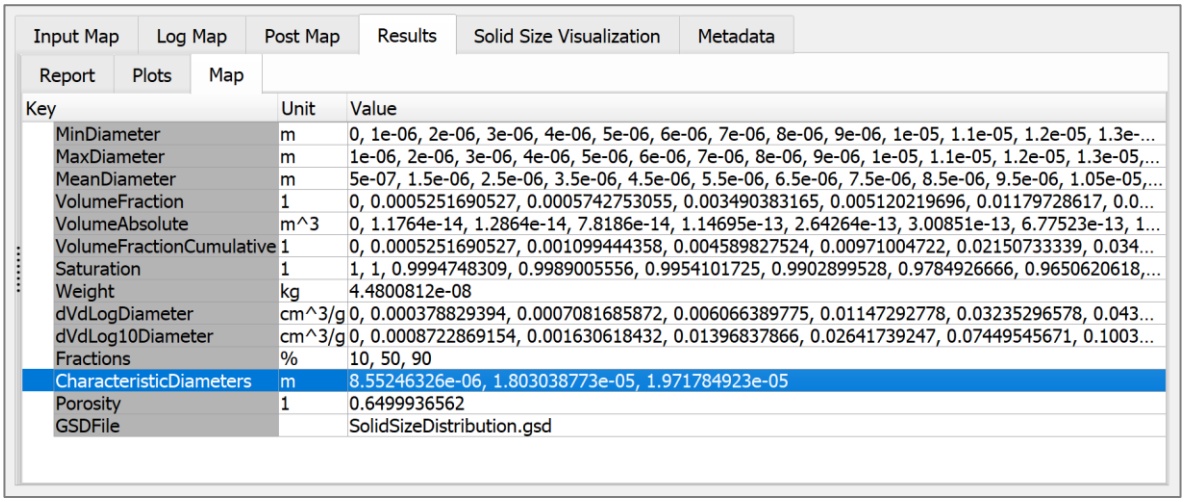


In the **Cumulative Histogram** plot, the red curve shows the volume fraction of solids smaller than a given diameter and the blue curve shows the solids larger than or equal to a given diameter. Both curves sum up to 100% for any given diameter.



As usual, the plots can be edited and saved as images or as text files by right-clicking on the graph area.

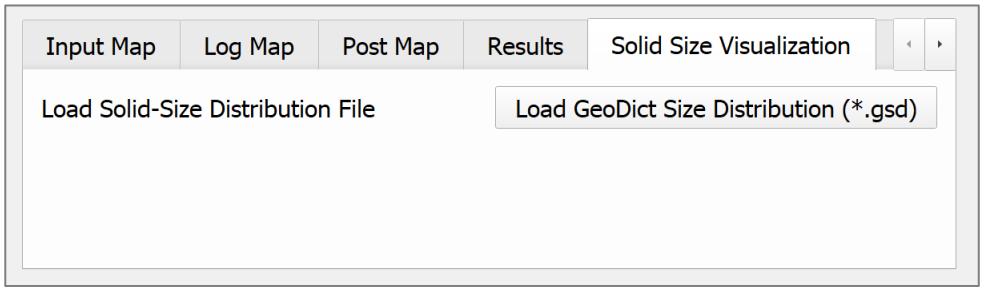
The **Results - Map** subtab gives access to the values of the computed parameters.

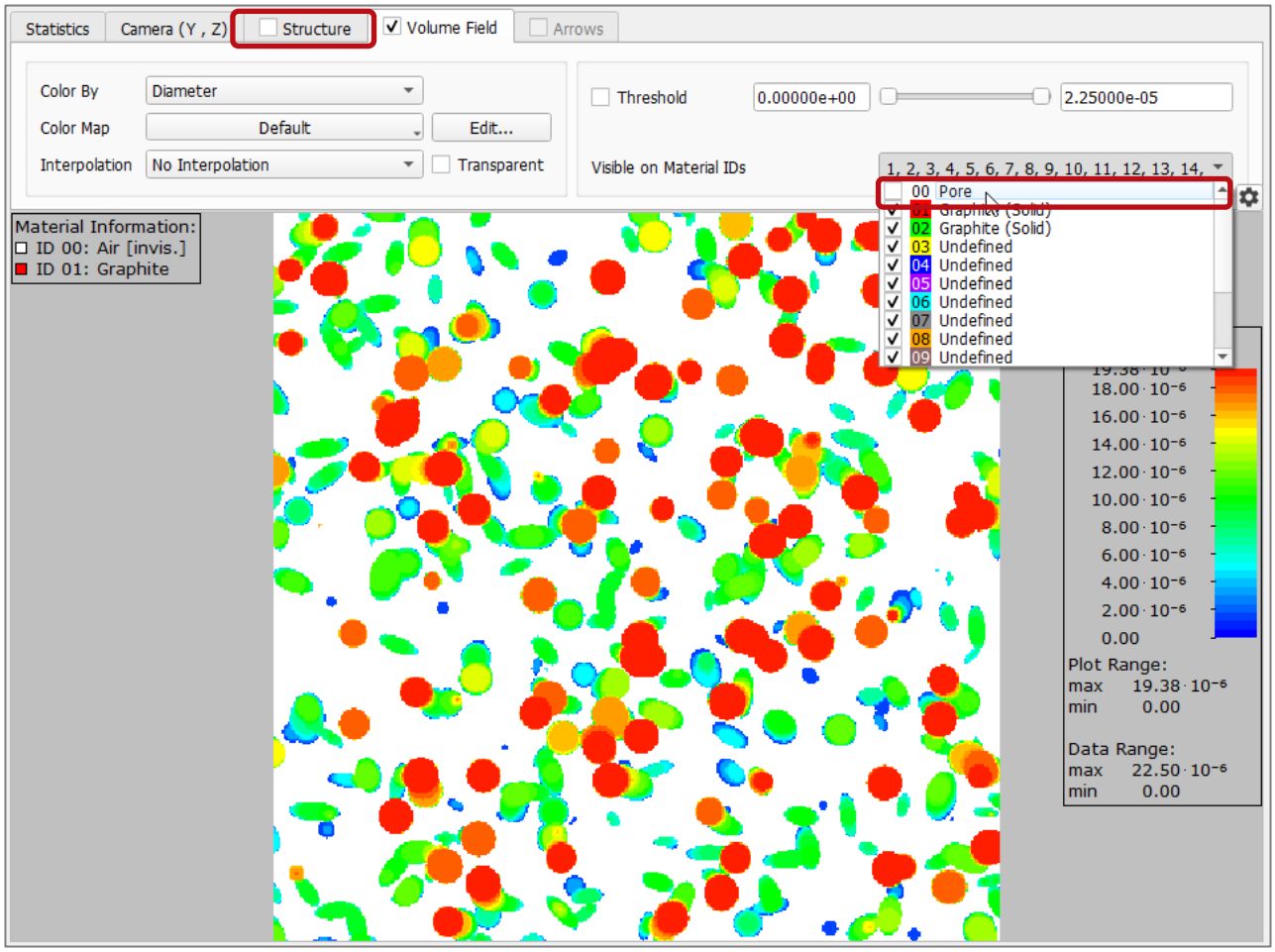


Key	Unit	Value
MinDiameter	m	0, 1e-06, 2e-06, 3e-06, 4e-06, 5e-06, 6e-06, 7e-06, 8e-06, 9e-06, 1e-05, 1.1e-05, 1.2e-05, 1.3e-...
MaxDiameter	m	1e-06, 2e-06, 3e-06, 4e-06, 5e-06, 6e-06, 7e-06, 8e-06, 9e-06, 1e-05, 1.1e-05, 1.2e-05, 1.3e-05,...
MeanDiameter	m	5e-07, 1.5e-06, 2.5e-06, 3.5e-06, 4.5e-06, 5.5e-06, 6.5e-06, 7.5e-06, 8.5e-06, 9.5e-06, 1.05e-05,...
VolumeFraction	1	0, 0.0005251690527, 0.0005742753055, 0.003490383165, 0.005120219696, 0.01179728617, 0.0...
VolumeAbsolute	m^3	0, 1.1764e-14, 1.2864e-14, 7.8186e-14, 1.14695e-13, 2.64264e-13, 3.00851e-13, 6.77523e-13, 1...
VolumeFractionCumulative	1	0, 0.0005251690527, 0.001099444358, 0.004589827524, 0.00971004722, 0.02150733339, 0.034...
Saturation	1	1, 1, 0.9994748309, 0.9989005556, 0.9954101725, 0.9902899528, 0.9784926666, 0.9650620618,...
Weight	kg	4.4800812e-08
dVdLogDiameter	cm^3/g	0, 0.000378829394, 0.0007081685872, 0.006066389775, 0.01147292778, 0.03235296578, 0.043...
dVdLog10Diameter	cm^3/g	0, 0.0008722869154, 0.001630618432, 0.01396837866, 0.02641739247, 0.07449545671, 0.1003...
Fractions	%	10, 50, 90
CharacteristicDiameters	m	8.55246326e-06, 1.803038773e-05, 1.971784923e-05
Porosity	1	0.6499936562
GSDFile		SolidSizeDistribution.gsd

Data Visualization

The distribution of pores is observed in the Volume Fraction/Pore 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)**.

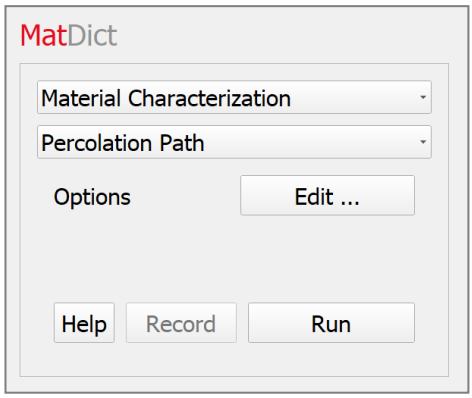


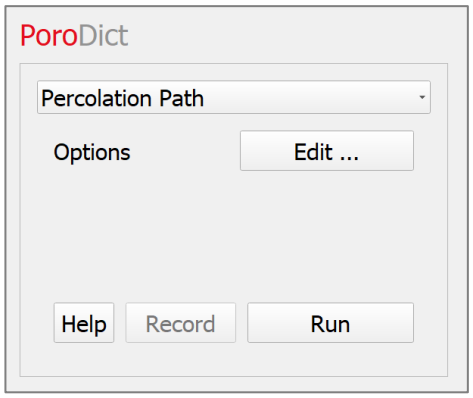


To see the solid size distribution inside of the structure, it is recommended to deactivate visualization of the structure itself. This can be done by unchecking **Structure** in the tab headers or alternatively in the **Data View** settings. Additionally, the visualization of the result field in the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

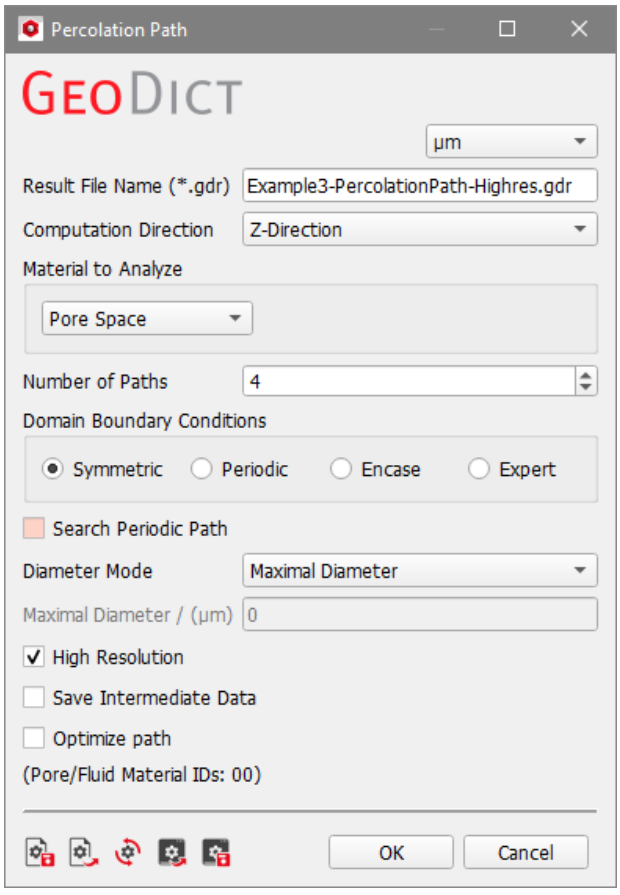
PERCOLATION PATH

The **Percolation Path** command is accessible from MatDict and PoroDict. It can find percolation paths in the pore space, or through a given material.





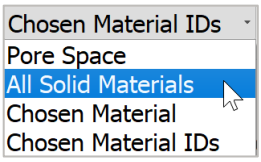
The Percolation Path dialog opens, and the necessary parameters can be entered by clicking the **Options' Edit...** button.



At the top of the dialog box, 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.

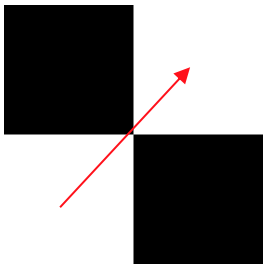
The diameter of pores and solids near the domain boundary is strongly influenced by the selected **Domain Boundary Conditions**. Here, the same boundary conditions as in the granulometry command are available. An example explaining the available options is given in the previous section on page 21.

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.

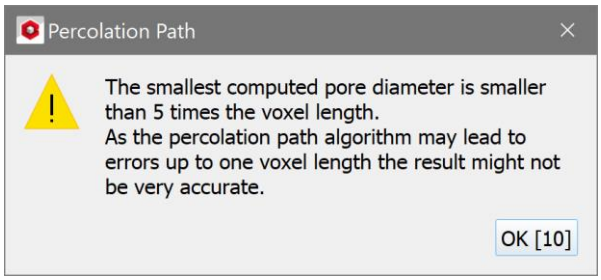
To run the calculations in **High Resolution** might be useful when the path space is expected to be narrow. The standard algorithm computes distances directly on the voxel grid, i.e. when determining a pore size, only the distances from the center of a pore voxel to the center of a solid voxel are taken 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.



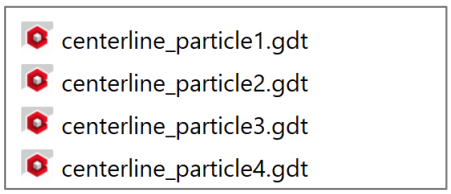
As an extreme example, the standard algorithm detects a percolation path across voxel edges as shown on the left. Using the **High Resolution** mode, no percolation path is found in such a situation, which is more accurate.

The disadvantage of the **High Resolution** mode is that the calculation runtime and memory usage may increase by a factor of eight.

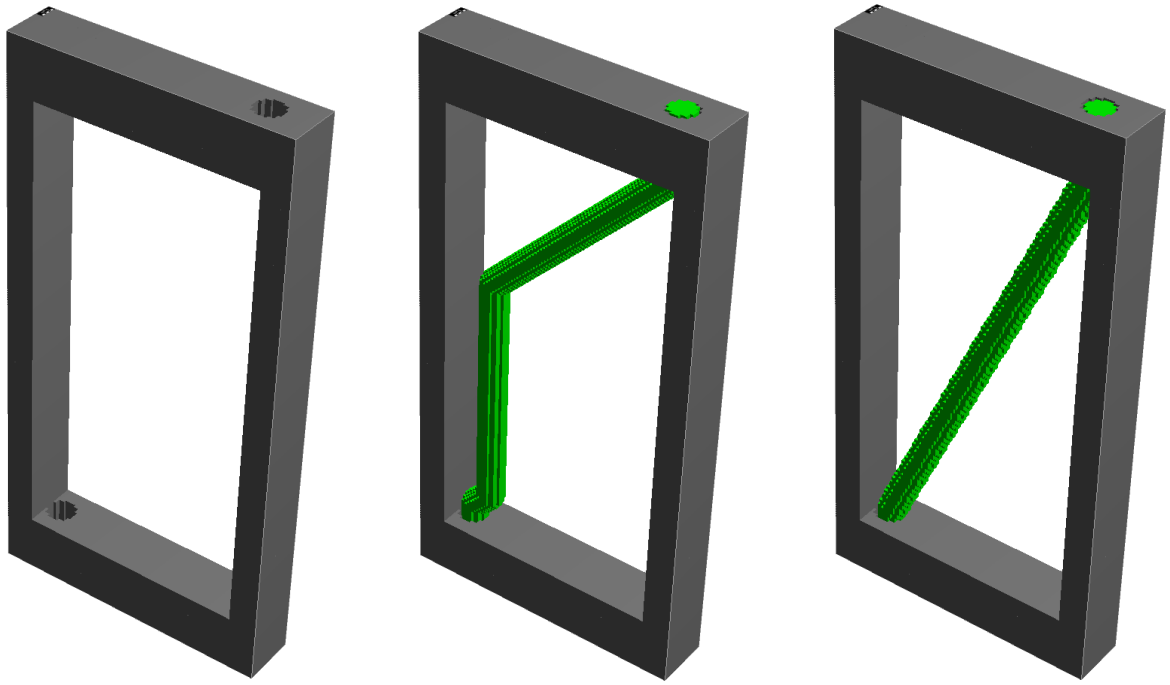
If the largest computed path is smaller than five voxel lengths, and the simulation was run in the standard mode, a warning message is shown. In this case, it is recommended to re-run the simulation in **High Resolution** mode.



When **Save Intermediate Data** 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).

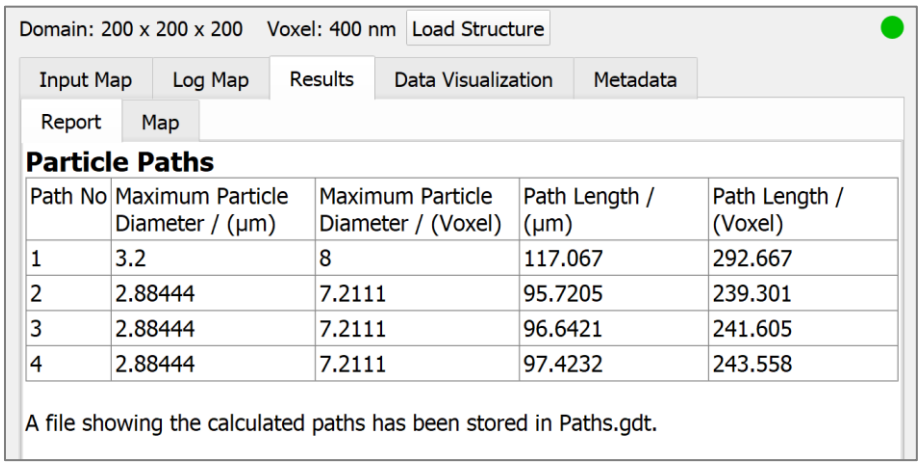


Structure without path

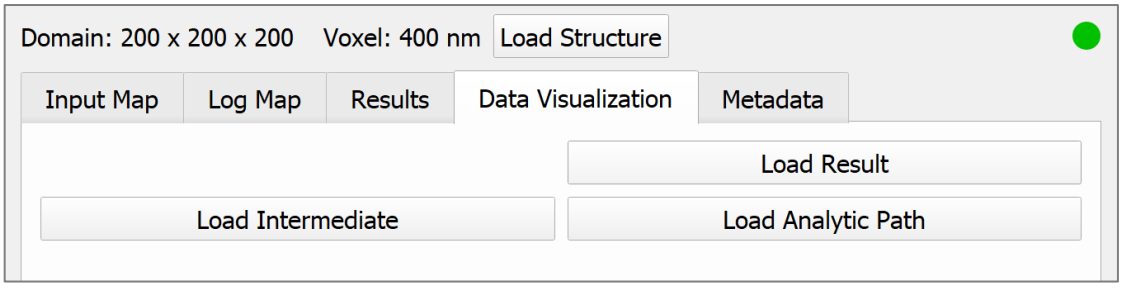
Click **OK** to close the Percolation Path dialog and start the command by clicking **Run**. The Result Viewer automatically opens at the end of the calculations.

RESULTS

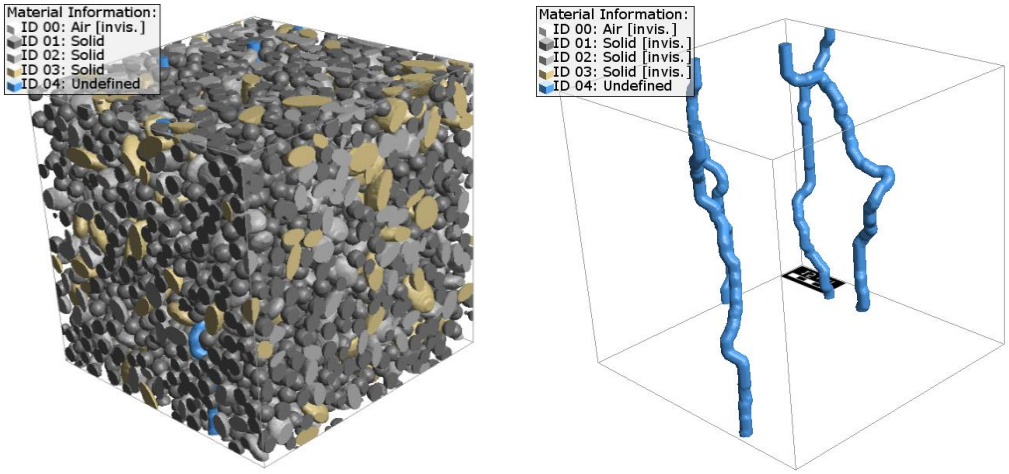
The **Results - Report** subtab includes the **Maximum Particle Diameter** (in µm and voxels) of spherical particles which may pass through the medium, as well as the **Path Length** (in µm and voxels) of the detected percolation path(s).



Under the **Data Visualization** tab, three options are available.

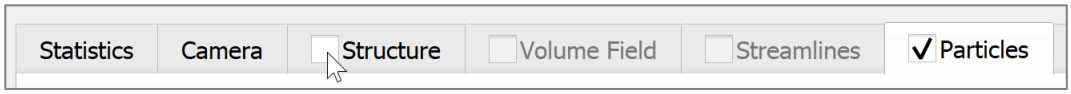


Click **Load Result** to show the percolation path(s) in the structure. Use **Settings** → **Color & Visibility Settings** → **visible**, to turn off the materials in the original structure (here Material ID 01: Solid, Material ID 02: Solid, Material ID 03: Solid) and see only the percolation path(s) (here Material ID 04: Undefined).

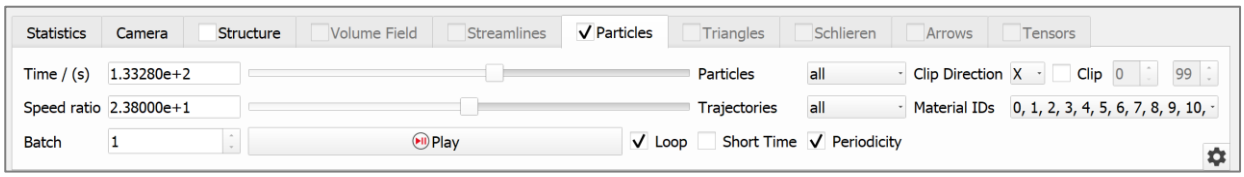


Alternatively, the percolation path can be visualized with animated spheres moving through the structure.

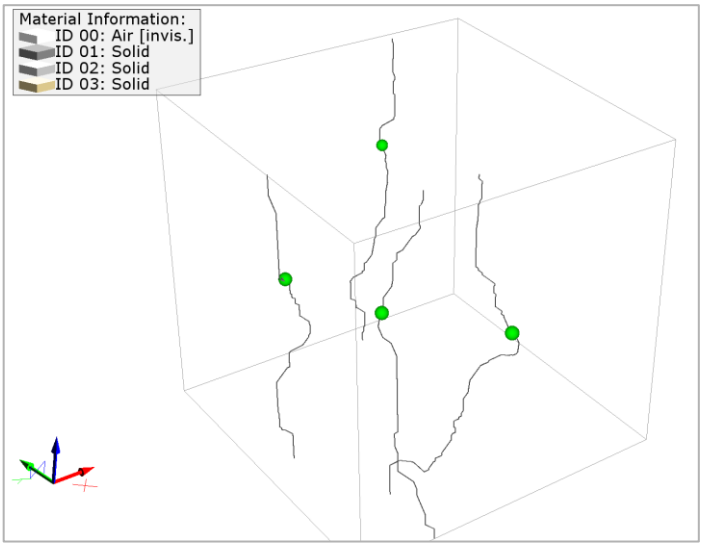
For this, reload the original structure by clicking **Load Structure** in the Result Viewer. Then, click **Load Analytic Path** under the Data Visualization tab. Deactivate the structure visualization by unchecking the **Structure** button in the Visualization tabs panel.



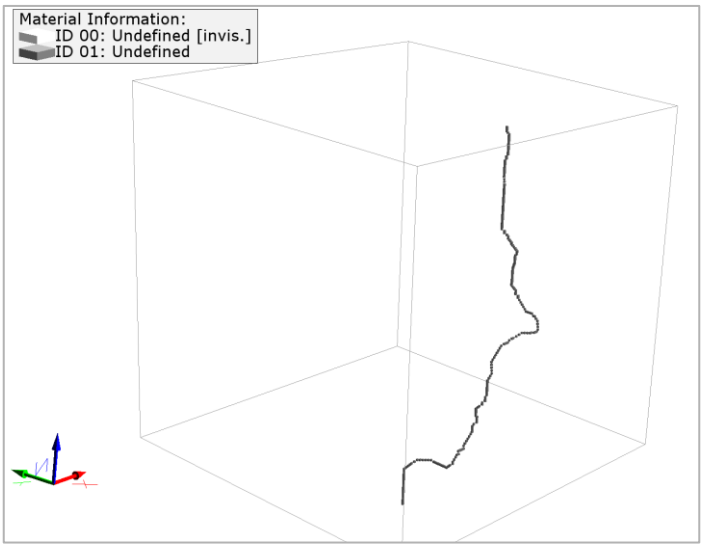
In the Visualization panel, above the Visualization area, click **Play** under the **Particles** tab. For convenience, check **loop** and, for the **Trajectories**, select to show **all**.



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



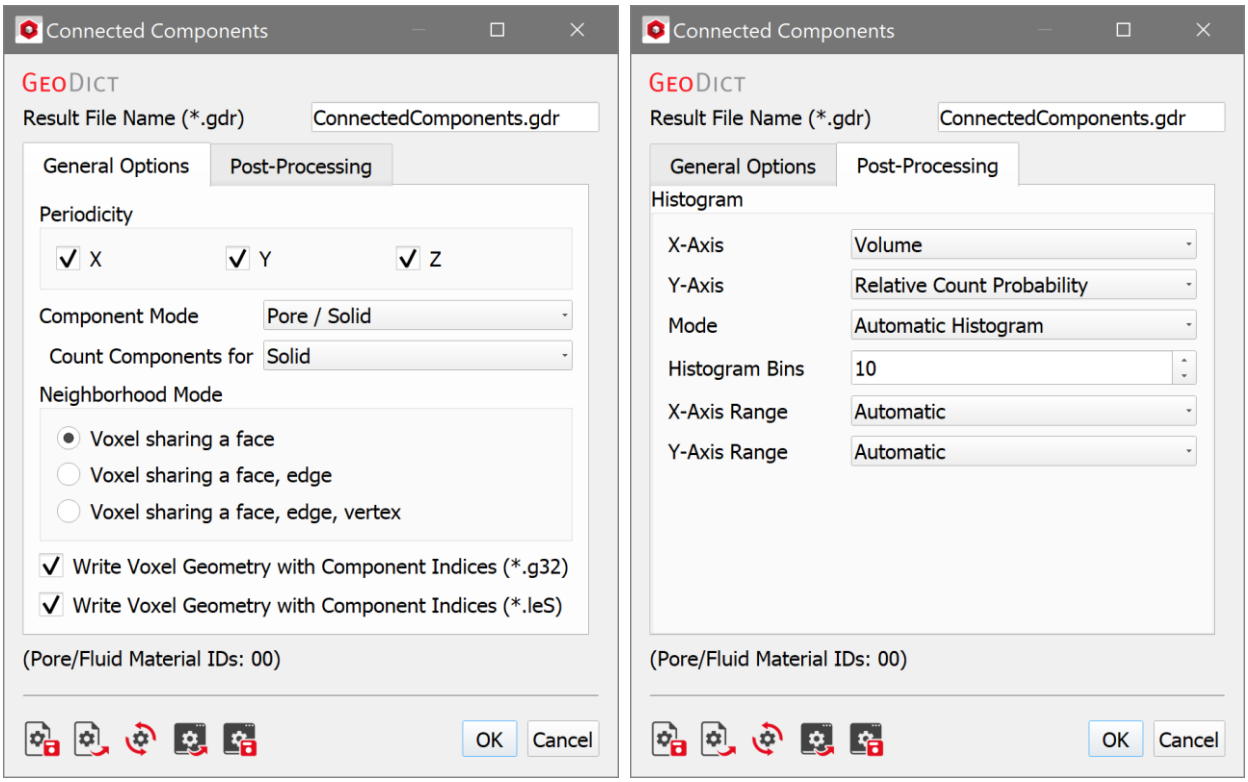
The last option, **Load Intermediate**, is only available if **Save Intermediate Data** was switched on when running the simulation. It loads a structure file that contains the center line of the path with the maximal diameter.



Connected Components

Through 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 or the same material ID.

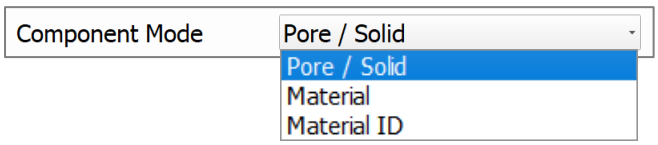
The **Connected Components** dialog opens when clicking the **Options' Edit...** button and includes the **General Options** and the **Post-Processing** tabs.



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

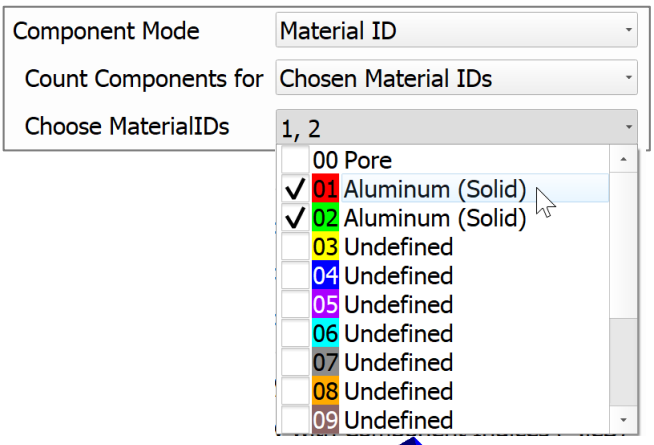
General Options

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.

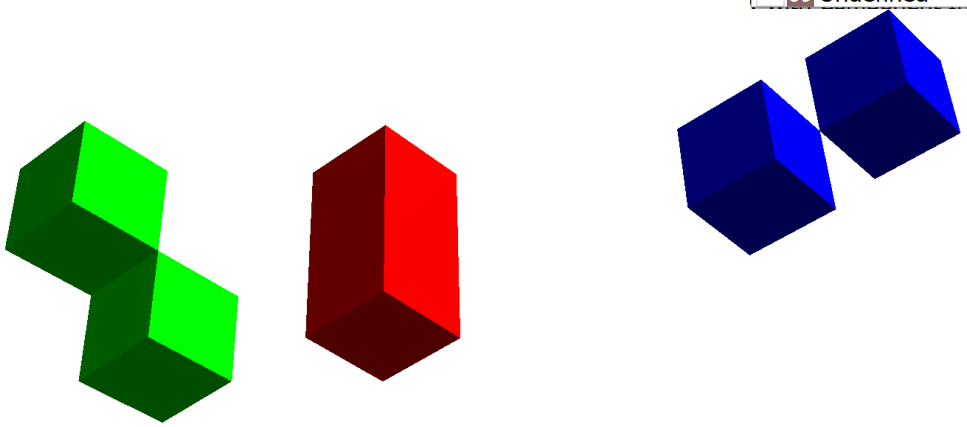


If the **Component Mode** is set to **Material ID**, all voxels belonging to one component must have the same material ID. If it is set to **Material**, all voxels belonging to one component must belong to the same material. If it is set to **Pore / Solid**, the distinction happens only between solid 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 box.

While the **Component Mode** defines which parts may belong to one component, set what is counted and reported with **Count Components for**. 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 from 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 from one component, and the blue voxels form one component.

When checking **Write Voxel Geometry with Object 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 Object 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 below in the Results section.

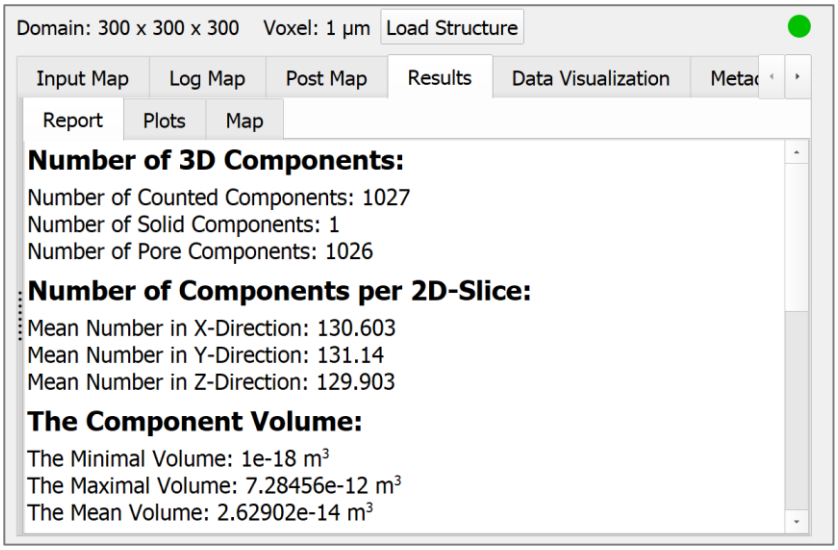
RESULTS

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 box in the upper part of the **Result Viewer** can be collapsed (and expanded) by pulling up (or down) the dotted line under the box.

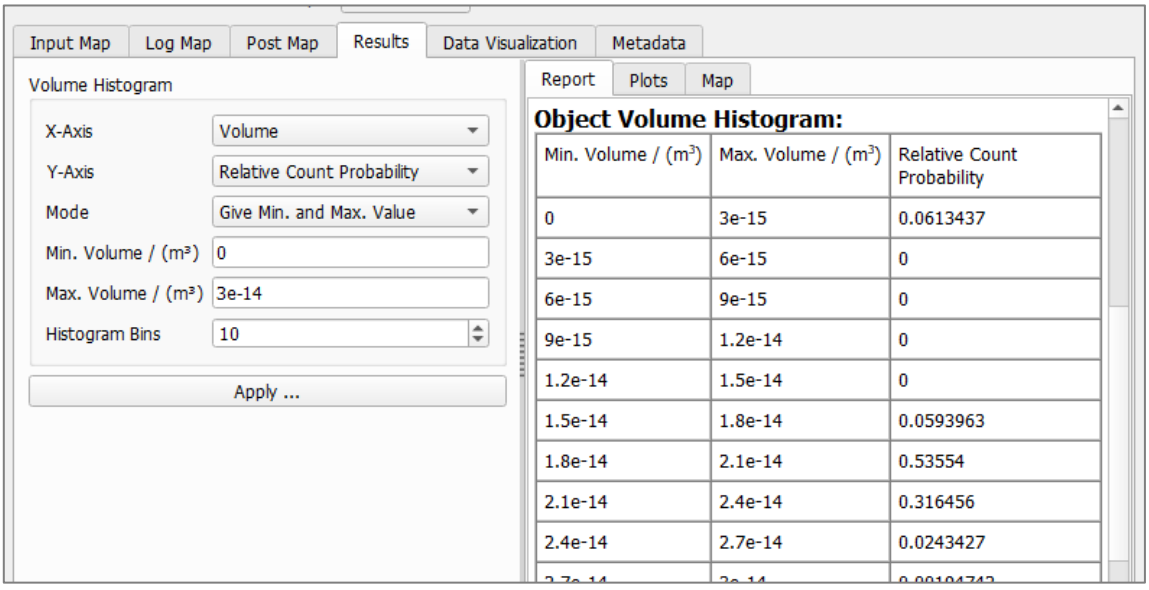
The same applies to the left panel of the **Results** tab, which can be collapsed (and expanded) by pulling left (or right) the dotted line between the post-processing options and the **Results** – **Report** subtab.

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.



As a post-processing step, the settings of the object volume histogram can be 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 adapt the values in the **Results** tabs.

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



POST-PROCESSING

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.

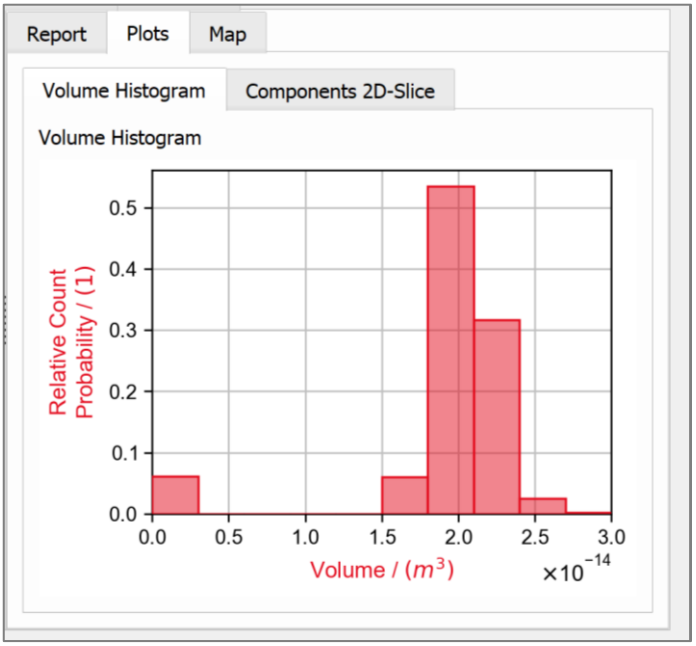
The histogram **Mode** offers the choice between generating an **Automatic Histogram** without further specifications or to **Give Min. and Max Value** for the parameter defined in the X-Axis pull-down menu (Volume or Equivalent Diameter). Either **Min. Volume** and **Max. Volume** or **Min. Diameter**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

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

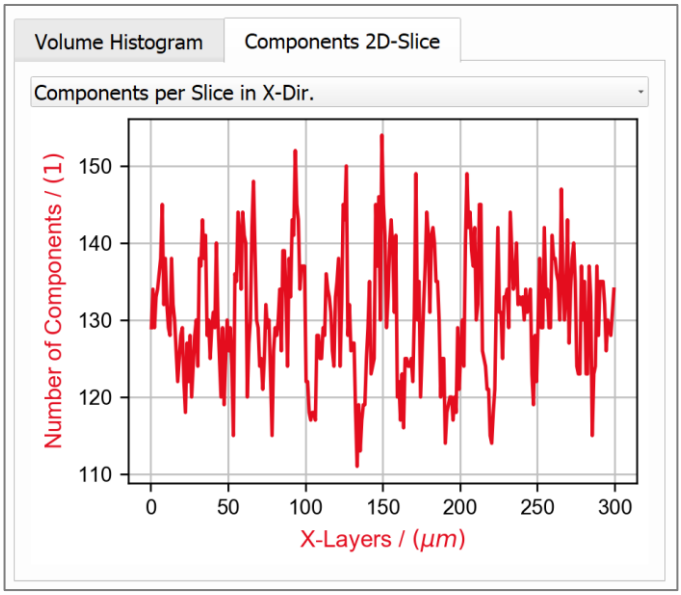
The object volume histogram is shown under the **Result - Plots** subtab. In the plot, the values for each bin are visualized as bars.

The parameters **X-Axis Range** and **Y-Axis Range** can be used to adjust the area shown in the plot. If **X-Axis Range** is set to **Automatic**, the whole range of the **Object Volume Histogram** table is plotted.

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

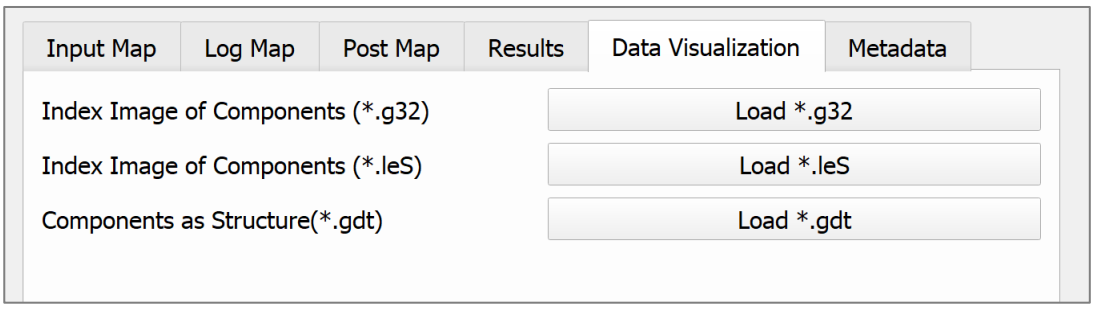


Under the **Plots** tab, also the computed **Number of Components per 2D Slice** is visualized by three graphs.



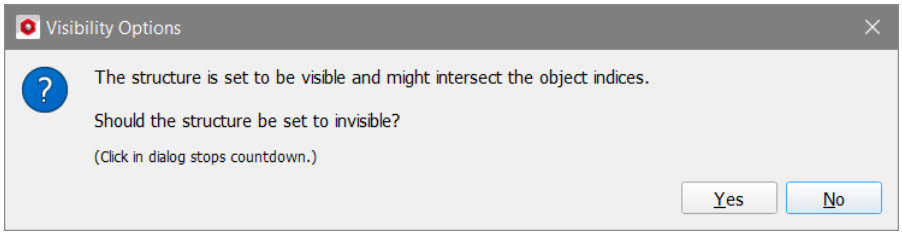
Data Visualization

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



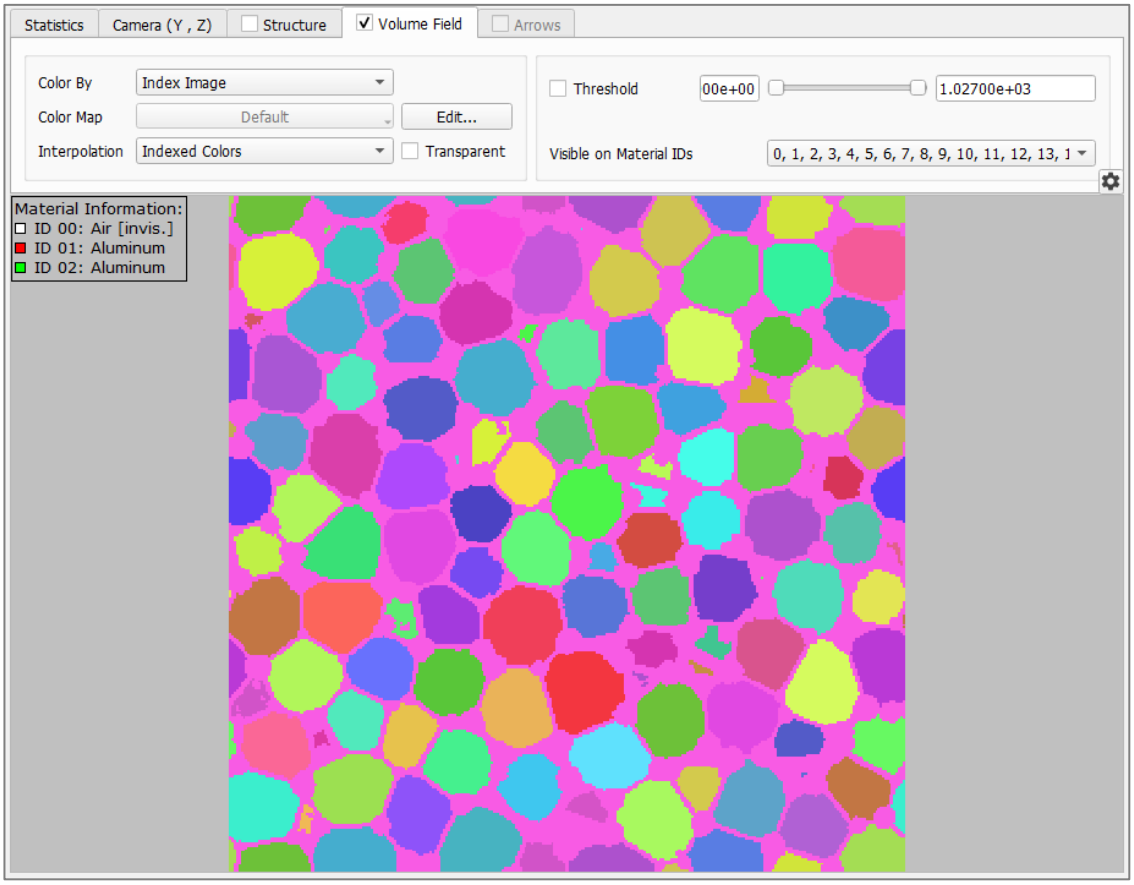
The first option is to load the index image in *.g32 or *.leS format. These files are 3D images, where for every voxel the index number of the corresponding component is stored. For example, if the structure consists of 1027 components, the file will contain numbers from 1 to 1027. Click **Load *.g32**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

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



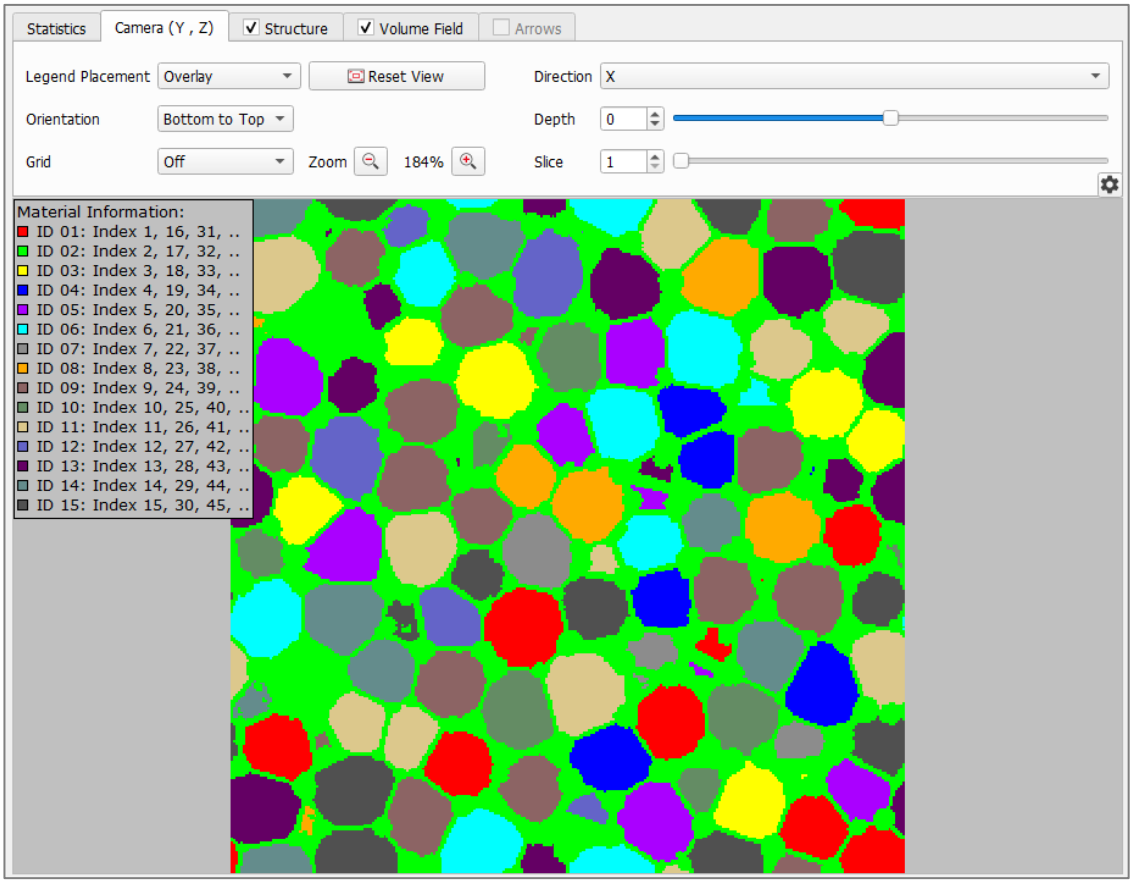
For the visualization of the index image, it is recommended to set the structure visualization to invisible, so that the indices can also be seen in the solid parts of the structure.

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 second option is to load the components as a structure file in GeoDict's *.gdt file format. This format supports only 16 different material IDs.

Every component is assigned a material ID based on the index number as shown in the following picture.

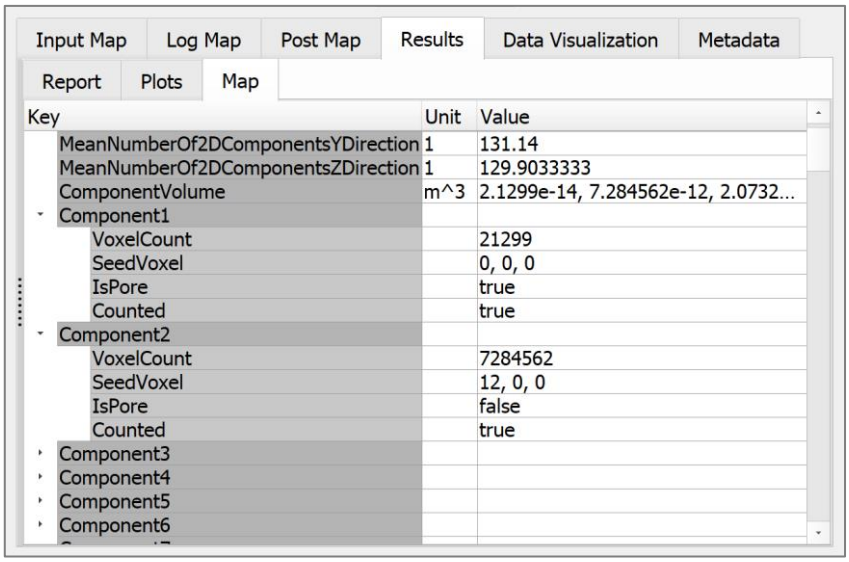


Be aware that neighboring components might get assigned to the same ID. In the example, every 15th foam cell gets assigned to the same ID as the cell walls, and therefore disappears in the visualization.

Result Map

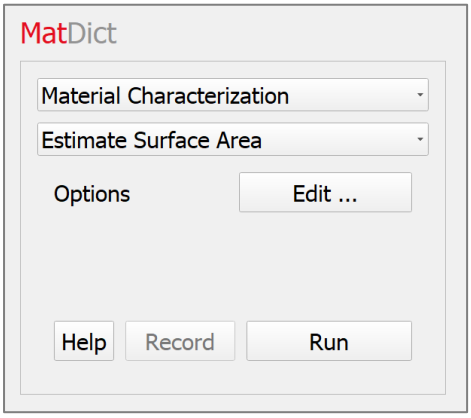
The result map additionally contains the details for every found component:

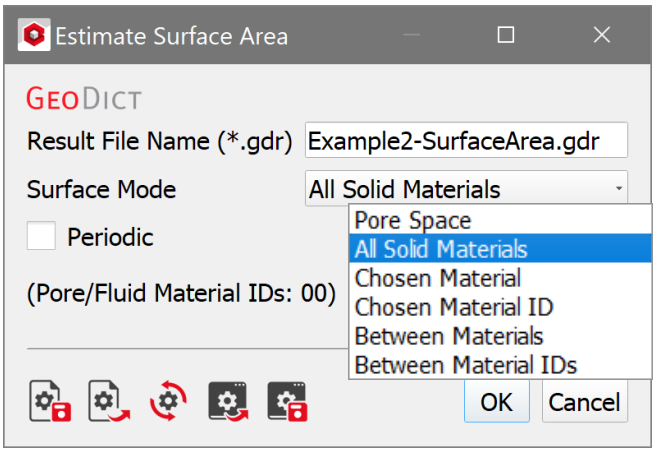
- **VoxelCount** states the number of voxels inside of a component.
- **SeedVoxel** is an arbitrary voxel inside of this component.
- **IsPore** states if this component is pore or solid.
- **Counted** states if this component is counted.



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.



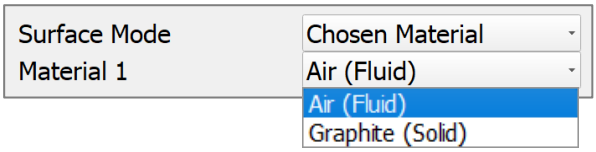


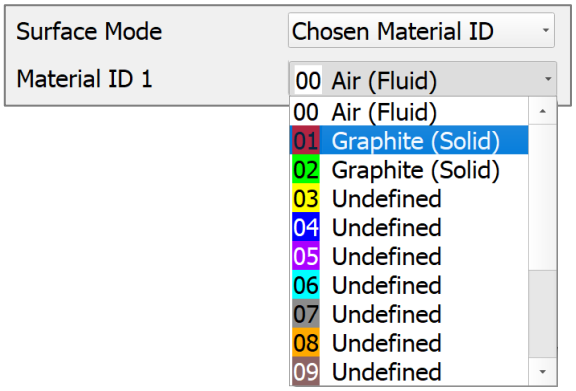
At the top of the dialog box, enter the **Result File Name**. The result file is saved in the chosen project folder (**File** → **Choose Project Folder**, in the menu bar).

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).

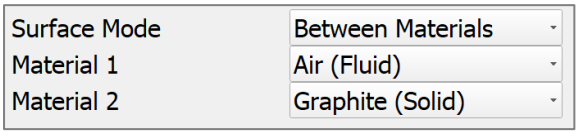
Pore Space computes the surface of the pore space, and returns the same result as **All Solid Materials**, which computes the surface of all solid materials combined to one material. Especially, **All Solid Materials** does not include the inner surfaces between different solid materials or material IDs.

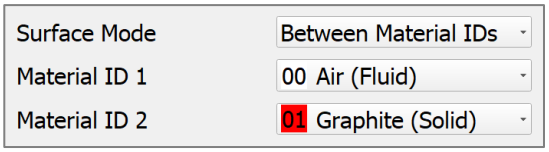
If **Chosen Material** or **Chosen Material ID** is selected, choose the desired material (material ID) from the pull-down menu that appears below.





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





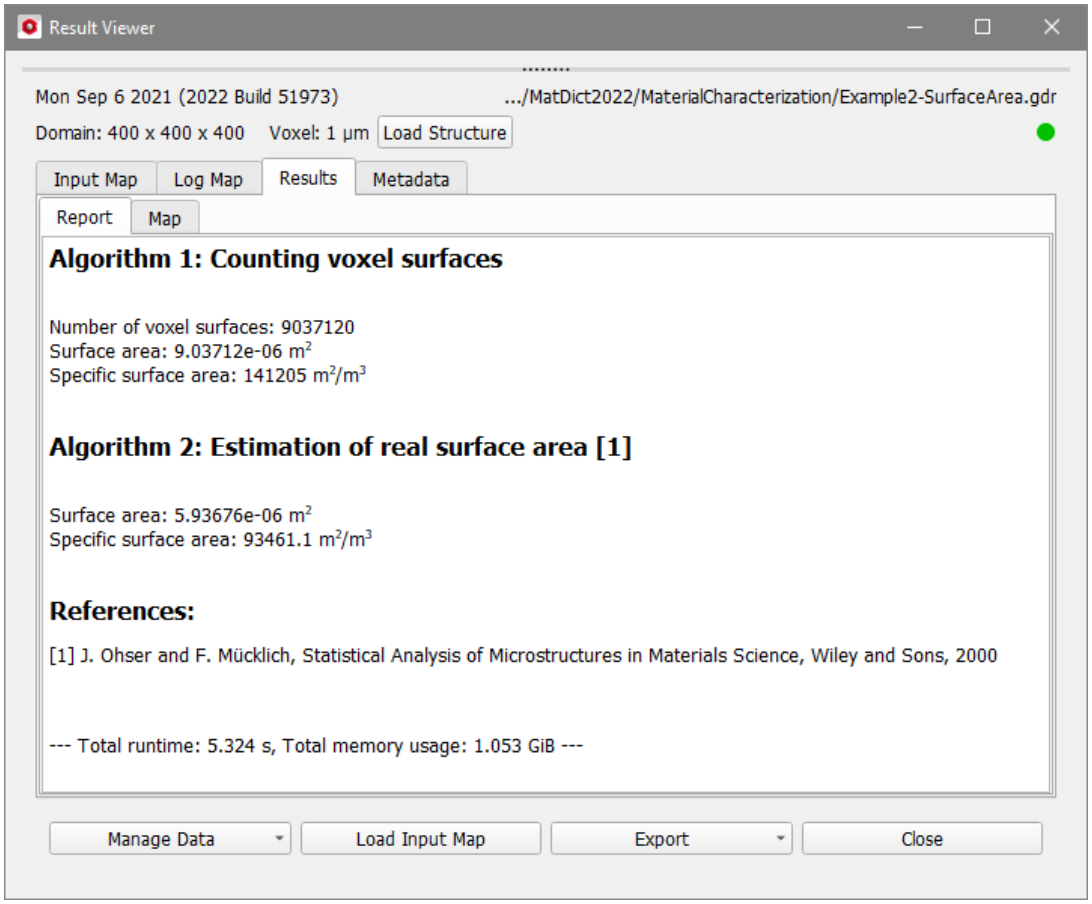
Selecting **Periodic**, the algorithm estimates the surface area assuming that the structure is periodic, so that the material that ends on one side of the volume reappears on the opposite side.

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.

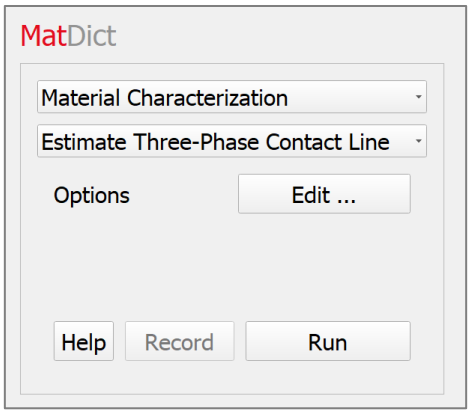


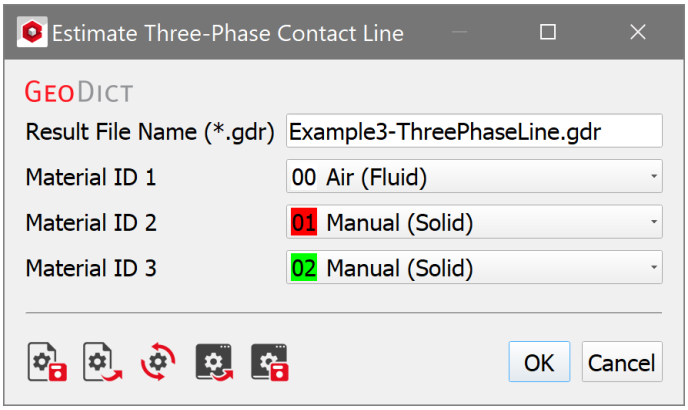
Algorithm 2 estimates the real surface area, originating from statistical image analysis, where the determination of the four Minkowski measures (Volume, Surface Area, Integral of mean curvature, Integral of total curvature) from voxelized images is an essential task.

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.

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.





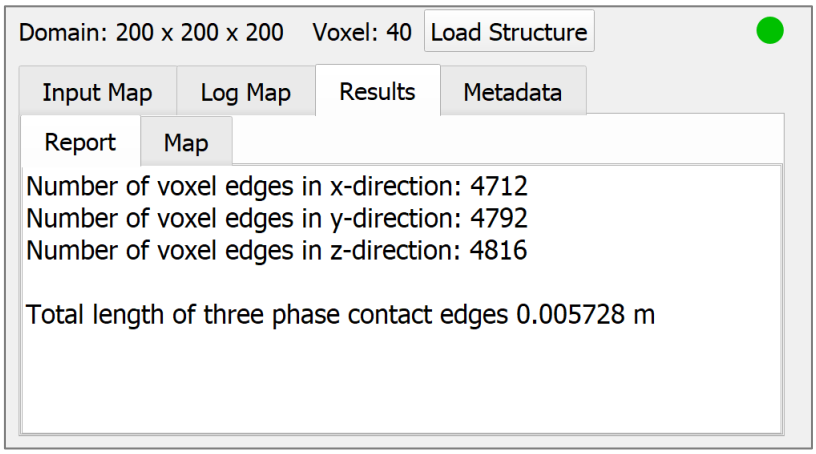
Through the **Material ID 1**, **Material ID 2**, and **Material ID 3** pull-down menus, the three-phase material IDs for which the **Three-Phase Contact Line** length should be computed are selected.

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.

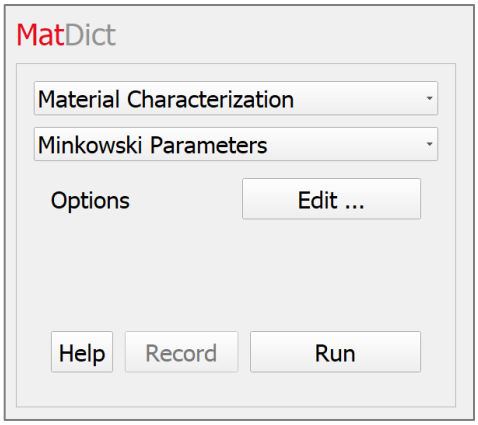
In this algorithm, all voxel edges are found that are adjacent to all three materials.

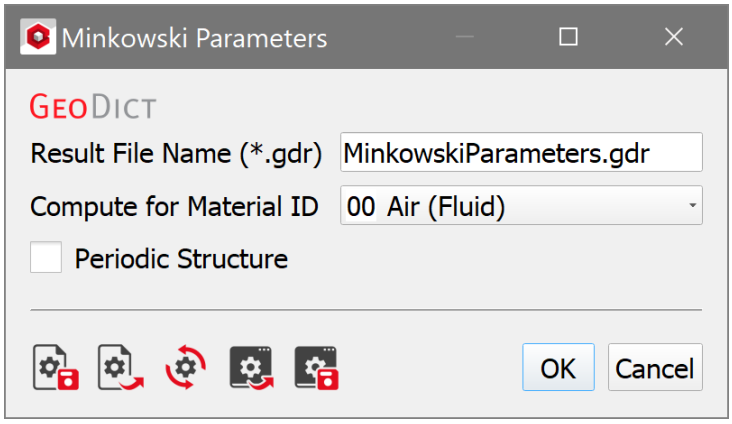
The report contains the computed values for **Number of voxel edges in x-, y-, and z-direction**, as well as the **Total length of three-phase contact edges**, which is computed by multiplying the sum of the above numbers with the voxel length.



MINKOWSKI PARAMETERS

To compute **Minkowski Parameters**, the needed parameters can be entered by clicking the **Options' Edit...** button.





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.

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:

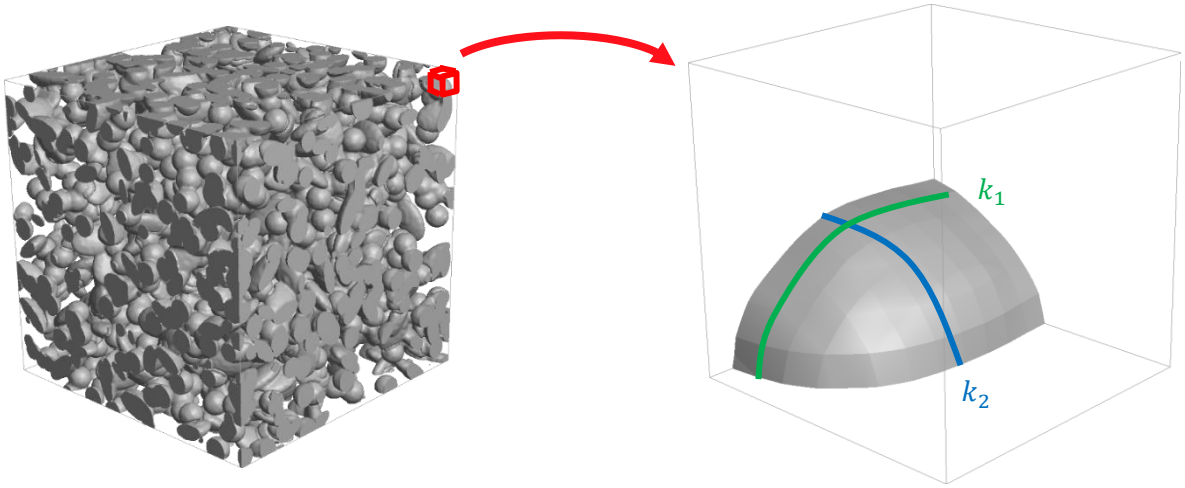
- The parameter **Volume Fraction** is the volume fraction of the chosen Material ID.
- The **Surface Area** is the boundary between the chosen Material ID and all other Material IDs. It is computed as in **Algorithm 2** of the **Estimate Surface Area** command.
- The **Integral of Mean Curvature** describes the mean curvature of the selected Material ID.

$$C_M(X) = \frac{1}{2}\int_{\delta X}\left(\frac{1}{k_1}+\frac{1}{k_2}\right)ds$$

- The **Integral of Total Curvature** describes the total curvature of the selected Material ID.

$$C_T(X) = \int_{\delta X}\left(\frac{1}{k_1 k_2}\right)ds$$

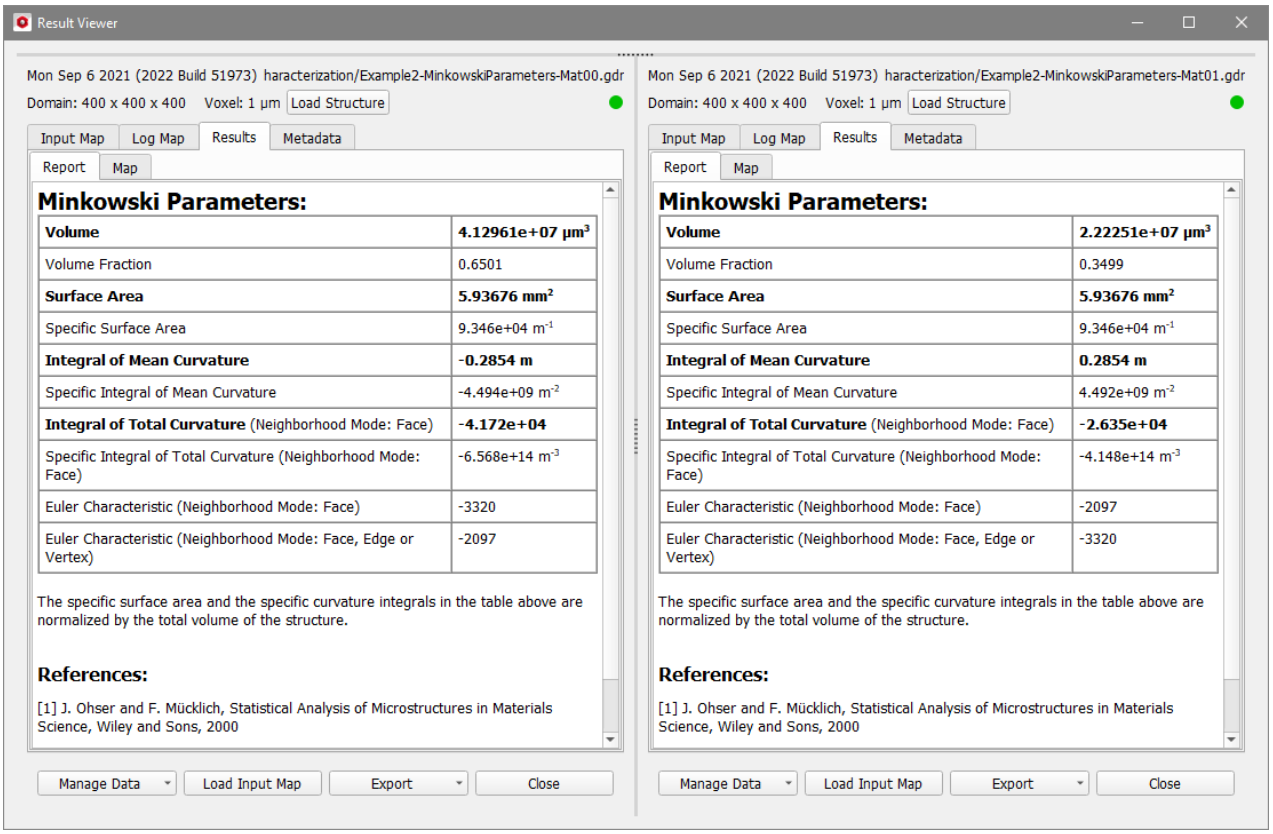
where X is the chosen material ID, s is a surface element of the chosen Material ID and the parameters k_1 and k_2 are defined as the two principal curvatures from the respective surface element.



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.

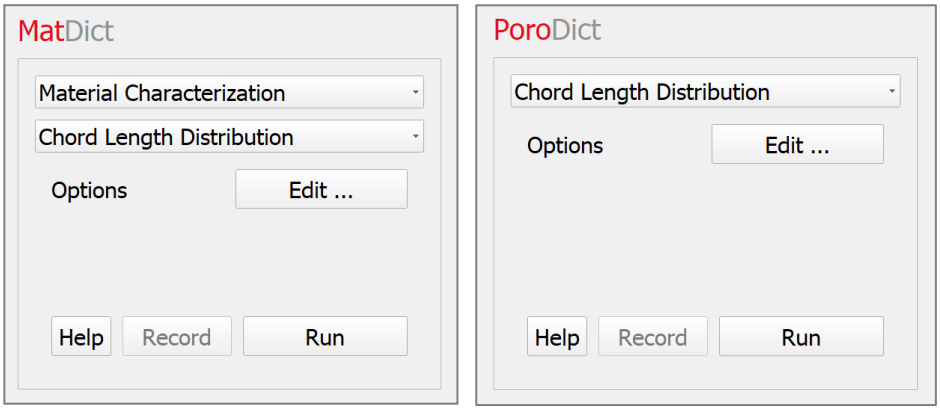
The **Euler Characteristic** (E) is a topological number, that describes to what extend the structure is connected. It equals $\frac{1}{4\pi}$ times the integral of total curvature. This results in $E = N - L + C$, where N is the number of objects, L is the number of loops and C is the number of cavities.



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).

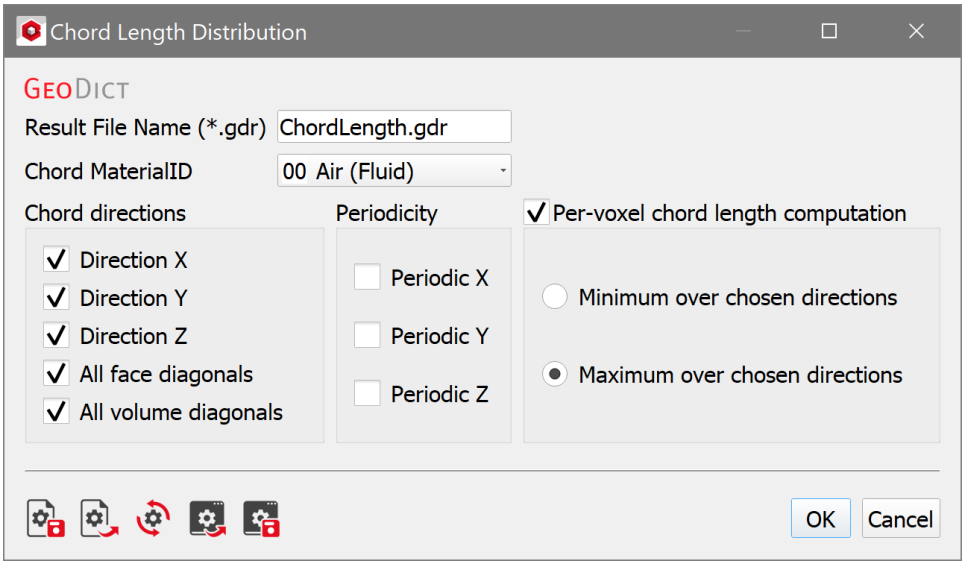
CHORD LENGTH DISTRIBUTION

The **Chord Length Distribution** command is accessible from MatDict and PoroDict. After selecting **Chord Length Distribution** from the pull-down menu, the settings for the calculations can be modified through the **Edit...** button.



In the **Chord Length Distribution** dialog box, 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 (**X**, **Y** or **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:

Report | Plots | Map

Warning: 491 chords of infinite length did not count for mean chord length and L10/L50/L90 in Z-direction

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, **Minimum over chosen directions** or **Maximum over chosen directions** must be selected.

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.

Under the **Report** tab, the **Mean Chord Length(s)**, 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) and the percentile of a particular length in the distribution (P10, P50, P90).

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).

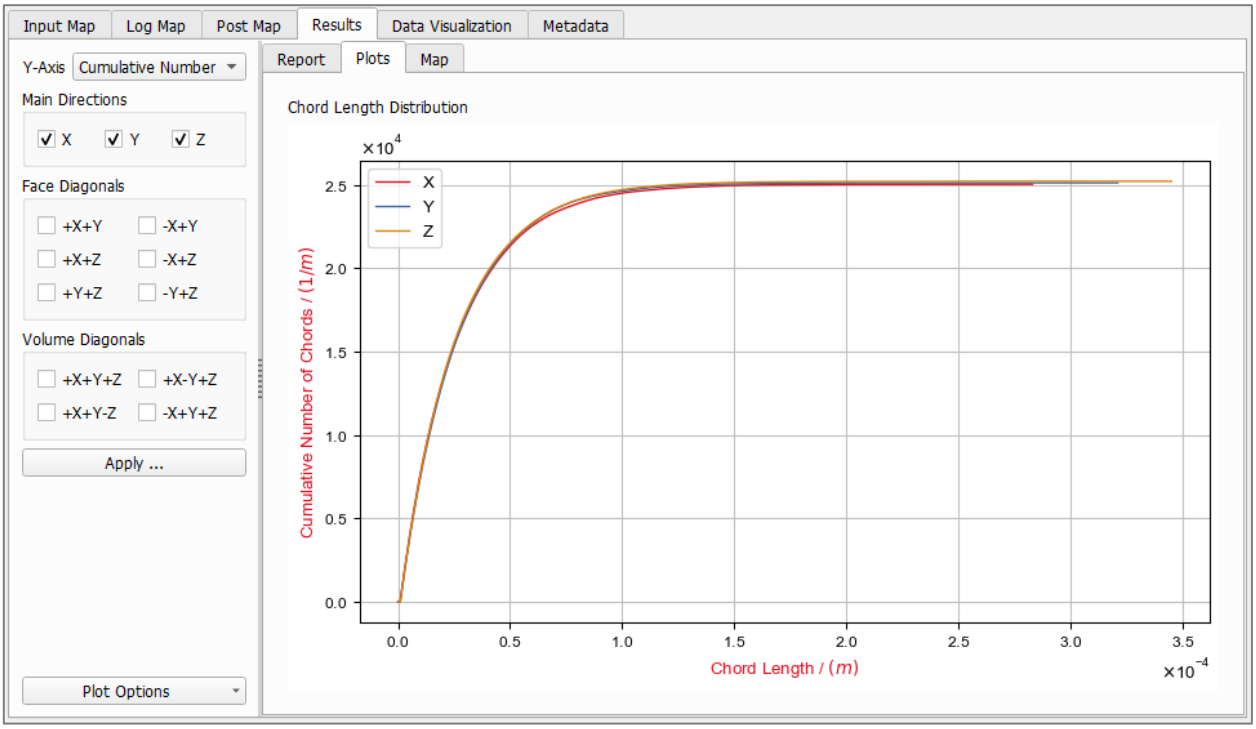
Chord Length Distribution

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

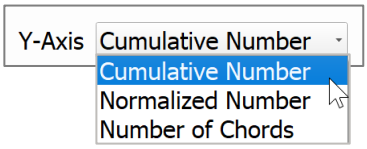
For example, a L10 of 2.6 µm means that 10% of all chords are smaller than this length. A L50 of 17.4 µm) means that 50% of all chords are smaller than this length. A L90 of 58.6 µm means that 90% of all chords are smaller than this length.

A P10 of 3e-6 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 can be seen under the **Results-Plots** subtab



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.

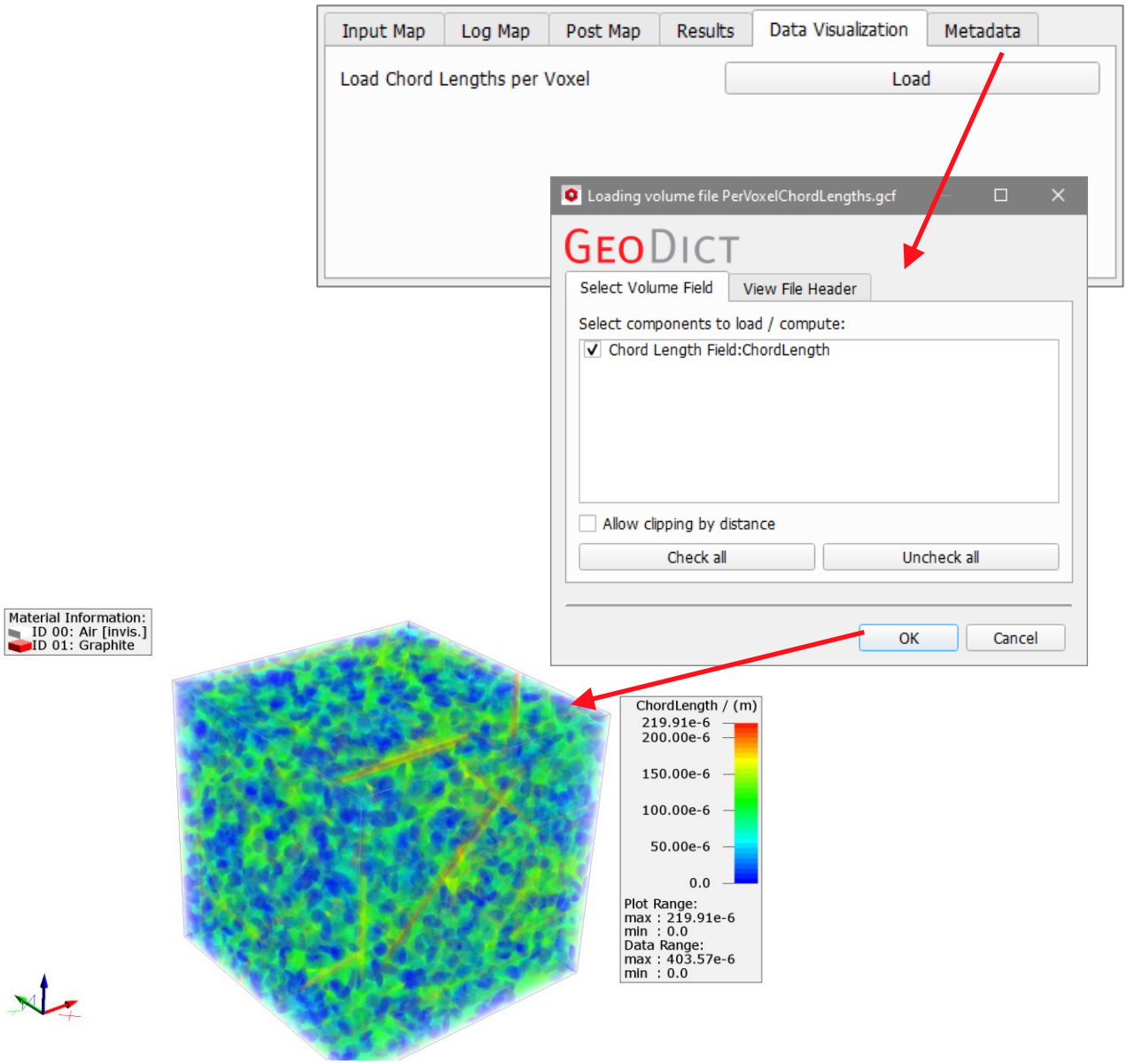
Alternatively, the normalized number of chords can also be obtained from the number of chords histogram. For example, the normalized number of chords in X-direction can be computed as follows: First, the number of chords is divided by NY*NZ to obtain the number of chords per ray. Then, this number is normalized by NX*voxel length to obtain the number of chords per meter. In the last step, this number must again be normalized by the voxel length to reflect the histogram bin size. 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.

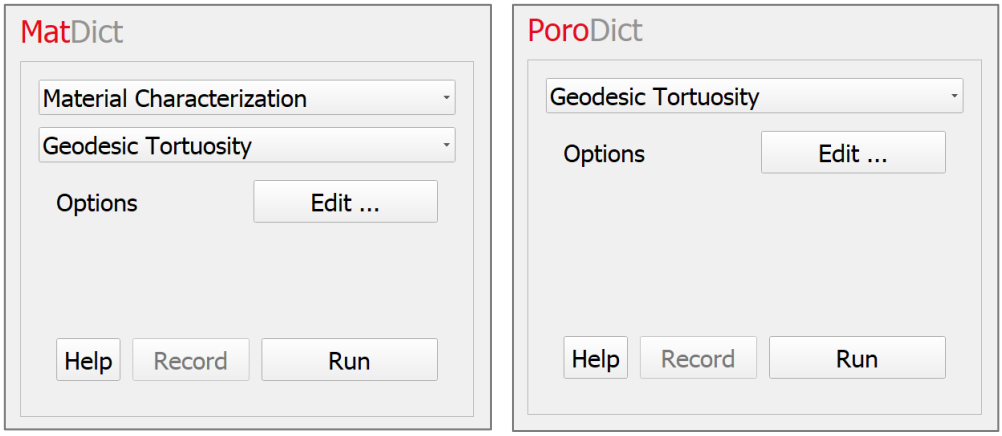
DATA VISUALIZATION

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 44).



GEODESIC TORTUOSITY

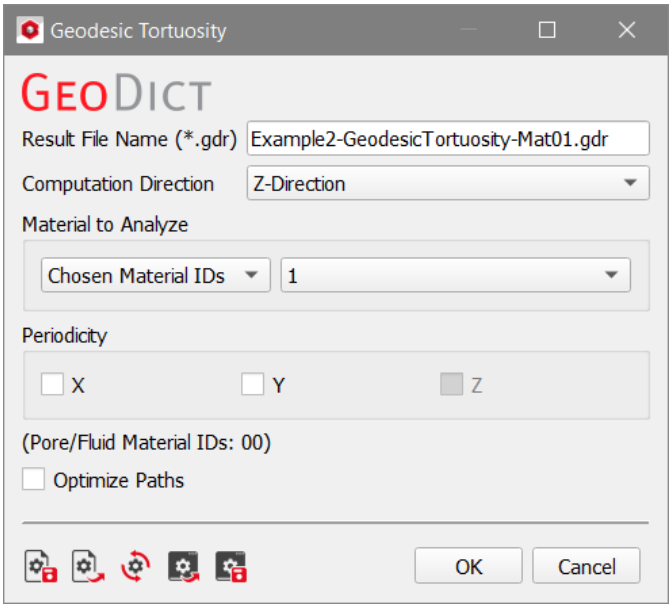
The **Geodesic Tortuosity** command is accessible from MatDict and PoroDict. It computes the tortuosity of paths crossing the material, either through pore space or through solid materials.



In the **Geodesic Tortuosity** dialog, set the direction of the paths by selecting the **Computation Direction**.

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

The algorithm will search for paths in the selected **Material to Analyze**, which can be **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 option **Optimize Paths** is explained on p. 27.

RESULTS

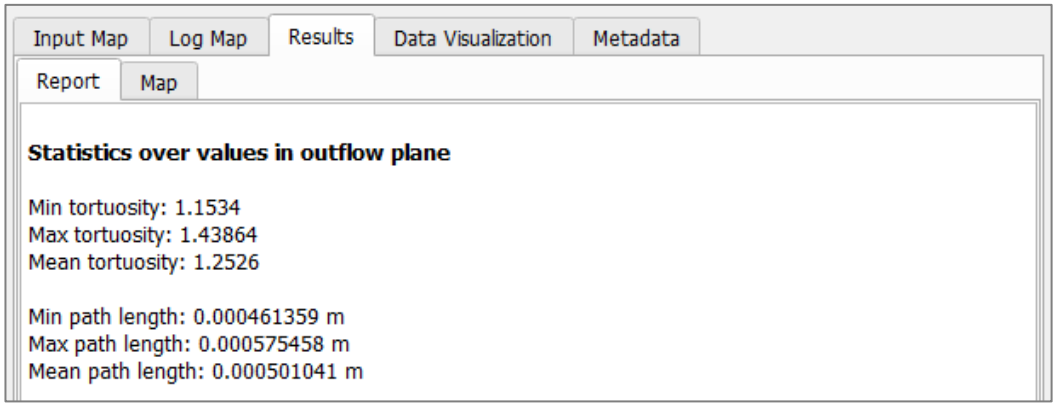
Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis.

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

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

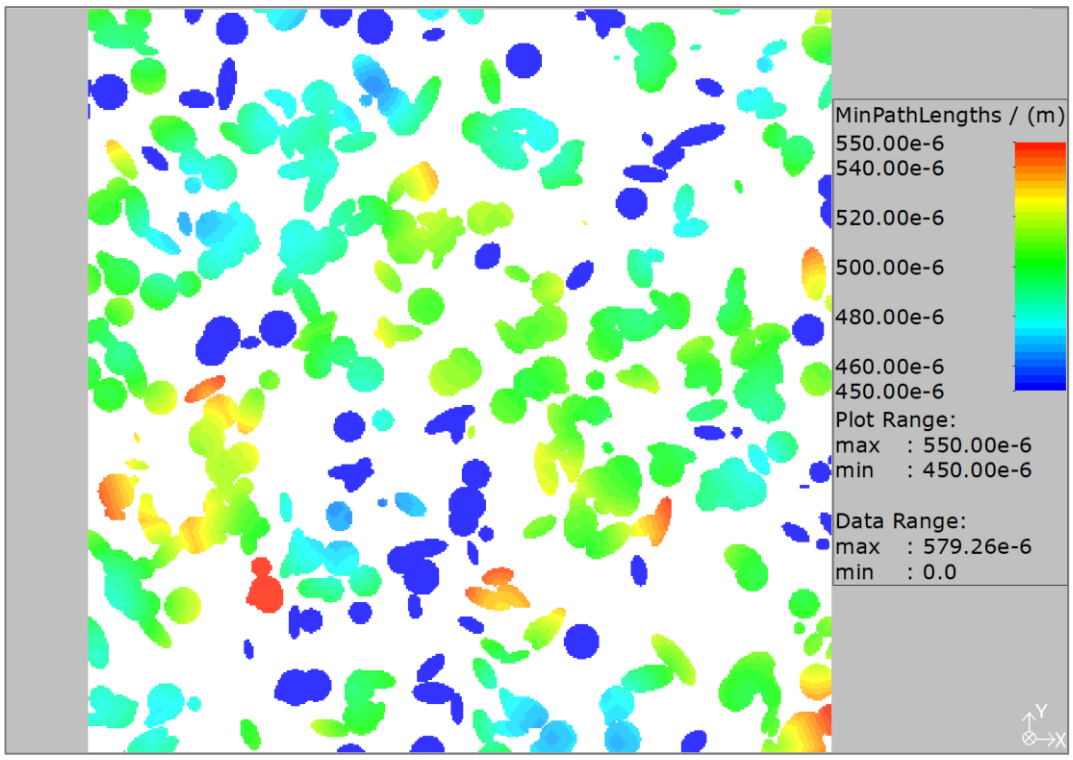
The Result Viewer opens at the end of the calculation.

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



DATA VISUALIZATION

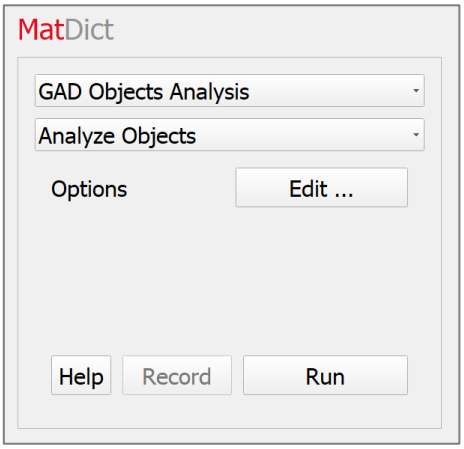
When clicking the **Load** button under the **Data Visualization** tab, a scalar field is loaded that contains for each voxel inside the selected material the shortest path distance between this voxel and the inflow plane. Therefore, on the inflow plane all voxels contain the value 0. On the outflow plane, the voxel values show the computed path lengths as shown below and their local distribution around the mean value of 501 µm



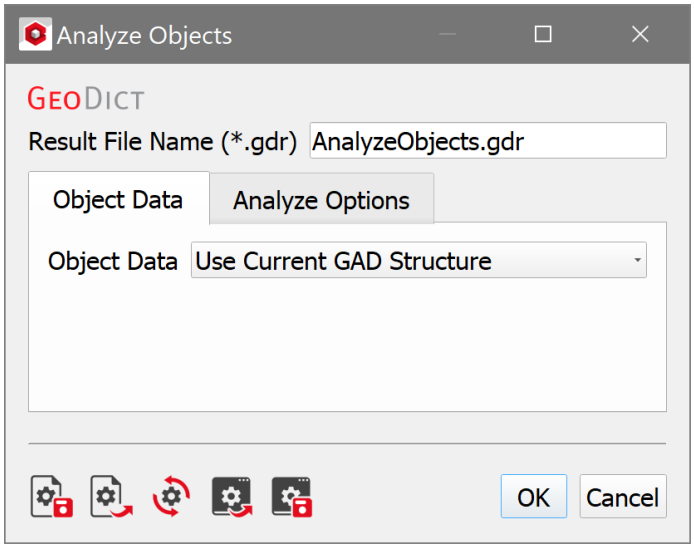
GAD Objects Analysis

Analyze Objects

With the **Analyze Objects** command it is possible to analyze how the geometrical objects forming the 3D micro-structure, e.g. fibers, spheres or ellipsoids, 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 box opens when clicking the **Options' Edit...** button and includes the **Object Data** and the **Analyze Options** tabs.



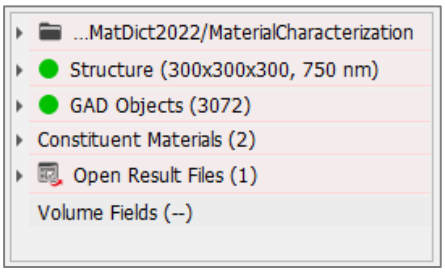
At the top of the dialog box, enter a name for the **Result File Name**.

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.

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

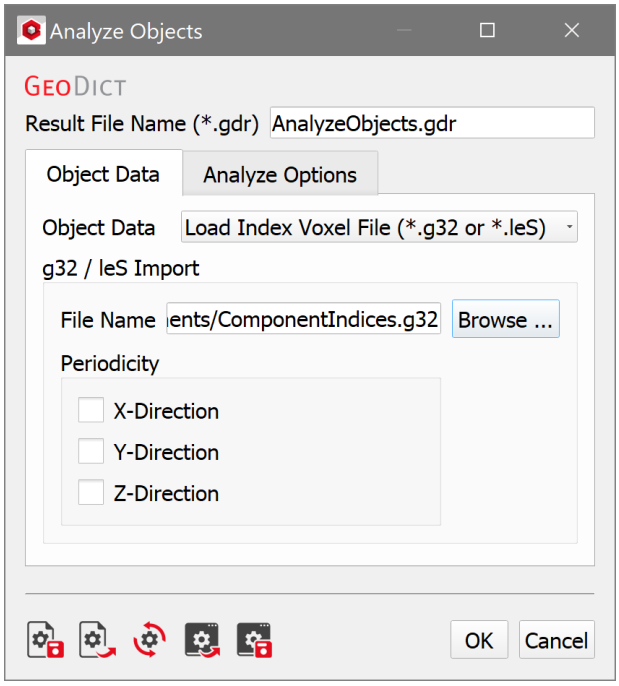


   To use the current object information, set **Object Data** to **Use Current GAD Structure.**

2. The second option is to load a voxel geometry with object indices (*.**g32 or *.leS File**).

   These files are the result of object analysis commands in GeoDict, e.g. MatDict's Connected Components analysis.

   To use this option, set **Object Data** to **Load Index Voxel File (*.g32 or *.leS)** and click **Browse...** to choose a file.



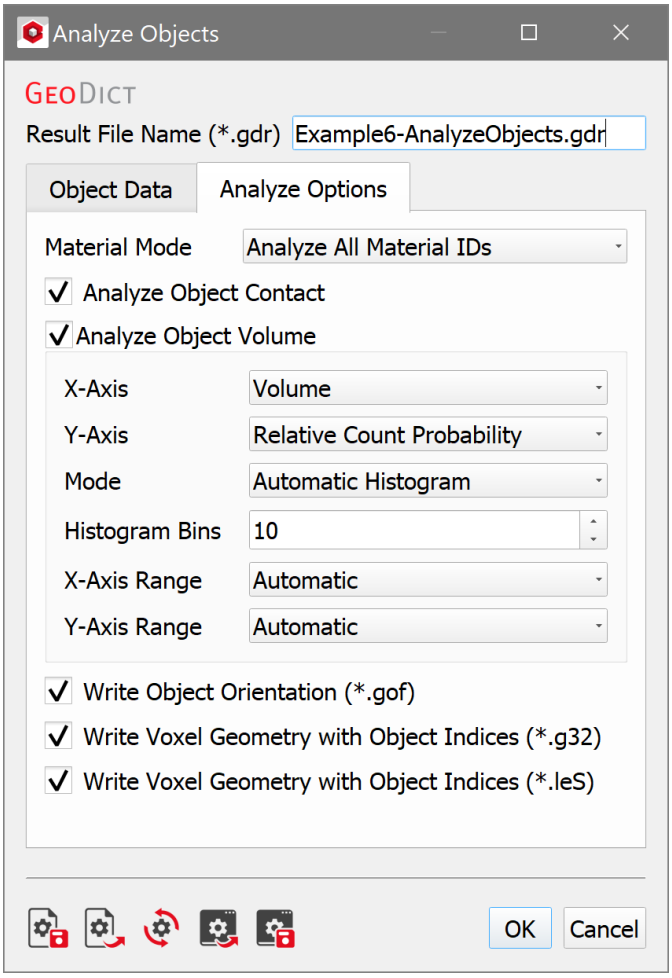
Analyze Options

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

In the **Material Mode** pull-down menu, choose to **Analyze All Material IDs** present in the structure or only one material (**Analyze Selected Material ID**). For the analysis of a single selected material ID, that material ID must be chosen from the corresponding pull-down menu.

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

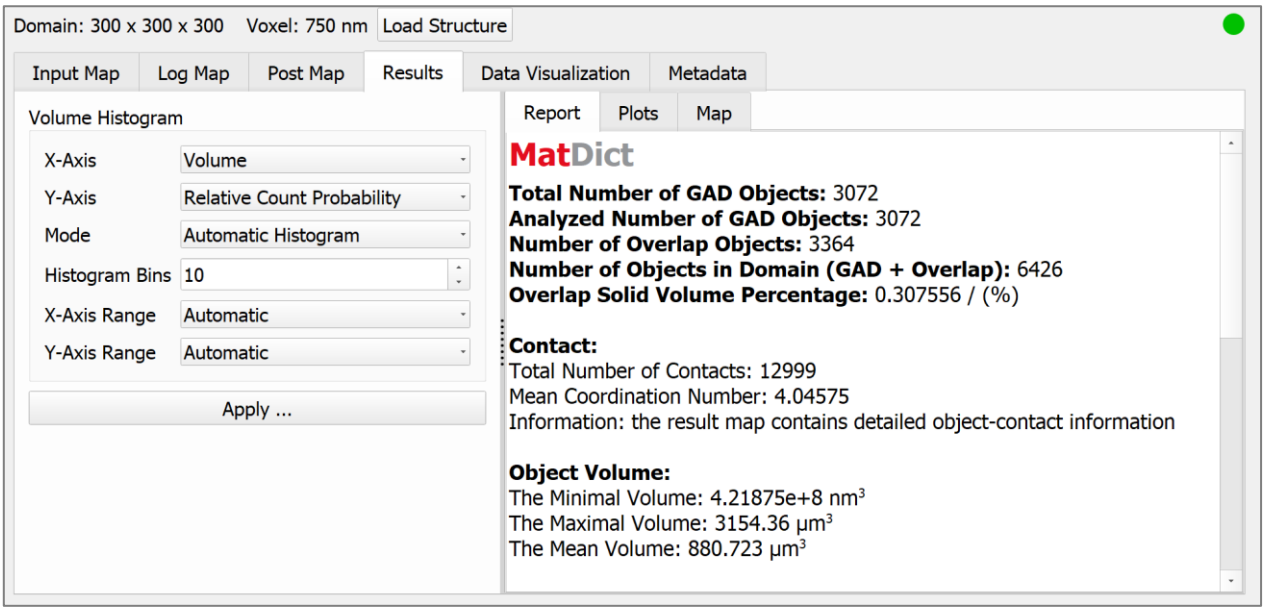


When checking **Write Object Orientation (*.gof)**, the data on the orientation of the objects is saved to a file with the same name as the result file (**Result File Name**) with the ending *.gof.

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.

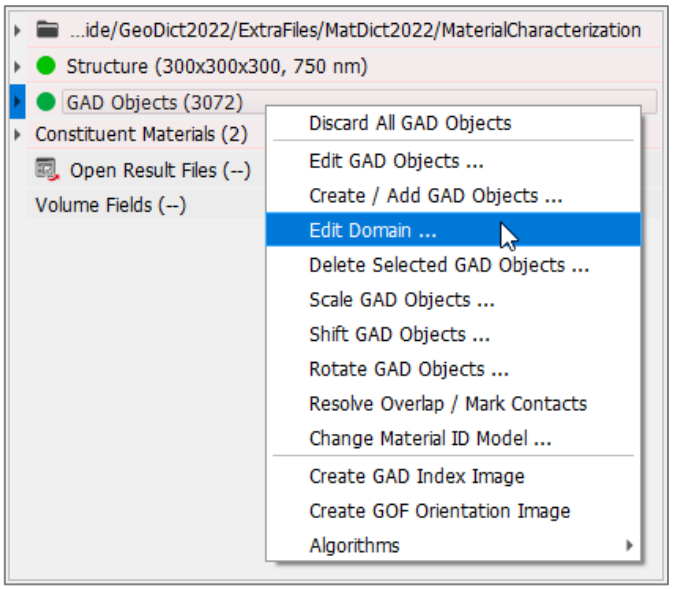


In the **Results - Report** subtab, the following values are reported:

- **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 number of objects inside of 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 of this User Guide for a more detailed description of this command.



If **Analyze Object Contact** was checked (see page 50), the total number of contacts and the mean coordination number is 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)

Under the **Results - Map** subtab, more detailed results for all contacts are available:

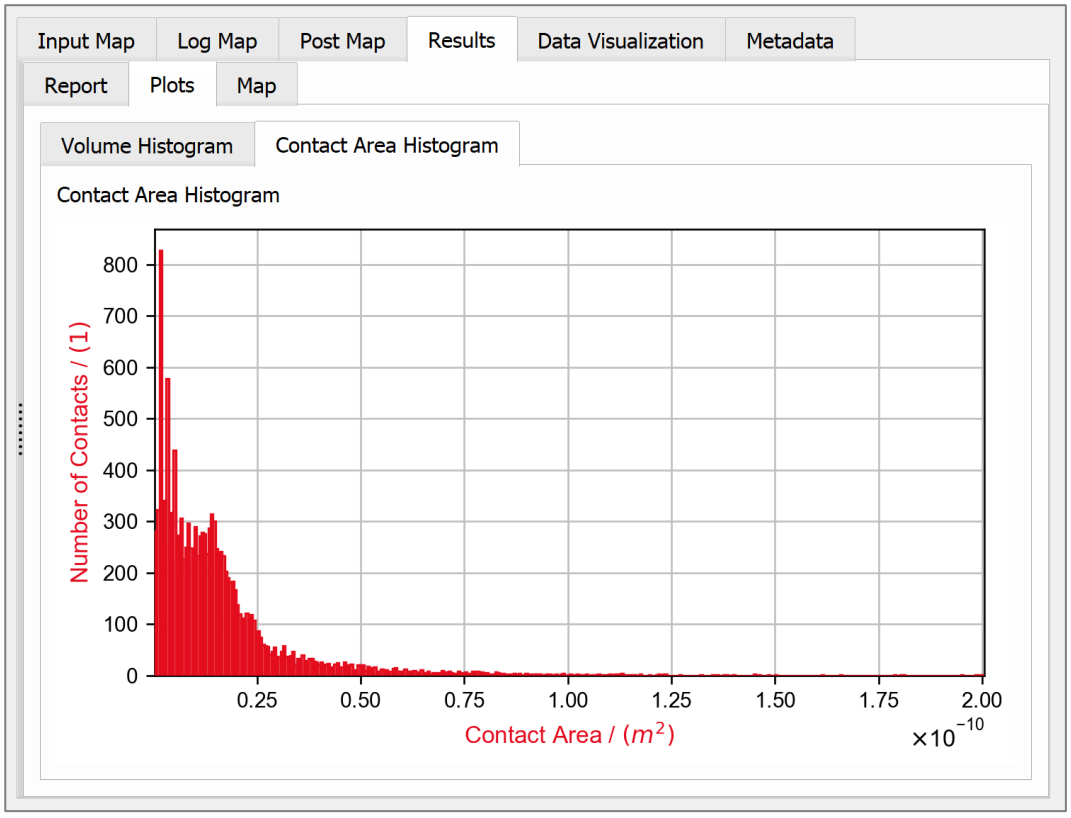
Input Map | Log Map | Post Map | Results | Data Visualization | Metadata

Report | Plots | Map

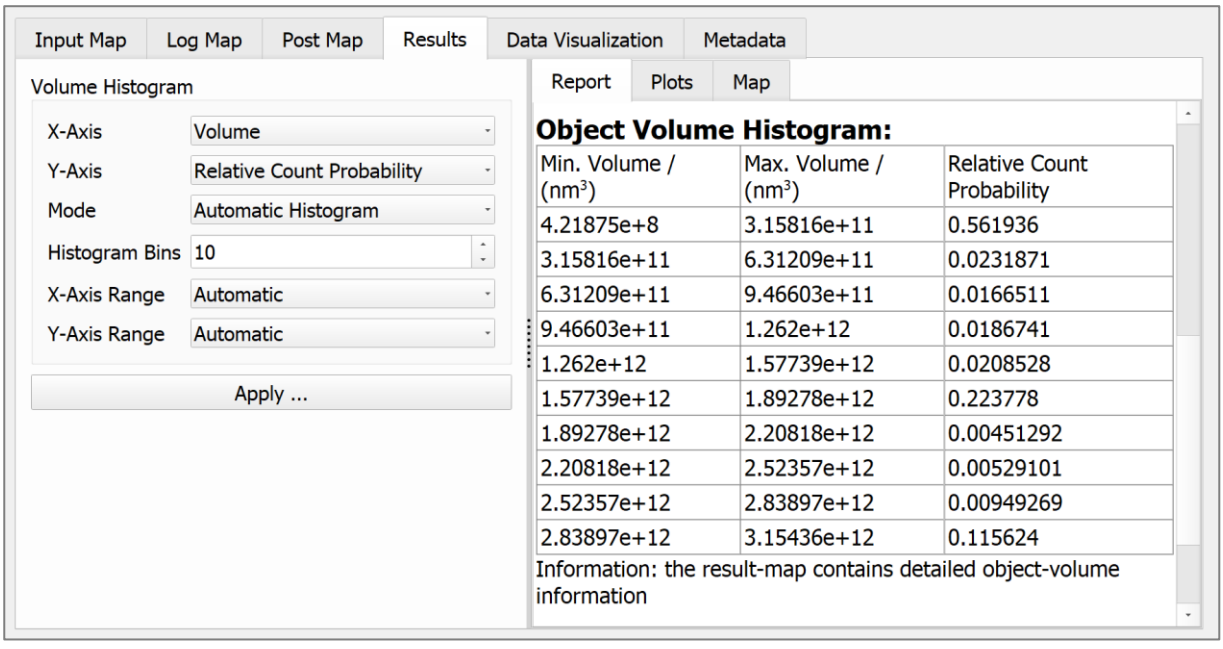
Key	Unit	Value
MeanCoordinationNumber		4.045751634
Contact		
TotalNumberOfContacts		12999
TotalContactFaces		354238
MaximumContactFaces	1	356
MinimumContactFaces	1	1
MeanContactFaces	1	27.25117317
ContactAreas	m^2	5.625e-13, 1.125e-12, 1.6875e-12, 2.25e-12, 2.8125e-12, 3.375e-12, 3.9375e...
NumberOfContacts	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, 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, 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:



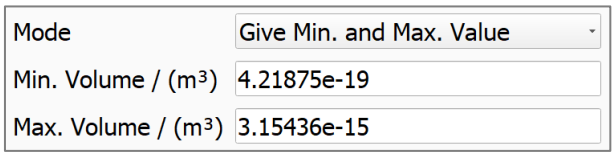
If **Analyze Object Volume** was checked (see page 50), the minimal, maximal, and mean volume are stated in the **Object Volume** section. Furthermore, an **Object Volume Histogram** table is plotted based on the **Volume Histogram** settings defined in the post-processing panel on the left-hand side 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**).

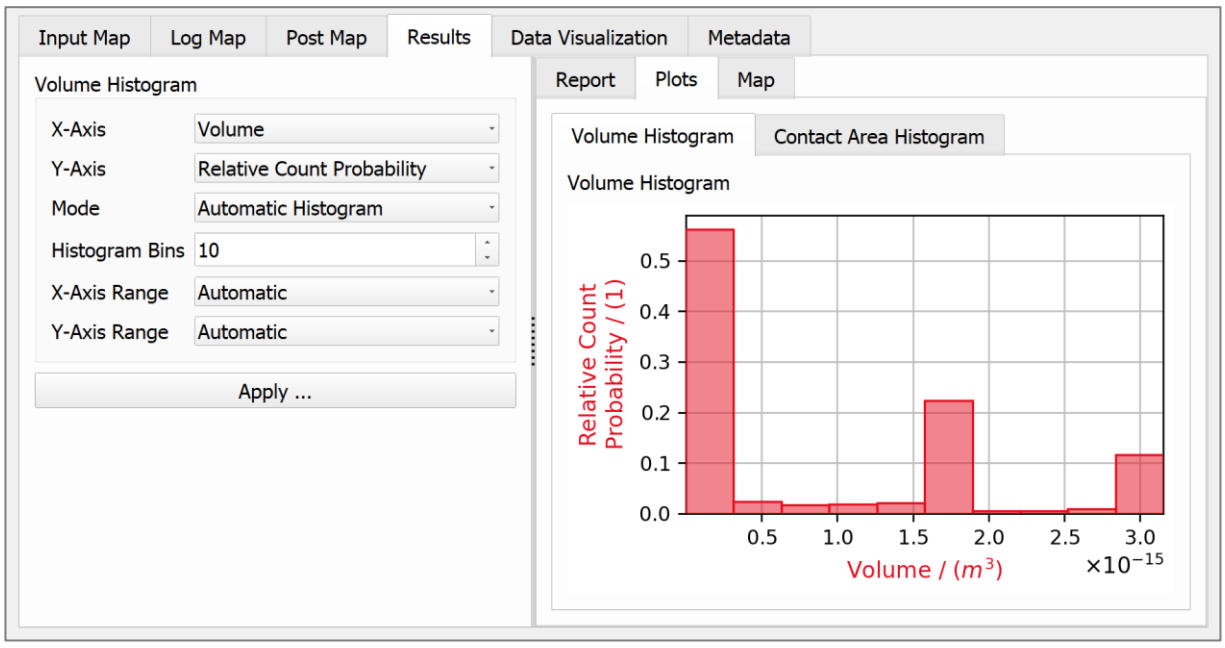
For the **Y-Axis** pull-down menu, the **Relative Count Probability** provides the number of components in each bin normalized to the total number of components. The **Cumulative Count Probability** is the sum of the Relative Count Probability over all bins starting from the smallest bin. **Relative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



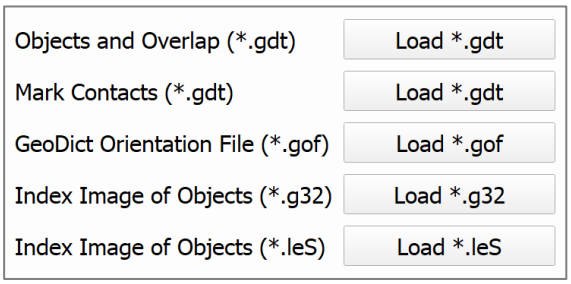
The parameters **X-Axis Range** and **Y-Axis Range** can be used to adjust the area shown in the plot. **If X-Axis Range** is set to **Automatic**, the whole range of the **Object Volume Histogram** table is plotted.

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

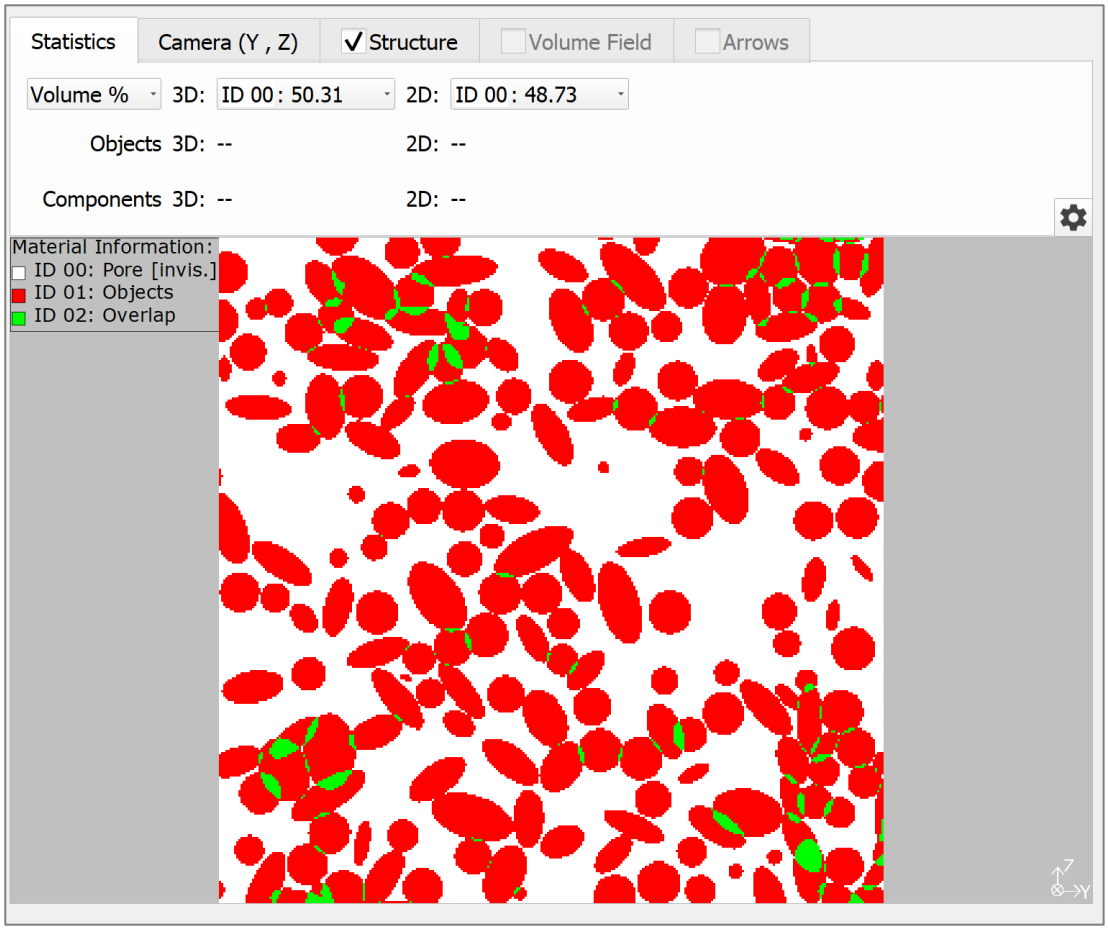
Data Visualization

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

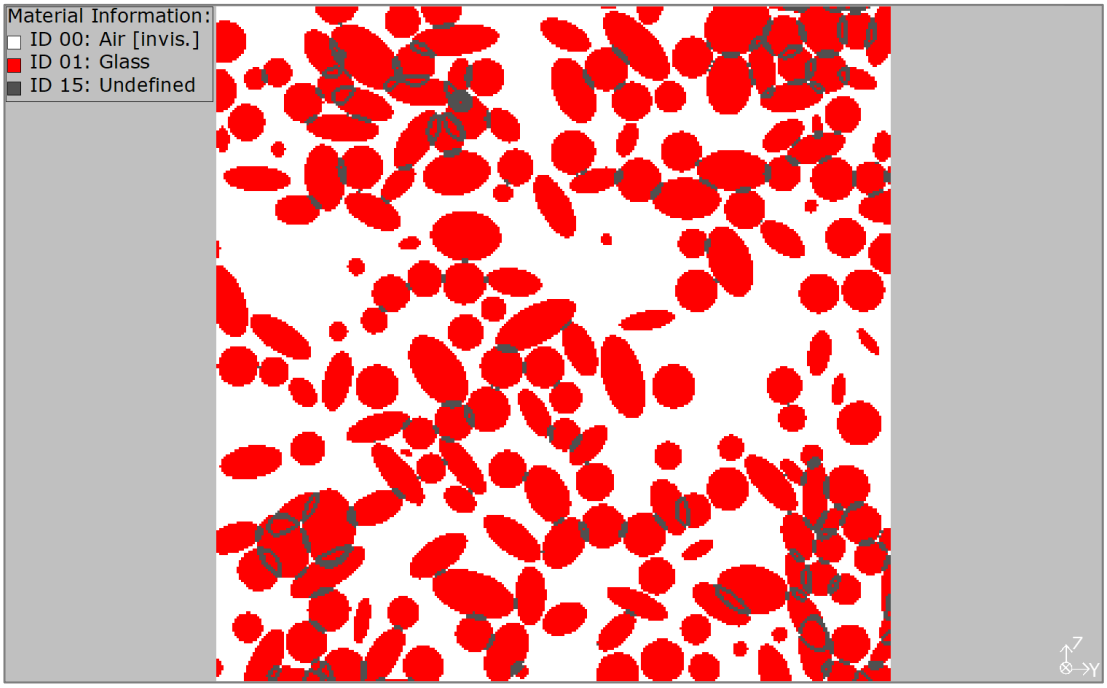
If **Use Current GAD Structure** was used as **Object Data** input, the Data Visualization tab offers visualization of object overlap and object orientation.



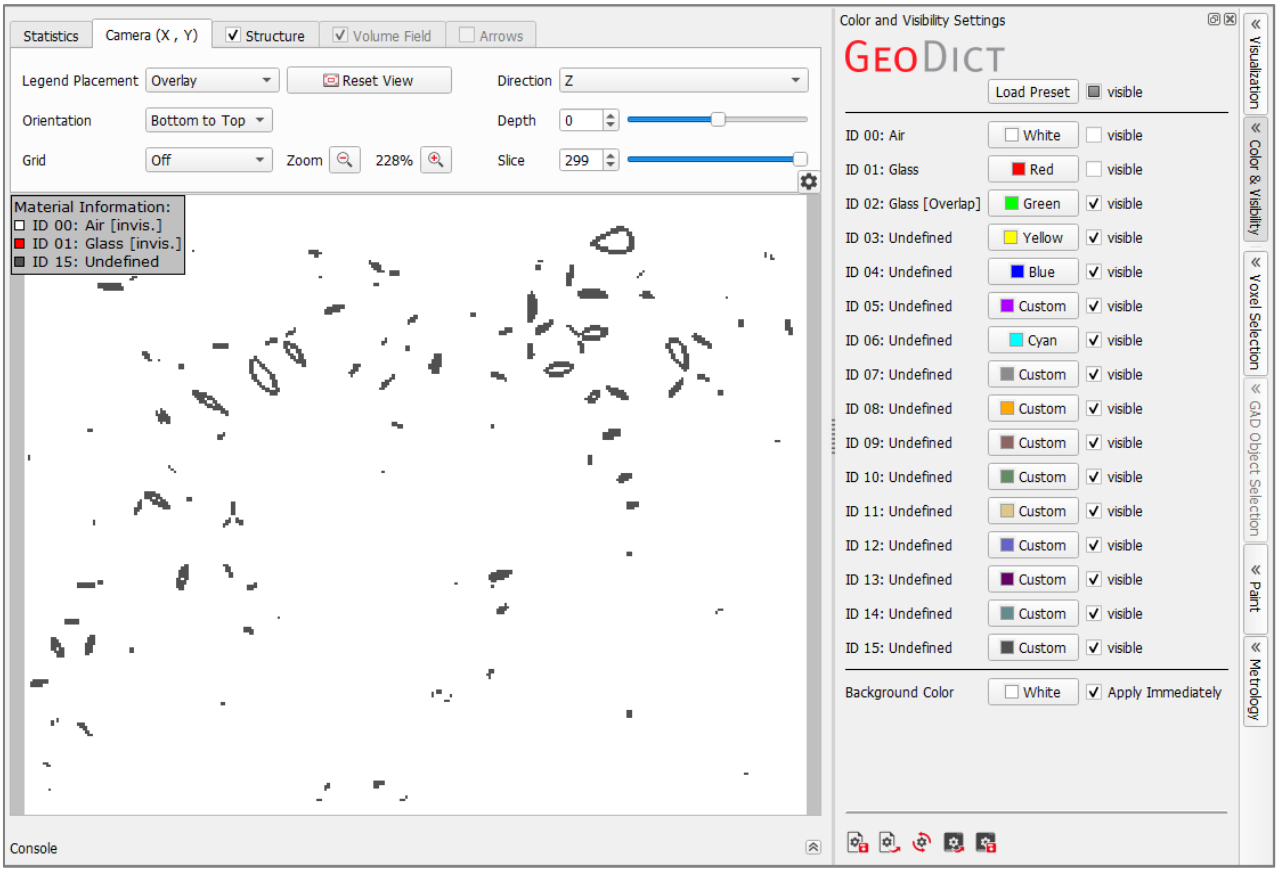
By clicking the **Objects and Overlap (*.gdt)**'s **Load *.gdt** button, the overlap between objects is displayed. All objects are assigned to Material ID 01 and the overlap is assigned to Material ID 02.



It is possible to visualize the contact voxels by clicking on the **Mark Contacts (*.gdt)**'s **Load *.gdt** button. All contact voxels will be marked with material ID 15:

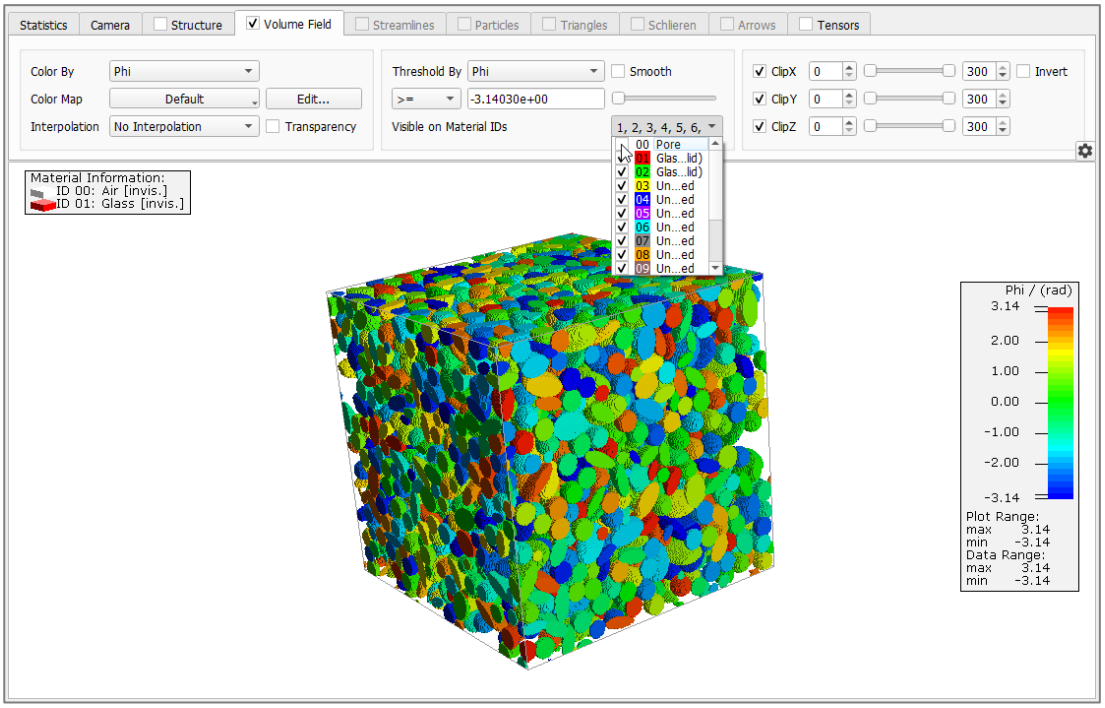


For the visualization of the labeled contacts only, select **Settings → Color & Visibility Settings** in the menu bar. Uncheck the visibility of all the material IDs in the structure model and check only the visibility of the Material ID 15.



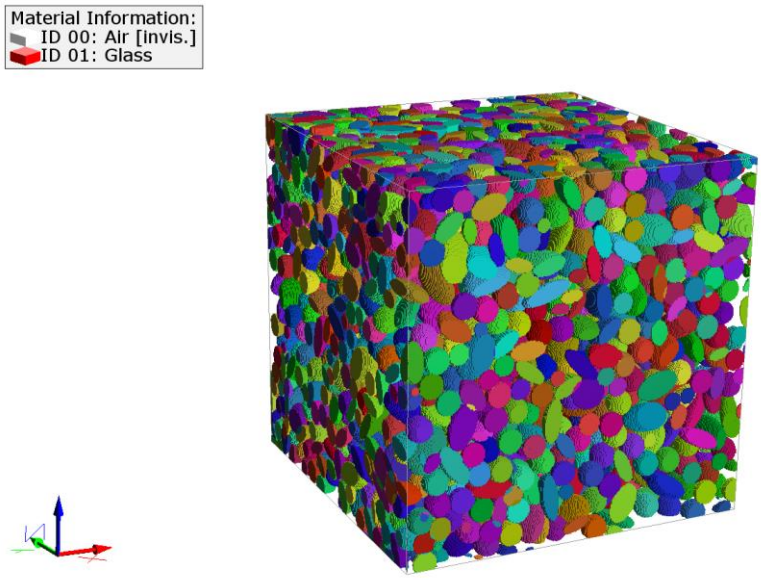
If **Write Object Orientation (*.gof)**was checked (see page 51), the orientation of the objects can be displayed by clicking the **Load** button for **GeoDict Orientation file (*.gof)**.

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



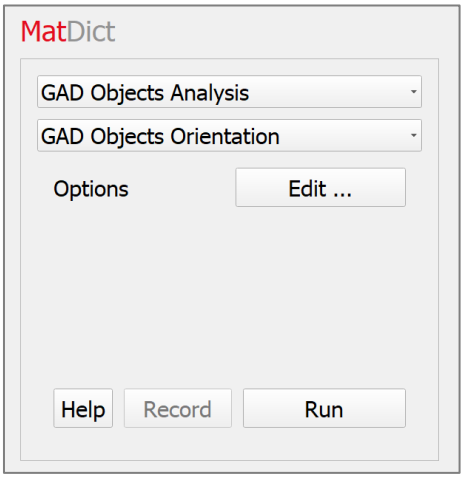
If **Write Voxel Geometry with Object Indices (*.g32)** or **Write Voxel Geometry with Object Indices and (*.leS)** was checked (see page 51), the index image of the identified objects is loaded by clicking on the **Load *.g32** or **Load *.leS** button.

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.

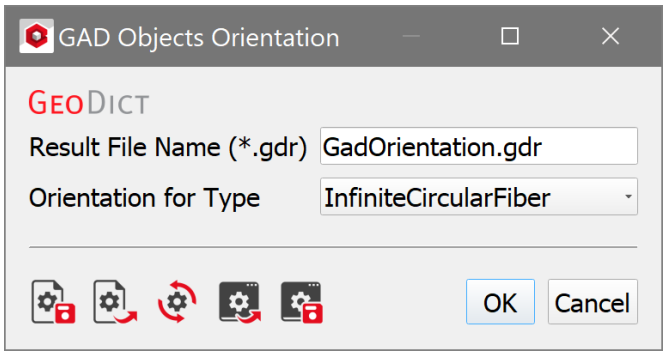


GAD-Objects Orientation

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



The **Gad-Object Orientation** dialog opens when clicking the **Options' Edit...** button.

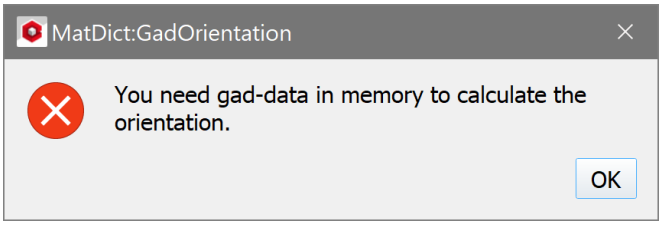


At the top of the dialog box, enter the **Result File Name**. The result file is saved in the chosen project folder (**File** → **Choose Project Folder**, in the menu bar).

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.

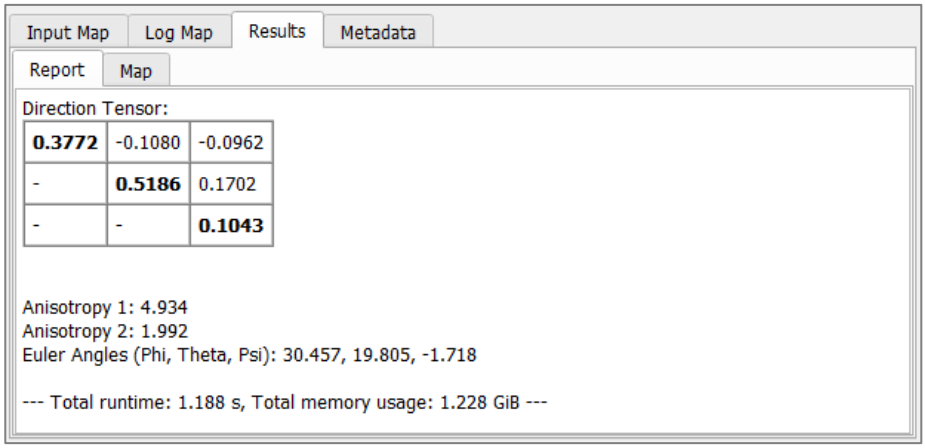
If no analytic data is available for the current structure, the object orientation analysis is not carried out after clicking **Run** in the MatDict section, and a warning message appears.

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



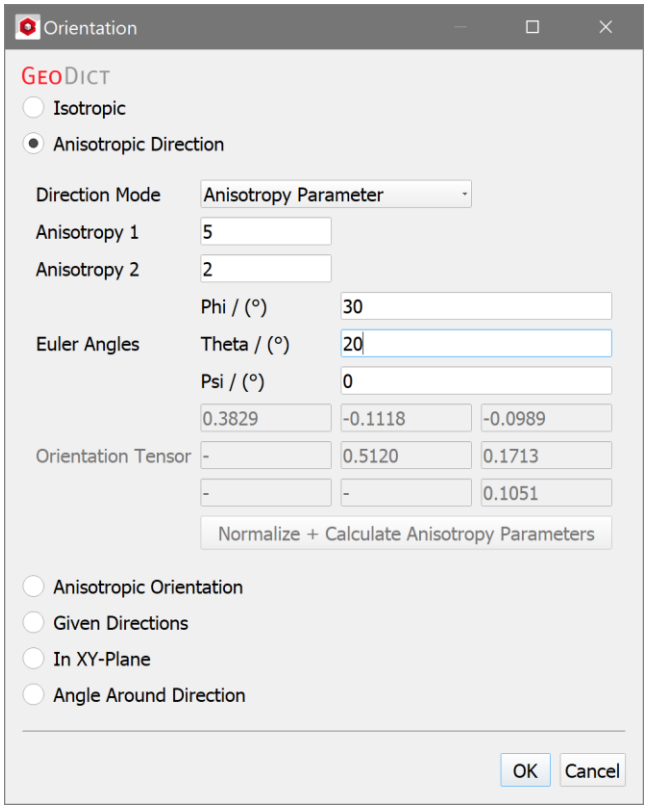
Results

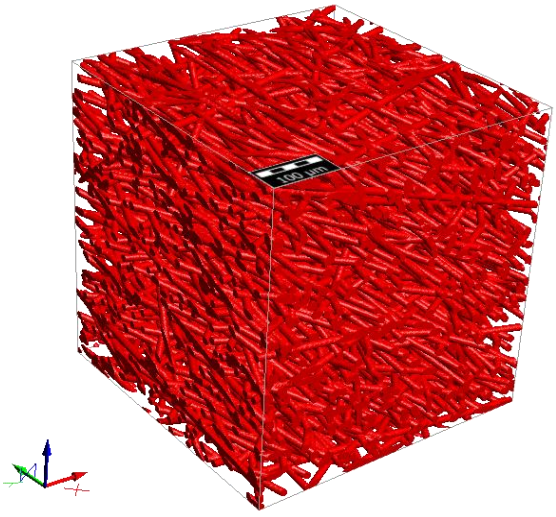
Click **OK** to input the entered parameters, and then click **Run** in the MatDict section to start the structure analysis. The result file (*.gdr) is opened in the **Result Viewer** after the computation is finished.



The definition of these parameters is the same as in the FiberGeo module. See the FiberGeo User Guide 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, if FiberGeo was used to generate the current 3D structure, MatDict **Gad-Objects Orientation** can be used to verify the orientation of the created structure. For example, the results shown above were achieved for a structure created with this target orientation:

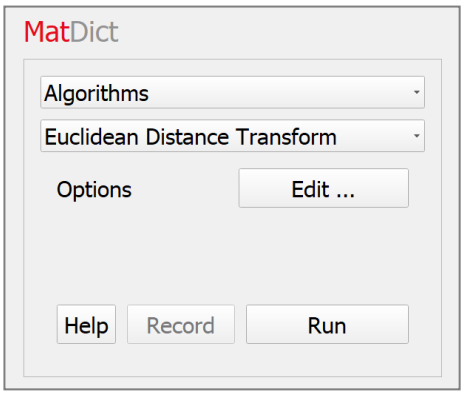


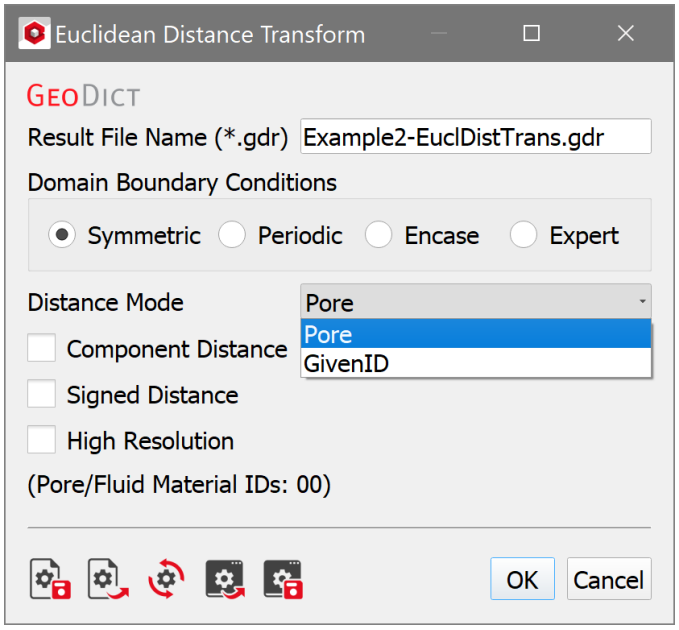


ALGORITHMS

EUCLIDEAN 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.

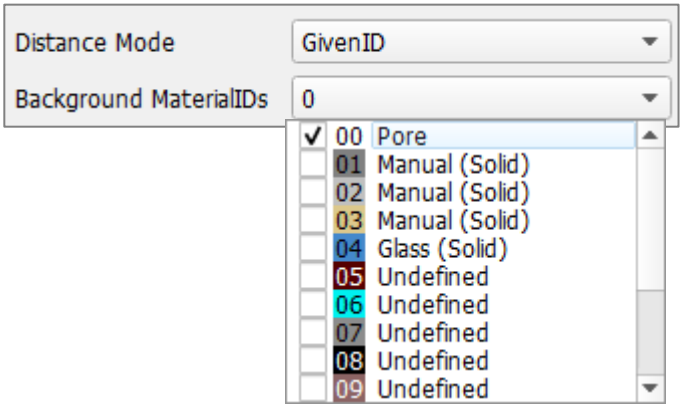




In the **Euclidean Distance Transform** dialog box, choose the **Result File Name**.

Decide which **Domain Boundary Conditions** should be used during the calculations. More detailed information about this feature is given on page 21.

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 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 27 for more explanations.

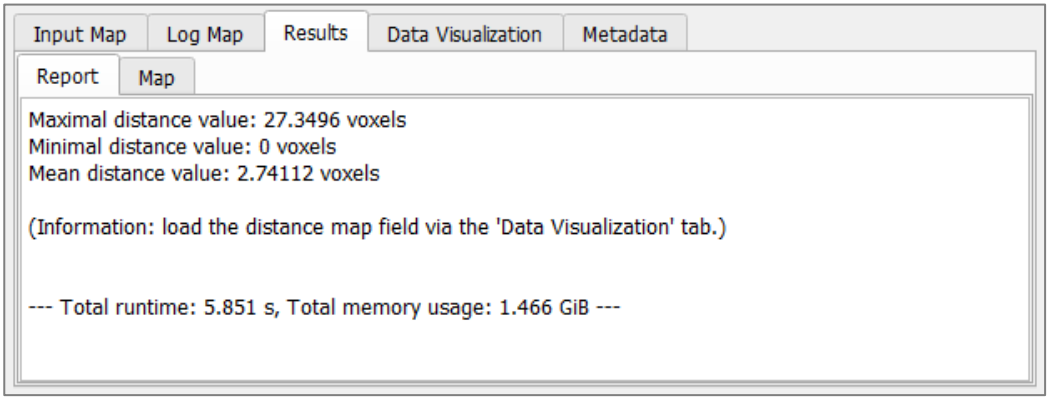
Results

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, this 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.



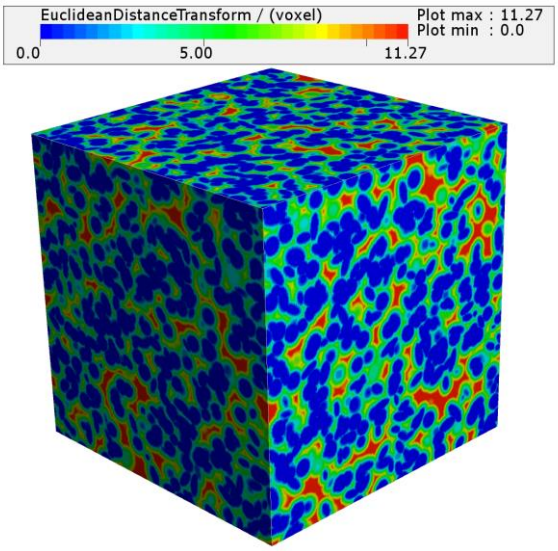
Data Visualization

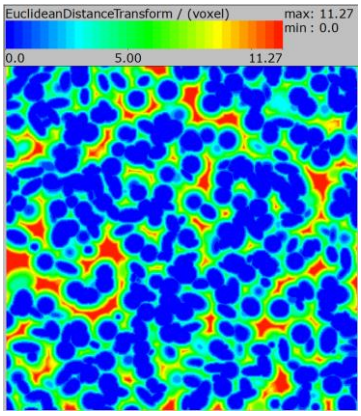
The **Euclidean Distance Transform** result can be visualized in 2D-Cross section view or 3D-Rendering when selecting the **Data Visualization** tab of the result file.

By clicking **Load *.dst**, the computed distance map is loaded into GeoDict.

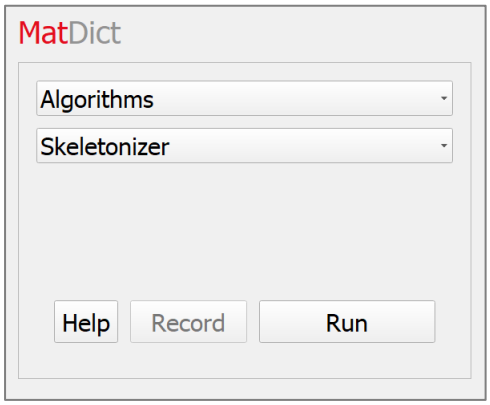
The **Volume Field** tab (in 2D Cross section view and in 3D Rendering) becomes selectable in the visualization panel above the Visualization area to fine-tune the visualization settings.

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

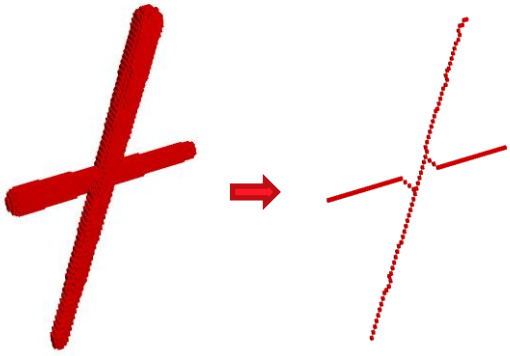

EuclideanDistanceTransform / (voxel)
Plot max : 11.27
Plot min : 0.0
0.0
5.00
11.27


EuclideanDistanceTransform / (voxel)
max: 11.27
min : 0.0
0.0
5.00
11.27

SKELETONIZER



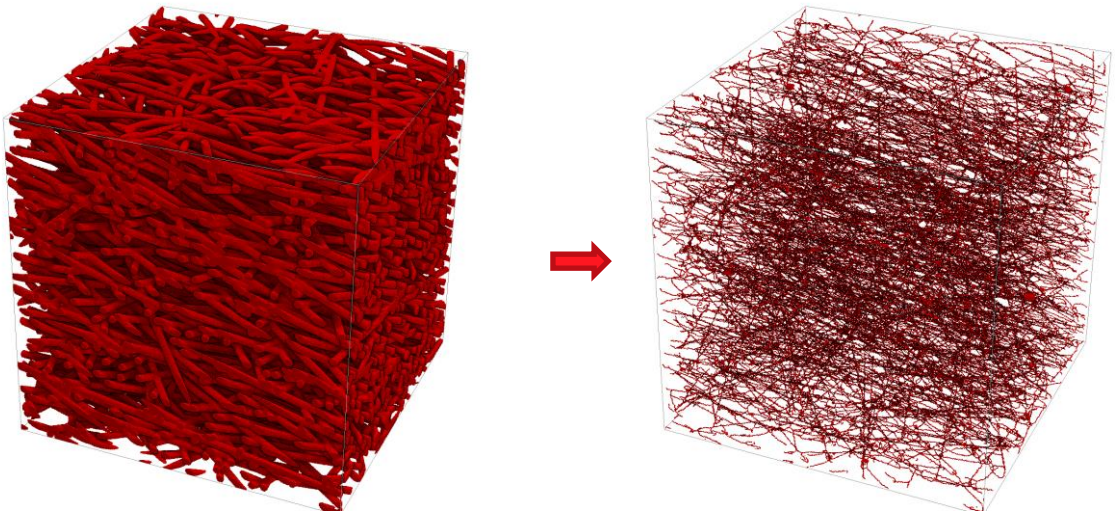
The **Skeletonizer** reduces a structure to its center lines. This command might be useful as an intermediate step in some workflows creating or analyzing certain structure types.



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.



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

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