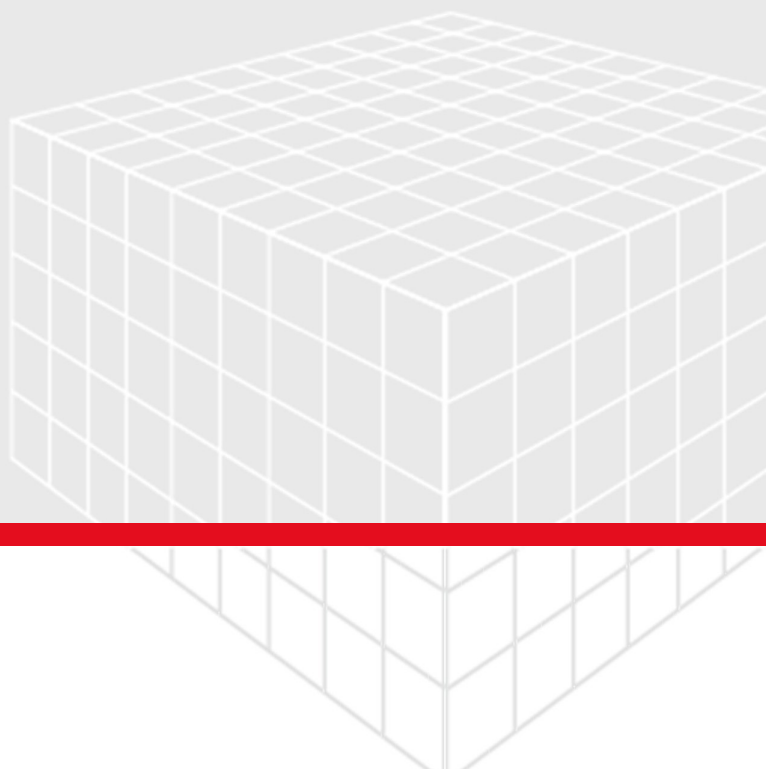


GrainGeo

User Guide

GEODICT Release 2026

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GEO DICT

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GrainGeo

1. GrainGeo	4
1.1 Create Grains	7
1.1.1 Options	7
1.1.2 Results	91
1.2 Pile Grains	95
1.2.1 Options	95
1.2.2 Results	118
1.3 Pack Analytic Spheres	121
1.3.1 Options	122
1.3.2 Results	135
1.4 Pile Analytic Spheres	141
1.5 Stochastic Field Thresholding	143
1.5.1 Options	143
1.5.2 Results	163
1.6 Distribute	165
1.7 Sinter & Crystallization	170
1.7.1 Options	170
1.7.2 Results	177
1.8 Grow Sediment	179
1.8.1 Options	179
1.8.2 Results	185
1.9 Roughen Surface	187
1.9.1 Options	187
1.9.2 Results	198
1.10 Add Binder	200
1.10.1 Options	200
1.10.2 Results	213
1.11 Grain GeoApps	216
1.11.1 Add Random Surface Cover	216
1.11.2 Bimodal Electrode	218
1.11.3 ElectrodeGeo	226
1.11.4 Catalyst Layer (PEM Fuel Cell)	228
1.11.5 Solid Oxide Electrode Generation	230
1.12 Gaussian Random Field Generator	238
1.12.1 Theoretical Background	239
1.12.2 Options	241
1.12.3 Results	251

1.13 References	255
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1 GrainGeo

The module GrainGeo creates detailed 3D models of granular structures, sintered materials, sphere packings and pilings with arbitrary object shapes.

Typical applications are replication of ceramics, soot particle filters, metamorphic rocks, polymer concrete, electrode materials, e.g., for Li-ion batteries. In general, the spectrum ranges from powders and piled granular structures to sintered materials with open or closed porosity, up to densely sintered composite materials.

The starting point for modeling a granular structure is to define initial parameters, such as grain size distribution, pore size distribution or grain shapes. By starting the creation process, randomly distributed grain structures, pilings of various digital grains and sphere packings are generated according to these parameters. Resulting target parameters are, e.g., the object volume percentage or the density of the final material. By varying the initial parameters, new materials can be created, and their properties can be optimized. Optionally, a result file (*.gdr) from GrainFind-**Identify Grains** can be loaded (see the GrainFind chapter) to set the initial parameters.

The structures can be further processed by a simulated sintering process, growing sediments, redistribution of the grains or by adding binder. Examples for possible structures are shown in the figure below.

1. Define and vary initial and target parameters

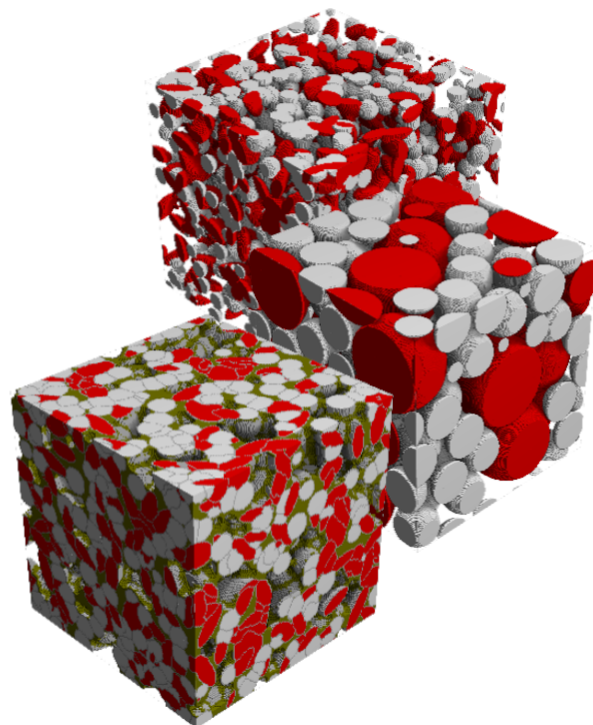
Structure Size, Grain Shape, SVP, Density, ...

2. Create granular microstructures

Create Grains, Pile Grains, Pack Analytic Spheres, ...

3. Postprocessing

Distribute, Sinter, Roughen, Add Binder, ...



For more complex examples, see the Grain GeoApps

With other GeoDict modules, the structures can be further analyzed and processed: Geometric properties like pore-size distribution (PoroDict) and transport properties like tortuosity, effective diffusion, and effective electrical and thermal conductivity (ConductoDict, DiffuDict) can be calculated. Flow resistivity (permeability, pressure drop), filter efficiency, filter capacity, and many more, can be computed using, e.g., FlowDict, FilterDict, and AddiDict. Mechanical

large deformation and stress/strain curves can be simulated using ElastoDict and the charging of battery electrodes can be analyzed with BatteryDict.

The generated models are available as 3D images and can be exported for further processing using additional software. Using ExportGeo-CAD, the structures can be meshed and exported as well.



New in GeoDict 2026

- In [Stochastic Field Thresholding](#)^[150] random fields based on Laplacian (Exponential) correlation functions are available.
- Additionally in [Stochastic Field Thresholding](#)^[145] you can compute and threshold squared random fields and their inverse.
- Packing analytical spheres can now be [parallelized](#)^[129]. Using 16 threads instead of 1 leads to a speedup by a factor of about 10 even for complicated sphere distributions.
- For the [Gaussian Random Field Generator](#)^[247] also Exponential functions were added.
- [GeoApps](#)^[216] are reorganized. The GeoApps of previous GeoDict versions are now transformed into [Create Presets](#)^[8] or [Pile Presets](#)^[96], or are moved to the Scripting Examples. Instead, other GeoApps are added in the GrainGeo section.

Learn to use GrainGeo:

- [Create Grains](#)^[7]
Generate granular structures with user-defined parameters.
- [Pile Grains](#)^[95]
Simulate grains falling, rotating, and finally settling to create the structure. Arbitrary objects can be chosen as grains.
- [Pack Analytic Spheres](#)^[121]
Create dense sphere packings close to the maximal possible packing density given a fixed number of spheres and a user defined distribution of sphere sizes.
- [Pile Analytic Spheres](#)^[141]
Is faster and might lead to denser packings than Pile Grains, but it is limited to spheres.
- [Stochastic Field Thresholding](#)^[143]
Creates a structure by segmenting a user-defined stochastic field following selected threshold criteria.
- [Distribute](#)^[165]
Grains can be redistributed in the domain to create a more homogeneous material.
- [Sinter & Crystallization](#)^[170]
Simulate a sintering process by compressing the structure currently in memory. The packing

Learn to use GrainGeo:

density is maximized, and grain boundaries can be formed.

- [Grow Sediment](#)¹⁷⁹
New material is added to the existing objects.
- [Roughen Surface](#)¹⁸⁷
The surfaces of objects in the granular structure are roughened with small grains.
- [Add Binder](#)²⁰⁰
Adds material in the shape of a concave meniscus in locations where objects in the structure are close together. The addition of binder in granular structures can be modeled this way.
- [Grain GeoApps](#)²¹⁶
Several GeoApps are available from the GrainGeo section.
- [Gaussian Random Field Generator](#)²³⁸
Generate Gaussian random fields. They can also follow the correlations of a 3D scan.
- [References](#)²⁵⁵
List of references used in the GrainGeo topic.



Join the conversation

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

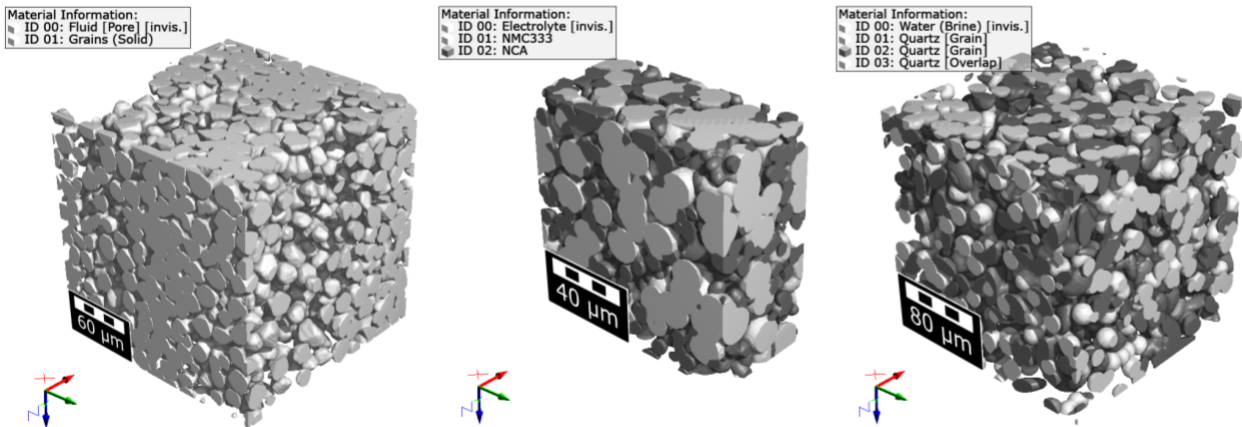
Find illustrative application examples on the [website](#).

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

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

1.1 Create Grains

Use **Create Grains** to generate granular structures. Define the grains shapes, orientation and distribution throughout the domain. Set the size and resolution of the structure and the constituent materials. You can create the objects either in an empty domain or add them to already existing structures.



The Create Grains command:

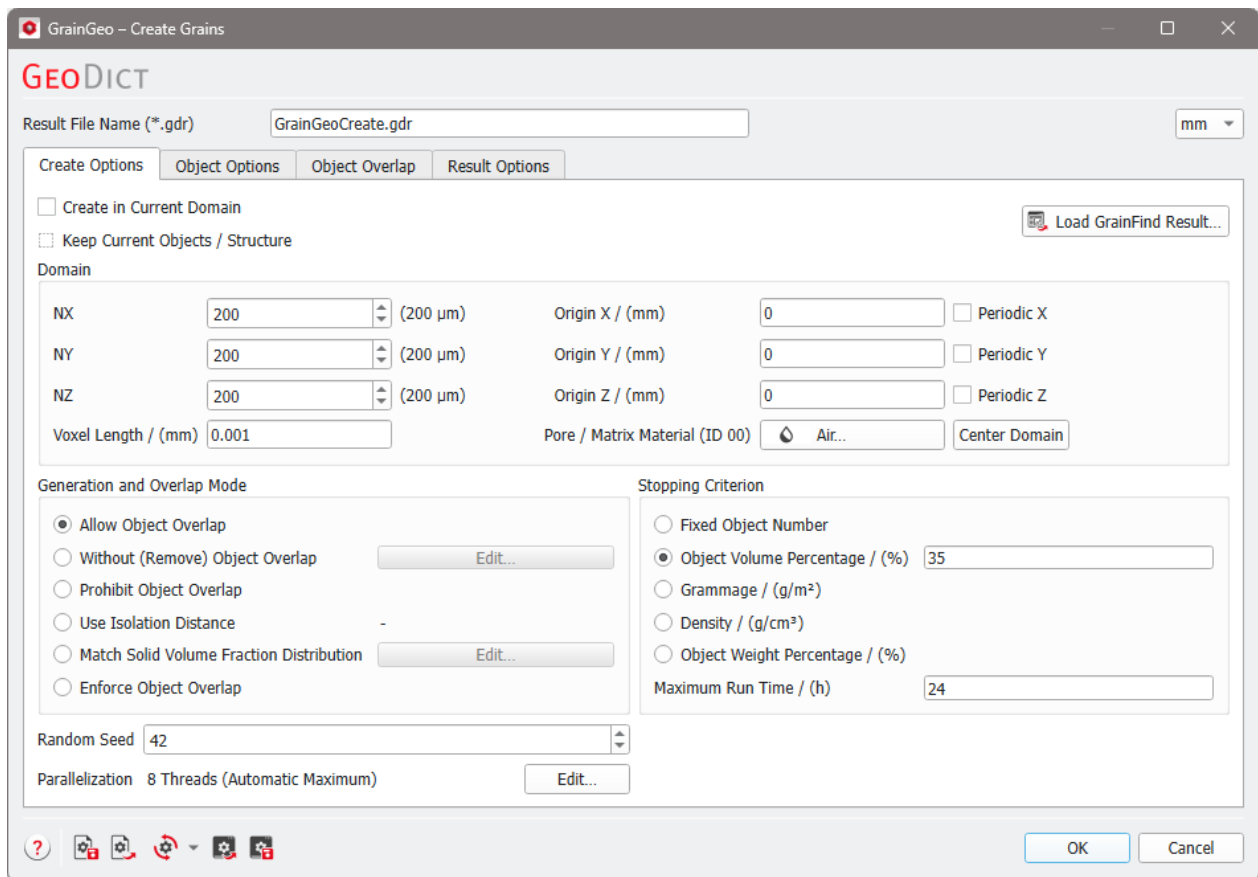
- [Options](#)⁷
Set the parameters for your structure generation.
- [Results](#)⁹¹
Inspect the result file in the Result Viewer.

1.1.1 Options

At the top left of the dialog, the name for the file containing the generation results can be entered in the **Result File Name (*.gdr)** box. The default name can be kept, or a new name can be chosen, fitting the current project.

The result files are saved in the chosen project folder (**File** → **Choose Project Folder**, in the **Menu bar**). If a GeoDict result file (*.gdr) with the given name already exists in the project folder, a warning message is shown at the start of the creation process. You can either decide to rename the chosen file name to a new one, to cancel the generation process, to overwrite or to back up the old file. When nothing is selected, GeoDict uses the **Back-Up** option after a waiting time.

The available units (m, cm, mm, μm, nm and Inch) are selectable from the pull-down menu at the top right of the dialog. When the units are changed, the entered values are adjusted automatically.



The parameters are organized into tabs:

- [Create Options](#)⁹
Determine general properties of the resulting structure, such as size, position, resolution, and solid volume fraction.
- [Object Options](#)³⁷
Define the geometrical properties of individual object types such as cross-section, length, and orientation. Up to eight different object types can be used in one structure.
- [Object Overlap](#)⁸⁷
Define how the IDs of different materials and objects are assigned. This is relevant for overlap operations performed on the structure and to define different materials with respective properties in the structure.
- [Result Options](#)⁹⁰
Determine if intermediate geometries are saved.

Different Create Grains Presets

In the bottom of the dialog find several helpful options.



Opens the corresponding User Guide section.

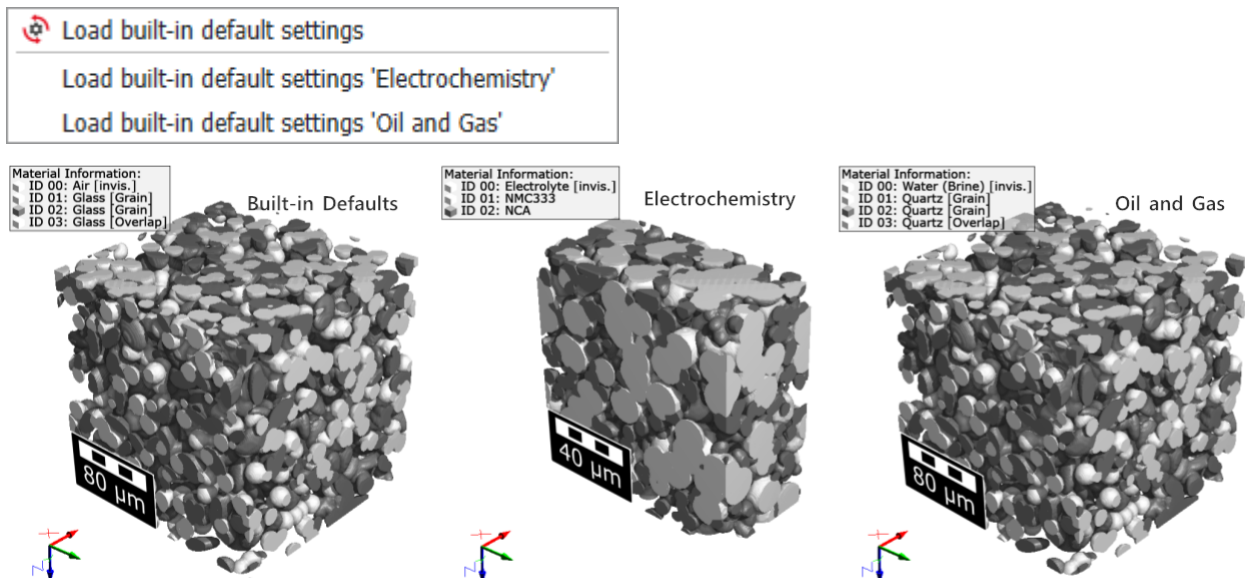
	Saves the settings to a GeoDict settings file (*.gps).
	Loads the settings from a GeoDict settings file (*.gps) or a GeoDict result file (*.gdr).
	Resets all parameter settings to the built-in default settings.
	Resets all parameter settings to the saved start-up settings.
	Saves the current parameter settings as start-up settings.

Each option is explained by a tooltip which appears when resting the mouse over the icon.

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

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

In GrainGeo Create find the presets **Electrochemistry** and **Oil and Gas**. Choose the presets and inspect the entered parameters in the different tabs if they are a better base for your applications. For the Oil and Gas preset only the materials are changed. For the Electrochemistry version also domain, object and overlap parameters are changed.



Create Options

Determine general properties of the resulting structure, such as size, position, resolution, and solid volume fraction. The parameters are grouped into three panels and five to six single parameters, three structure options at the top and two to three general options at the bottom. The parameter temperature is only shown, if a corresponding [stopping criterion](#)³⁰ is selected.

The screenshot shows the 'Create Options' dialog box in GrainGeo. It is organized into several sections:

- Domain:** Includes input fields for NX, NY, and NZ (all set to 200 μm), Voxel Length / (mm) (0.001), Origin X / (mm), Origin Y / (mm), and Origin Z / (mm) (all set to 0). There are checkboxes for Periodic X, Y, and Z. A 'Pore / Matrix Material (ID 00)' dropdown is set to 'Air...'. A 'Center Domain' button is also present.
- Generation and Overlap Mode:** Contains radio buttons for 'Allow Object Overlap' (selected), 'Without (Remove) Object Overlap', 'Prohibit Object Overlap', 'Use Isolation Distance', 'Match Solid Volume Fraction Distribution', and 'Enforce Object Overlap'. There are 'Edit...' buttons for the 'Without (Remove) Object Overlap' and 'Match Solid Volume Fraction Distribution' options.
- Stopping Criterion:** Contains radio buttons for 'Fixed Object Number', 'Object Volume Percentage / (%)' (selected, set to 35), 'Grammage / (g/m²)', 'Density / (g/cm³)', 'Object Weight Percentage / (%)', and 'Maximum Run Time / (h)' (set to 24).
- Random Seed:** A dropdown menu set to 42.
- Parallelization:** A dropdown menu set to '8 Threads (Automatic Maximum)' with an 'Edit...' button.

The parameters are organized in the following groups:

- [Structure Options](#)¹⁰
Create in a current domain and keep current objects or the current structure.
- [Domain](#)¹¹
Define the domain parameters, such as resolution, periodicity, and matrix material.
- [Generation and Overlap Mode](#)¹⁷
Decide about removing overlap and following solid volume fraction distributions.
- [Stopping Criterion](#)³⁰
Define according to which criteria the object generation should be stopped.
- [General Options](#)³⁴
Define parallelization, temperature, and random seed.

Structure Options

At the top of the **Create Options** tab, find options to load GrainFind results and to keep the current domain and structure.

This screenshot shows the top section of the 'Create Options' dialog box, specifically the 'Structure Options' area. It contains two checkboxes: 'Create in Current Domain' and 'Keep Current Objects / Structure'. To the right of these checkboxes is a button labeled 'Load GrainFind Result...'.

Create in Current Domain and Keep Current Objects / Structure

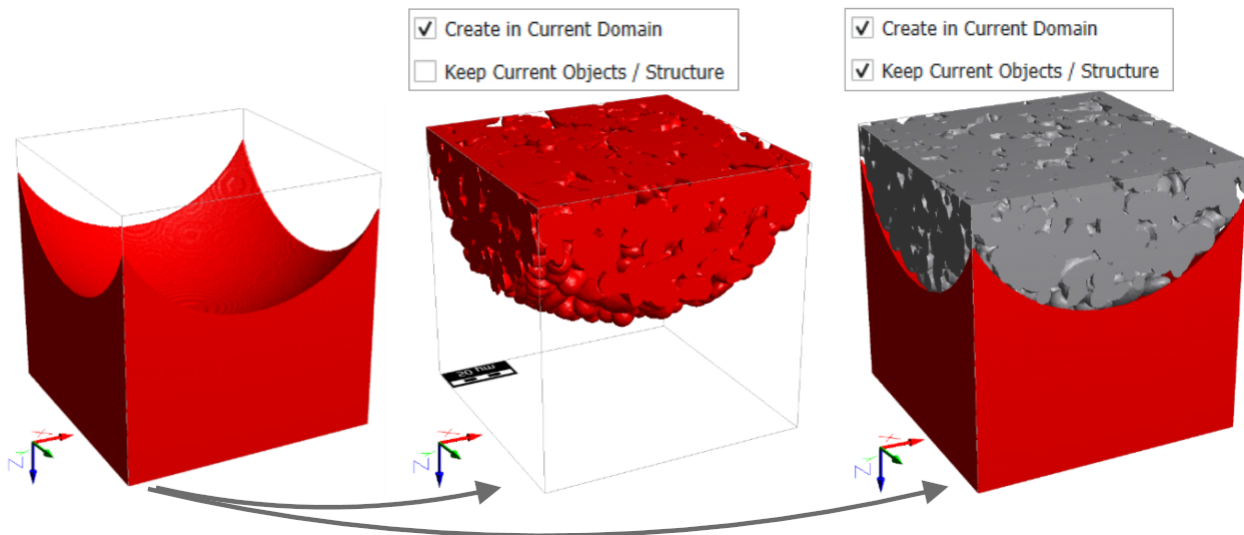
Create in a current domain with or without keeping the current objects or the structure. When checking **Create in Current Domain** the structure currently in memory is considered during the generation of a new structure. Additionally, when **Keep Current Objects / Structure** is

checked, the structure in memory is kept and combined with the newly generated granular structure.

This feature is used in combination with checking **Prohibit Object Overlap** or **Prohibit Overlap with Current Objects** in the [Generation and Overlap Mode](#)¹⁷ panel. By this, complex models of granular structures can be generated. For example, you can make copper spheres cover a mold that is later discarded.

Once **Create in Current Domain** is checked, the parameters grouped under the **Domain** panel are inactive, including the voxel length, because they are taken from the structure already in memory.

In the example below, a previously generated mold (current object / structure) is present in memory while spheres are added. **Prohibit Overlap with Current Structure** is checked to avoid the spheres from entering the mold, but the spheres can overlap each other. The spheres are automatically assigned as Material ID 02, while keeping the initial structure (with Material ID 01).



If the spheres should not overlap each other, nor the mold, either **Prohibit Object Overlap** or **Without (Remove) Object Overlap** should be checked. Learn more about these options in the [Generation and Overlap Mode](#)¹⁷ topic.

Load GrainFind Results

If **GrainFind Identify Grains** was applied for example to a segmented gray value image, the result file (*.gdr) can be loaded into GrainGeo to generate a statistical digital twin. The parameters can be altered after loading the result. How to do this is described in the GrainFind User Guide in the chapter Connecting GrainFind Analysis Results with GrainGeo.

Domain

The **Domain** panel contains the parameters defining the structure size (**NX**, **NY**, and **NZ**) in combination with the resolution (**Voxel Length**), as well as the **Origin** parameters, the **Periodicity** check boxes, the **Center Domain** button, and the **Pore / Matrix Material** button.

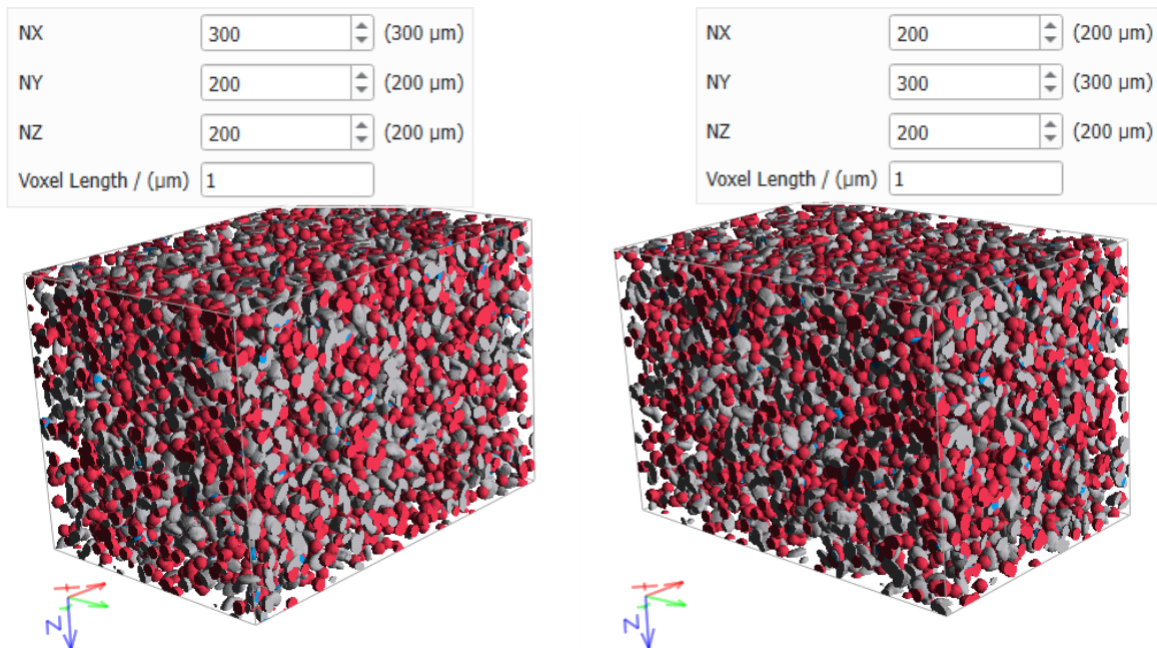
Domain					
NX	200	(200 μm)	Origin X / (mm)	0	☐ Periodic X
NY	200	(200 μm)	Origin Y / (mm)	0	☐ Periodic Y
NZ	200	(200 μm)	Origin Z / (mm)	0	☐ Periodic Z
Voxel Length / (mm)	0.001		Pore / Matrix Material (ID 00)	Air...	Center Domain

✓ NX, NY, NZ, and Voxel Length

The internal representation of a structure in GeoDict consists of rectangular 3D arrays of cubes, hereafter called volume elements or voxels.

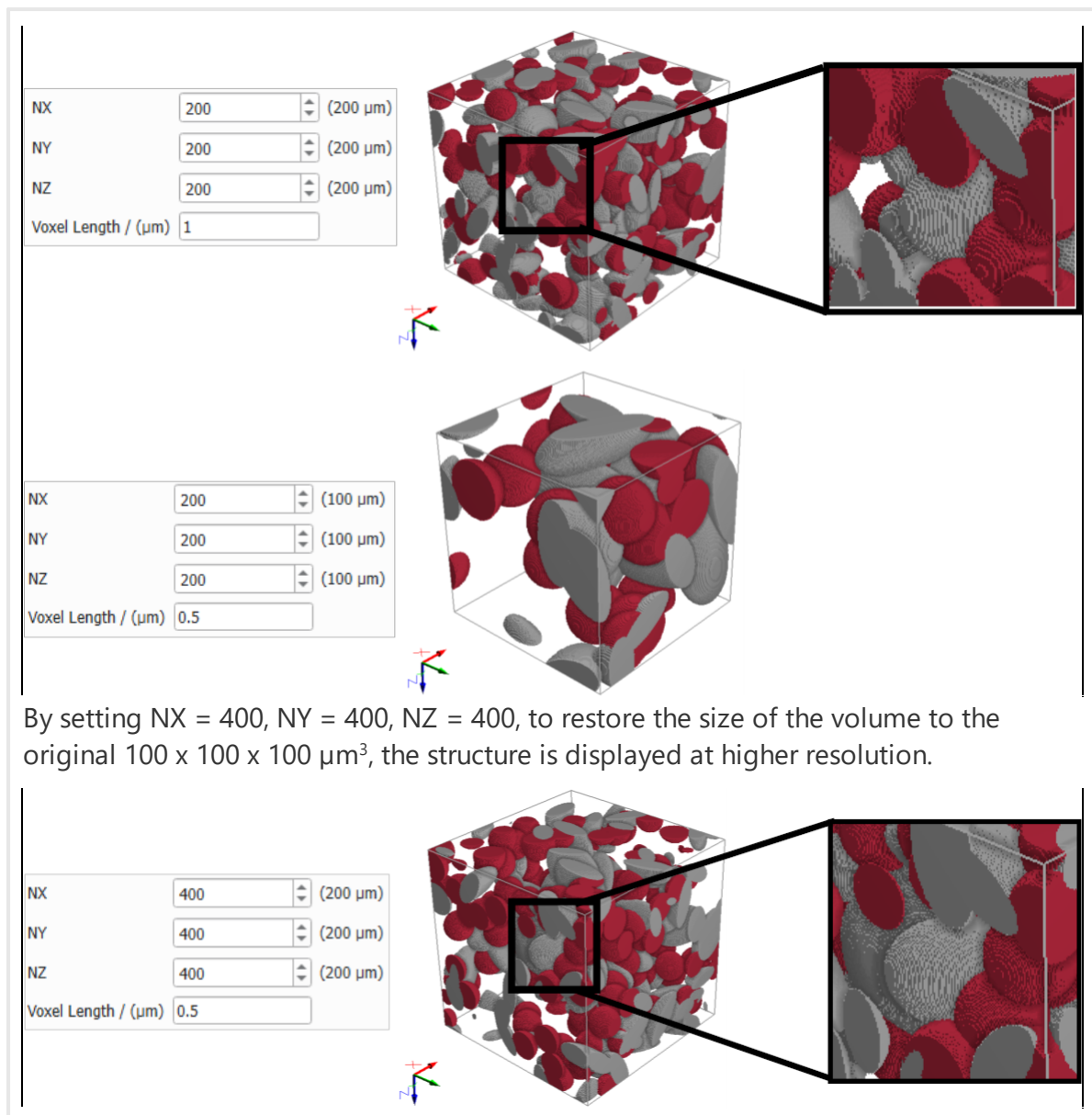
NX, **NY**, and **NZ** are the number (N) of voxels in X, Y, and Z directions.

The **Voxel Length** is the size of one voxel in the chosen units. Varying the values for **NX**, **NY**, and **NZ** has the effect of changing the size of the structure in the given direction.



Low values for **Voxel Length** in combination with high values for **NX**, **NY**, and **NZ** increase the resolution, but also increase computational time. After setting the values of **NX**, **NY**, **NZ**, and **Voxel Length**, the physical structure size is automatically displayed in the chosen units (here μm).

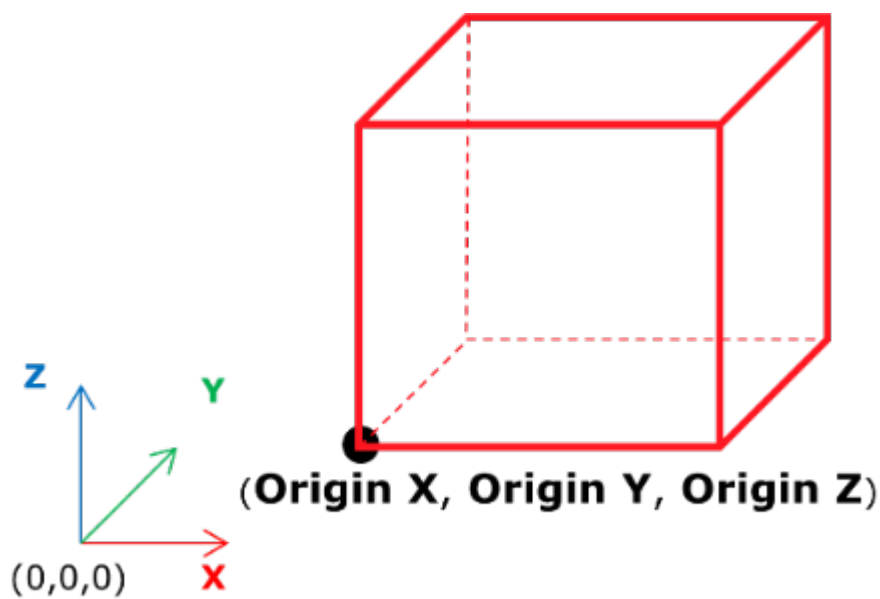
The following example shows how starting with $\text{NX} = 200$, $\text{NY} = 200$, $\text{NZ} = 200$ ($100 \times 100 \times 100 \mu\text{m}^3$, at voxel length $0.5 \mu\text{m}$), and decreasing the Voxel Length from $0.5 \mu\text{m}$ to $0.25 \mu\text{m}$ has the effect of refining the structure by increasing the resolution, while decreasing the size of the volume to $50 \times 50 \times 50 \mu\text{m}^3$.



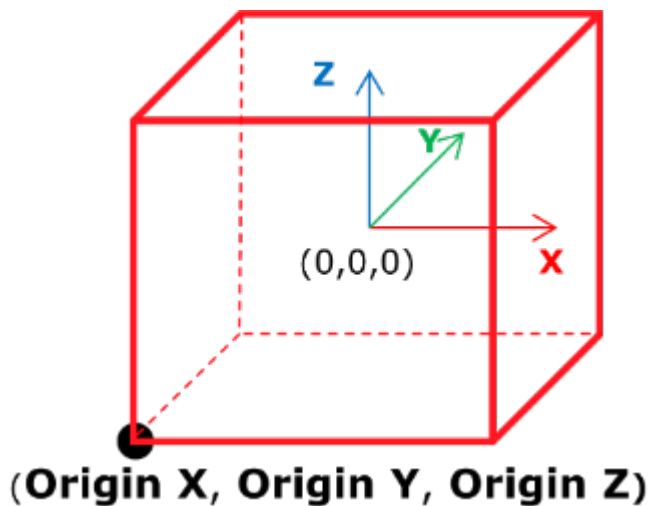
By setting NX = 400, NY = 400, NZ = 400, to restore the size of the volume to the original $100 \times 100 \times 100 \mu\text{m}^3$, the structure is displayed at higher resolution.

✓ Origin X, Origin Y, and Origin Z

The **Origin X**, **Origin Y**, and **Origin Z** parameters, together with the **Center Domain** button, determine the placement of the structure in the physical space. Zero values for Origin X, Origin Y, and Origin Z mean that the point with (0, 0, 0) coordinates is located at the lower left corner of the structure.



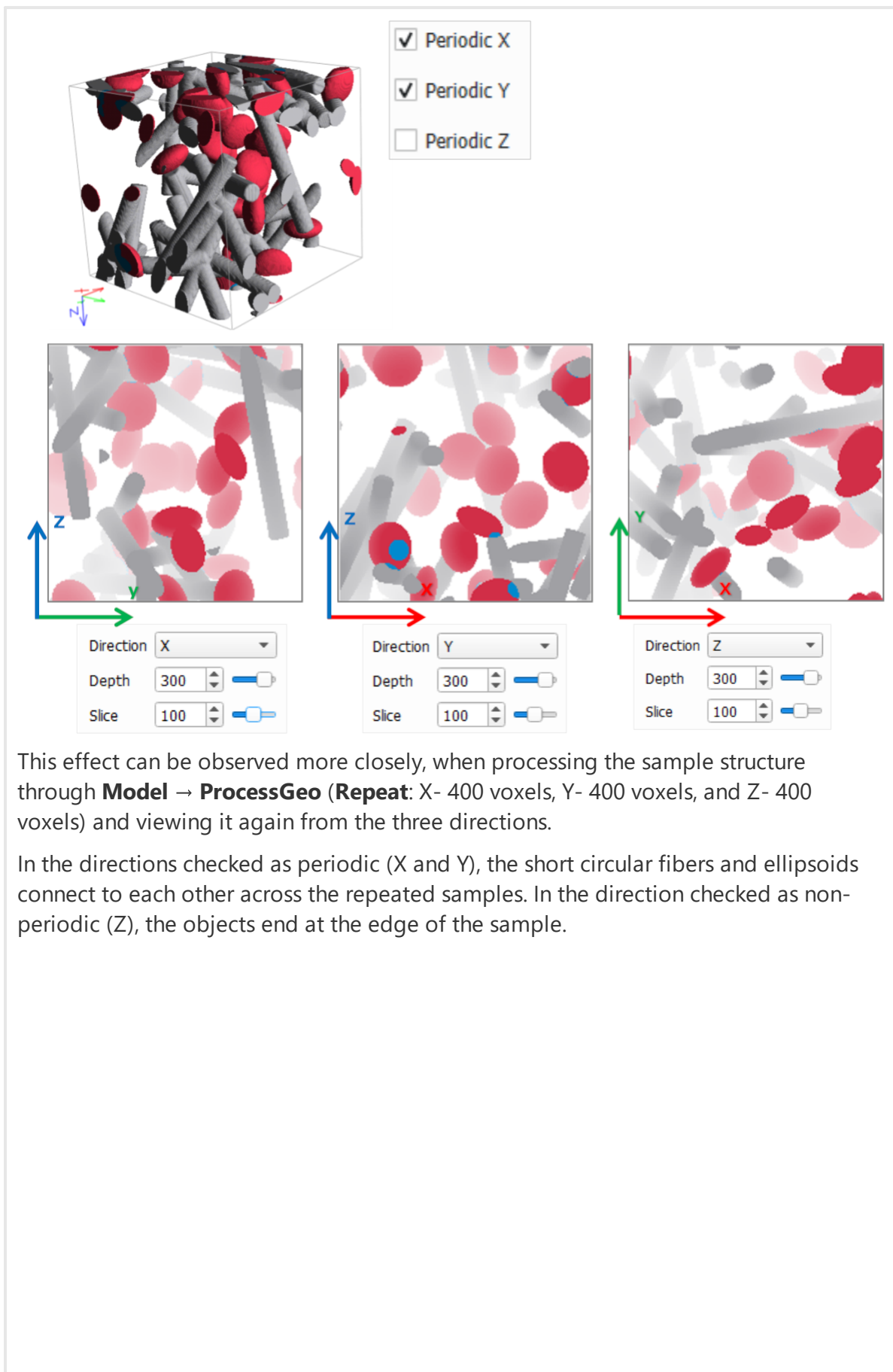
When clicking the **Center Domain** button, the (0, 0, 0)-point is set to the center of the structure as shown below.

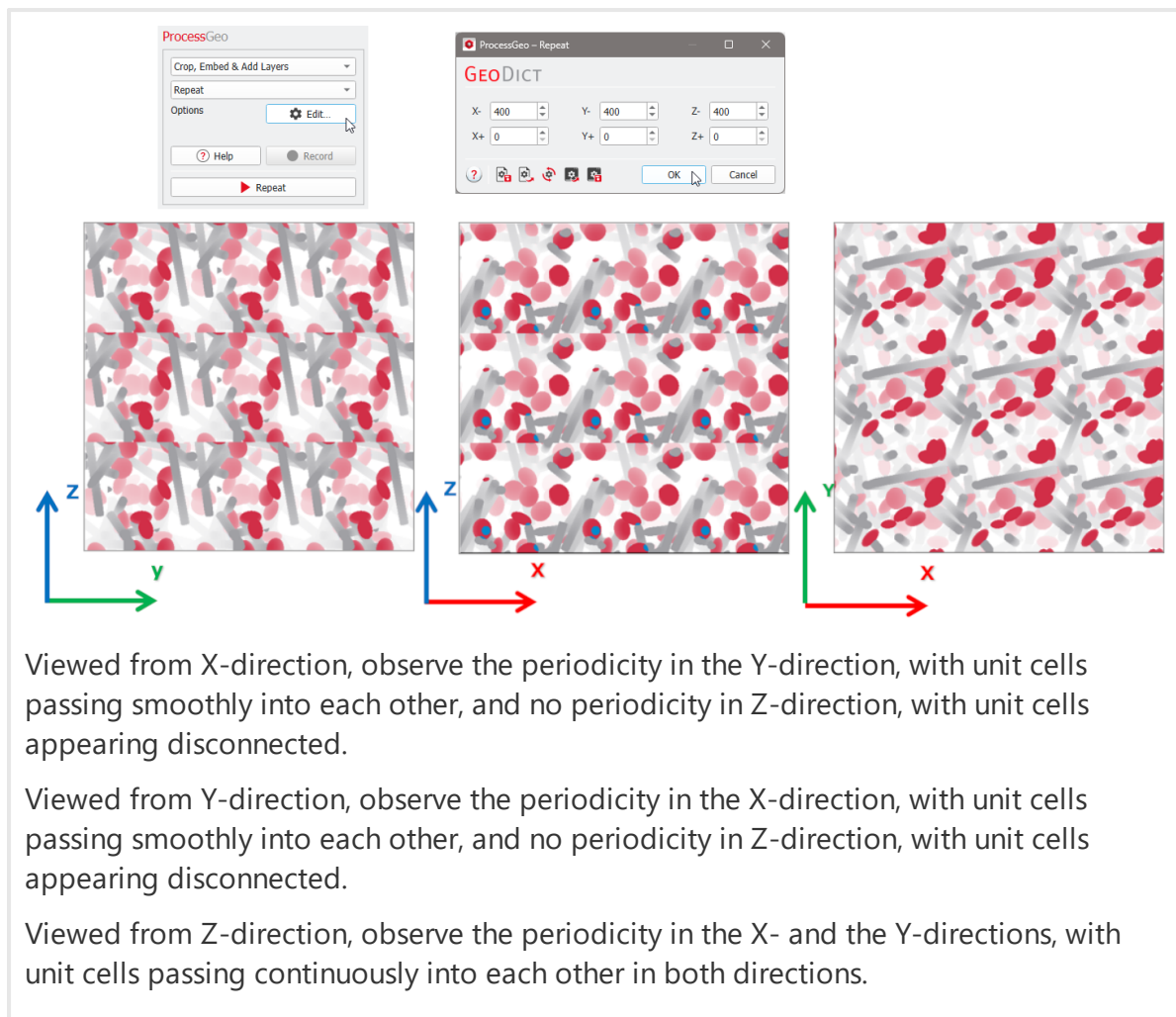


☒ Periodicity

Checking the **Periodic X**, **Periodic Y**, and **Periodic Z** boxes allows the generation of structures which are periodic in one or several directions. Periodicity has the effect, that objects ending on one side of the volume reappear on the opposite side, so that merging of several volumes with periodic objects results in a repetitive complex.

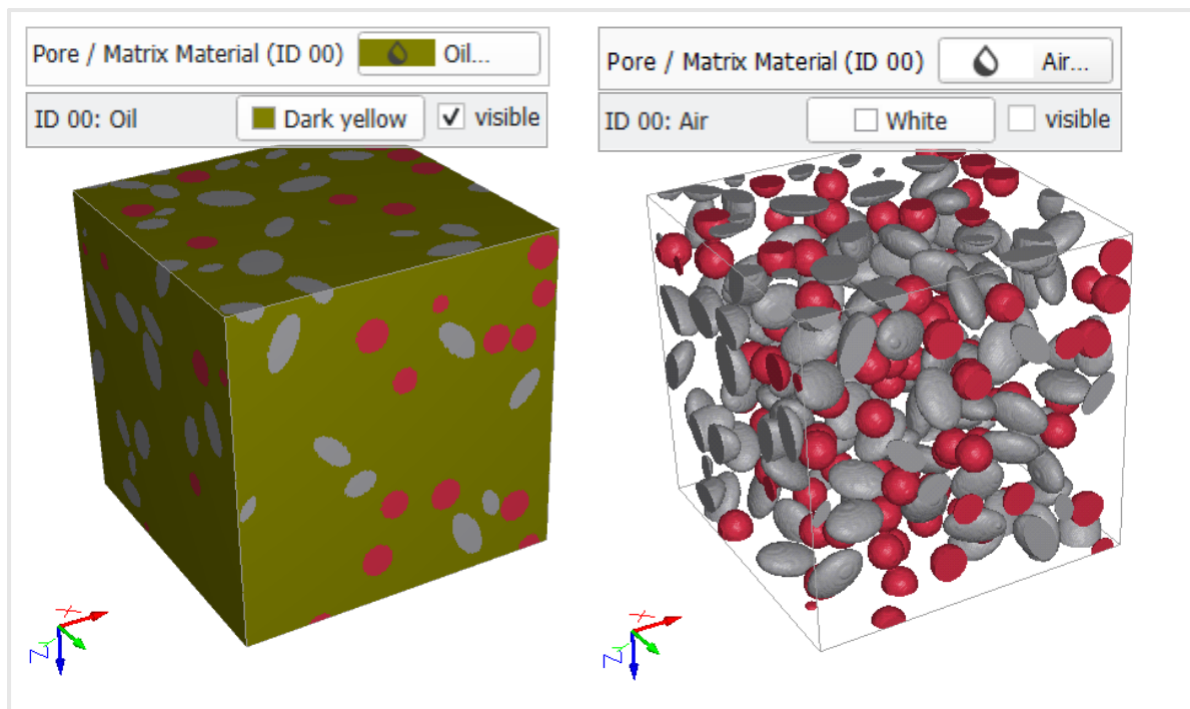
Checking the Periodic X and Periodic Y boxes, but leaving un-checked the Periodic Z box, has the following effect on the periodicity of a generated granular structure.





✓ Pore / Matrix Material and Density

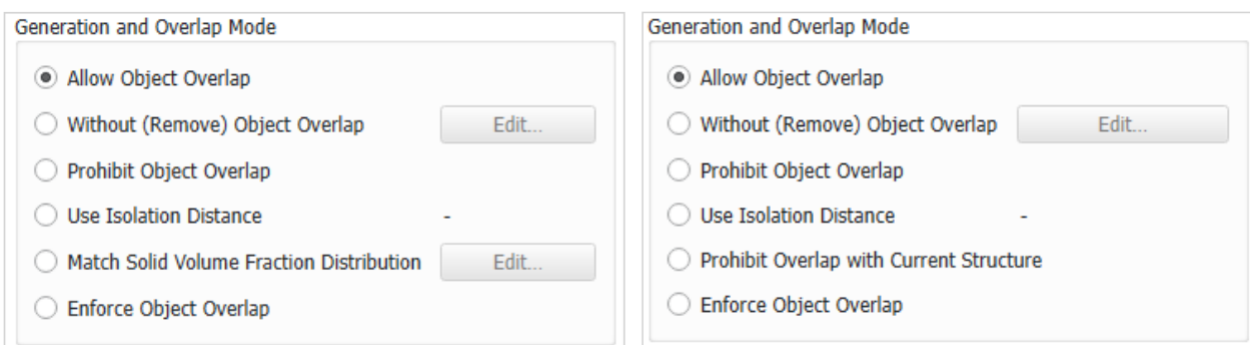
When the material with ID 00 is chosen to be **Pore**, the objects are embedded in empty pore space. Alternatively, the material filling the pore space can be a **Solid**, a **Porous** medium, or **Fluid**, in which the structural objects are embedded. The physical properties of the pore / matrix material can be attributed for simulations. The color and the visibility / invisibility can be chosen independently of the material.



Generation and Overlap Mode

The options in the **Generation and Overlap Mode** panel control the relative position among objects. It is possible to choose between **Allow Object Overlap**, **Without (Remove) Object Overlap**, **Prohibit Object Overlap**, **Use Isolation Distance**, **Match Solid Volume Fraction Distribution**, and **Enforce Object Overlap**.

If checking **Create in Current Domain**, **Prohibit Overlap with Current Structure** appears instead of **Match Solid Volume Fraction Distribution**. The objects in the newly generated structure can intersect with each other but not with those of the already existing structure.



Know how! The algorithm under **Allow Object Overlap** is fast, especially for big structures and, in most cases, leads to excellent results.

If you choose **Remove Object Overlap**, the generation time may be longer when generating structures with high solid volume percentages. The objects are first positioned in the structure allowing overlap. Afterwards they are moved to remove overlap as good as possible.

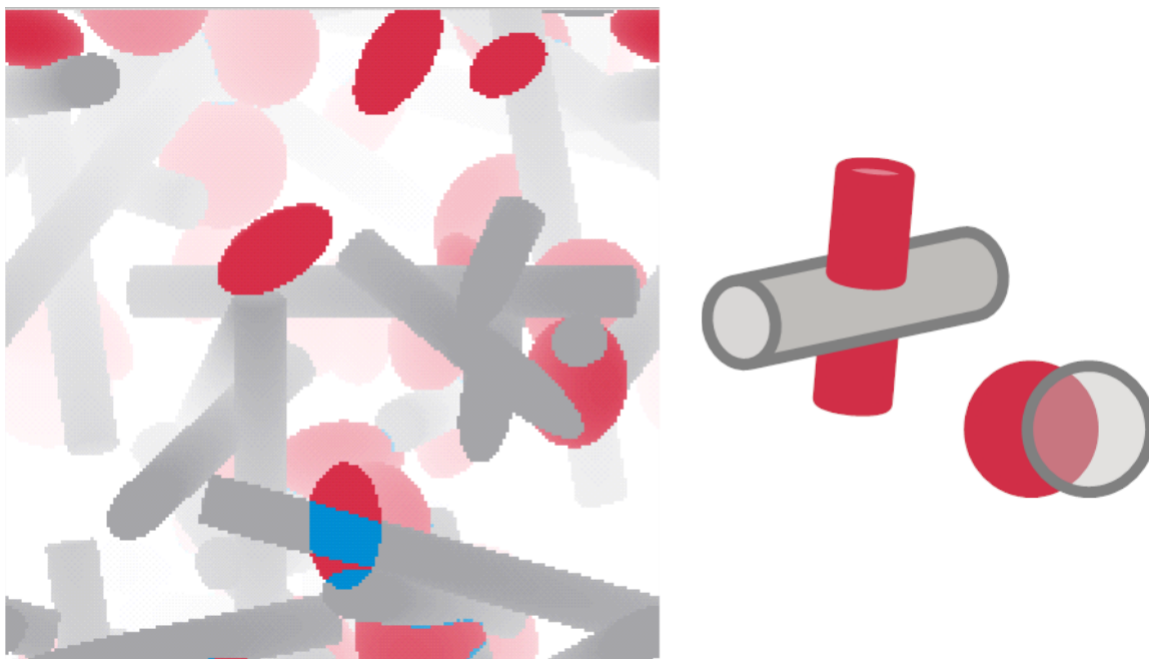
Prohibit Object Overlap or **Prohibit Overlap with Current Structure** directly position the objects one after the other without overlap. This is fast for low densities, but may be very slow or even unfeasible when generating dense geometries since the positioning of new non overlapping objects might be geometrically impossible.

For the same reasons, with **Use Isolation Distance**, the generation time may be long, or the generation might be impossible depending on the chosen value for the isolation distance and the selected value for stopping criterion. Then, use the isolation distance option in the Remove Object Overlap dialog.

Generally, structures with overlapping objects can be used for processes in the pore space, as filtration and flow simulation. For simulations of mechanical properties, structures without overlap should be generated.

✓ Allow Object Overlap

Objects may overlap when selected.



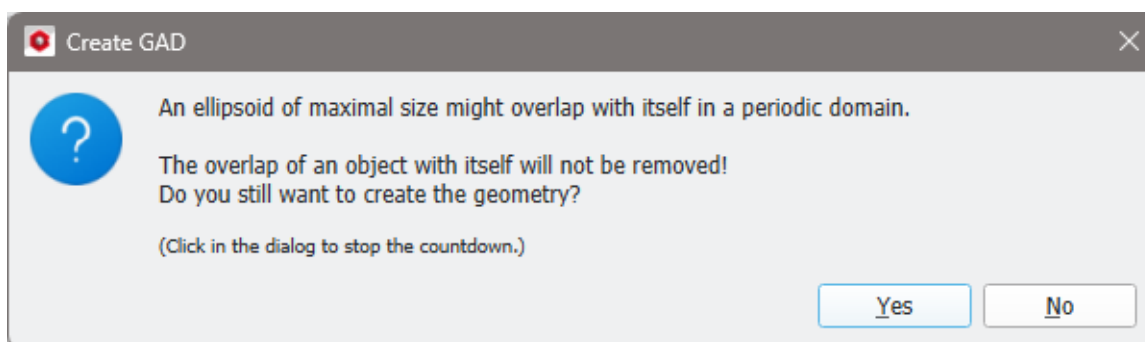
✓ Without (Remove) Object Overlap

Checking **Without (Remove) Object Overlap** eliminates existing overlaps after the generation step.

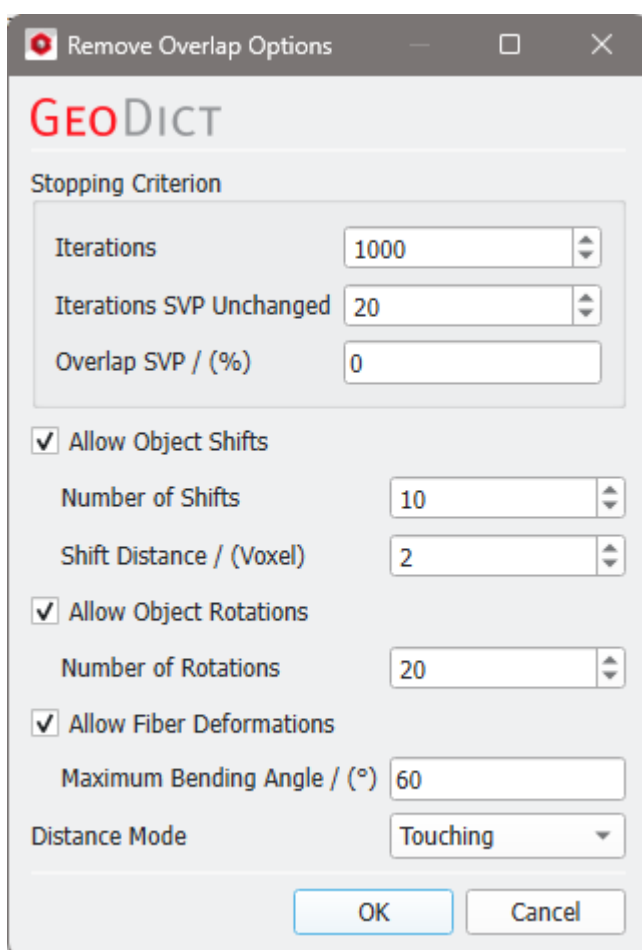
i Note! The statistical properties might change slightly after removing overlap.

Overlaps can be removed from periodic structure models with objects smaller than the domain size or non-periodic structure models with arbitrary object sizes. In a periodic

domain, objects which are longer than the domain might overlap with themselves. This type of overlap cannot be removed. In this case, a message appears:



The way in which the overlap removal occurs can be controlled through the **Remove Overlap Options** accessible via the **Edit...** button.



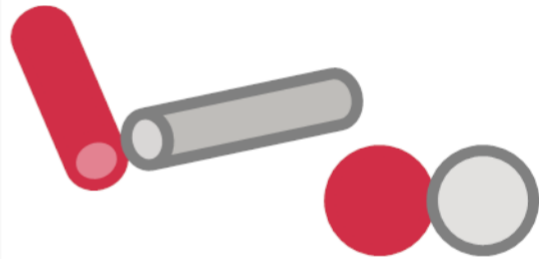
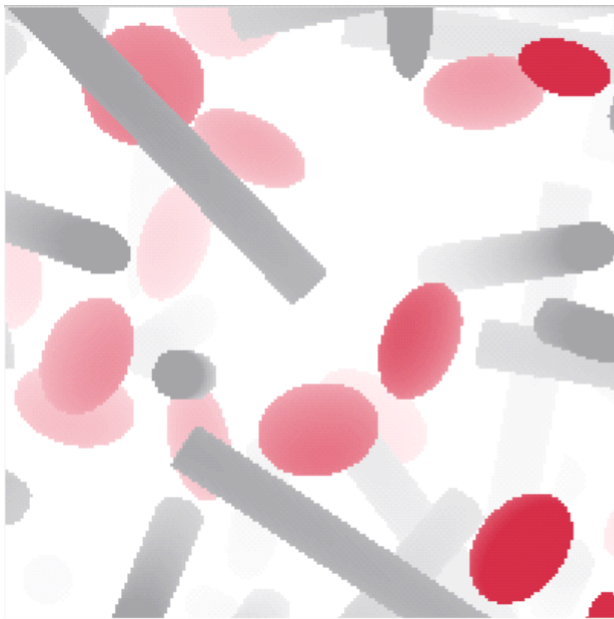
In the **Remove Overlap Options** dialog, the following parameters can be set:

- **Iterations:** Defines after how many iterations the removal stops.
- **Iterations SVP Unchanged:** The removal stops if the SVP (Solid Volume Percentage) remained unchanged during this number of iterations.

- **Overlap SVP / (%)**: Defines the final allowed Overlap SVP.
- **Allow Object Shifts**: Check if shifting the objects should be an allowed operation for overlap removal. Define the **Number of Shifts** per iteration and the maximal **Shift Distance** in voxel per iteration.
- **Allow Object Rotations**: Check if rotating the objects should be an allowed operation for removal. Define the maximal **Number of Rotations** allowed per iteration. Objects will be rotated in all directions, where the maximal rotation angle per iteration is one degree.
- **Allow Fiber Deformations**: Check if bending fibers should be an allowed operation for overlap removal. Define the **Maximum Bending Angle** allowed between two segments. Each fiber consists of several segments. The center points of the segment connections are shifted in all directions, while the other shape parameters, as, e.g., fiber length and segment length are kept constant. The maximal point shift distance is the same as for the object shift. This option is only applied to fibers, as other objects do not consist of segments.
- **Distance Mode**: The pull-down menu offers four options:
 - The objects can be **Touching** (distance zero).
 - Enter a maximal **Defined Overlap** allowed for the objects.
 - Enter a minimal **Defined Isolation** distance for the objects.
 - **Avoid Contacts** means a defined isolation of one voxel volume diagonal.

Prohibit Object Overlap

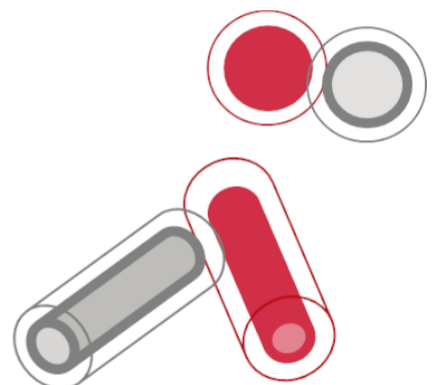
Objects may touch but not overlap when selected. In this case, the overlap of the objects is prohibited during the creation process. This option might lead to longer run times compared to **Remove Objects Overlap**. It only works for low volume percentages.



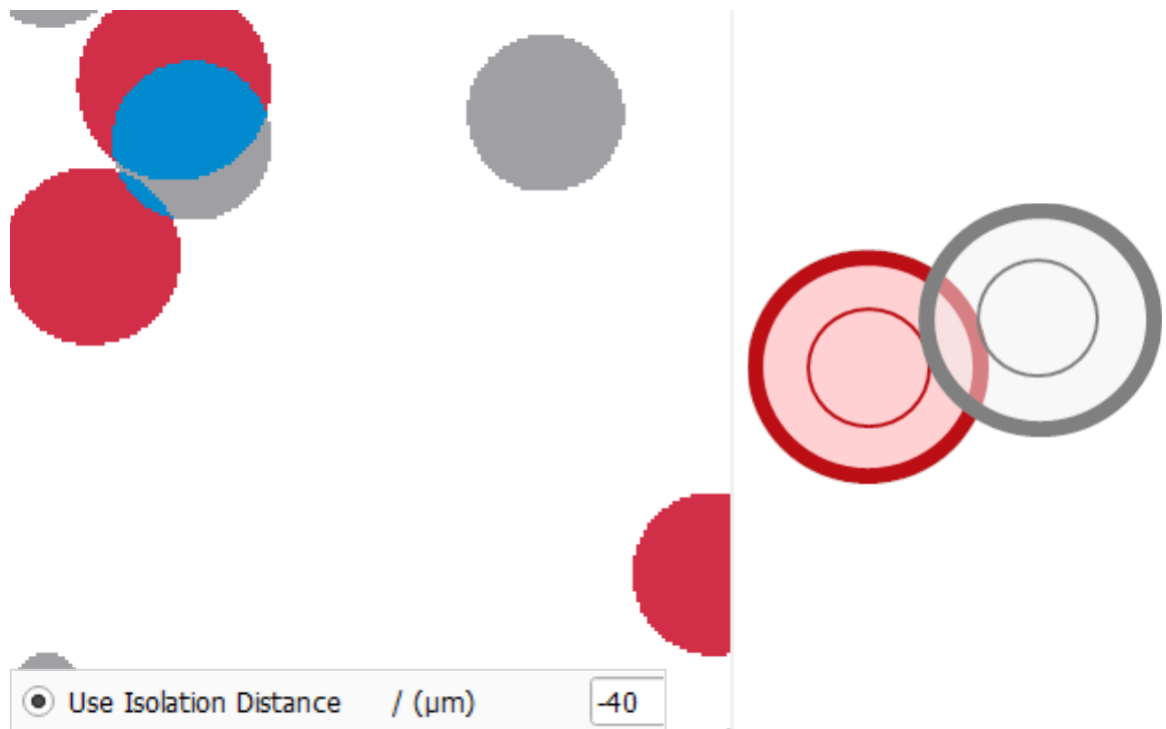
As mentioned above, objects longer than the domain might overlap themselves if a periodic domain is selected.

✓ Use Isolation Distance

Inserting a positive value, the gaps between objects have at least this preset distance. When set to negative values (e.g., $-40\ \mu\text{m}$), the effect is that the objects may overlap by maximally $40\ \mu\text{m}$ (showing in a different color, here blue). While the distance mode **Defined Isolation** in **Remove Overlap** considers the objects, the **Use Isolation Distance** option only considers the voxel structure, and thus works for all object types.



Negative values for the isolation distance are useful to model synthetic objects that melt, or objects that deform at their touching points.



✓ Match Solid Volume Fraction Distribution

For certain applications it is necessary to create statistically distributed inhomogeneities, e.g., to generate a bimodal distribution of objects. The **Match Solid Volume Fraction (SVF) Distribution** option allows to create such structures with an inhomogeneous solid volume distribution. Objects are shifted and rotated to optimally match a SVF distribution given by a Gaussian random field. This takes place after the generation step. Consider that **Periodicity** is checked automatically for all directions. This is a prerequisite for the **Match Solid Volume Fraction** algorithm.

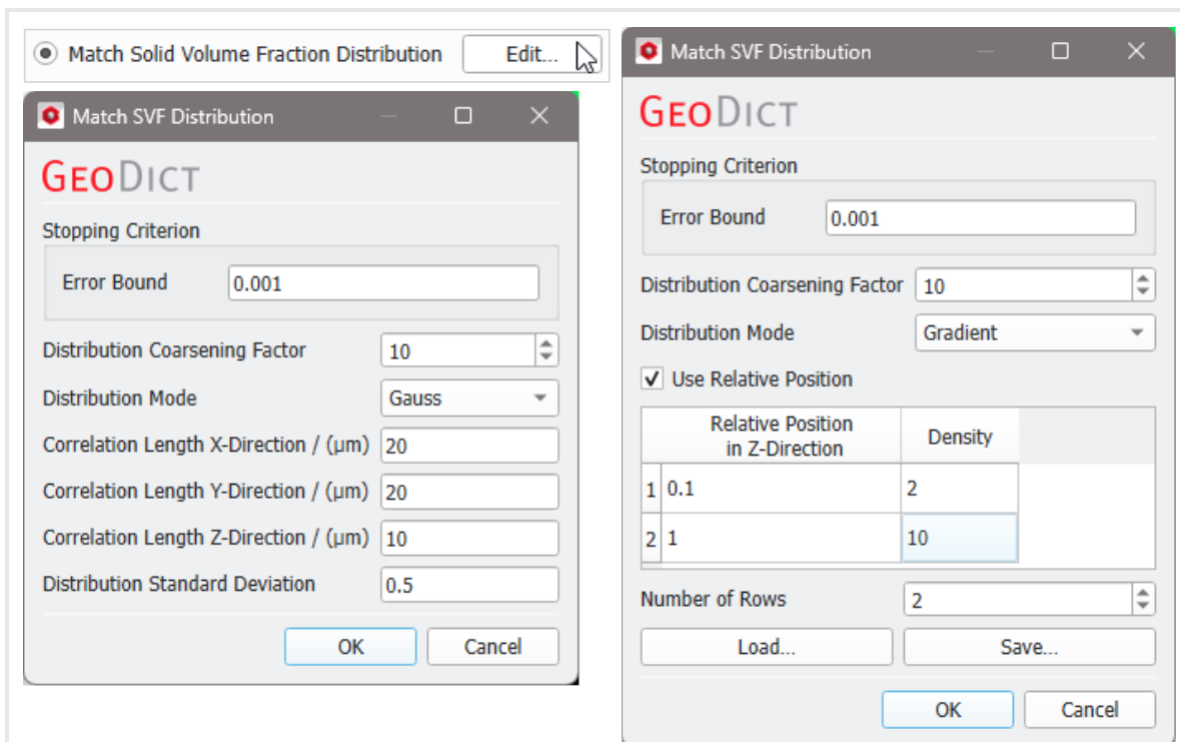


Note!

- Using this feature, overlap cannot be entirely removed during structure generation. After the solid volume fraction distribution algorithm was applied, a few steps of **Remove Overlap** are applied. The object's movement during that operation is limited such that the desired distribution is kept.
- As the SVF distribution is matched after generating the objects fitting the **Stopping Criterion**, the resulting values can differ from the inserted parameters for the **Stopping Criterion**. This is because the structure is generated with overlap and the amount of overlap can change when Objects are shifted.

- The distribution for **Center** defined in the **Object Options** tab will also be affected strongly by matching the SVF distribution after generating the grain structure with the specified center distribution. The difference between the **Center Distribution** and the **Match SVF Distribution** is explained below.
- It is recommended to generate the structure without using the **Center Distribution** option under the **Object Options** tab when using this algorithm. The objects will be moved afterwards, matching the given SVF distribution not considering the initial center distribution anymore. The center distribution is often used to generate inlet and outlet. This can also be achieved using a Gradient distribution here. However, if you need inlet and outlet while using a Gaussian distribution, add them later either with **GadGeo - Edit Domain** or with **ProcessGeo - Embed** to avoid cropped objects.
- It is possible to reuse an existing stochastic field describing the desired SVF distribution. For this, first generate the structure with the mode **Allow Overlap** and then use the **Match SVF distribution** algorithm in GadGeo. Open the **GadGeo** section by selecting **Model** → **GadGeo** from the menu bar. Select **Algorithms** from the first pull-down menu and then **Match SVF Distribution** from the second.
- For large structures, the feature needs a large amount of memory as a volume field is loaded in GeoDict additional to the structure file.

The SVF distribution can be controlled through the **Match SVF Distribution** dialog accessible via the **Edit ...** button.



In the **Match SVF Distribution** dialog, the following parameters can be set:

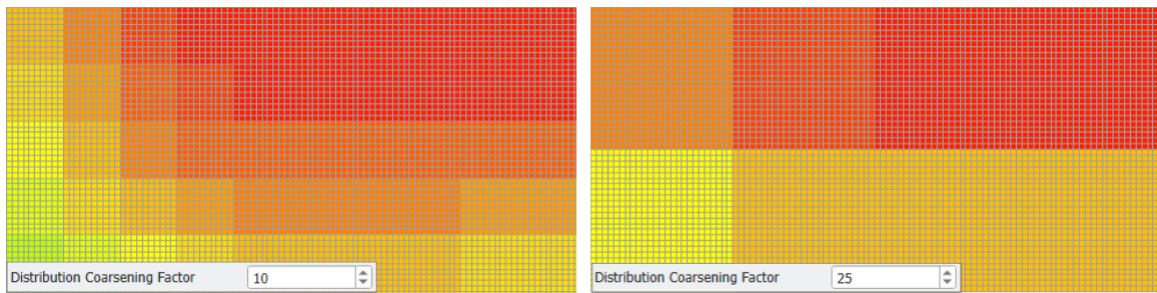
Stopping Criterion: Define the **Error Bound** to determine when the SVF matching should be stopped. When the normalized relative change of solid volume fraction is smaller than the given error bound, the algorithm is stopped.

Distribution Coarsening Factor: The SVF distribution is matched using a coarser version of the created Gaussian random field. The value must be small enough to resolve the heterogeneity of the structure. A larger value leads to a shorter run-time. If the Distribution Coarsening Factor is set to 1, the Gaussian random field is generated with the same resolution as the grain structure. The coarsening factor must be a divisor of the domain size in voxels for each of the three dimensions.

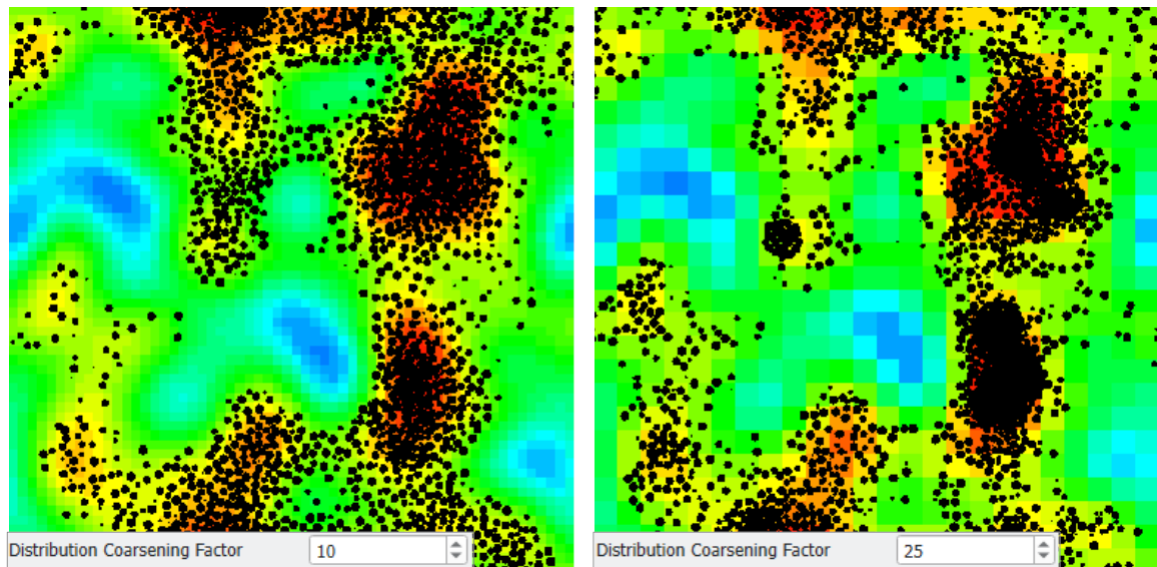
For a structure with a domain size of 2048x1024x512 voxels and a voxel length of 1 μ m a coarsening factor of 32 leads to a random field of 64x32x16 voxels with a voxel length of 32 μ m.

Keep in mind, that the coarsening factor also determines how many voxels remain to resolve the correlation lengths. The correlation length should be resolved with at least three or four voxels. Otherwise, the random field is too coarse to accurately resolve the correlation length. Consider the example above with a correlation length of 128 μ m and a coarsening factor of 32. Then, $128/32 = 4$ voxels remain to resolve one feature of the random field.

In the example below, with the grid turned on under the Camera tab in 2D view, observe the influence of the coarsening factor on the volume field. For a coarsening factor of 10, each color box has 10x10x10 voxels.



A smaller coarsening factor leads to a smoother distribution of the objects, which you can observe in the grain structure example below.



Distribution Mode: For distribution select **Gauss** or **Gradient** from the pull-down menu. The following parameters are different for these two options.

- **Gauss:**

- **Correlation Length:** The correlation length is a measure for the inhomogeneity of the material. The parameters for X-, Y- and Z-Direction determine the correlation length of the Gaussian random field, which defines the SVF distribution. It is recommended to select a value significantly smaller than the domain size in the corresponding direction to see an effect. For a constant SVF in one direction choose the corresponding domain size as correlation length.
- **Distribution Standard Deviation:** Define the relative standard deviation of the created SVF distribution. Relative means relative to the given object solid volume percentage. A larger value leads to a larger difference between the regions of low and high density. Using the relative standard deviation instead of the absolute standard deviation allows using the same Gaussian field for different solid volume percentages.

Distribution Mode	Gauss
Correlation Length X-Direction / (μm)	20
Correlation Length Y-Direction / (μm)	20
Correlation Length Z-Direction / (μm)	10
Distribution Standard Deviation	0.5

- **Gradient:**

- **Use Relative Position:** If checked, the left column values from 0 to 1 correspond to locations in the structure. In the Z-direction, the value 0 is at the origin and the value 1 is at end of the domain. If not checked, the values in the left column correspond to absolute values in the given unit.
- **Distribution Table:** The right column assigns relative density values at the locations defined in the left column, e.g., the value 10 means that there are five times more objects at $Z = 1$ than at $Z = 0.1$, with a density value of 2. The object density increases and decreases smoothly between the given locations in the Z-direction.
- **Number of Rows:** The number of rows in the distribution gradient can be increased or decreased to enter as many pairs of position and density as desired.
- **Load/Save:** The density distribution can be saved to and loaded from a .txt file.

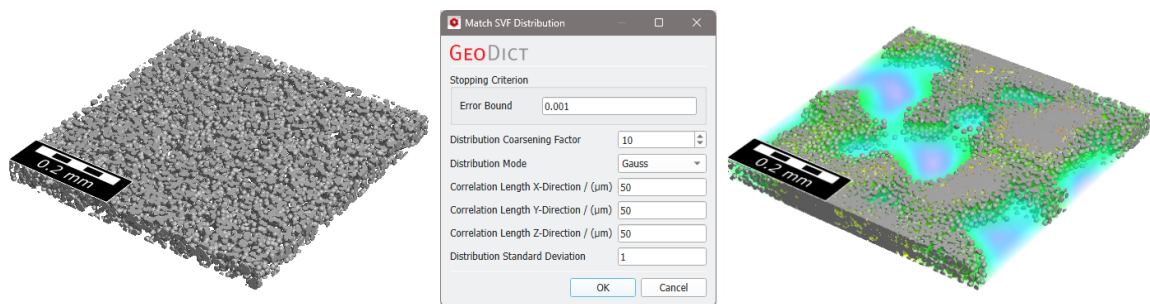
Distribution Mode	Gradient
☒ Use Relative Position	
Relative Position in Z-Direction	Density
1 0.1	2
2 1	10
Number of Rows	
2	
Load...	Save...

Example - Gauss

In the following example, grains are generated in a domain of 600x600x50 μm .

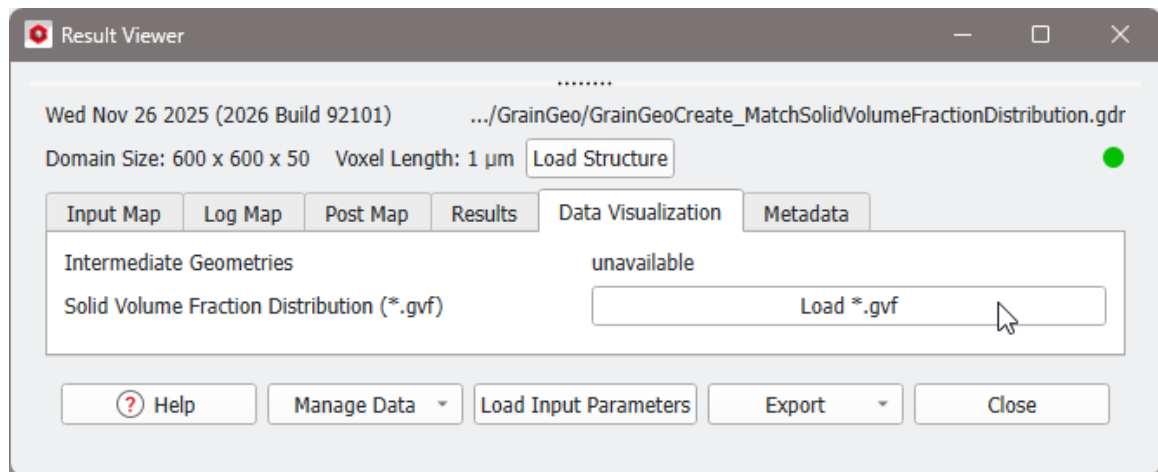
For the left structure, **Allow Object Overlap** is checked and no SVF distribution is matched.

The right structure was generated with the same parameters, except for matching the SVF distribution shown below.

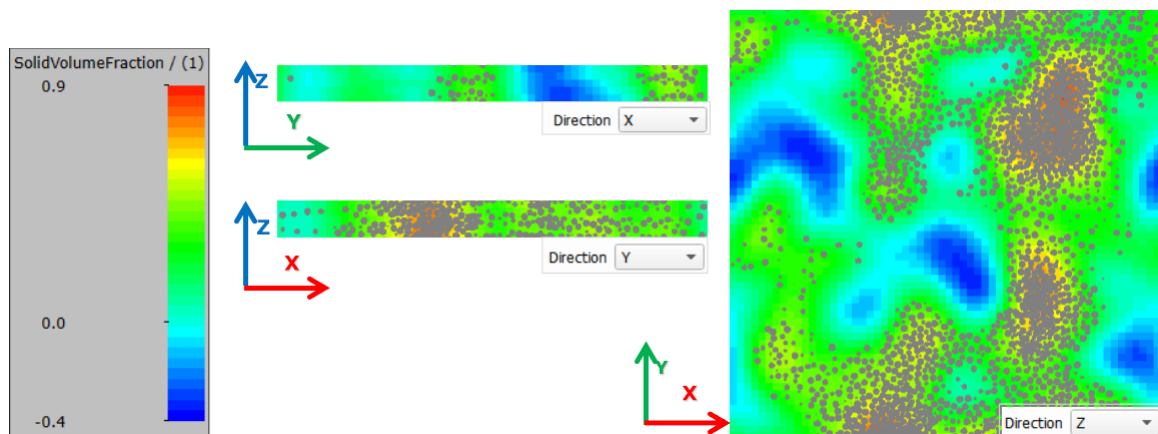


After generating a structure matching a SVF distribution a volume field describing the used Gaussian random field is saved in the result folder.

Select **File** → **Load Volume Field ...** from the menu bar to load it or choose the **Data Visualization** tab in the **Result Viewer** of the (*.gdr) result file and click **Load *.gvf**.



For the example from above, the resulting Gaussian random field is shown below in 2D view from all three directions.



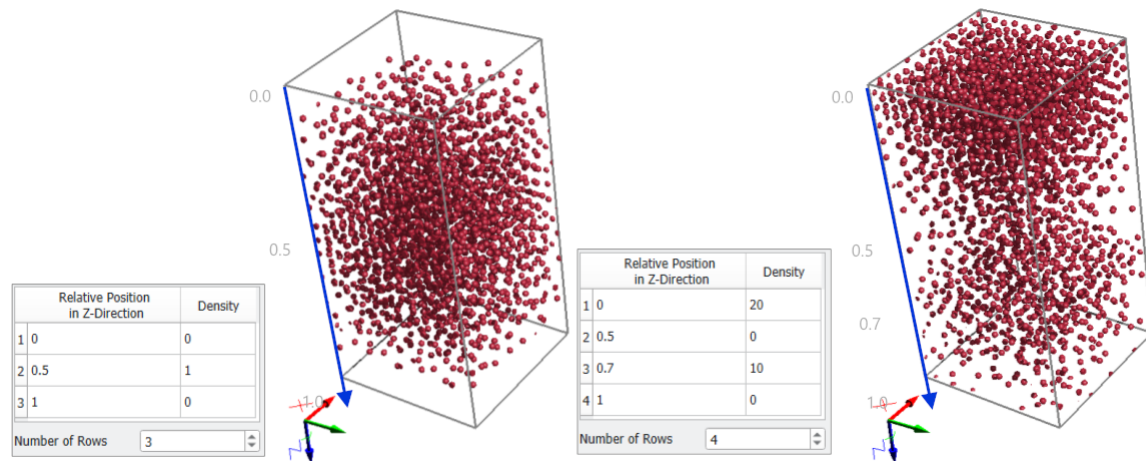
Viewed from X-direction a high correlation in Z-direction is observed, as the structure size in this direction equals the Correlation Length Z. In Y-direction a more inhomogeneous SVF distribution was generated, as the structure size in Y-direction (600 µm) is 12 times the Correlation Length Y (50 µm).

Viewed from Y-direction a similar observation can be obtained. Still, the distribution in Z-direction is very homogeneous, whereas it has low correlation in X-direction.

From Z-direction, the structure is very inhomogeneous, due to small Correlation Length values for X and Y (50 μm) compared to the structure size in these directions (600 μm).

Example - Gradient

In the following example observe how the objects are distributed corresponding to the given **Gradient**.

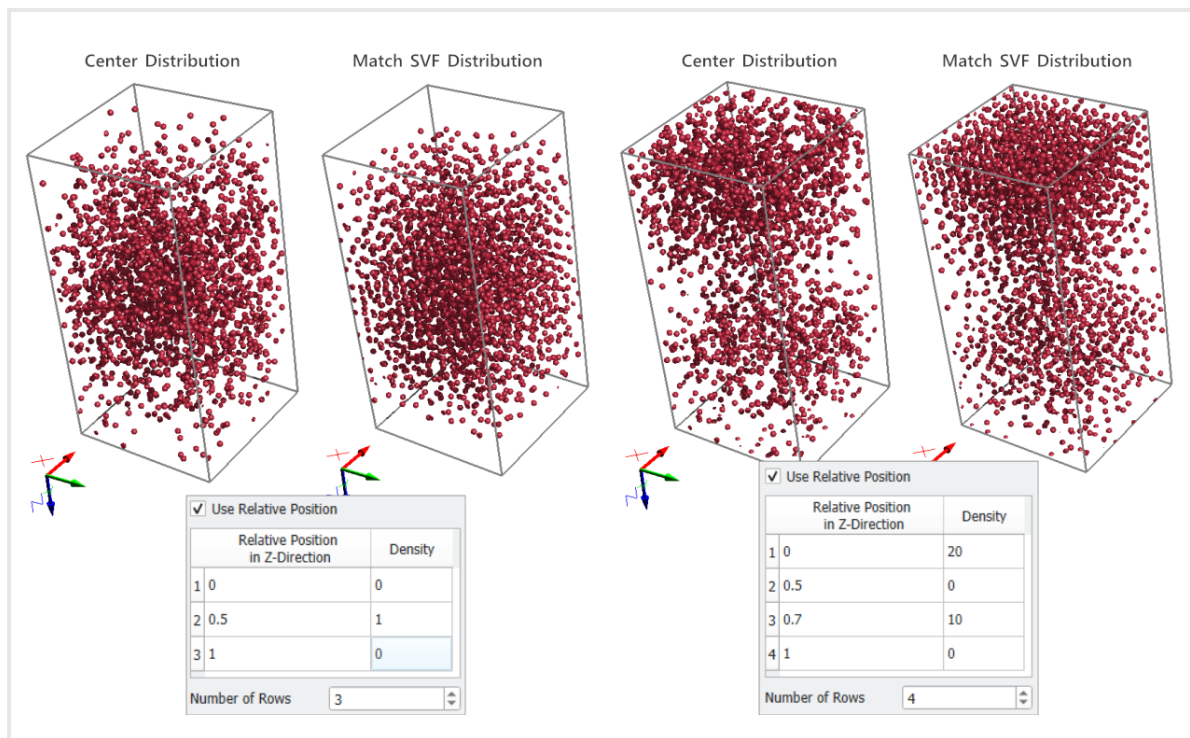


The objects in the first example on the left have the highest density in the center of the Z-axis. Towards both ends of the domain in Z-direction the objects become fewer. This corresponds to the density values 0 for the relative positions $Z=0$ and $Z=1$ and a density of 1 for the relative position $Z=0.5$.

The second example on the right shows a density distribution in Z-direction with 4 rows. A density of 20 for position $Z=0$ leads to twice as many objects near the top as objects in the lower third with a density value of 10 for position $Z=0.7$. Towards the center and the bottom, the objects become fewer for a density value of 0.

This feature is different from the [Density Distribution for Center](#)^[49], to be found in the [Object Options](#)^[48]. The Match SVF Distribution is a post-processing step, and the grains are moved till they match the given solid volume fraction distribution.

For the **Center Distribution**, the object centers are placed according to the given distribution which is much faster and does not change the orientation of the objects, but leads to a different solid volume fraction distribution and the distribution is not as smooth as with **Match SVF Distribution**.

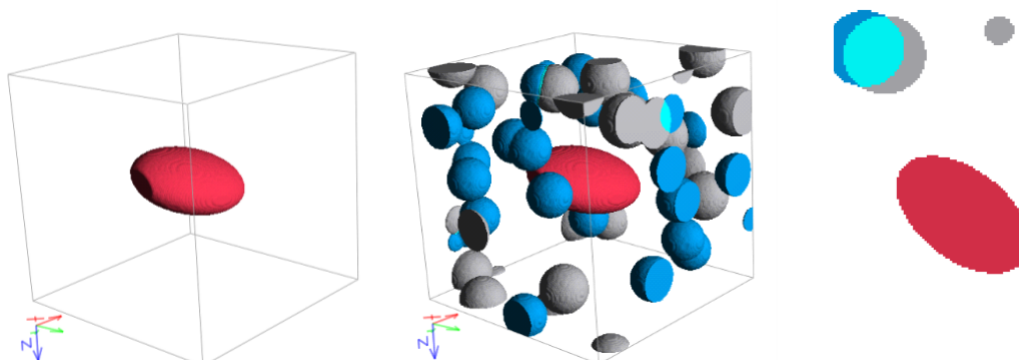


✓ Prohibit Overlap with Current Structure

If checking [Create in Current Domain](#)^[10], **Prohibit Overlap with Current Structure** appears instead of **Match SVF Distribution**. The objects in the newly generated structure can intersect with each other but not with those of the already existing structure.

Observe this effect in a structure with one (red) ellipsoid over which a new structure with blue and gray spheres is generated.

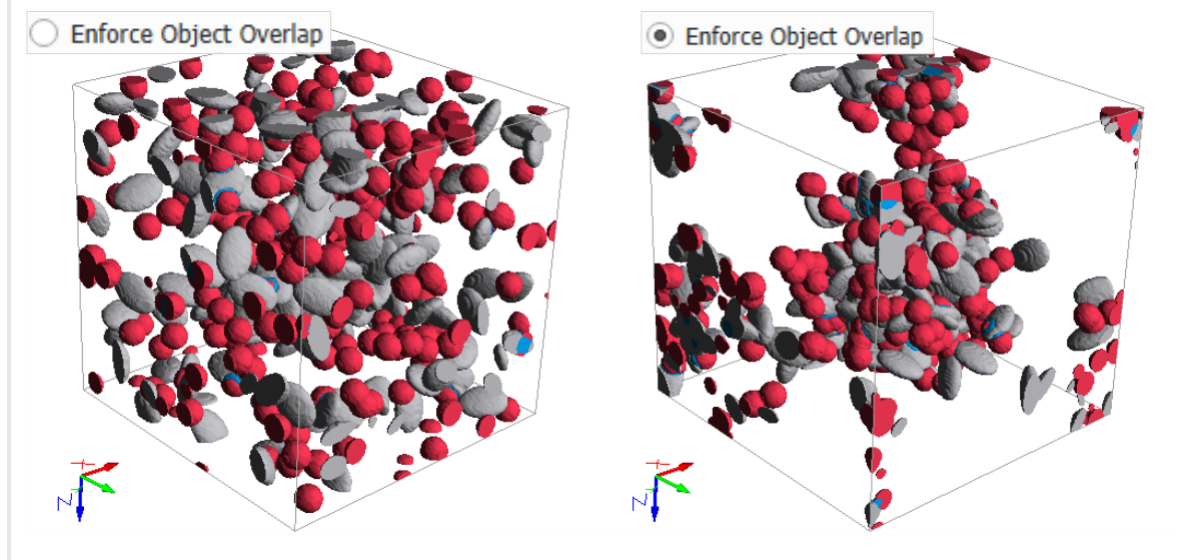
Whereas the blue and gray spheres overlap with each other, they do not overlap with the red ellipsoid.



✓ Enforce Object Overlap

The objects are required to join each other, forming one large, connected component. This effect is obvious when the structures [object volume percentage](#)^[31] is low (here

10%), i.e., the objects do not already form a connected component.



Stopping Criterion

The parameters in the **Stopping Criterion** panel define according to which criteria the object generation should be stopped. The available parameters are **Fixed Object Number**, **Object Volume Percentage / (%)**, **Grammage / (g/m²)**, **Density / (g/cm³)** or **Object Weight Percentage / (%)**. Additionally, when the **Maximal Run Time / (h)** is expired, the process is stopped even when the desired stopping criterion cannot be achieved.

Stopping Criterion

☐ Fixed Object Number
 ☒ Object Solid Volume Percentage / (%)
☐ Grammage / (g/m²)
 ☐ Density / (g/cm³)
 ☐ Object Weight Percentage / (%)

Maximum Run Time / (h)

When **Grammage**, **Density** or **Object Weight Percentage** are chosen as stopping criterion, the temperature must be set as additional parameter. The density of the constituent materials will be set with respect to the chosen temperature based on the Material Database.

When choosing **Fixed Object Number** or **Object Volume Percentage**, the temperature parameter is not available.

If checking **Create in Current** and [Keep Current Objects / Structure](#)^[10] only the criteria [Fixed Object Number](#)^[31], [Add Object Solid Volume Percentage](#)^[31] and [Maximum Run Time](#)^[33] are available.

Stopping Criterion

☐ Fixed Object Number

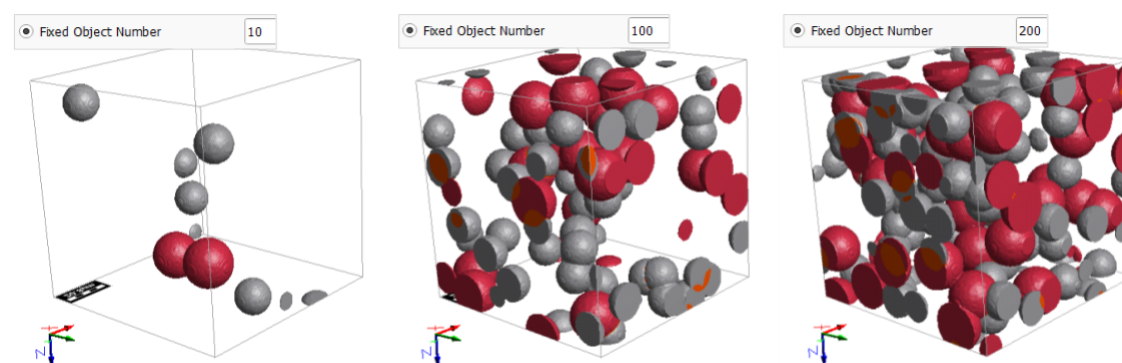
☒ Add Object Solid Volume Percentage / (%)

Maximum Run Time / (h)

✓ Fixed Object Number

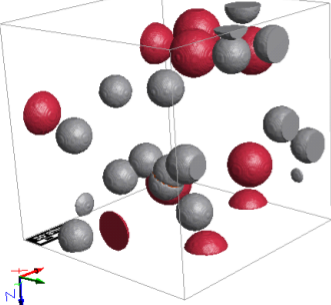
When **Fixed Object Number** is chosen as stopping criterion, GrainGeo places the given number of objects in the structure and then the generation stops.

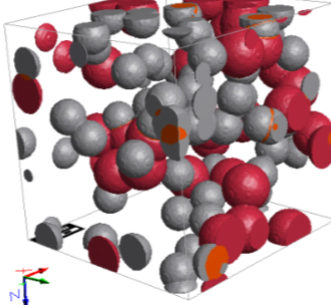
Observe the effect of setting a fixed number of objects (10, 100, or 200) as stopping criterion, for the generation of a structure with two types of spheres. All other parameters are left untouched.

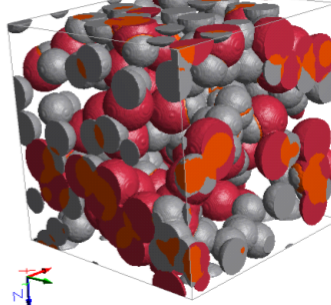


✓ (Add) Object Solid Volume Percentage

Object Solid Volume Percentage determines the fraction of the total volume in percent that the structure should have. Accepted values range from 0% to 100%. For example, a structure with an **Object Volume Percentage** of 40% consists of 40% spheres and 60% void space. Porosity is then defined as $(1 - \text{Object Volume Percentage} / 100)$. Observe the difference in a structure when varying the volume percentage from 5%, to 20% and finally to 40%, while all other parameters are left unchanged.

☒ Object Volume Percentage / (%) 5
 

☒ Object Volume Percentage / (%) 20
 

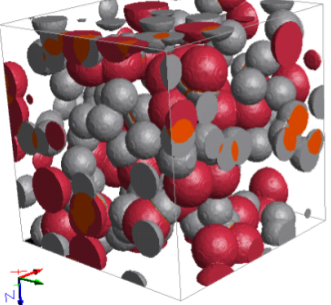
☒ Object Volume Percentage / (%) 40
 

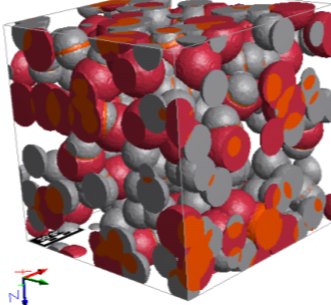
If **Create in Current** and [Keep Current Objects / Structure](#)¹⁰ are selected, the parameter changes to **Add Object Solid Volume Percentage**. Only the added solid volume percentage counts, i.e., only the objects not overlapping with the current structure are considered for the stopping criterion. Therefore, it is important to prevent overlap, for example by checking [Prohibit Overlap with Current Structure](#)²⁹.

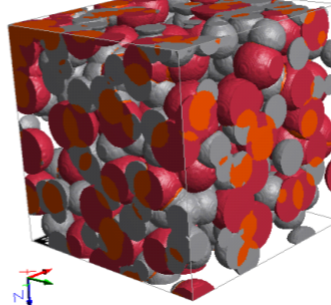
✓ Grammage

The **Grammage / (g/m²)** determines the mass per unit area (in the XY-Plane) of the resulting structure. When **Grammage** is chosen as stopping criterion, the [density](#)³⁸ (g/cm³) of the object material(s) must be defined for each object type and chosen material in the object panels under the **Object Options** tab and the [temperature](#)³⁴ must be set in the **Create Options** dialog, below the **Stopping Criterion** panel.

Observe the effect of increasing the **Grammage** from 60 g/m² to 120 g/m², whereas all other parameters are left unchanged.

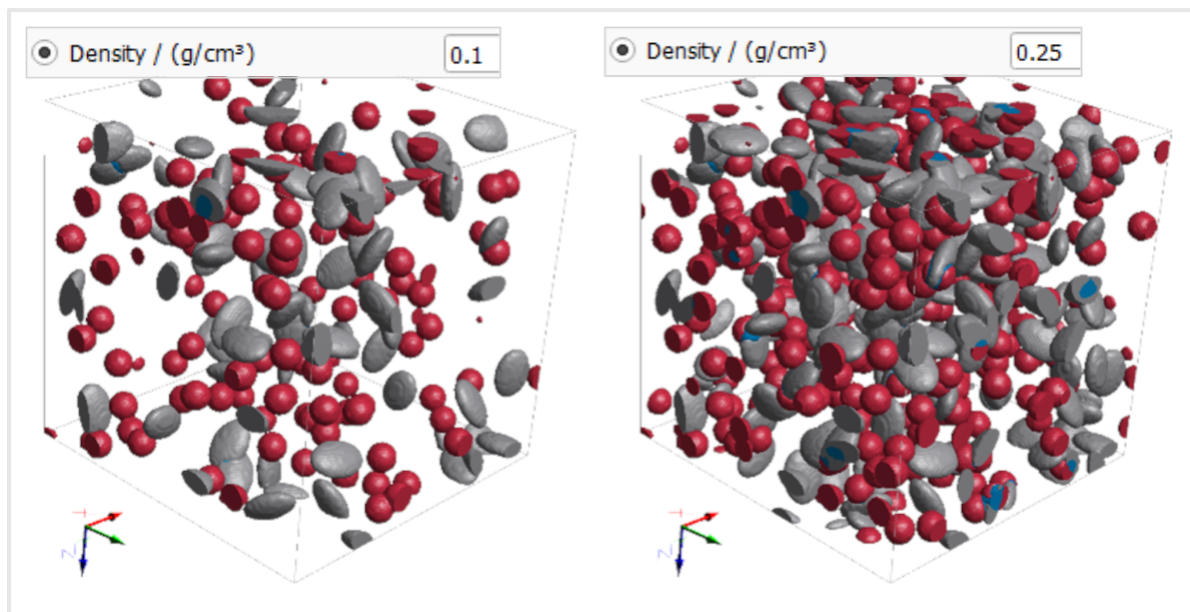
☒ Grammage / (g/m²) 60
 

☒ Grammage / (g/m²) 90
 

☒ Grammage / (g/m²) 120
 

✓ Density

The **Density / (g/cm³)** of the resulting structure depends on the densities of the constituent materials. In the following simple example, the **Matrix Density** is 0 (for vacuum), and the two grain types have the densities 3.1 g/cm³ and 1.0 g/cm³. The **Density** of the structure is set to 0.10 g/cm³ and to 0.25 g/cm³. It cannot be set smaller than the lowest occurring density (here 0 g/cm³) or larger than the highest occurring density (here 3.1 g/cm³).



✓ Object Weight Percentage

The **Object Weight Percentage** determines the weight of the created object in relation to the weight of the whole structure (including the matrix material). The calculation is only possible when the density of the **Pore / Matrix Material** is greater than zero. Otherwise, an error message will appear.

✓ Maximum Run Time

The **Maximum Run Time (h)** becomes important when generating complex structures with elevated solid volume fraction. When **Prohibit Object Overlap** has been checked, the required number of objects in the structure may become unattainable. In that case, the structure generation is stopped after the time entered in **Maximum Run Time** has passed and the achieved structure is considered as the result. The analysis of the GDR result file shows any disparity between the achieved result values and the desired ones.

✓ How to know if the stopping criterion is achieved?

The relationship of the variables **Fixed Object Number**, **Object Solid Volume Percentage**, **Grammage** and **Weight Percentage** can be observed in the Result Viewer of the result file, under the **Results - Report** subtab.

In this example, a **Count** (Fixed Object Number) of 52 corresponds to a **Volume** (Object Volume Percentage) of 10.35%, a **Grammage** of 50.46 g/m² and a **Density** of 0.2523 g/cm³.

Input Map	Log Map	Post Map	Results	Data Visualization	Metadata
Report	Plots	Map			
Absolute object distribution:					
	Count	Volume / (%)	Grammage / (g/m ²)	Density / (g/cm ³)	Weight / (%)
Total	realized: 52 target: --- error: ---	realized: 10.35 target: --- error: ---	realized: 50.46 target: --- error: ---	realized: 0.2523 target: 0.2500 error: 0.0023	realized: 0.00 target: --- error: ---
Object type 1	realized: 32 target: --- error: ---	realized: 7.09 target: --- error: ---	realized: 43.94 target: --- error: ---	realized: 0.2197 target: --- error: ---	realized: 0.00 target: --- error: ---
Object type 2	realized: 20 target: --- error: ---	realized: 3.26 target: --- error: ---	realized: 6.53 target: --- error: ---	realized: 0.0326 target: --- error: ---	realized: 0.00 target: --- error: ---
Stopping criterion error: 0.93 %					

General Options

Define the general parameters temperature, random seed and parallelization.

Random Seed	42	Temperature	20	°C
Parallelization	8 Threads (Automatic Maximum) Edit...			

Temperature

When **Grammage** (or **Density** or **Object Weight Percentage**) is chosen as **Stopping Criterion**, a temperature can be entered. The temperature is considered for materials with temperature dependent density.

Choose the temperature in Kelvin, Celsius, or Fahrenheit.

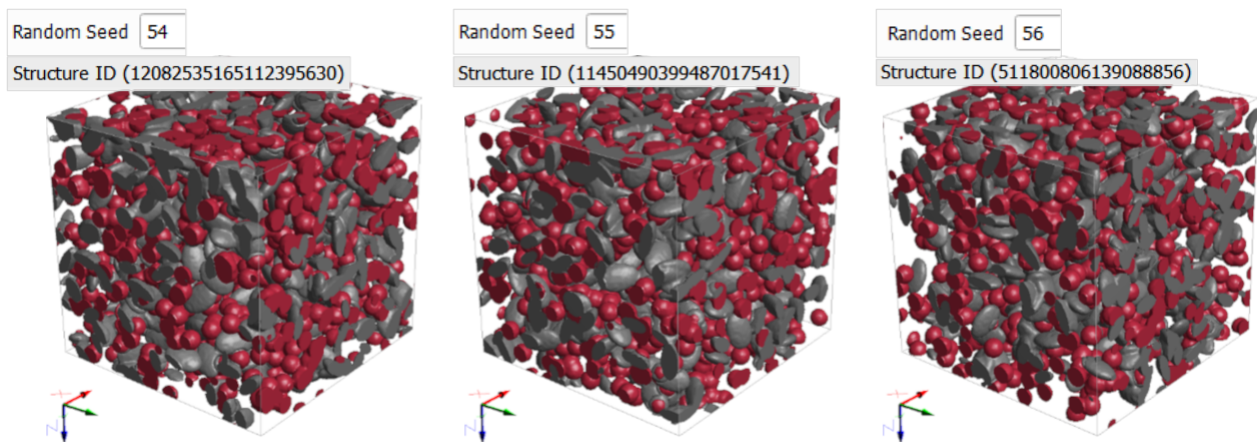
Temperature	20	°C
		K °C °F

Random Seed

Random Seed initializes the random number generator behind the structure generator. Changing its value produces different sequences of random numbers and hence, different realizations of the specified structure. If all settings are equal, generating with the same **Random Seed** value produces exactly the same structure, as shown by the **Structure ID** number in the Status section. The **Random Seed** is a non-negative integer number, it increases automatically with every generation run.

Varying the **Random Seed** allows generating different samples of the same structure for a

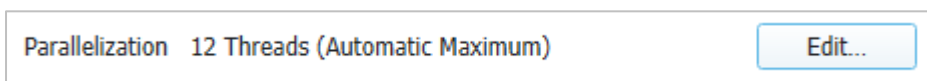
series of experiments. In the following examples, all parameters are unchanged while the random seed is modified with every generation run.



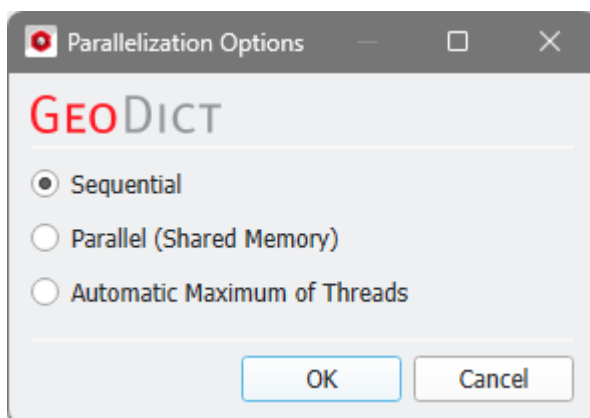
Parallelization

Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

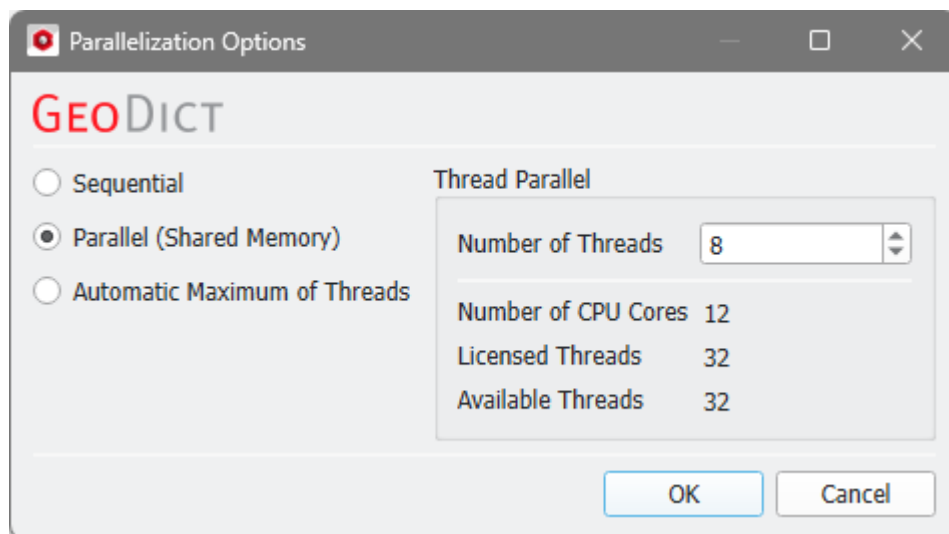
The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.



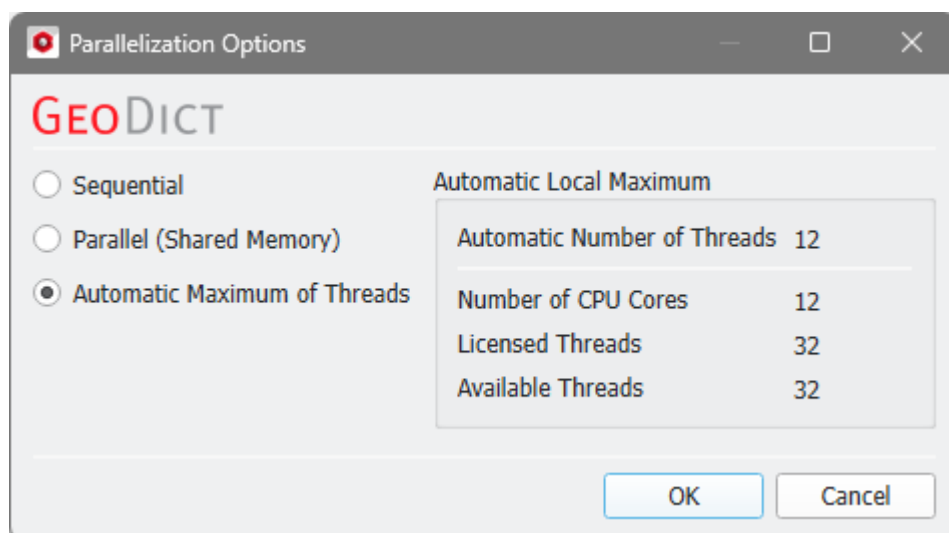
Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.

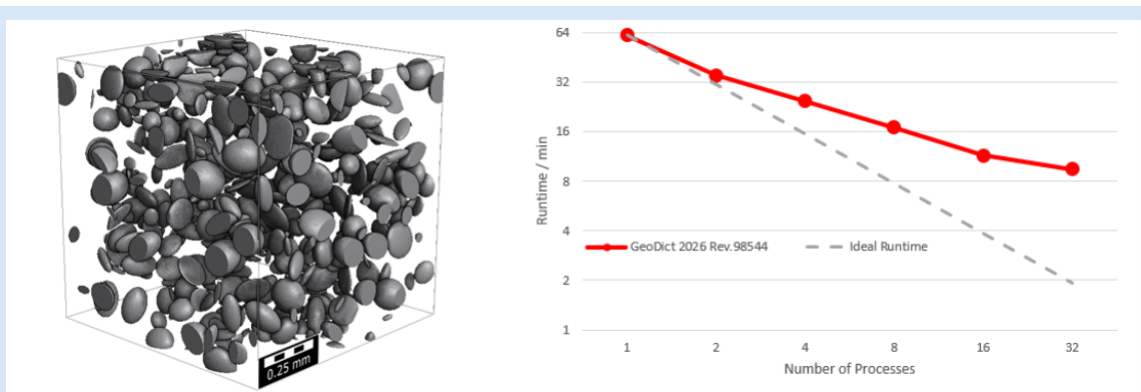


The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.



Parallelization Benchmark Results

As an example for the parallelization, the complete overlap in a granular structure is removed with different number of processes. The computation is run on a server with 2 x Intel E5-2697A v4 processors with 16 cores each, running with a maximum of 3.60 GHz, and 1 TB RAM. The large grain structure has size 1000^3 voxels and 10 % object volume percentage. [Remove Overlap](#)¹⁷ is used with stopping criterion 0% remaining overlap.



The memory usage was 2.1 GB. As can be observed, the parallelization reduces the runtime significantly. With four processes, the runtime is already reduced by over 60%.

Object Options

In the **Object Options** tab you can define the geometrical properties of your object types. Add up to eight different object types to your structure.

The object type parameters for the generation of granular structures are organized and listed in three columns. In the left one define the [Object Type](#)^[38] together with its percentage and material, the center column shows a [scheme](#)^[41] of the chosen object type's parameters and in the right one you can edit the [object parameters](#)^[48]. In the bottom, find the options to choose additional object types and how the object percentage should be given.

The parameters are organized in the following groups:

- [Object Type and Percentage](#)^[38]
Add objects of different types, define their percentages in the structure and their materials.
- [Available Object Types](#)^[41]

The parameters are organized in the following groups:

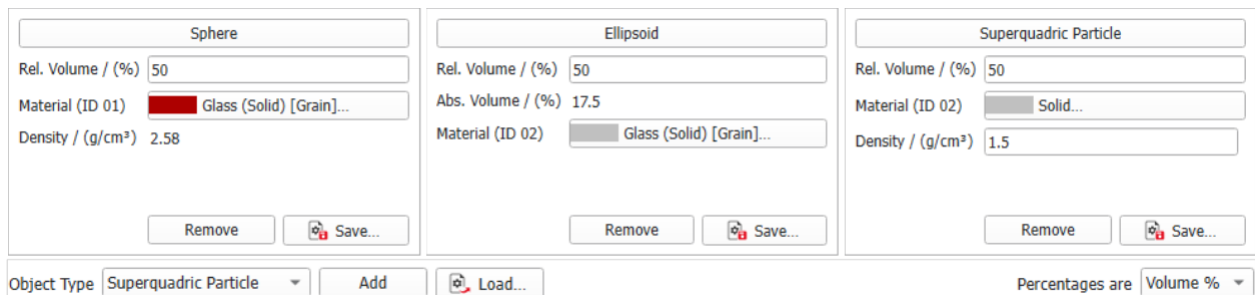
An overview of all available object types and their parameters.

- [Object Parameters](#) 48

Define the different parameters for the object types.

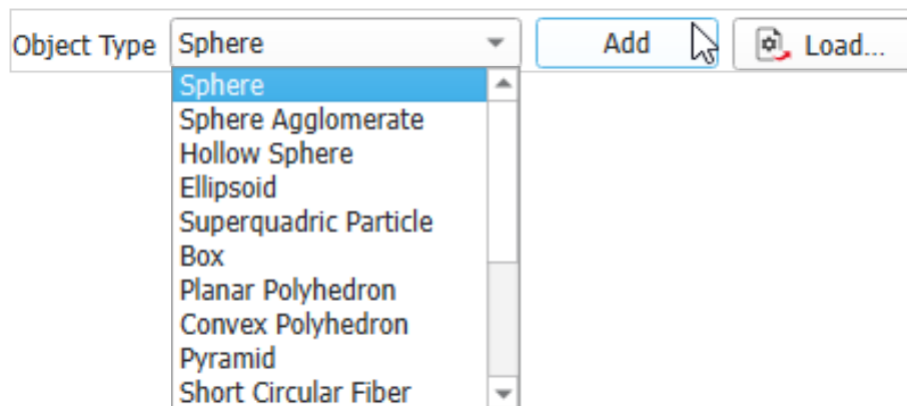
Object Type and Percentage

For all objects, the left column of the panel contains the name of the object type, the object percentage in the structure, and the material.



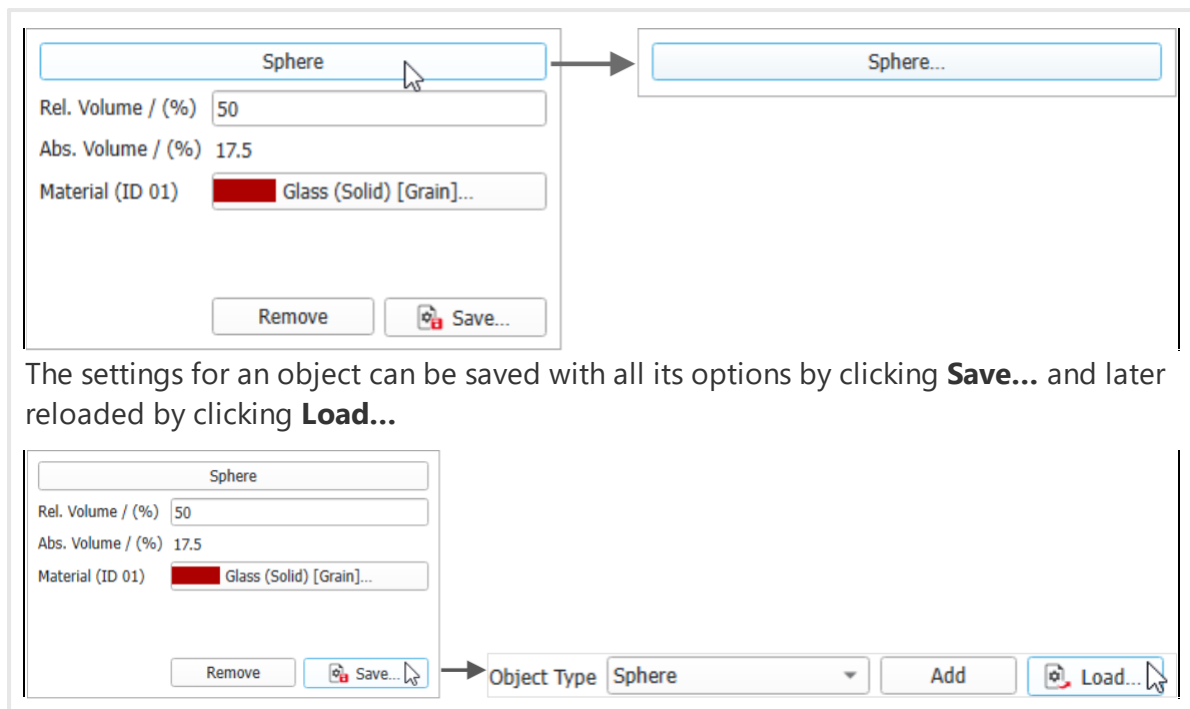
✓ Adding and removing object types

Sphere and **Ellipsoid** are the two default **Object Types**. At the bottom left of the dialog box, clicking **Add** inserts other object types chosen from the **Object Type** pull-down menu (Sphere Agglomerate, Superquadric Particle, Polyhedrons, etc.).



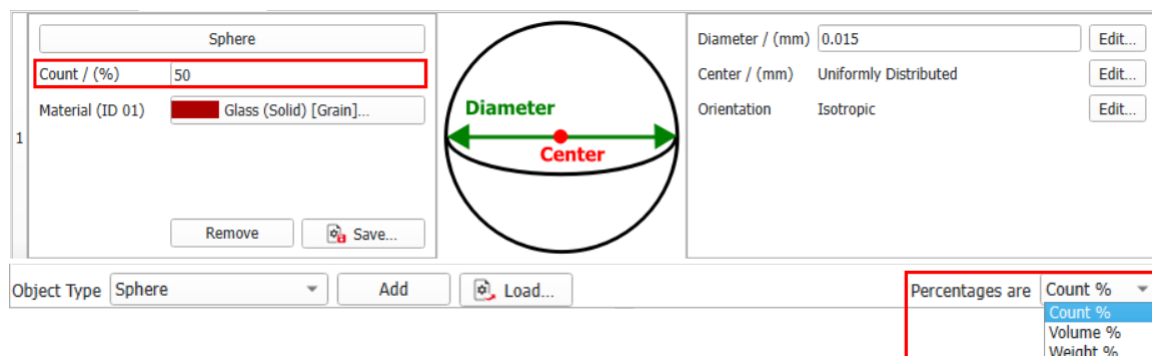
Unwanted object types can be discarded when clicking **Remove** in the left column for that object type.

Clicking on the object type name minimizes the object panel, and clicking on it again when minimized, expands it. A scroll bar at the right allows to navigate up and down in the list of chosen object types.



✓ Percentage

The percentage of a certain object type can be specified as **Count %**, **Volume %**, or **Weight %**, as selected from the pull-down menu at the bottom right of the dialog box.



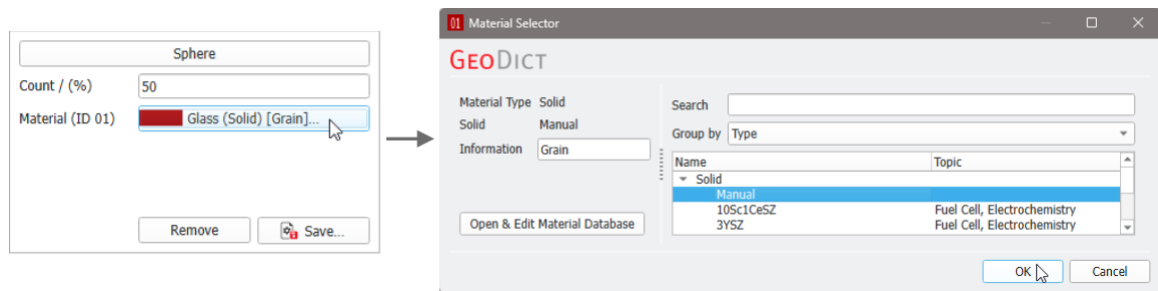
✓ Rel. Volume and Abs. Volume

If [Volume](#)^[39] is selected for **Percentages**, enter the **Relative Volume**. If [Fixed Object Number](#)^[31] or [\(Add\) Object Solid Volume Percentage](#)^[31] is chosen as **Stopping Criterion**, the **Absolute Volume** is automatically computed and given below.

The image shows two side-by-side screenshots of the GrainGeo interface for configuring a 'Sphere' object. Both panels have a 'Sphere' title bar. The left panel is configured with 'Grammage / (g/m²)' set to 40. It shows 'Rel. Volume / (%)' as 85, 'Material (ID 01)' as a red square labeled 'Grain (Solid)...', and 'Density / (g/cm³)' as 2.58. The right panel is configured with 'Fixed Object Number' set to 1000. It shows 'Rel. Volume / (%)' as 85, 'Abs. Volume / (%)' as 22.037037, 'Material (ID 01)' as a red square labeled 'Grain (Solid)...', and 'Density / (g/cm³)' as 2.58. Both panels have 'Remove' and 'Save...' buttons at the bottom.

✓ Material

Material designates the constituent material assigned to the object type used in the structure. Clicking on the material gives access to selecting the desired material from the GeoDict Material Database. When none of the materials available in the database fit the preferred specifications, **Manual** should be chosen.



To match realistic material colors for visualization in a certain application, or to distinguish the constituting materials more easily, the colors of the materials can be changed through **Settings** → **Color & Visibility Settings** in the Menu bar, or by unfolding the **Color & Visibility** sidebar next to the GeoDict visualization area as described in the Visualization User Guide.

✓ Density and Weight

When **Grammage** is chosen as **Stopping Criterion** or **Weight %** is chosen for **Percentages**, the material **Density / (g/cm³)** of that object type appears. For materials included in the GeoDict Material Database, the density is automatically entered. For other materials (manual, user-defined), the density must be entered manually.

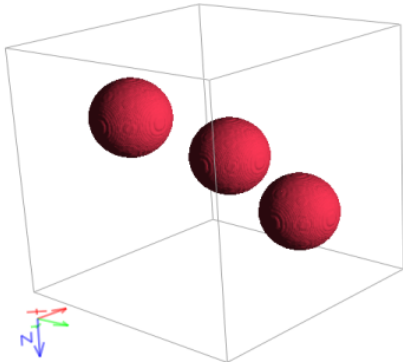
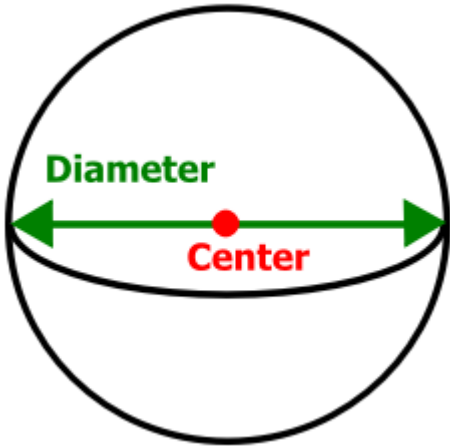
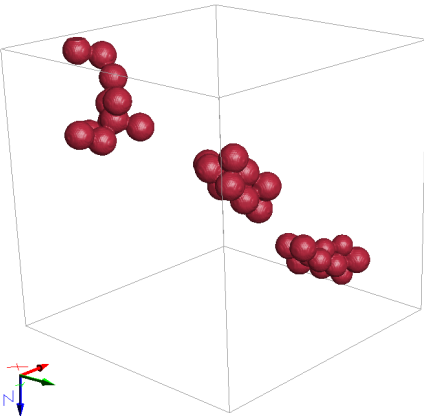
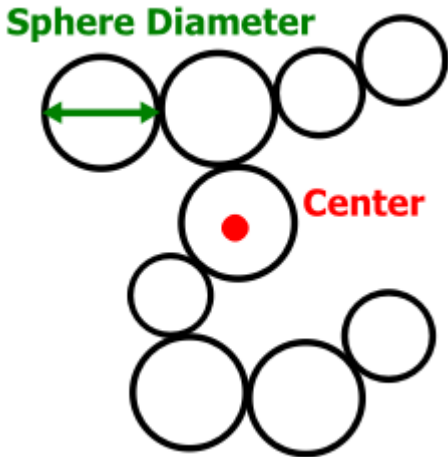
The object **Density**, given in g/cm³, is an intrinsic property of the selected object type, affecting the final weight of the granular structure. The density of objects is intimately related to the **Grammage** / (g/m²) of the created granular structure. When denser objects are used, and the grammage is unchanged, less objects of this type appear in the object structure.

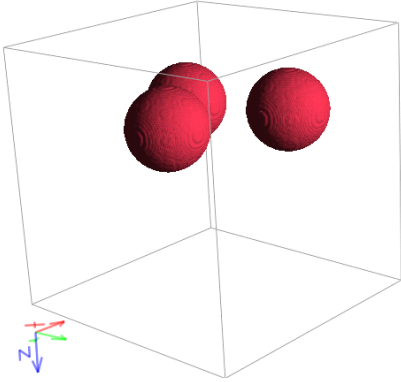
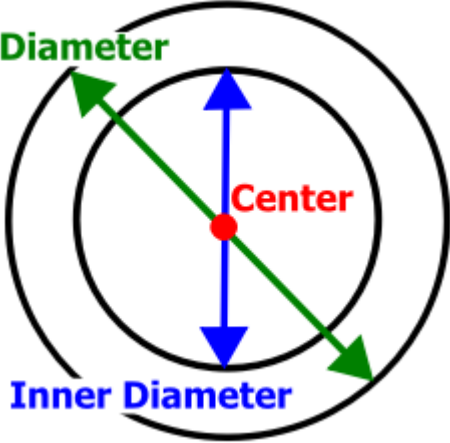
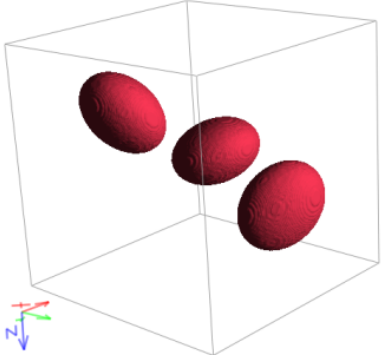
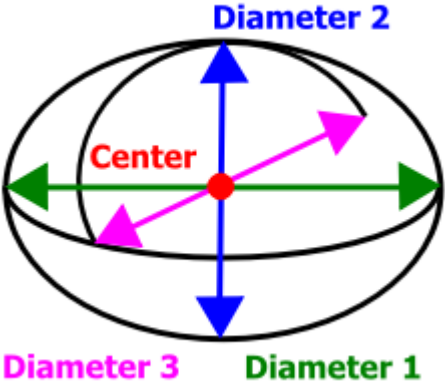
Vice versa, when the same object type is used but an increase in grammage should be achieved, the structure must contain more objects.

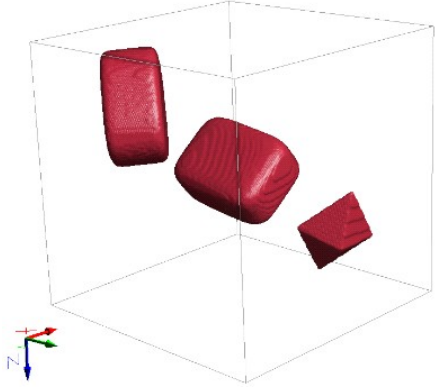
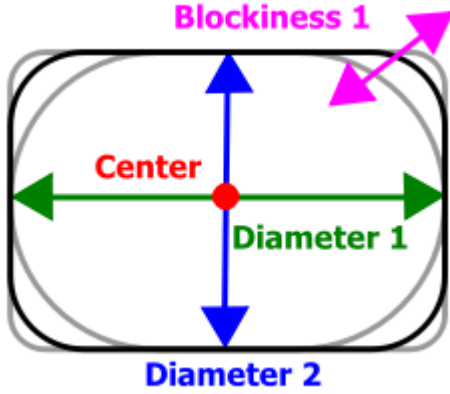
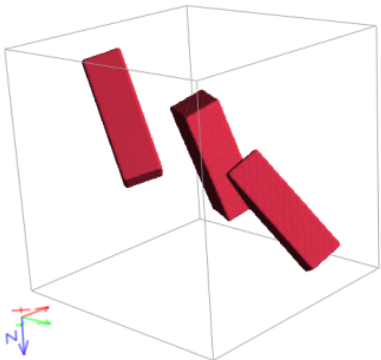
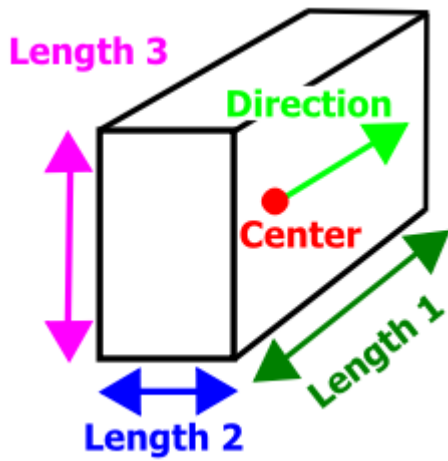
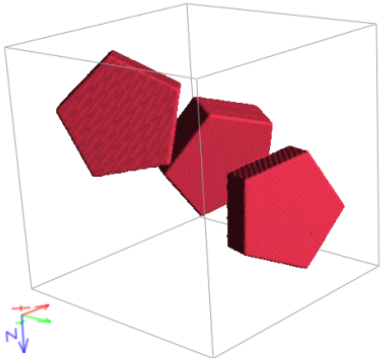
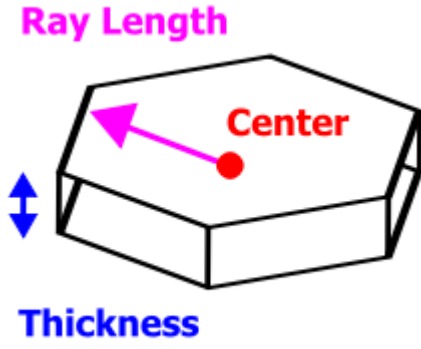
Available Object Types

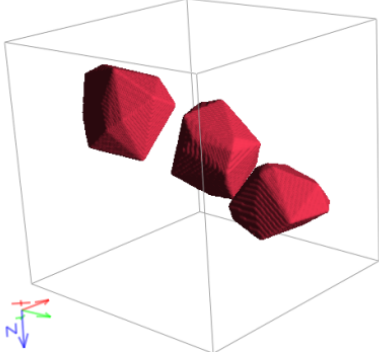
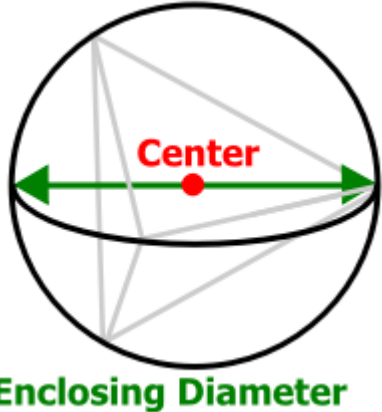
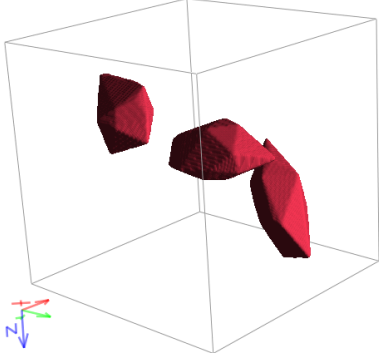
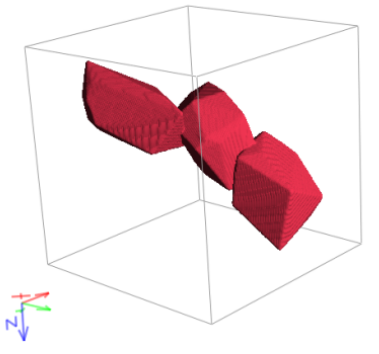
The **Object Type** is selected from the pull-down menu at the lower left under the **Object Options** tab. After selecting, click **Add** to include this object type. If the wrong object type has been added, discard it by clicking **Remove**.

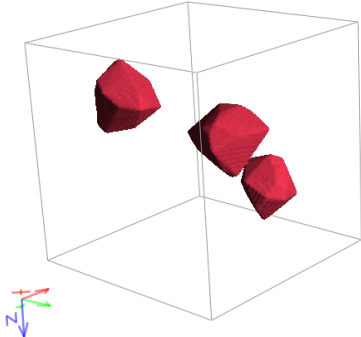
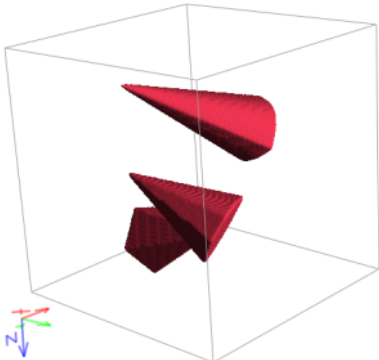
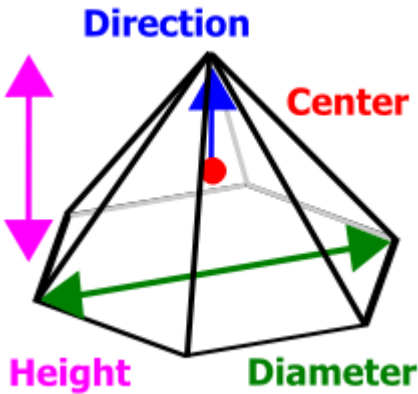
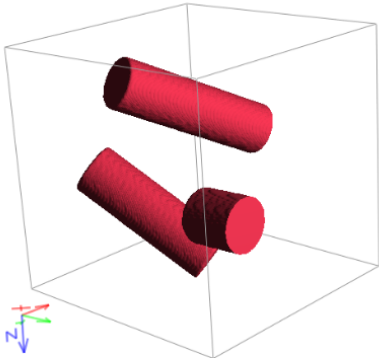
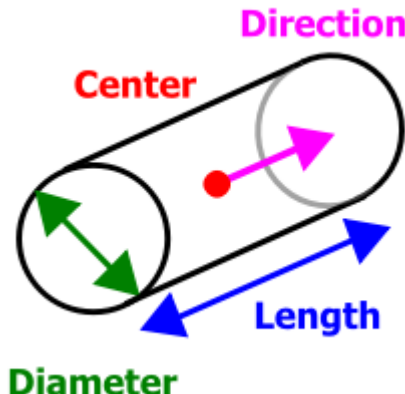
The following table summarizes the object types that can be used with **GrainGeo Create** and **Pile** commands: **Sphere**, **Sphere Agglomerate**, **Hollow Sphere**, **Ellipsoid**, **Superquadric Particle**, **Box**, **Planar Polyhedron**, **Convex Polyhedron**, **Pyramid**, **Short Fibers** (**Circular**, **Hollow**, **Rosetta**, **Elliptical**, **Cellulose**, **Rectangular**, and **Angular**), and their combinations (**Combined Objects**).

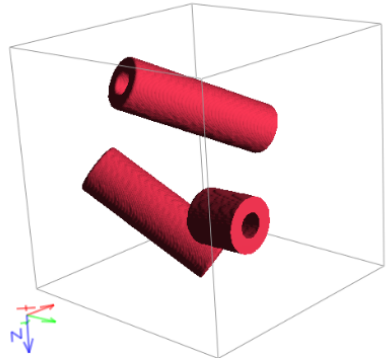
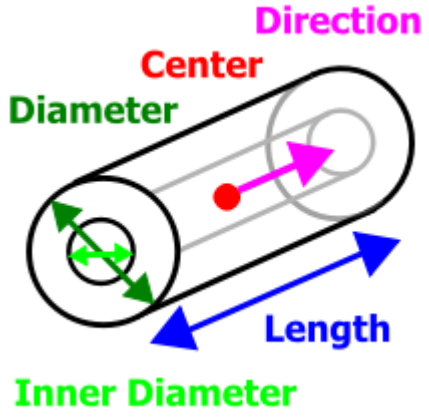
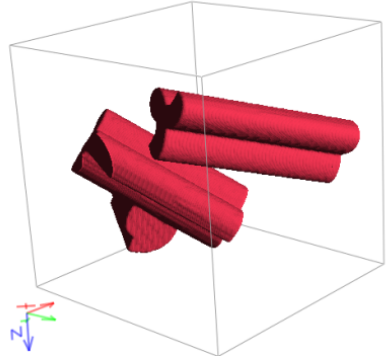
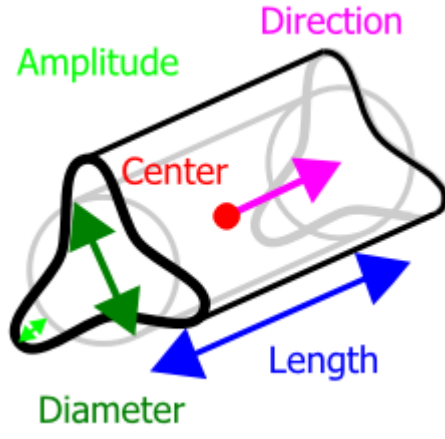
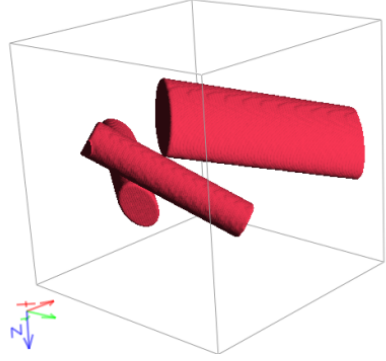
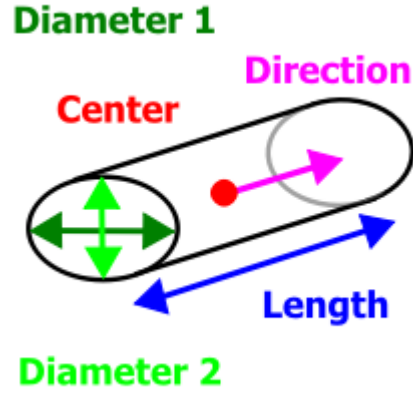
Object Type	Example	Defining parameters
Sphere		
Sphere Agglomerate		

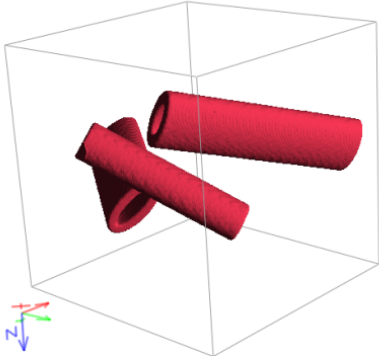
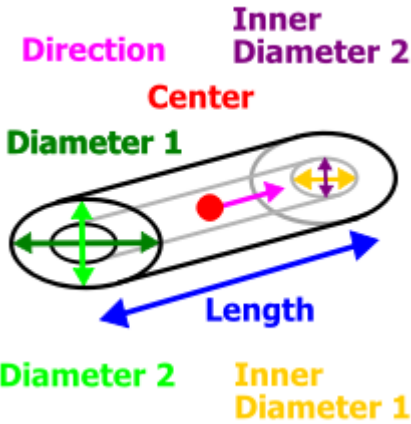
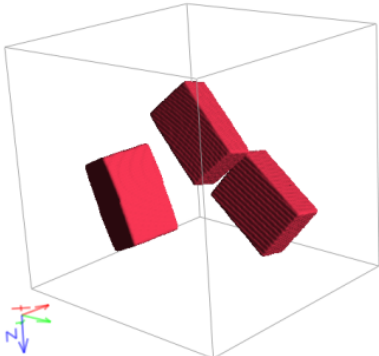
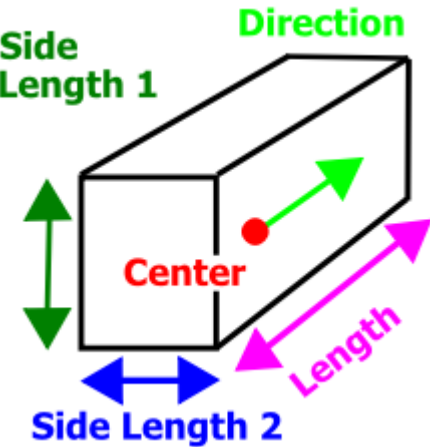
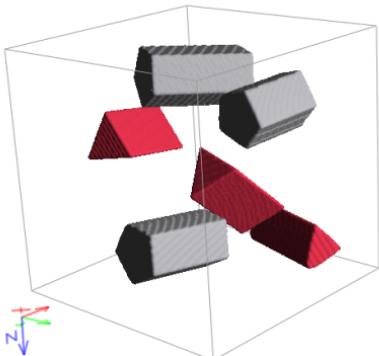
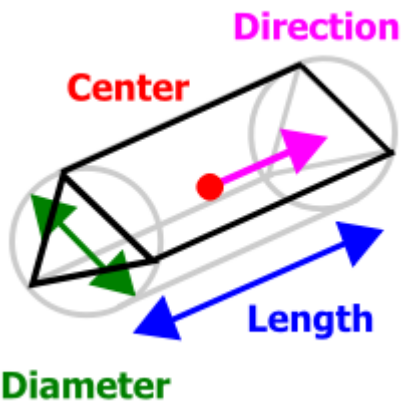
Object Type	Example	Defining parameters
Hollow Sphere	 	
Ellipsoid	 	

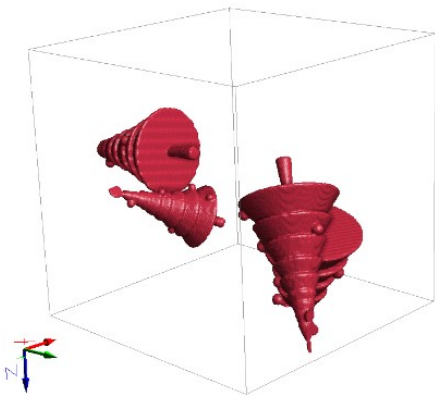
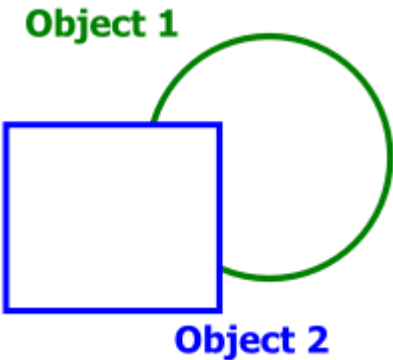
Object Type	Example	Defining parameters
Superquadric Particle		
Box		
Planar Polyhedron		

Object Type	Example	Defining parameters
Convex Polyhedron Enclosing Object: Sphere		
Convex Polyhedron Enclosing Object: Ellipsoid		
Convex Polyhedron Enclosing Object: Box		

Object Type	Example	Defining parameters
Convex Polyhedron Enclosing Object: Pyramid		
Pyramid		
Short Circular Fiber		

Object Type	Example	Defining parameters
Short Hollow Fiber		
Short Rosetta Fiber		
Short Elliptical Fiber		

Object Type	Example	Defining parameters
Short Cellulose Fiber		
Short Rectangular Fiber		
Short Angular Fiber Red: 3 edges Gray: 5 edges		

Object Type	Example	Defining parameters
Combined Object		

Object Parameters

The right column of the **Object Type** panel contains the parameters controlling the geometrical and physical properties of each object type of the granular structure.

Some object parameters can only be set for specific object types, e.g., **Number of Edges** and **Ray Length** are only applicable for planar polyhedrons. Other parameters are common to several objects, such as, e.g., **Diameter**, **Center**, **Length**, or **Orientation**.

Size Mode Independent Diameter 1 / (mm) 0.02 Edit... Diameter 2 / (mm) 0.02 Edit... Diameter 3 / (mm) 0.01 Edit... Center / (mm) Uniformly Distributed Edit... Orientation Isotropic Edit...	Size Mode Independent Diameter 1 / (mm) 0.03 Edit... Diameter 2 / (mm) 0.015 Edit... Diameter 3 / (mm) 0.015 Edit... Blockiness 1 5 Blockiness 2 2 Center / (mm) Uniformly Distributed Edit... Orientation Isotropic Edit...
General Enclosing Object Enclosing Object Sphere Enclosing Object Diameter / (mm) 0.01 Edit... Enclosing Object Orientation Isotropic Edit...	Scaling Factor / (1) 1 Edit... Center / (mm) Uniformly Distributed Edit... Orientation Isotropic Edit... Combined Object (*.gad) Browse...

Learn about the object parameters:

- [Center](#) 

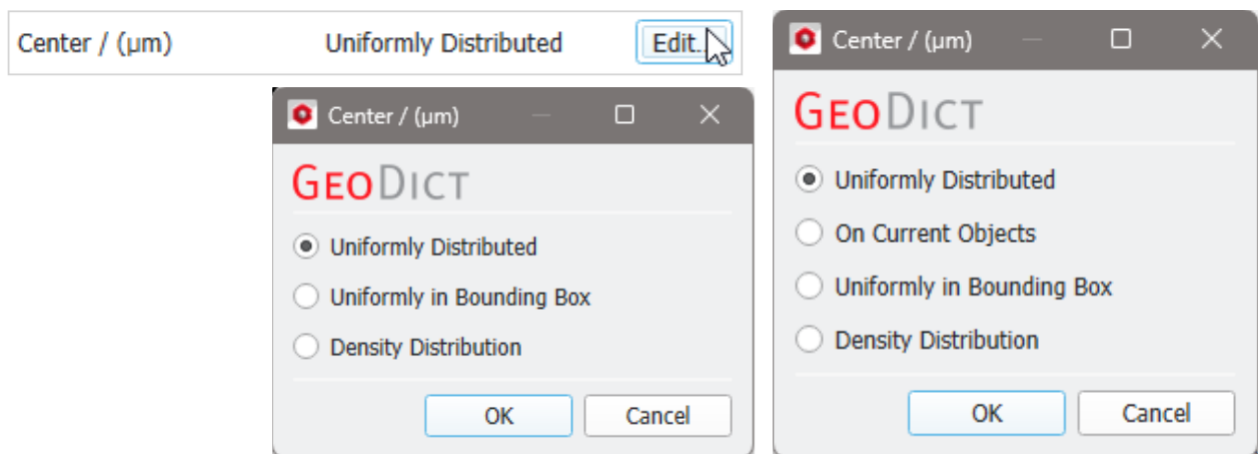
Define how the object's centers should be distributed throughout the domain.

Learn about the object parameters:

- [Shape Parameters](#)⁵⁴
Define the object's shapes through various parameters.
- [Orientation](#)⁶⁵
Define how the objects should be oriented in the domain.
- [Distribution](#)⁸¹
Define a constant value or a distribution for different object parameters.

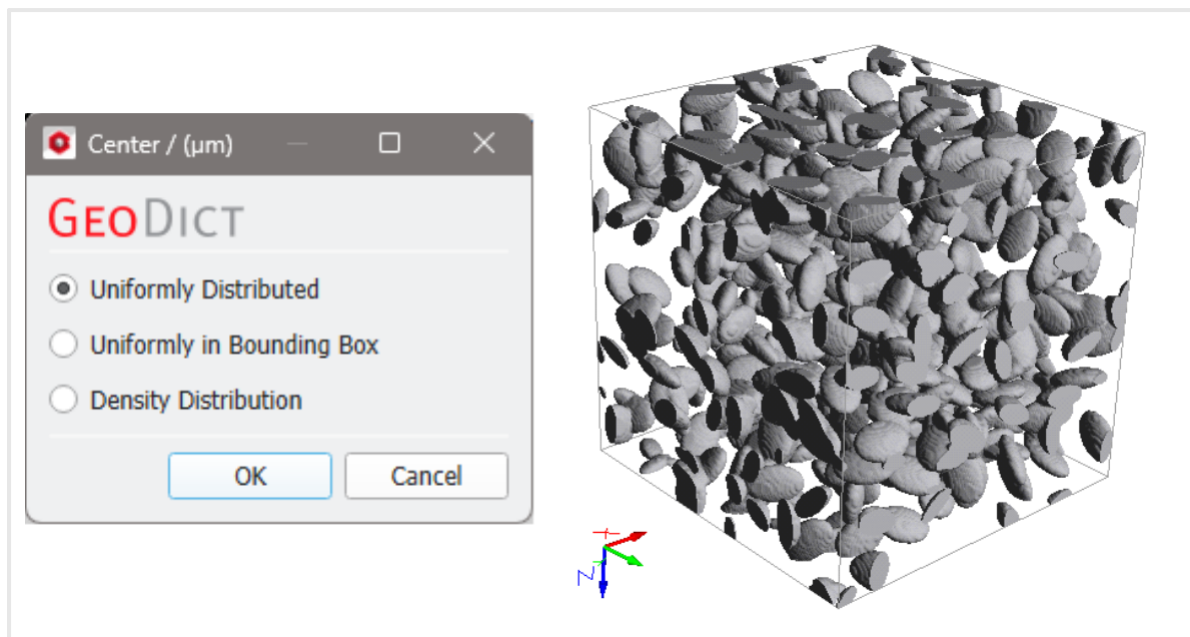
Center

Define how the object's centers should be distributed throughout the domain. The **Center** can be set to distribute **Uniformly, On Current Objects** (when [Create in Current Domain](#)¹⁰ is checked under **Create Options**), **Uniformly in Box**, or to follow a **Density Distribution**. The position of short and curved objects in a generated structure can be controlled by adjusting the position of their **Center** through the **Edit...** button.



✓ Uniformly Distributed

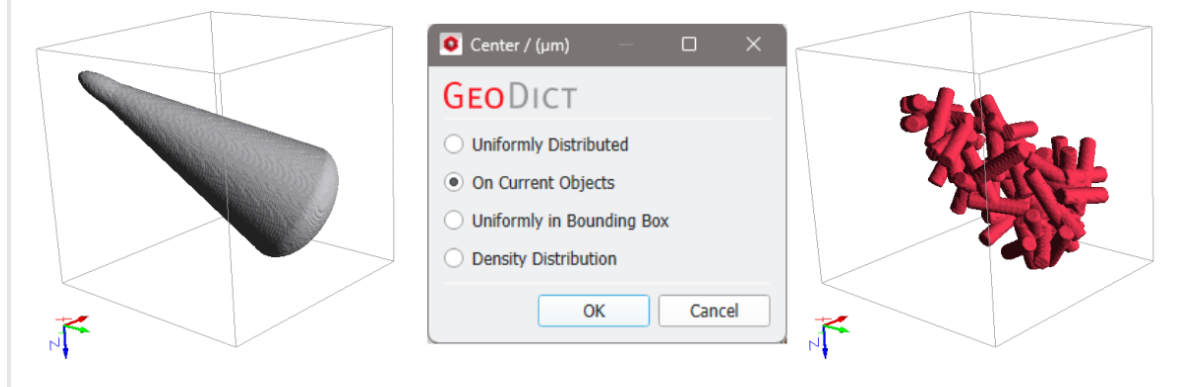
When **Uniformly Distributed** is checked, the random object center values are uniformly distributed across the whole structure. The uniform distribution of the centers is clearly observed in the example below.



✓ On Current Objects

After having selected [Create in Current Domain](#) under the **Create Options** tab, the centers can also be positioned **On Current Objects**.

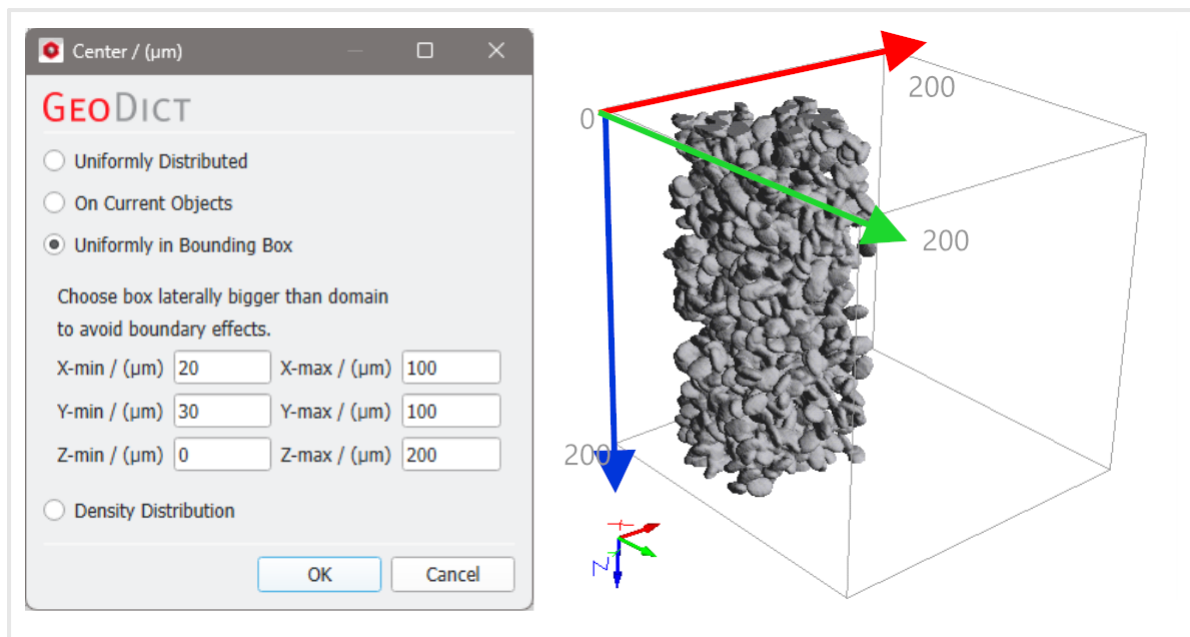
Observe the placement of short circular objects' centers on a conical structure generated with GadGeo, when **On Current Objects** is chosen in the **Center** dialog.



✓ Uniformly in Box

With **Uniformly in Box** checked, the values entered for X-min, X-max, Y-min, Y-max, Z-min, and Z-max limit the distribution of the center position to certain areas. These directionally limiting values define a volume in which the structure occurs.

For a 200 x 200 x 200 μm structure, the values in the **Center** dialog limit an area in which the respective ellipsoid center is positioned between 20 μm and 100 μm in the X-direction, 30 μm and 100 μm in the Y-direction, and between the origin (0 μm) and the end of the domain in the Z-direction.



✓ Density Distribution

The **Density Distribution** table describes the [probability](#) of a random center taking certain position values in Z-direction.

Note! The center density distribution should be defined with monotonously increasing Z-values. If Z is non-monotonic or monotonously decreasing, the values are ordered as needed after closing the dialog.

Relative Position in Z-Direction		Density
1	0	0
2	0.5	2
3	0.2	0
4	1	10
Number of Rows		4

Relative Position in Z-Direction		Density
1	0	0
2	0.2	0
3	0.5	2
4	1	10
Number of Rows		4

When checking **Use Relative Position** in the density distribution table, the left column values from 0 to 1 correspond to locations in the structure. In the Z-direction, the value 0 is at the origin and the value 1 is at end of the domain.

The right column assigns relative density values at these locations. The value 20 means that there are ten times more objects in $Z = 1$ than in $Z = 0.1$, with a density value of 2. The object density increases and decreases linearly between the given locations in the Z-direction.

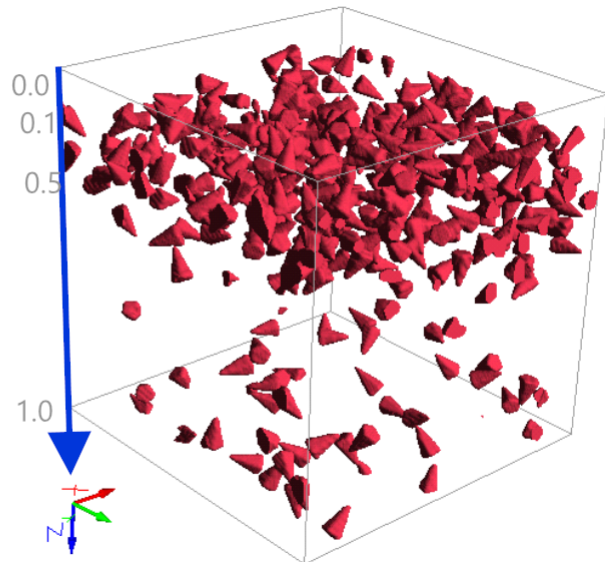
Observe how, with the values entered in the table ($0.1 \rightarrow 20$, $0.5 \rightarrow 0$, and $1 \rightarrow 2$), most pyramids occupy an area in the structure near the Z-origin ($Z = 0.1$), then there is an area almost empty of pyramids in the middle ($Z = 0.5$), and only some pyramids are at the end of the domain in Z-direction ($Z = 1$).

☒ Density Distribution

☒ Use Relative Position

	Relative Position in Z-Direction	Density
1	0.1	20
2	0.5	0
3	1	2

Number of Rows:



With **Use Relative Position** unchecked, the left column values of the density distribution table correspond to absolute locations in the structure.

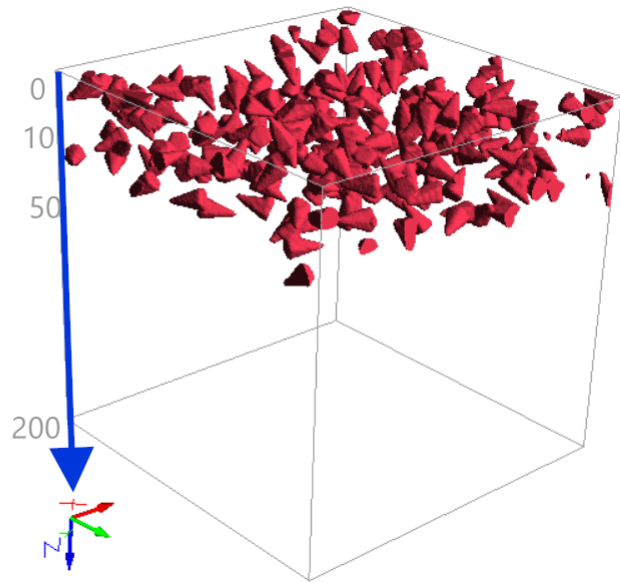
In the Z-direction, in a structure of size $200 \times 200 \times 200 \mu\text{m}$, the value 0 is at the origin and the value 200 is at the end of the domain. The right column assigns density values at these locations, where 0 means that pyramid centers are absent at that location, and 1 means that pyramid centers are present at the location.

The object density increases and decreases linearly between the given locations in the Z-direction. Therefore, in the following example, the position 50, where a sharp transition is desired, is given twice: once with positive density and once with density of 0.

☒ Density Distribution

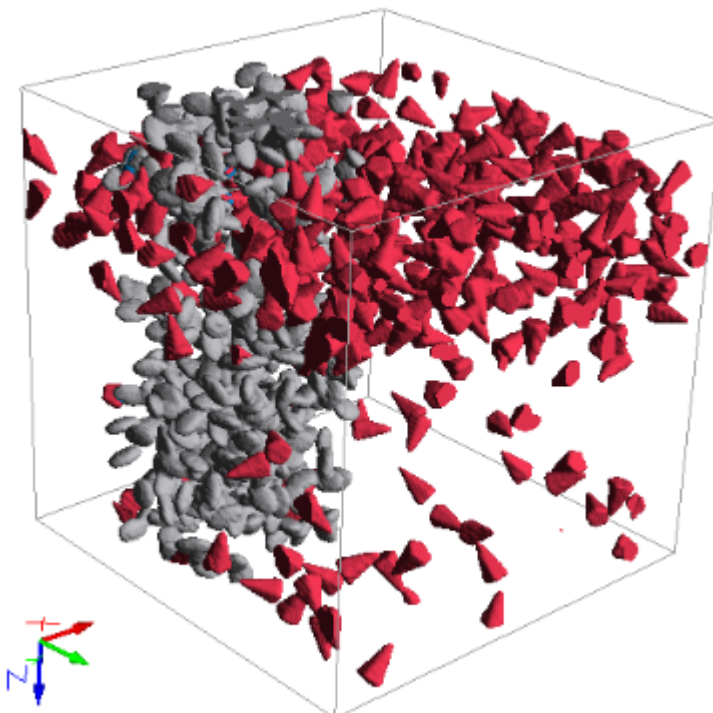
☐ Use Relative Position

	Absolute Position in Z-Direction / (mm)	Density
1	0	0
2	10	1
3	50	1
4	50	0
5	200	0



As before, with orientation, the distribution of centers can be separately set for each object type so that differently distributed object types may coexist within the same structure.

In the following example, observe that the gray ellipsoids are distributed **Uniformly in Box**, whereas the red pyramids follow a **Density Distribution**.



Shape Parameters

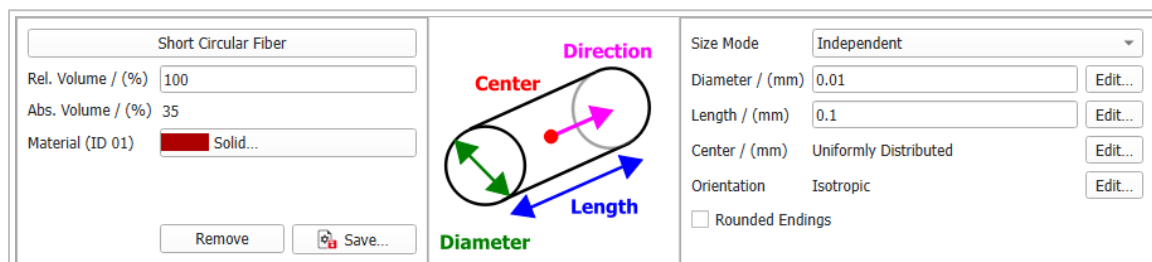
Define the object's shapes through various parameters. For each object type the object's **Center**⁴⁹ distribution and the **Orientation**⁶⁵ can be defined as explained in the corresponding topics.

Size Mode

The object types **Ellipsoid**, **Superquadric Particle**, **Box**, **Convex Polyhedron** (Enclosing Objects Ellipsoid, Box and Pyramid), **Pyramid**, and all **Fiber** types have the parameter **Size Mode**. From the pull-down menu three options can be selected. Here you can decide if the different diameter and length parameters of one object type should be interdependent.

✓ Independent

All diameter, height and length parameters are independent from each other, and thus have their own values and distributions available through their **Edit...** buttons.



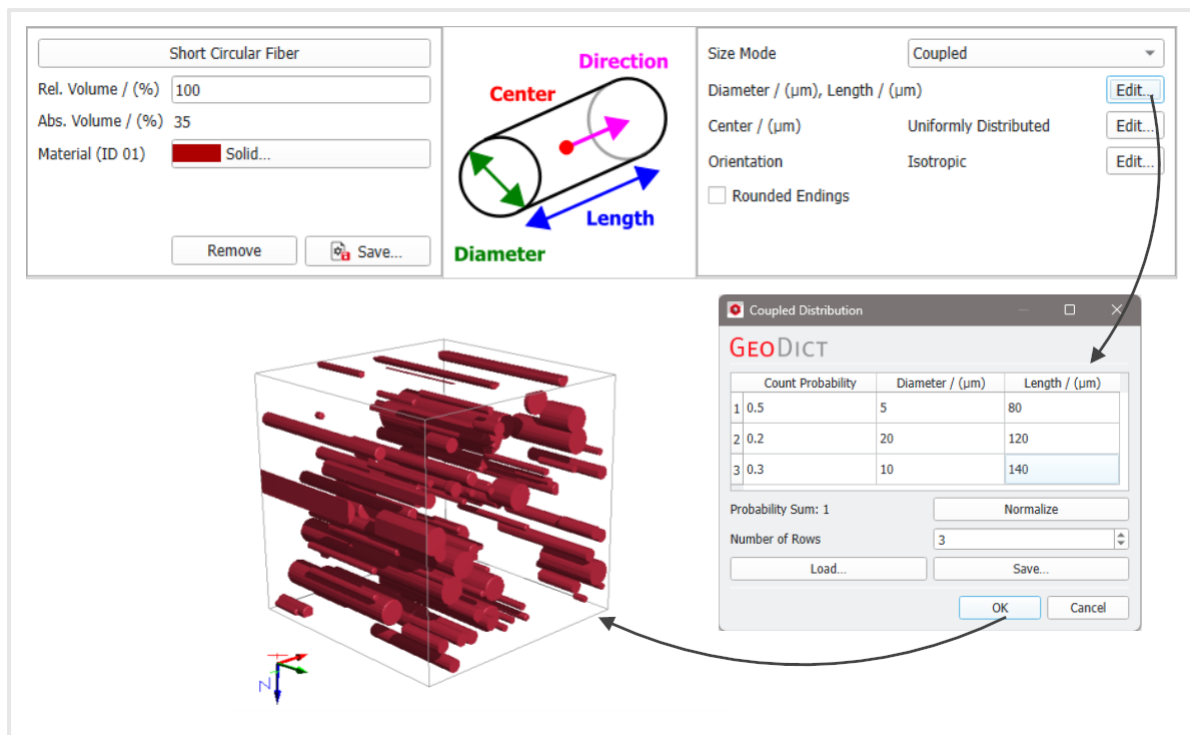
The screenshot shows the 'Short Circular Fiber' configuration window. On the left, there are fields for 'Rel. Volume / (%)' (100), 'Abs. Volume / (%)' (35), and 'Material (ID 01)' (Solid...). In the center, a diagram of a fiber is shown with labels: 'Center' (red dot), 'Direction' (pink arrow), 'Length' (blue arrow), and 'Diameter' (green arrow). On the right, the 'Size Mode' is set to 'Independent'. Below it, there are four rows of parameters: 'Diameter / (mm)' (0.01), 'Length / (mm)' (0.1), 'Center / (mm)' (Uniformly Distributed), and 'Orientation' (Isotropic). Each row has an 'Edit...' button. At the bottom, there is a checkbox for 'Rounded Endings' which is currently unchecked. 'Remove' and 'Save...' buttons are at the bottom left.

✓ Coupled

The different diameter/height/length parameters are coupled. Clicking the **Edit...** button for these parameters, the coupling can be defined in the distribution table.

The following structure, entirely made of short circular fibers, is generated with the coupled values for diameter and length entered in the coupled distribution table shown here. Observe the three distinct diameter-length combinations of short circular fibers:

- 50% with diameter 5 μm and length 80 μm ,
- 20% with diameter 20 μm and length 120 μm , and
- 30% with diameter 10 μm and length 140 μm .



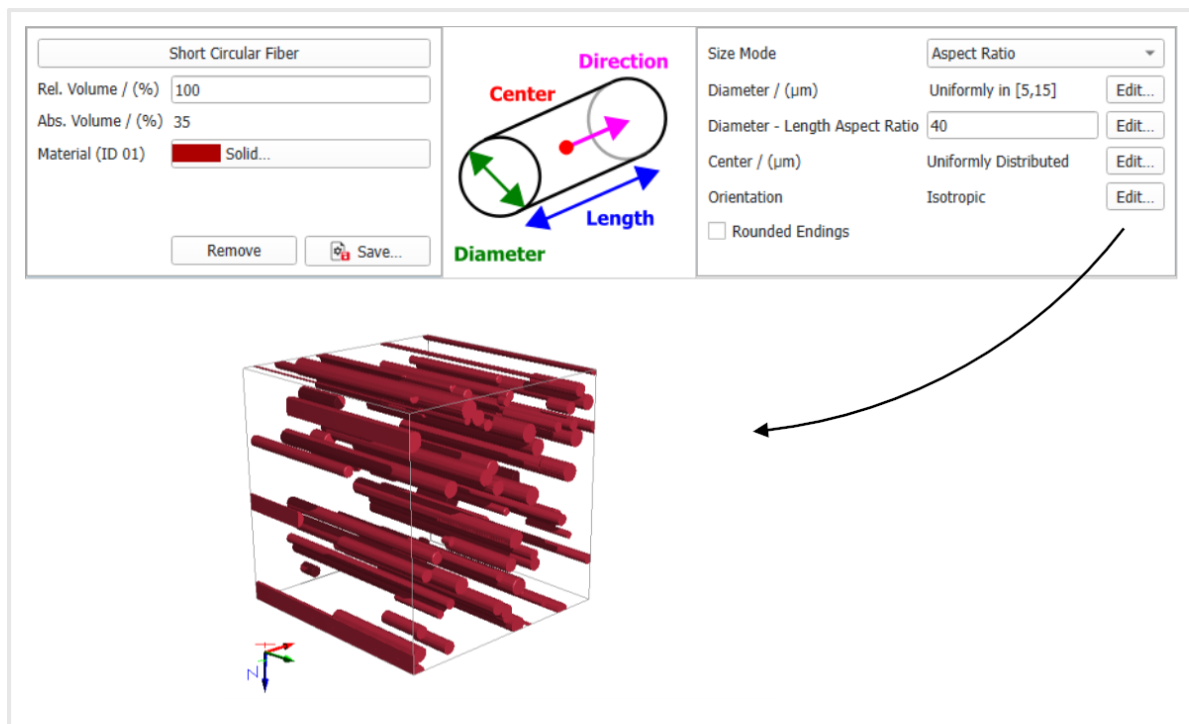
✓ Aspect Ratio

The different diameter/length parameters are given with an aspect ratio. They depend on the first given Diameter (or Length for some object types). The resulting diameter/length value then is the aspect ratio multiplied with the first parameter value, for example:

$$\text{Length} = \text{Diameter 1} \cdot \text{Aspect Ratio} \quad (1)$$

where Aspect Ratio is short for Diameter 1 - Length Aspect Ratio.

This way, you can, for example, generate fibers with a diameter [distribution](#)⁸¹ keeping the same aspect ratio to their length as shown below.

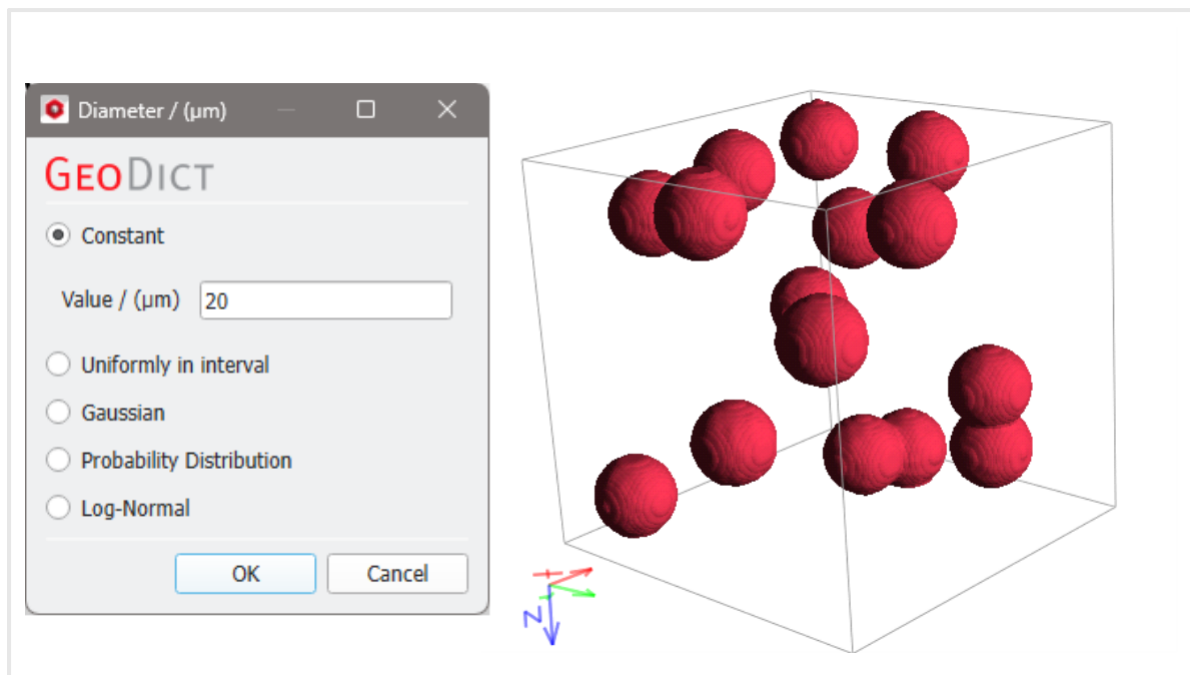


Object Specific Shape Parameters

✓ Sphere and Hollow Sphere

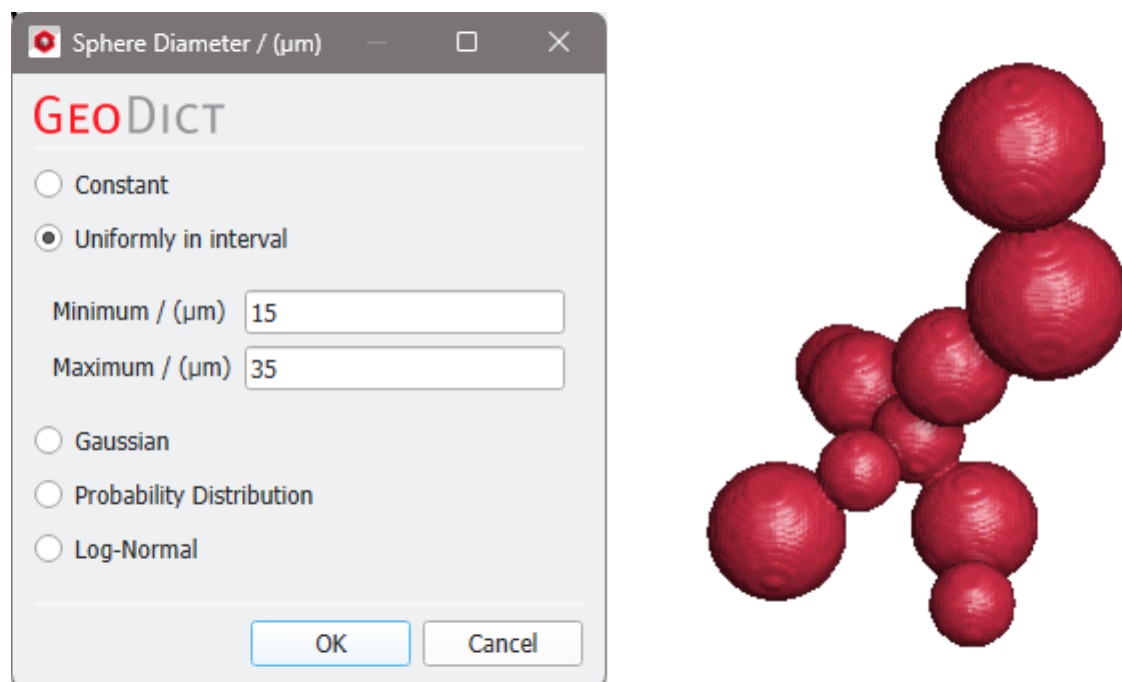
Spheres are defined by one **Diameter** value. **Hollow Spheres** additionally are defined by the **Wall Thickness**.

The **Diameter** and **Wall Thickness** values can be edited by clicking **Edit...** to open the corresponding dialog. They can be set to a **Constant** value, or to follow a [diameter distribution](#)⁸¹: **Uniformly in interval**, **Gaussian**, **Probability Distribution**, or **Log-Normal** (Log-Normal).



✓ Sphere Agglomerate

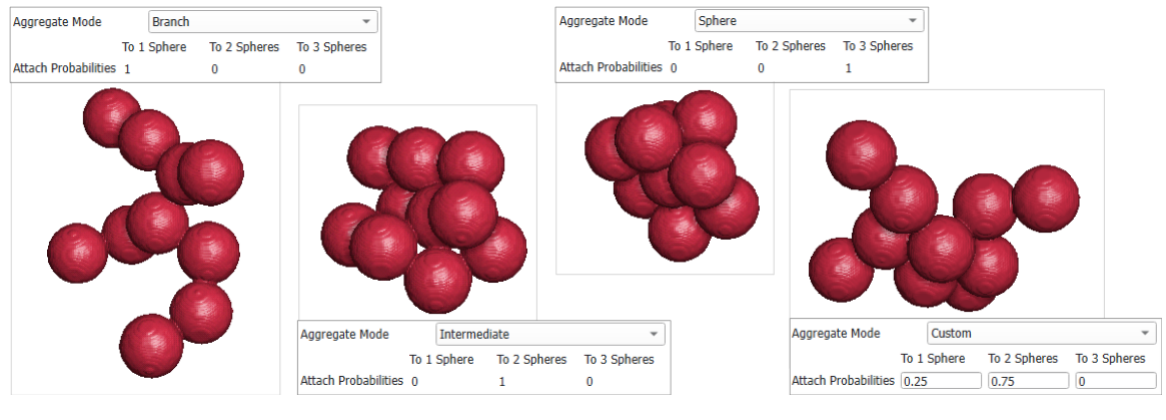
For **Sphere Agglomerates** the **Sphere Diameter** can be different for the spheres belonging to the same agglomerate.



The **Number of Spheres** defines how many spheres build one agglomerate. The value can either be constant or follow a [distribution](#) .

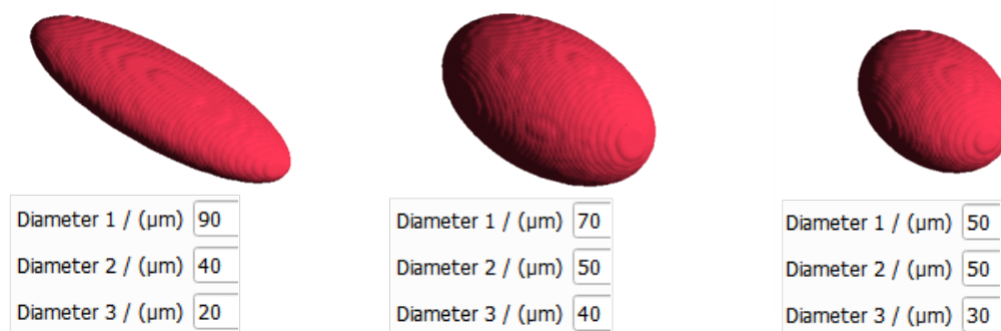
The **Aggregate Mode** defines how the spheres are agglomerated. They can be agglomerated **Branch** like, **Sphere** like, an **Intermediate** state between those two or you define your **Custom** aggregate mode by editing the **Attach Probabilities**. The

attach probabilities are automatically normalized to sum up to 1 after closing the dialog and define with which probabilities one sphere is attached to 1, 2 or 3 other spheres.



✓ Ellipsoid

Ellipsoids are defined by three diameters (**Diameter 1**, **Diameter 2**, and **Diameter 3**) which control the shape and size of the object. The values can either be constant or follow a [distribution](#)⁸¹.



✓ Superquadric Particle

Superquadric Particles are defined by three diameters (**Diameter 1**, **Diameter 2**, and **Diameter 3**) and the two blockiness parameters (**Blockiness 1** and **Blockiness 2**) which control the shape and size of the object.

The diameters can either be constant or follow a [distribution](#)⁸¹.

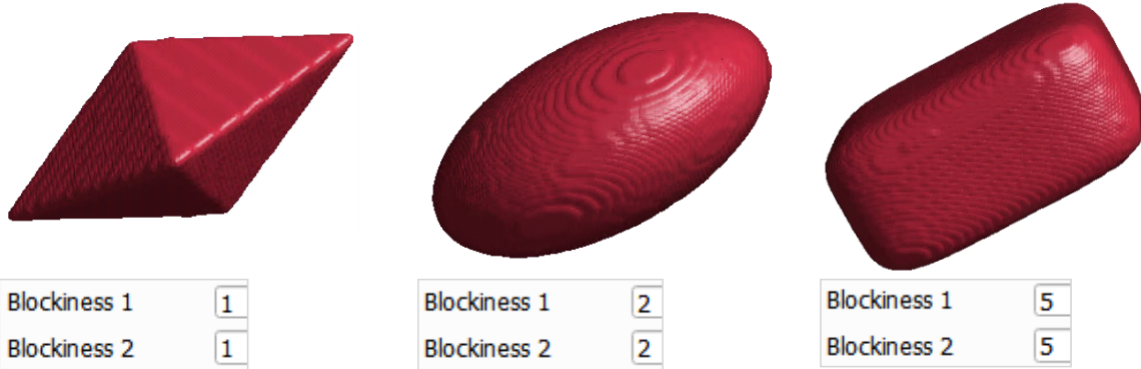
The surface of a **Superquadric Particle** is implicitly defined by the formula:

$$\left(\left| \frac{x}{d_1} \right|^{b_2} + \left| \frac{y}{d_2} \right|^{b_2} \right)^{\frac{b_1}{b_2}} + \left| \frac{z}{d_3} \right|^{b_1} = 1$$

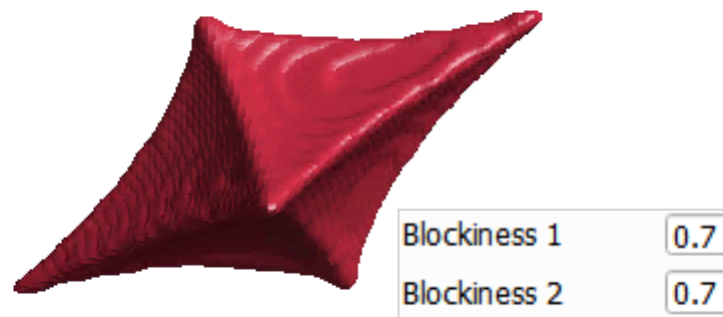
(2)
Superquadric
Particle
Surface

The three **Diameter** values correspond to the diameters d_1 , d_2 , d_3 in the formula, **Blockiness 1** to the exponent b_1 and **Blockiness 2** to the exponent b_2 .

For exponents $b_1 = b_2 = 1$ the particle takes the shape of an octahedron, exponents $b_1 = b_2 = 2$ lead to an ellipsoidal shape, and for higher exponents the shape approaches a rectangular box.

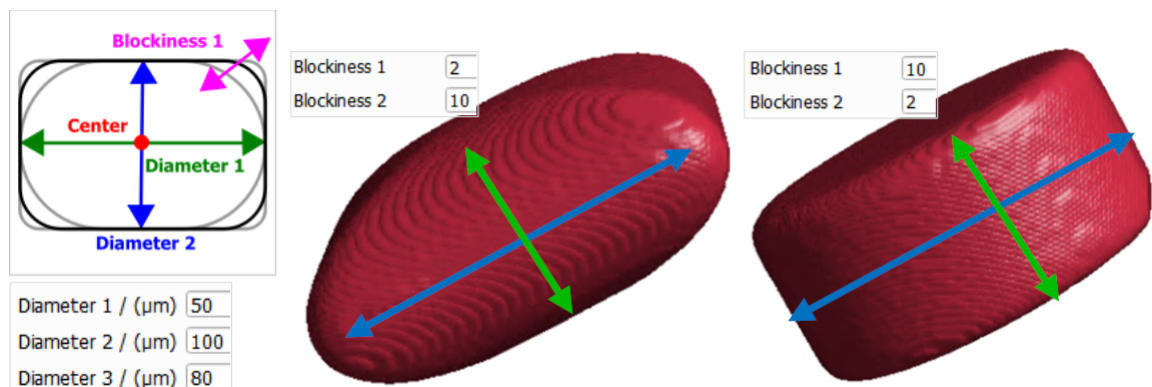


Parameters between 0 and 1 lead to a concave surface and might decrease the size defined by the diameters. Thus, it is recommended to use values of at least 0.5.



Blockiness 1 describes the shape in the plane defined by **Diameter 1** and **Diameter 2** as shown on the right and the plane described by **Diameter 1** and **Diameter 3**.

Blockiness 2 describes the shape in the plane described by the diameters **Diameter 2** and **Diameter 3**.



The three values of **Length** for **Boxes** are editable by clicking **Edit...** and choosing the desired settings in the **Length** dialog.

The **Length** can be set to take a **Constant** value, or to follow a [distribution](#)⁸¹ (**Uniformly in interval**, **Gaussian**, **Probability Distribution**, or **Log-Normal**).

Boxes are defined by **Length 1**, **Length 2**, and **Length 3** which control the shape and size of the object.

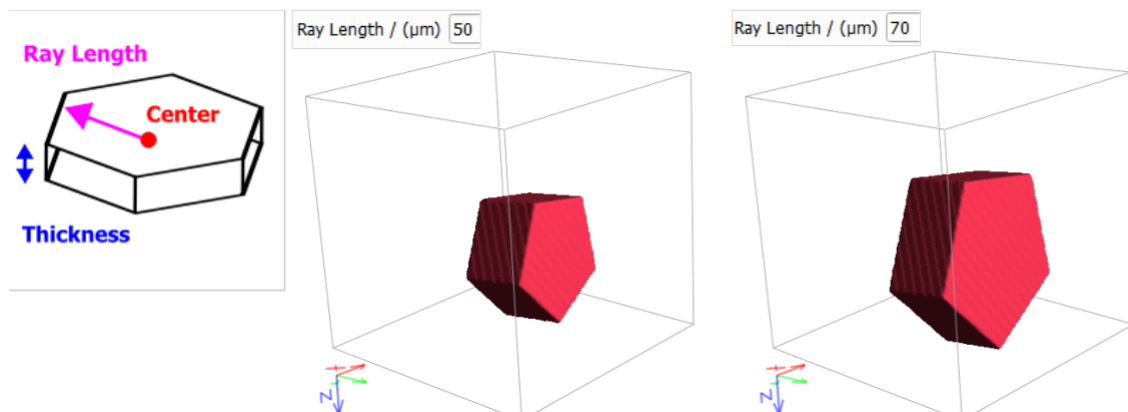


✓ Planar Polyhedrons

For planar polyhedrons, define the **Thickness**, the **Number of Edges** and the **Ray Length**.

All three parameters can be set to take a **Constant** value, or to follow a [distribution](#)⁸¹.

The **Ray Length** is the distance from the center of the object to any of the edges.



✓ Convex Polyhedron

For a **Convex Polyhedron**, the shape determining parameters depends on the chosen

Enclosing Object to be defined in its tab. For a [Box](#)^[59], [Sphere](#)^[56], [Ellipsoid](#)^[58] or [Pyramid](#)^[62] as **Enclosing Object**, the respective diameters must be set as described in their respective sections.

General
Enclosing Object

Center / (μm)
Uniformly Distributed
Edit...

Point Mode
Volume

Number of Random Points
20
Edit...

☒ Match Enclosing Object Volume

General
Enclosing Object

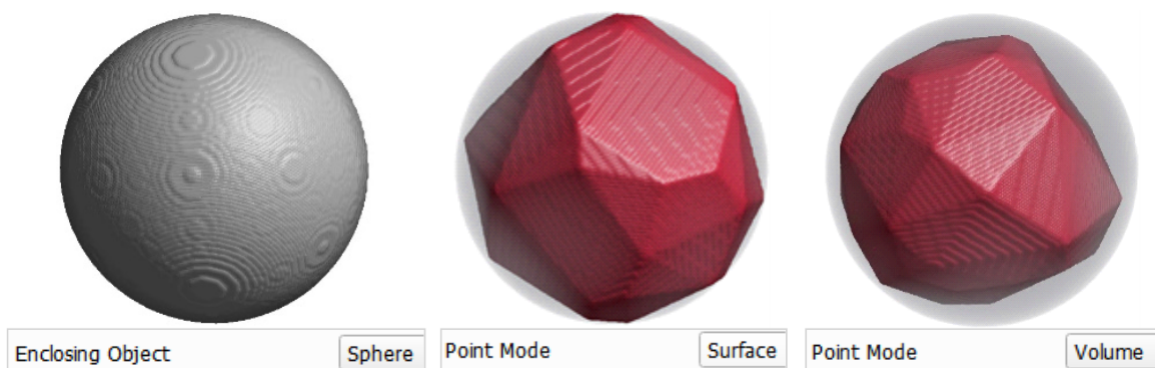
Enclosing Object
Sphere

Sphere
Ellipsoid
Box
Pyramid

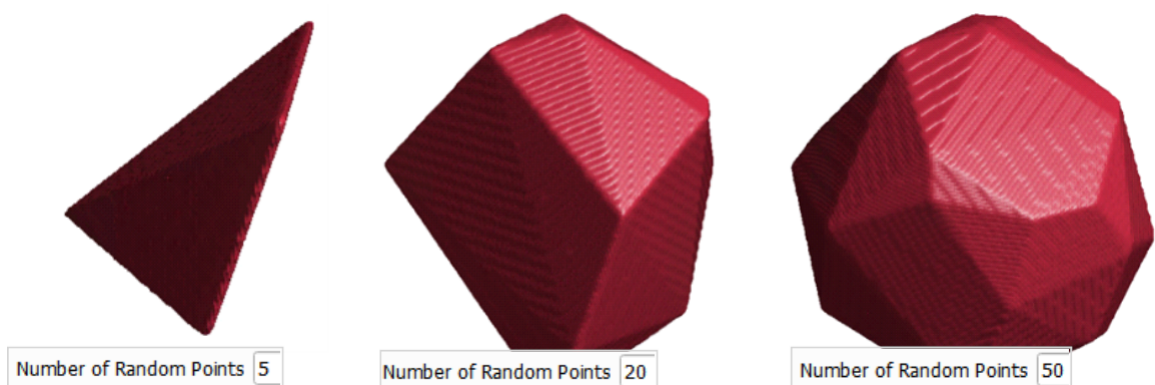
Enclosing Object Diameter / (μm)
10
Edit...

Enclosing Object Orientation
Isotropic
Edit...

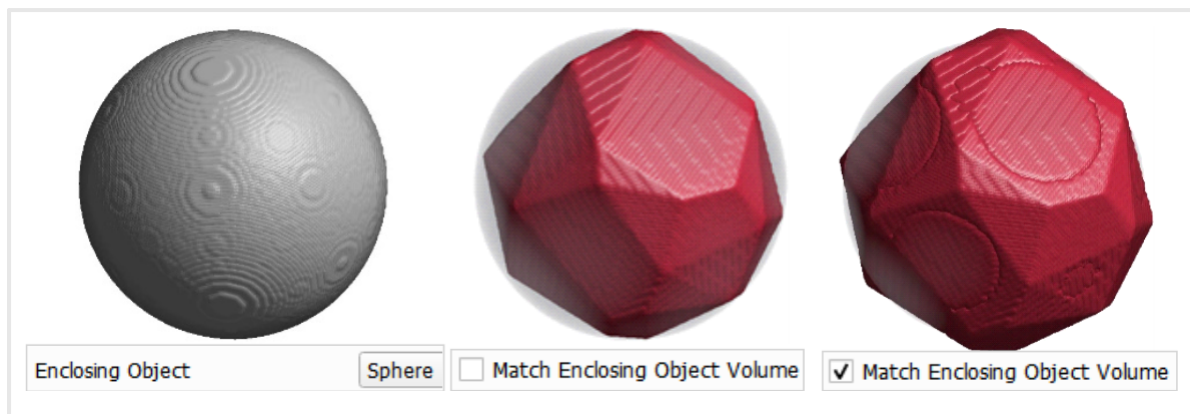
The **Point Mode** defines if the vertices of the polyhedron can be defined anywhere inside the **Volume** of the enclosing object, or if they must lay on its **Surface**.



To generate a **Convex Polyhedron**, several random points (**Number of Random Points**), serving as vertices of the polyhedron, are placed inside the chosen **Enclosing Object**.



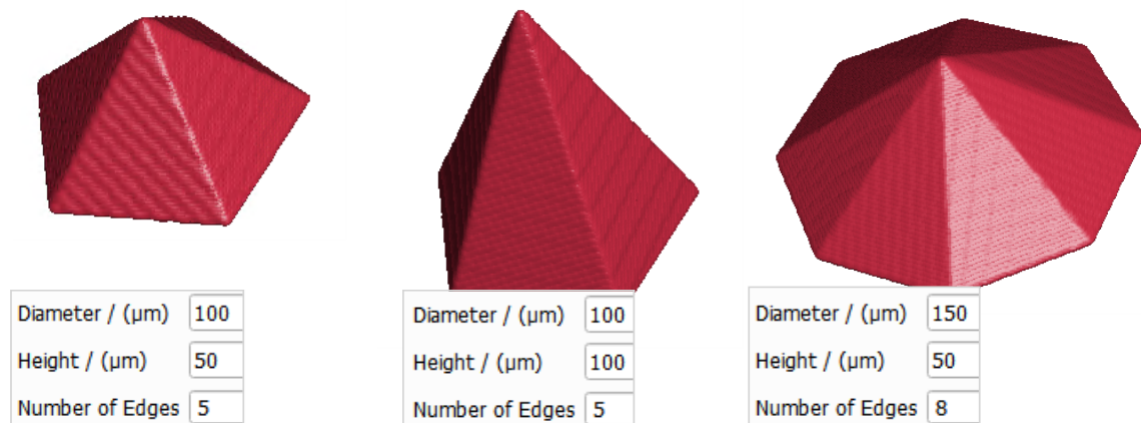
Additionally, checking **Match Enclosing Object Volume** scales the object size until the volume is as big as the volume of the enclosing object. Leaving this option unchecked always leads to a smaller volume.



✓ Pyramid

Pyramids are defined by their **Diameter**, **Height**, and **Number of Edges**.

The values of **Diameter** and **Height** are editable by clicking **Edit...** and choosing the desired settings in the opening dialog. They can be set to take a **Constant** value, or to follow a [distribution](#) ⁸¹ (**Uniformly in interval**, **Gaussian**, **Probability Distribution**, or **Log-Normal**).



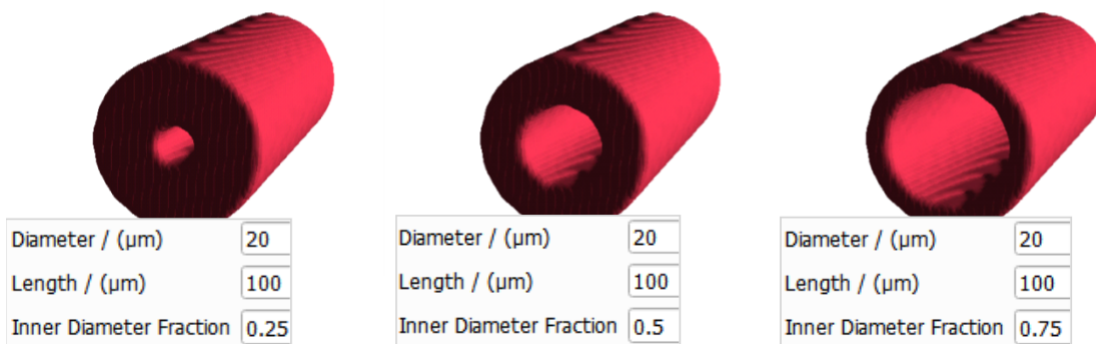
✓ Short Fibers

The values of **Length** and **Diameter** for all **Short Fibers**, as well as the **Side Length** of short rectangular fibers are editable by clicking **Edit...** and choosing the desired settings in the opening dialog.

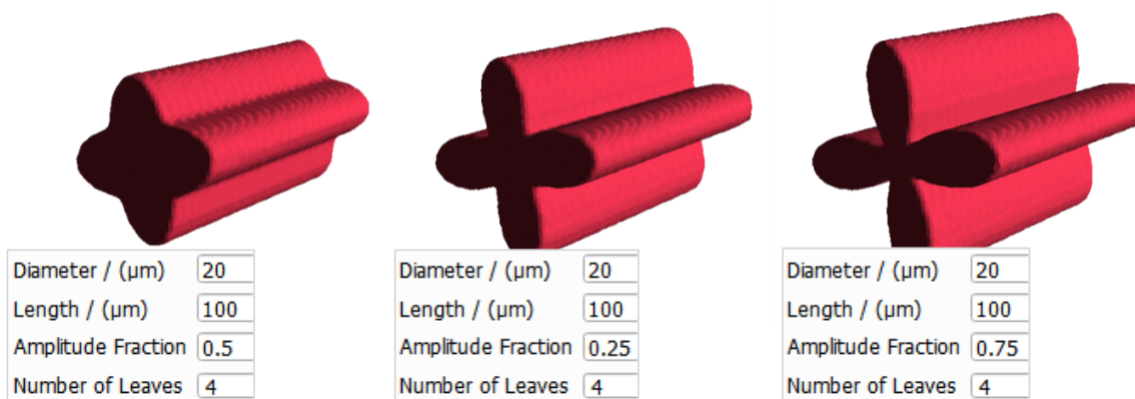
The **Length**, **Diameter**, and **Side Length** can be set to take a **Constant** value, or to follow a [distribution](#) ⁸¹ (**Uniformly in interval**, **Gaussian**, **Probability Distribution**, or **Log-Normal**).

For **circular fibers** only **Diameter** and **Length** define the shape.

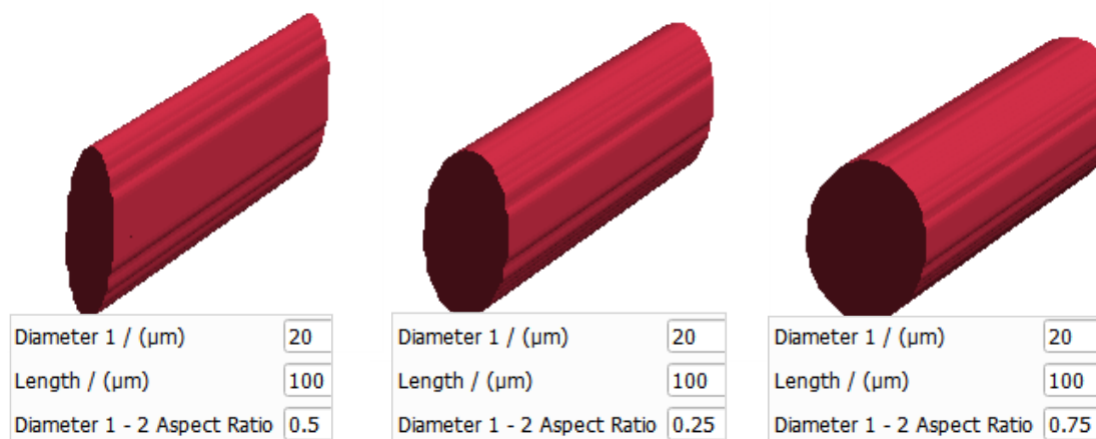
For **non-circular fibers**, the diameter and length but also other parameters control their shape. For a hollow fiber, the **Inner Diameter Fraction** defines the ratio of the entered (outer) diameter to the inner diameter.



For fibers with **Rosetta** cross-section, the **Amplitude Fraction** determines the length of the Rosetta leaves, and the **Number of Leaves** defines how many leaves the Rosetta has.



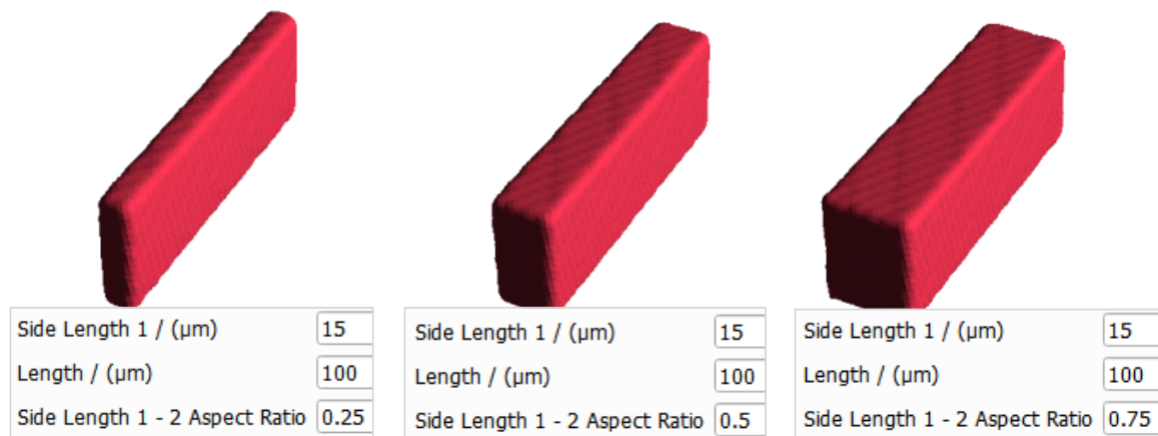
For **short elliptical fibers**, defined by two diameters, the **Diameter 1 - 2 Aspect Ratio** is the relationship between the longer diameter **Diameter 1** and the shorter diameter **Diameter 2**.



For **short cellulose fibers**, defined by two diameters and two inner diameters, the **Diameter 1 - 2 Aspect Ratio** is the relationship between the longer diameter **Diameter 1** and the shorter diameter **Diameter 2**. The **Inner Diameter Fraction**

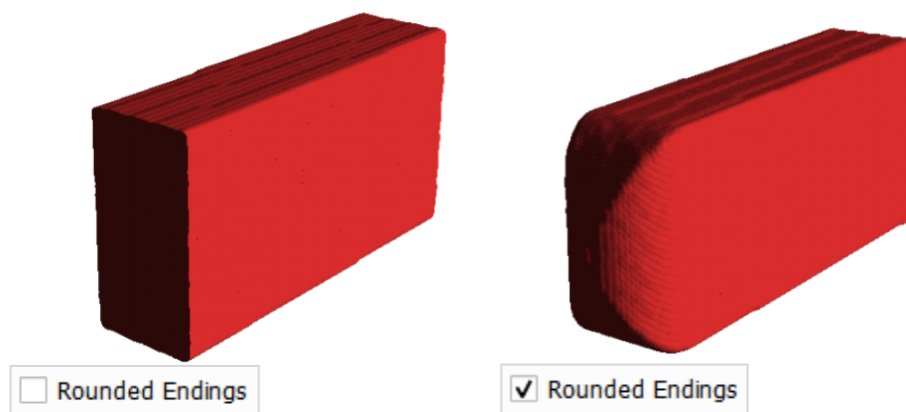
defines the inner diameter similar as for the hollow fiber shown above. Since the cellulose fiber has an elliptical shape, two inner diameters are defined, where the inner diameter 1 is defined by the product of diameter 1 and the inner diameter fraction and the inner diameter 2 depends on the diameter 2 in the same way.

For short rectangular fibers, the **Side Length 1** and the **Side Length 1 - 2 Aspect Ratio** can be entered.



For **short angular fibers** the **Number of Edges** of the fiber cross-section must be defined.

All short fibers with any cross-section can be created with or without rounded ends by checking or leaving un-checked the **Rounded Endings** box. Observe the variation in the shape of the short rectangular fibers after checking the **Rounded Endings** box.



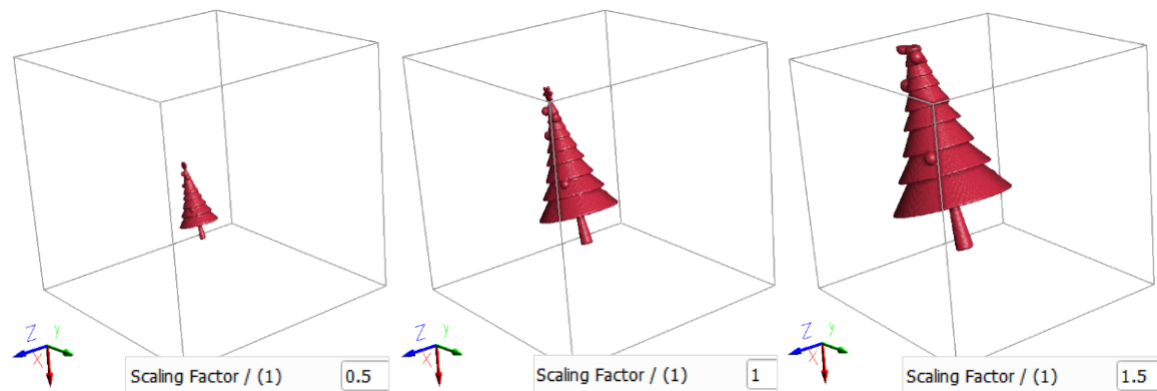
✓ Combined Object

Combined Objects are created through the combination of two or more objects (which have the same or different object types). They must be generated beforehand with GadGeo and saved in GAD-format. To learn how to generate combined objects with GadGeo refer to the GadGeo User Guide.

Click **Browse ...** in the right column of the **Object Type** panel to select and import combined objects from a *.gad-file. The Christmas tree example for combined objects is included in the installation folder.

OS (C:) > Program Files > Math2Market GmbH > GeoDict 2026 > Examples > GrainGeo > Piling of Complex Objects

The **Scaling Factor** controls the size of the objects. A scaling factor of 1 generates the selected combined object with original size.



Orientation

All objects in the generated structure have either isotropic or anisotropic orientation. The **Orientation** of an object type in a generated structure can be set by clicking the **Edit...** button. The orientation can be separately set for each object type so that differently oriented objects may coexist within the same structure.

In the **Orientation** dialog, objects can be defined to be Isotropic, have a certain **Anisotropic Direction**, **Anisotropic Orientation**, **Given Directions**, to be oriented **In XY-Plane** or have a maximum **Angle Around Direction**.

For all object types, it is possible to control the object direction (isotropic or anisotropic) and the position of the cross-section with respect to the XY-plane as well.

Size Mode: Independent

Diameter / (mm): 0.01 Edit...

Length / (mm): 0.1 Edit...

Center / (mm): Uniformly Distributed Edit...

Orientation: Isotropic Edit...

☐ Rounded Endings

Orientation

GEODICT

☒ Isotropic

☐ Anisotropic Direction

☐ Anisotropic Orientation

☐ Given Directions

☐ In XY-Plane

☐ Angle Around Direction

OK Cancel

Isotropic

In an Isotropic orientation, all directions have the same probability.

Anisotropic Direction

When checking **Anisotropic Direction** and selecting **Anisotropy Parameter** from the **Direction Mode** pull-down menu, the **Anisotropy Parameters** (Anisotropy 1 and Anisotropy 2), as well as the **Phi**, **Theta** and **Psi Euler Angles** for the three-dimensional rotation of anisotropic objects can be defined.

In this case, the positions of cross-sections to the XY-plane are isotropic (and not entered).

☒ Anisotropic Direction

Direction Mode: Anisotropy Parameter

Anisotropy 1: 1

Anisotropy 2: 1

Euler Angles: Phi / (°): 0, Theta / (°): 0, Psi / (°): 0

Orientation Tensor: 0.3333, 0.0000, 0.0000; -, 0.3333, 0.0000; -, -, 0.3334

Normalize + Calculate Anisotropy Parameters

✓ Anisotropy Parameters

The **Anisotropy Parameters**, **Anisotropy 1** (a_1) and **Anisotropy 2** (a_2), allow to define the orientation of the objects. **Anisotropy Parameters** and the [Orientation Tensor](#)⁷³ are equivalent representations for the orientation, and GeoDict can compute one from the other automatically. The objects are created with random orientations, following a distribution defined by the given parameters.

The Algorithm

For each object, a random direction is computed

$$d = \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

which follows an isotropic distribution. Afterwards, the anisotropy parameters are used to influence these orientations. Before normalization, the resulting vector for the object orientation is:

$$d_a = \begin{pmatrix} x_a \\ y_a \\ z_a \end{pmatrix} = \begin{pmatrix} a_1 x \\ a_1 a_2 y \\ z \end{pmatrix}$$

(3)
Anisotropic
orientation
vector

With normalization follows:

$$d_{normalized} = \frac{1}{|d_a|} d_a = \frac{1}{\sqrt{(a_1 x)^2 + (a_1 a_2 y)^2 + z^2}} \begin{pmatrix} a_1 x \\ a_1 a_2 y \\ z \end{pmatrix}$$

(4)
Normalized
anisotropic
orientation
vector

Before normalization, **Anisotropy 1** controls the first two coordinates, while **Anisotropy 2** only affects the second coordinate and none of them changes the third. After normalization, the anisotropy parameters both have impact on all three coordinates, where the influence on the object direction differs. Whereas high values for **Anisotropy 1** lead to objects parallel to the XY-plane, high values for **Anisotropy 2** result in objects oriented in Y-direction. Objects oriented in Z-direction are obtained by low values for **Anisotropy 1**, and low values for **Anisotropy 2** result in objects parallel to the XZ-plane.

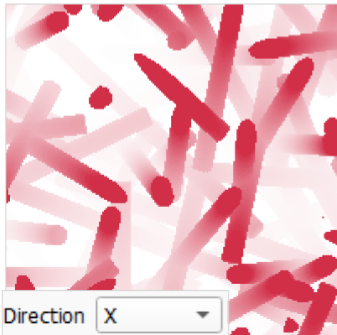
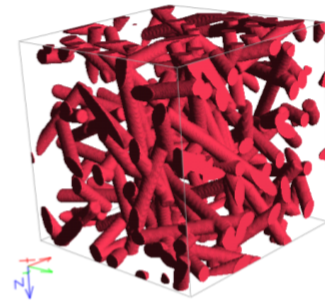
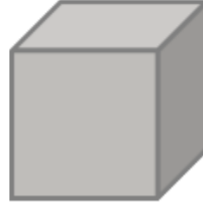
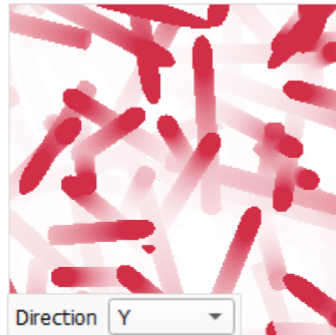
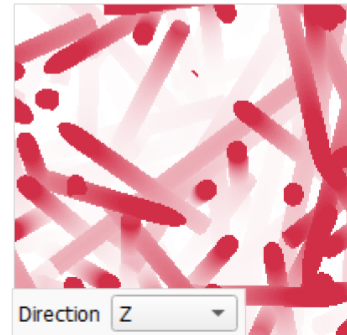
In the following, five main cases for the anisotropy parameters are described:

1. **Anisotropy 1 = Anisotropy 2 = 1 (Isotropic material)**

The object orientation is isotropic. All directions have the same probability, as the direction obtained from the random algorithm is not changed:

$$d_a = \begin{pmatrix} a_1 x \\ a_1 a_2 y \\ z \end{pmatrix} = \begin{pmatrix} 1 \cdot x \\ 1 \cdot 1 \cdot y \\ z \end{pmatrix} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = d$$

Anisotropy 1	1
Anisotropy 2	1

Direction Direction Direction

2. Anisotropy 1 < 1 and Anisotropy 2 = 1

Values smaller than 1 for **Anisotropy 1** lead to orientations in Z-direction, so that the objects are parallel to the YZ-plane and the XZ-plane when viewed from the X- or Y-direction. The smaller the value of **Anisotropy 1**, the more anisotropic the objects have.

For example, with the values 0.01 for **Anisotropy 1** and 1 for **Anisotropy 2** it follows:

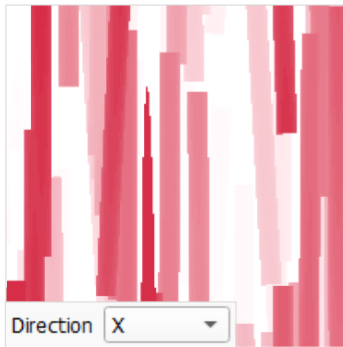
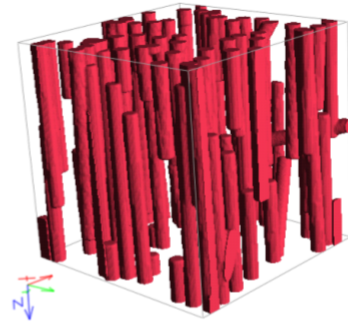
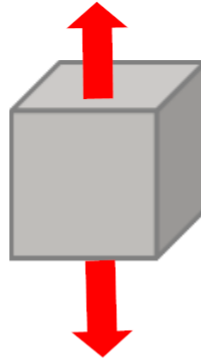
$$d_a = \begin{pmatrix} a_1 x \\ a_1 a_2 y \\ z \end{pmatrix} = \begin{pmatrix} 0.01 \cdot x \\ 0.01 \cdot y \\ z \end{pmatrix}$$

Thus, after normalization the direction vectors of the objects approximate the unit vector:

$$d_{normalized} = \frac{1}{\sqrt{0.0001 \cdot x^2 + 0.0001 \cdot y^2 + z^2}} \begin{pmatrix} 0.01 \cdot x \\ 0.01 \cdot y \\ z \end{pmatrix} \cong \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

That results in objects oriented in Z-direction.

Anisotropy 1	0.01
Anisotropy 2	1



3. Anisotropy 1 > 1 and Anisotropy 2 = 1

The objects are isotropic in the XY-plane (Z-slice). The higher the value of **Anisotropy 1**, the stronger is the anisotropy.

For example, with the values 100 for **Anisotropy 1** and 1 for **Anisotropy 2** it follows:

$$d_a = \begin{pmatrix} a_1 x \\ a_1 a_2 y \\ z \end{pmatrix} = \begin{pmatrix} 100 \cdot x \\ 100 \cdot y \\ z \end{pmatrix}$$

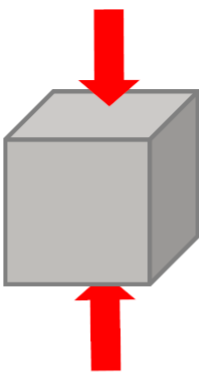
Thus, after normalization the direction vectors of the objects approximate the vector:

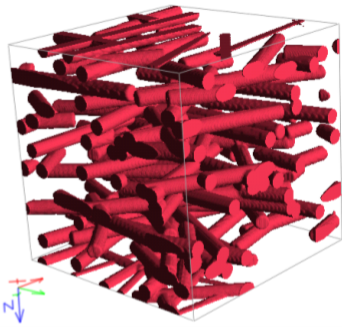
$$d_{normalized} = \frac{1}{\sqrt{10000 \cdot x^2 + 10000 \cdot y^2 + z^2}} \begin{pmatrix} 100 \cdot x \\ 100 \cdot y \\ z \end{pmatrix} \cong \begin{pmatrix} x \\ y \\ 0 \end{pmatrix}$$

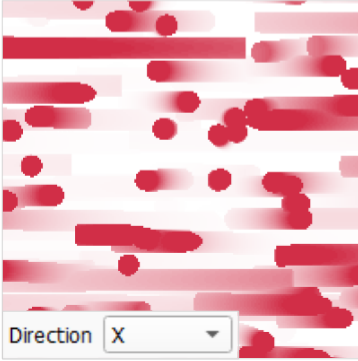
That results in objects oriented in the XY-plane.

Anisotropy 1

Anisotropy 2



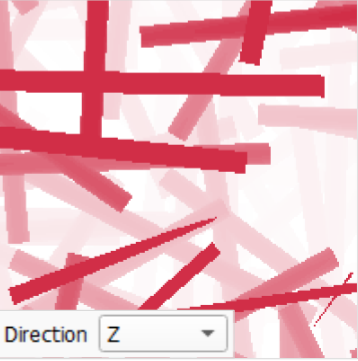




Direction X



Direction Y



Direction Z

4. Anisotropy 1 = 1 and Anisotropy 2 < 1

Small values for **Anisotropy 2** lead to objects oriented parallel to the XZ-plane. Observe that the objects are isotropic in the XZ-plane (Y-slice).

For example, with the values 1 for **Anisotropy 1** and 0.01 for **Anisotropy 2** it follows:

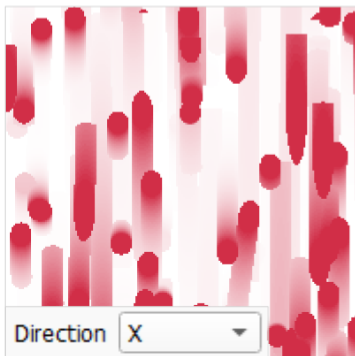
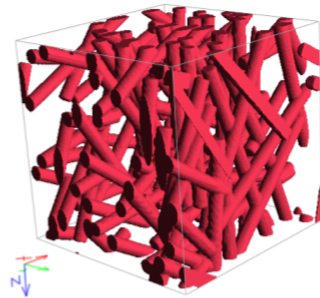
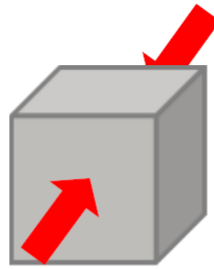
$$d_a = \begin{pmatrix} a_1 x \\ a_1 a_2 y \\ z \end{pmatrix} = \begin{pmatrix} x \\ 0.01 \cdot y \\ z \end{pmatrix}$$

Thus, after normalization the direction vectors of the objects approximate the vector:

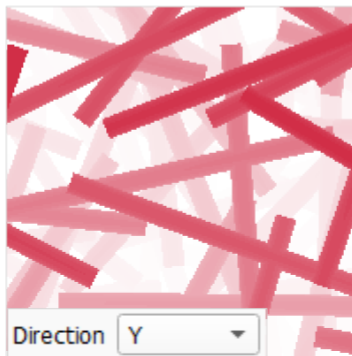
$$d_{normalized} = \frac{1}{\sqrt{x^2 + 0.0001 \cdot y^2 + z^2}} \begin{pmatrix} x \\ 0.01 \cdot y \\ z \end{pmatrix} \cong \begin{pmatrix} x \\ 0 \\ z \end{pmatrix}$$

That results in objects oriented in the XZ-plane.

Anisotropy 1	1
Anisotropy 2	0.01



Direction



Direction



Direction

5. Anisotropy 1 = 1 and Anisotropy 2 > 1

The higher the values for **Anisotropy 2**, the more the objects tend to be oriented along the Y-axis. Observe that the objects cut the XZ-plane (Y-slice), while they run parallel to the YZ-plane and the XY-plane when viewing them from the X- or the Z-direction.

For example, with the values 1 for **Anisotropy 1** and 100 for **Anisotropy 2**, it follows:

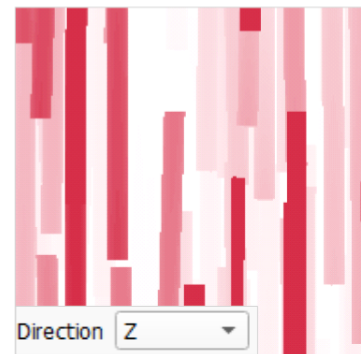
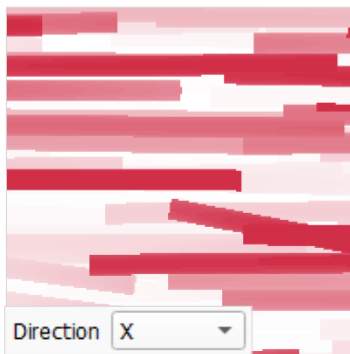
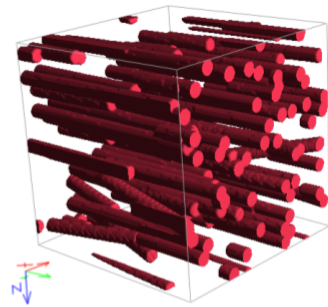
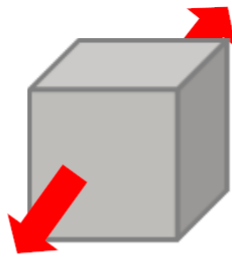
$$d_a = \begin{pmatrix} a_1 x \\ a_1 a_2 y \\ z \end{pmatrix} = \begin{pmatrix} x \\ 100 \cdot y \\ z \end{pmatrix}$$

Thus, after normalization the direction vectors of the objects approximate the unit vector:

$$d_{normalized} = \frac{1}{\sqrt{x^2 + 10000 \cdot y^2 + z^2}} \begin{pmatrix} x \\ 100 \cdot y \\ z \end{pmatrix} \cong \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

That results in objects oriented in Y-direction.

Anisotropy 1	1
Anisotropy 2	100

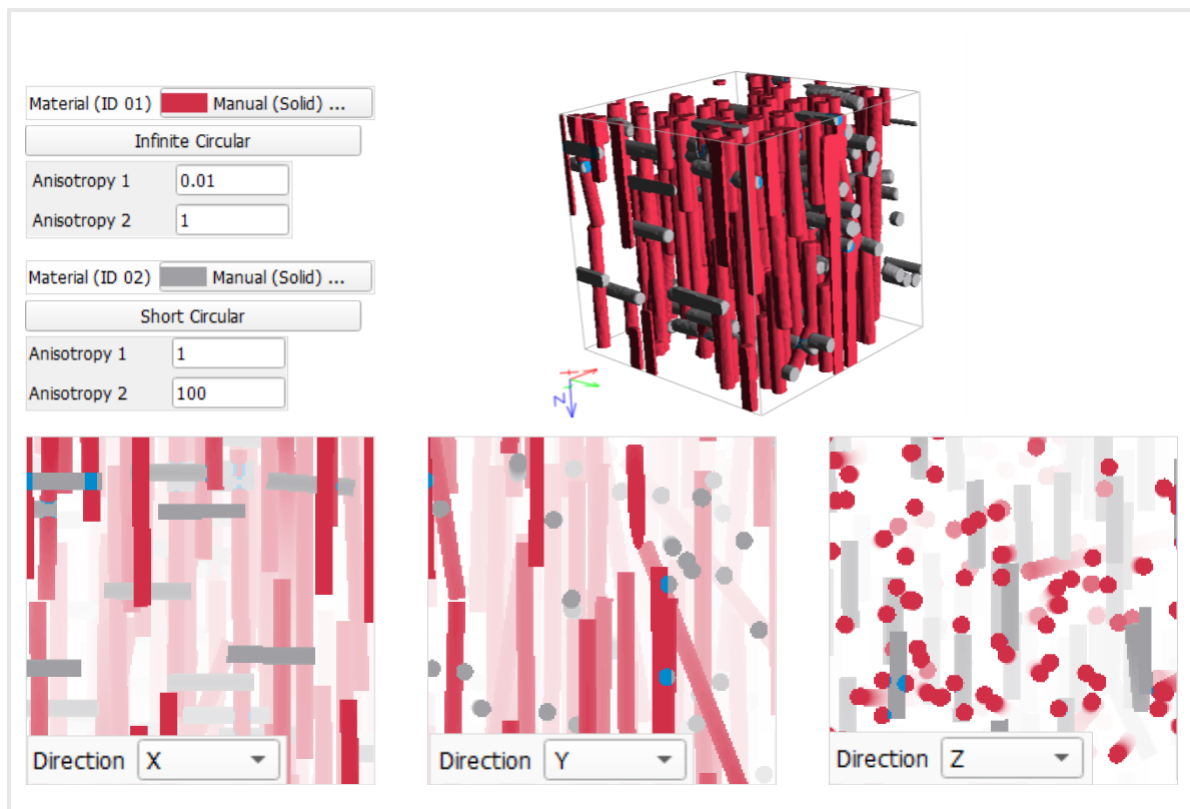


Different anisotropy values for different object types

As mentioned before, the orientation can be separately set for each object type so that differently oriented objects may coexist within the same structure. In the following structure, observe that **Anisotropy 1** and **Anisotropy 2** are set to 0.01 and 1 for the short circular (red) fibers. The short circular (gray) fibers have **Anisotropy 1** and **Anisotropy 2** of 1 and 100, respectively.

The red fibers tend to be oriented along the Z-axis, and the fibers run parallel when viewed from the X- or Y-direction.

The gray fibers tend to be oriented in the Y-axis and cut the XZ-plane, while they run parallel to the YZ-plane and the XY-plane, as observed from the X- or the Z-direction.

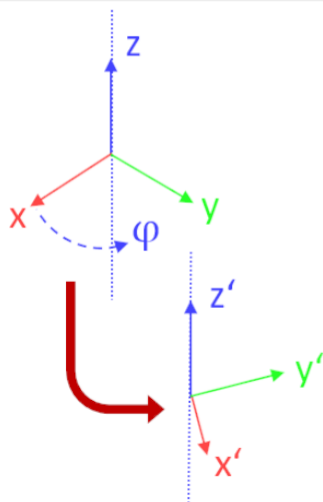


✓ Euler Angles

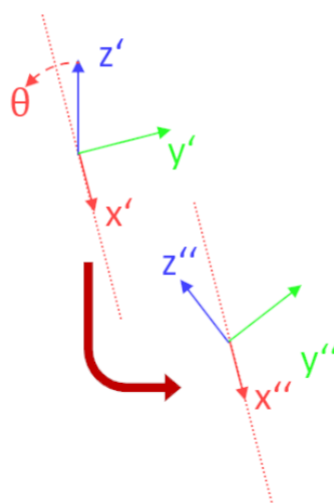
The [Euler rotation angles](#) are applied to the objects during the generation after applying the anisotropy parameters following the order **Phi** → **Theta** → **Psi**.

Euler Angles	Phi / (°)	90
	Theta / (°)	30
	Psi / (°)	30

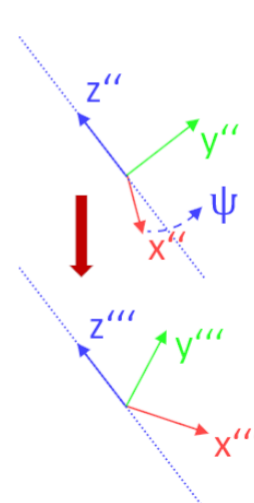
Z-axis fixed
Phi applies rotation around existing Z-axis



new X-axis fixed
Theta applies rotation around new X-axis



new Z-axis fixed
Psi applies rotation around new Z-axis



✓ Orientation Tensor

Alternatively, when selecting **Orientation Tensor** from the **Direction Mode** pull-down menu, the values for the orientation tensor for the anisotropic objects can be entered.

The **Orientation Tensor** provides an equivalent alternative to the combination of the **Anisotropy Parameters** and the **Euler Angles**.

☒ Anisotropic Direction

Direction Mode: Orientation Tensor

Anisotropy 1: 1

Anisotropy 2: 1

Phi / (°): 90.0000

Euler Angles: Theta / (°): 180.0000

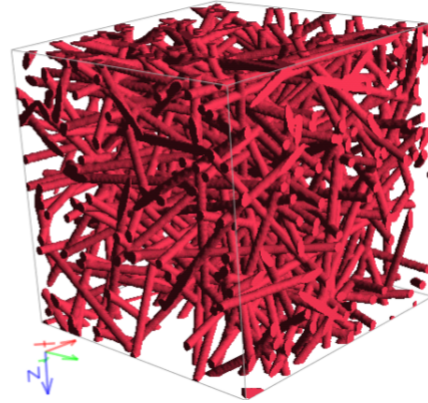
Psi / (°): 0.0000

0.3333 0.0000 0.0000

Orientation Tensor: - 0.3333 0.0000

- - 0.3334

Normalize + Calculate Anisotropy Parameters



Clicking the **Normalize + Calculate Anisotropy Parameters** button enters the adjusted values in the orientation tensor and the **Anisotropy 1** and **Anisotropy 2** boxes.

In detail, let

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

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

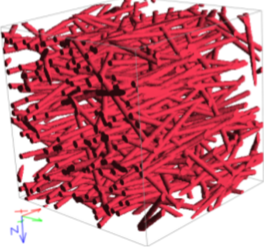
$$\mathbf{T} = \frac{1}{n} \left(\sum_{k=1}^n \mathbf{d}_k \mathbf{d}_k^T \right) = \frac{1}{n} \sum_{k=1}^n \begin{pmatrix} x_k x_k & x_k y_k & x_k z_k \\ y_k x_k & y_k y_k & y_k z_k \\ z_k x_k & z_k y_k & z_k z_k \end{pmatrix} = \begin{pmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{pmatrix} \quad (5) \text{ Orientation Tensor}$$

The diagonal elements define the orientation strength for the corresponding directions and sum up to 1. Thus, if for example **t₁₁=1** (and **t₂₂=t₃₃=0**), all objects are oriented in the X-direction. For **t₁₁=0** all objects are oriented normally to the X-direction and same values for all diagonal elements (**t₁₁=t₂₂=t₃₃=1/3**) result in a uniform distribution for the object orientation.

Observe the effect of changing the default values of the isotropic **Orientation Tensor** to obtain anisotropic structures oriented in the X-, Y-, or Z-direction.

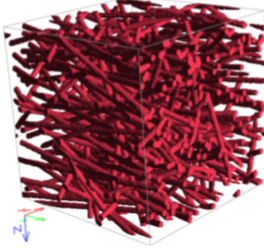
X-direction

0.7	0.0000	0.0000
-	0.15	0
-	-	0.15



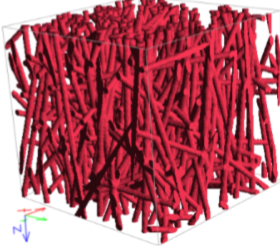
Y-direction

0.15	0.0000	0.0000
-	0.7	0
-	-	0.15



Z-direction

0.15	0.0000	0.0000
-	0.15	0
-	-	0.7



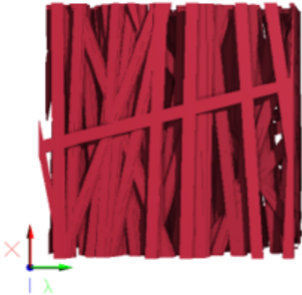
The extra-diagonal values define the statistical variation of the orientations given by the diagonal values. For example, if t_{11} has a high value near 1, and t_{12} has a relatively high value near 0.1, less fibers are oriented straight in X-direction than it is the case for a lower value for t_{12} .

Realized direction tensor:

0.8932	0.0130	-0.0001
-	0.1066	-0.0003
-	-	0.0002

Target direction tensor:

0.8995	0.0000	0.0000
-	0.1000	0.0000
-	-	0.0005

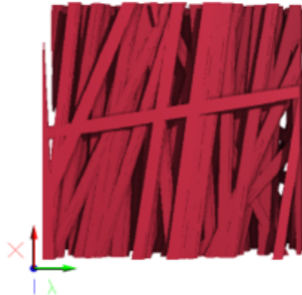


Realized direction tensor:

0.9006	0.1080	0.0003
-	0.0992	-0.0007
-	-	0.0002

Target direction tensor:

0.8995	0.1000	0.0000
-	0.1000	0.0000
-	-	0.0005



Clicking the **Normalize + Calculate Anisotropy Parameters** button, the **Orientation Tensor** is normalized, and the **Anisotropy values** and the **Euler Angles** are calculated and entered in the boxes above.

Anisotropic Orientation

To control not only the object direction, but also the position of the cross-section with respect to the XY-plane, check **Anisotropic Orientation** and select either [Anisotropy Parameter](#)^[66] or [Orientation Tensor](#)^[73] from the **Orientation Mode** pull-down menu. Since all other parameters are the same as for the [Anisotropic Direction](#)^[66], here only the **Profile Angle** is described.

☒ Anisotropic Orientation

Orientation Mode: Anisotropy Parameter

Anisotropy 1: 1

Anisotropy 2: 1

Euler Angles: Phi / (°): 0, Theta / (°): 0, Psi / (°): 0

Orientation Tensor: 0.3333, 0.0000, 0.0000, 0.0, 0.3333, 0.0000, 0.0, 0.0, 0.3334

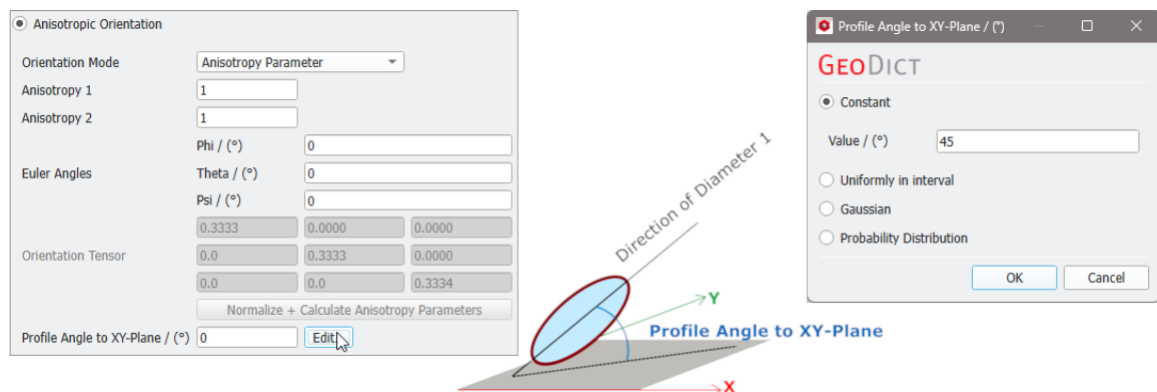
Normalize + Calculate Anisotropy Parameters

Profile Angle to XY-Plane / (°): 0 Edit...

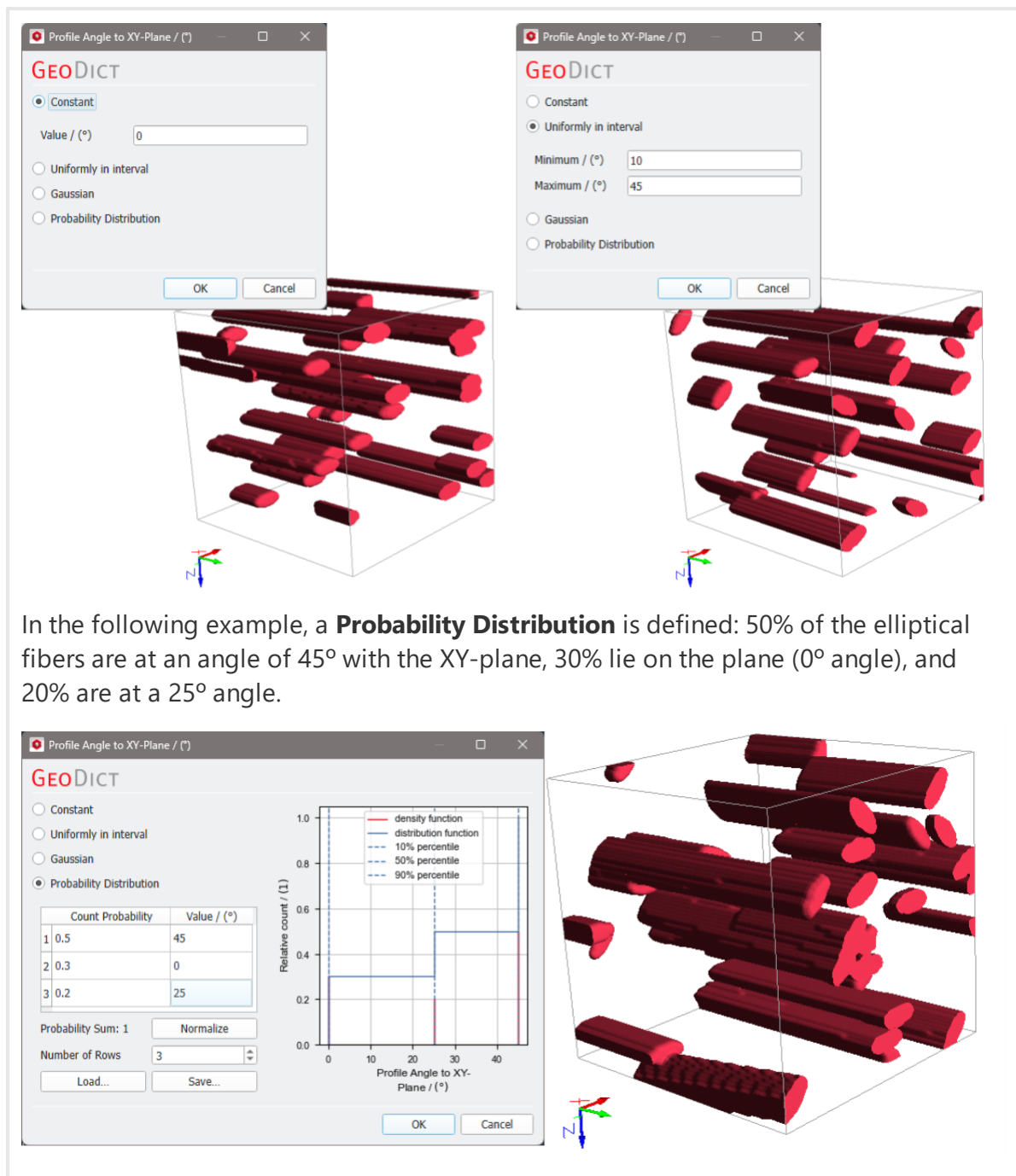
✓ Profile Angle to XY-Plane

The angle between the object cross section axis and XY-plane can be entered in the **Profile Angle to XY-Plane** dialog.

The object **Profile Angle to XY-Plane**, can be set to be a **Constant** value, or to follow a distribution (**Uniformly in interval**, **Gaussian**, or **Probability Distribution**).



Observe the effect of varying the **Profile Angle To XY-Plane** in a structure made of **Short Elliptical** fibers strongly oriented in the Y-axis (Anisotropy 1 = 1, Anisotropy 2 = 1000). Other parameters are unchanged.



In the following example, a **Probability Distribution** is defined: 50% of the elliptical fibers are at an angle of 45° with the XY-plane, 30% lie on the plane (0° angle), and 20% are at a 25° angle.

Given Directions

By checking **Given Directions**, a distribution gradient can be entered for different direction vectors for the objects in the generated structure.

☒ Given Directions

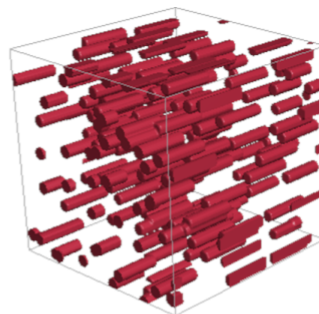
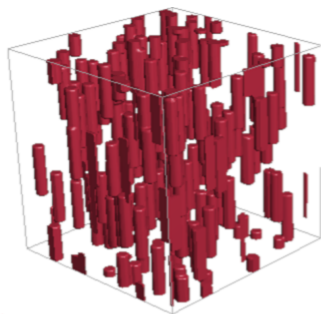
Count Probability	X-Dir.	Y-Dir.	Z-Dir.
1 1	0	0	1

Probability Sum: Normalize

Number of Rows

✓ Table: Count Probability and Number of Rows

In the left column the **Count Probability** can be entered. A value of 1 means all objects will have the given direction on the right. For example, a **Count Probability** of 1 for the direction vector 0, 0, 1 means that all objects follow the Z-direction, and 1, 0, 0 means that all objects follow the X-direction.



☒ Given Directions

Count Probability	X-Dir.	Y-Dir.	Z-Dir.
1 1	0	0	1

Probability Sum: Normalize

Number of Rows

☒ Given Directions

Count Probability	X-Dir.	Y-Dir.	Z-Dir.
1 1	1	0	0

Probability Sum: 1 Normalize

Number of Rows

If more rows are given via **Number of Rows**, every given direction will be applied to the generated objects with the corresponding count probability. In the following example observe how 80% of the short circular fibers are oriented in X-direction while the other 20% are oriented along the Z-axis.

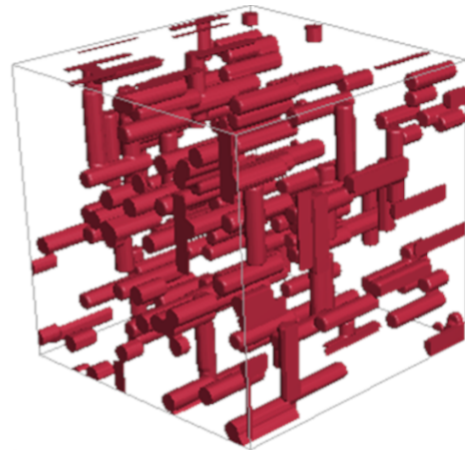
☒ Given Directions

	Count Probability	X-Dir.	Y-Dir.	Z-Dir.
1	0.2	0	0	1
2	0.8	1	0	0

Probability Sum: 1

Number of Rows: 2

Load... Normalize Save...



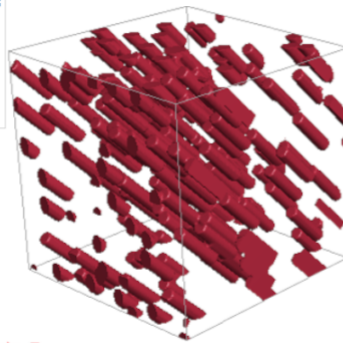
Every direction in the 3-dimensional space is possible, as seen in these examples:

	Count Probability	X-Dir.	Y-Dir.	Z-Dir.
1	1	1	0	1

Direction-tensor object type 1:

Realized direction tensor:

0.5000	0.0000	0.5000
-	0.0000	0.0000
-	-	0.5000

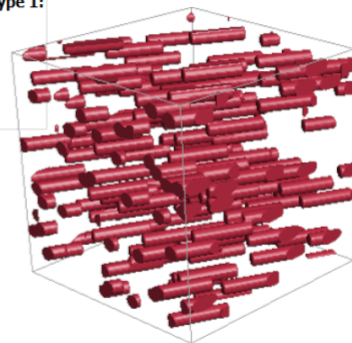


	Count Probability	X-Dir.	Y-Dir.	Z-Dir.
1	1	1	0.5	0

Direction-tensor object type 1:

Realized direction tensor:

0.8000	0.4000	0.0000
-	0.2000	0.0000
-	-	0.0000



✓ Normalize, Save and Load

Clicking the **Normalize** button ensures the **Count Probability** values sum up to one.

	Count Probability	X-Dir.	Y-Dir.	Z-Dir.
1	0.2	1	0	1
2	5	1	0.5	0
3	4	0	1	1

Probability Sum: 9.2

Normalize

	Count Probability	X-Dir.	Y-Dir.	Z-Dir.
1	0.0217391304	1	0	1
2	0.543478261	1	0.5	0
3	0.434782609	0	1	1

Probability Sum: 1

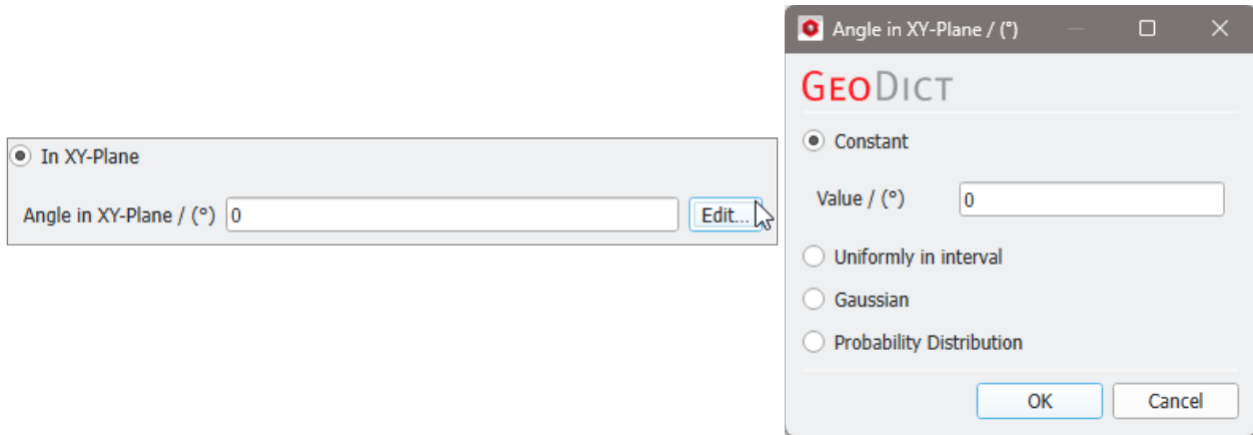
Normalize

The **Given Directions** distribution settings can be saved as text file and loaded by clicking **Save** and **Load**, respectively.

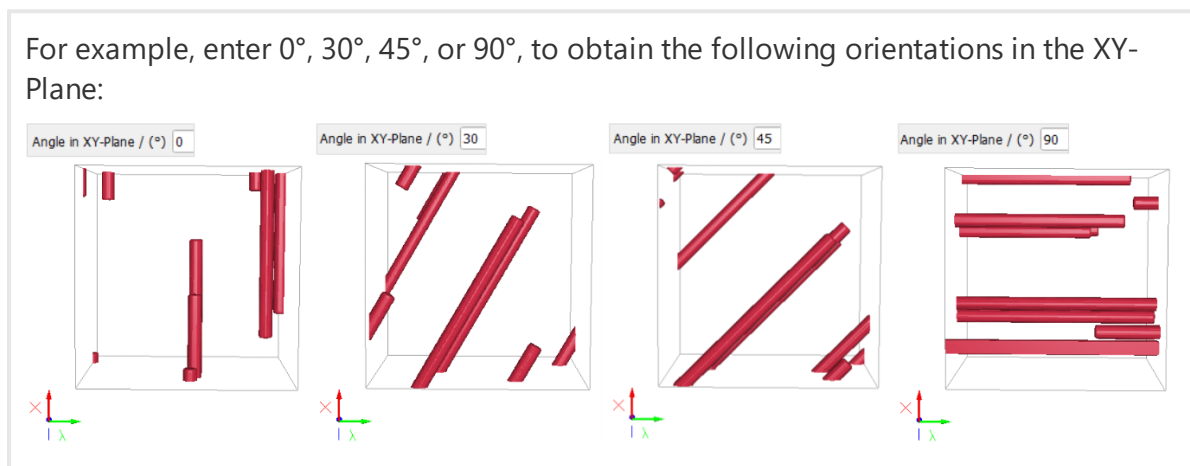
Load... Save...

In XY-Plane

By checking **In XY-Plane**, the angle of the objects main axis in the XY-Plane can be set. The objects lie in the XY-Plane and their main axis orientation in relation to the X-direction is controlled by the entered value. The **Angle in XY-Plane** can be set to be a **Constant** value, or to follow a distribution (**Uniformly in interval**, **Gaussian**, or **Probability Distribution**).



✓ Example



Angle Around Direction

If **Angle Around Direction** is checked, define the **Main Direction Vector** of the objects generated in the structure. The orientation of the objects can vary if an **Angle Around Direction** is given.

The **Angle Around Direction** defines the maximum angle the object orientation varies from the **Main Direction**. The **Angle Around Direction** can be set to be a **Constant** value, or to follow a distribution (**Uniformly in interval**, **Gaussian**, or **Probability Distribution**).

☒ Angle Around Direction

Main Direction Vector

Angle Around Direction / (°) [Edit...](#)

GEODict

☒ Constant

Value / (°)

☐ Uniformly in interval

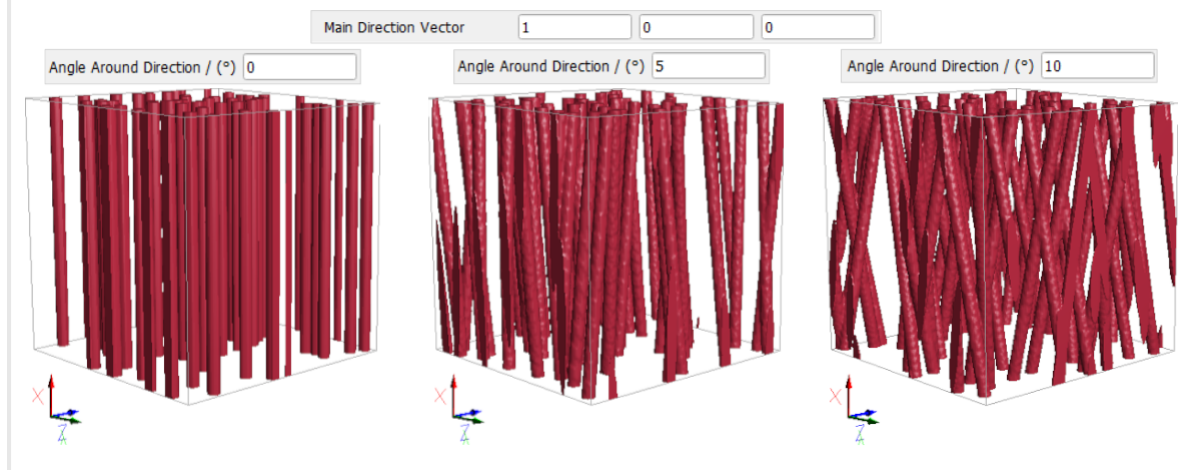
☐ Gaussian

☐ Probability Distribution

[OK](#) [Cancel](#)

✓ Example

Observe how the orientation varies in the following example with angles around direction of 0°, 5°, and 10° together with a **Main Direction Vector** of (1, 0, 0).



Distribution

Many object parameters, as for example the **Diameter**, the **Ray Length**, the **Side Length**, the **Wall Thickness**, and the **Scaling Factor** (for **Combined Objects**) can be set to a **Constant** value, or to follow a distribution (**Uniformly in interval**, **Gaussian**, **Probability Distribution** (user-defined), or **Log-Normal**).

Diameter / (μm)

GEODict

☒ Constant

Value / (μm)

☐ Uniformly in interval

☐ Gaussian

☐ Probability Distribution

☐ Log-Normal

[OK](#) [Cancel](#)

Length / (μm)

GEODict

☒ Constant

Value / (μm)

☐ Uniformly in interval

☐ Gaussian

☐ Probability Distribution

☐ Log-Normal

[OK](#) [Cancel](#)

Ray Length / (μm)

GEODict

☒ Constant

Value / (μm)

☐ Uniformly in interval

☐ Gaussian

☐ Probability Distribution

☐ Log-Normal

[OK](#) [Cancel](#)

Scaling Factor / (1)

GEODict

☒ Constant

Value / (1)

☐ Uniformly in interval

☐ Gaussian

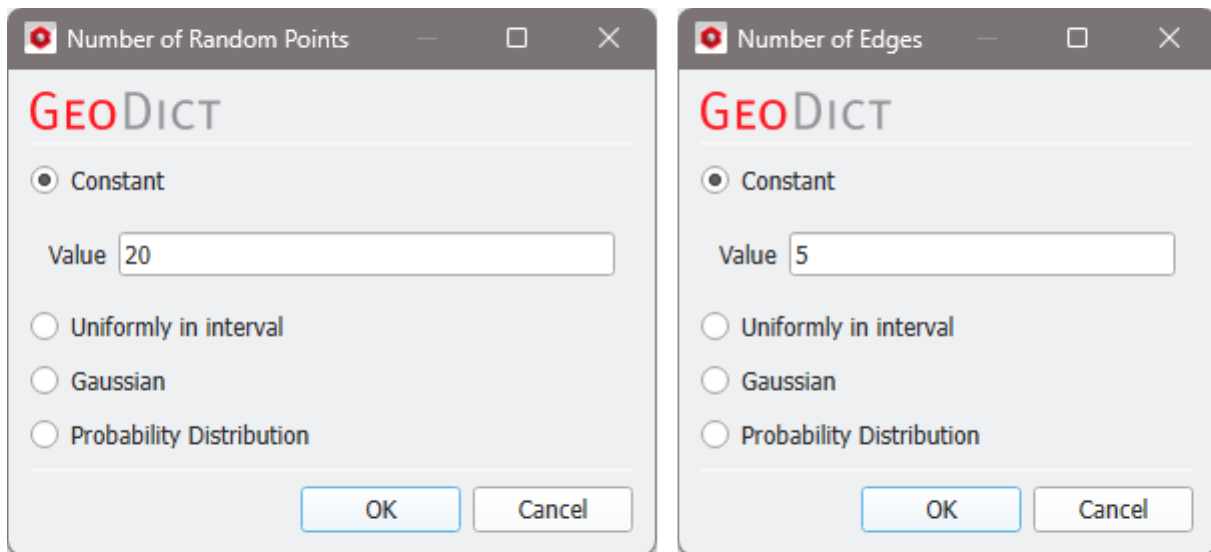
☐ Probability Distribution

☐ Log-Normal

[OK](#) [Cancel](#)

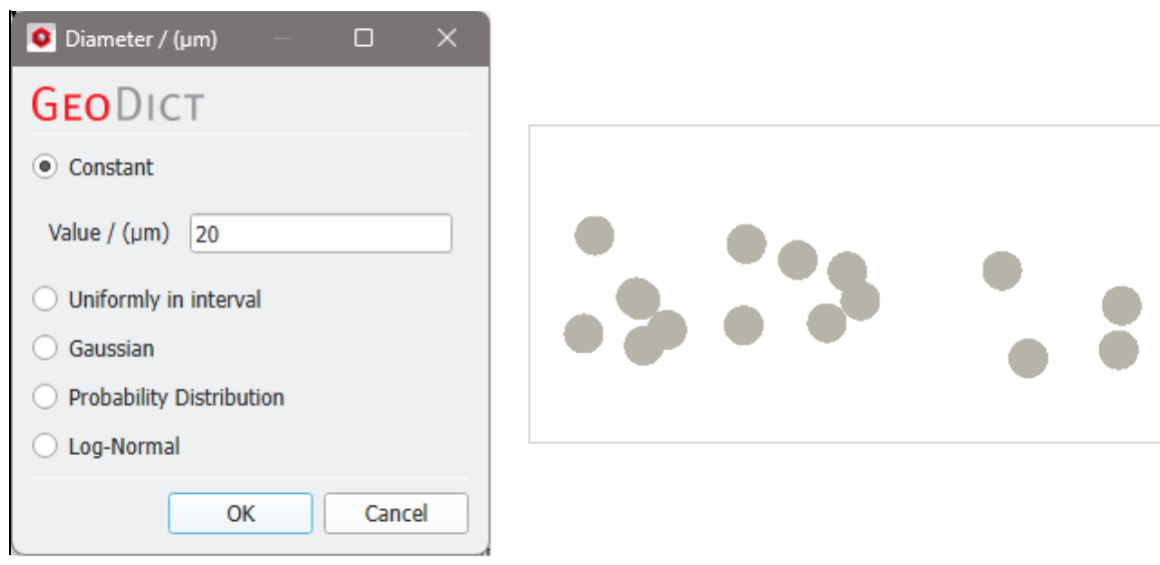
Other parameters as for example the **Number of Edges** (for **Planar Polyhedrons**) and the **Number of Random Points** (for **Convex Polyhedrons**) values can also set to be **Constant**, to

distribute **Uniformly in interval**, or to follow a **Gaussian** or user-defined **Probability Distribution**.



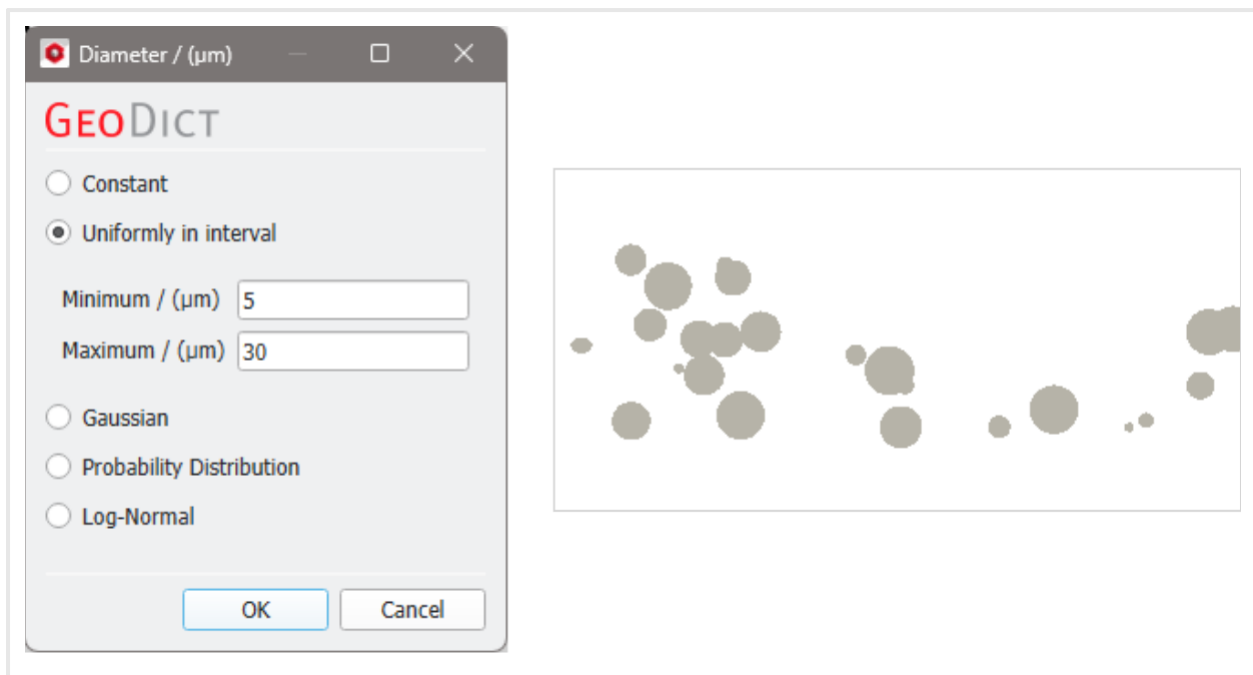
✓ Constant

Observe the effect of choosing the diameter to be **Constant** in the following example with only circular cross-section fibers. The generated structures are shown as 2D cross-section. To better observe the circular cross-section in 2D view, the fibers are all oriented perpendicular to the view direction.



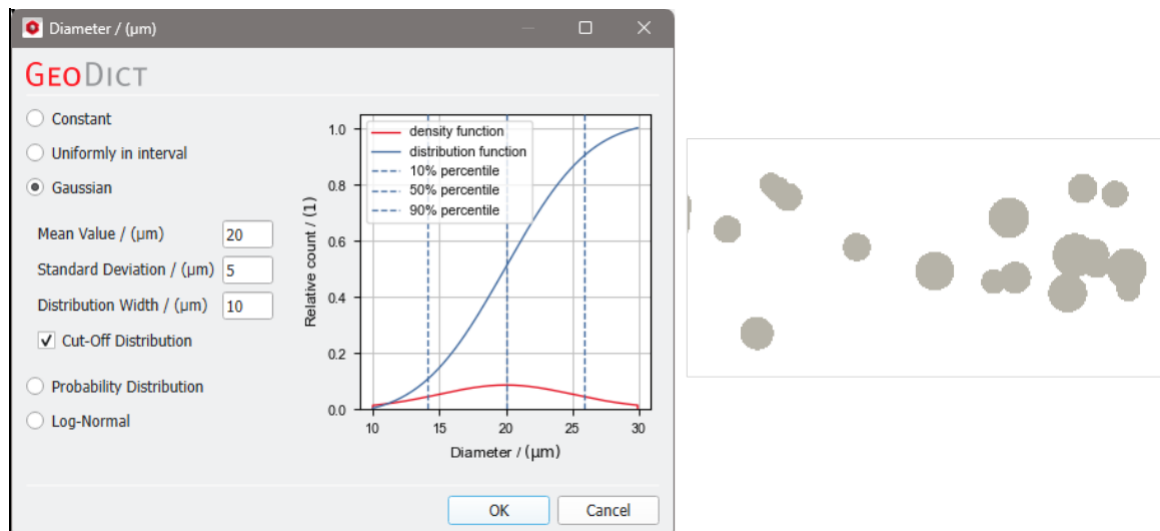
✓ Uniformly in interval

When selecting **Uniformly in interval**, and entering a **Minimum** value and a **Maximum** value, the random diameters are distributed within the given interval and every feasible diameter has the same probability.



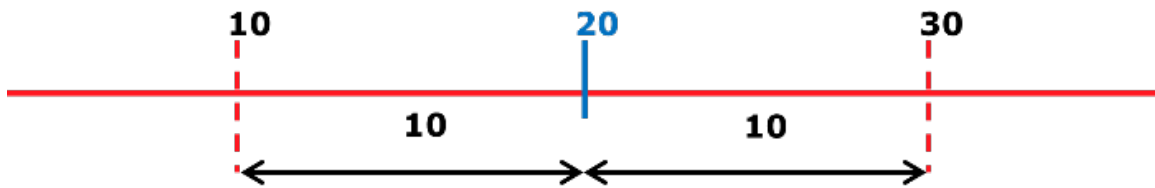
✓ Gaussian

Taking the **Gaussian** distribution, the random diameter, length, or side length values follow a bell-shaped distribution. The values cluster around the entered **Mean Value** but may vary according to the entered **Standard Deviation**.



The value in **Distribution Width** corresponds to the interval on both sides of the mean value limiting the random diameter or angle values that are accepted.

As an example, a **Distribution Width** value of 10 means that the values may vary only - 10 to +10 from the given **Mean Value**.



You can set the parameters so that negative values would be possible. Then, the negative values are ignored and only the range of possible values is generated. For example, a mean value of 20 and a distribution width of 25 would lead to values between 1 and 45.

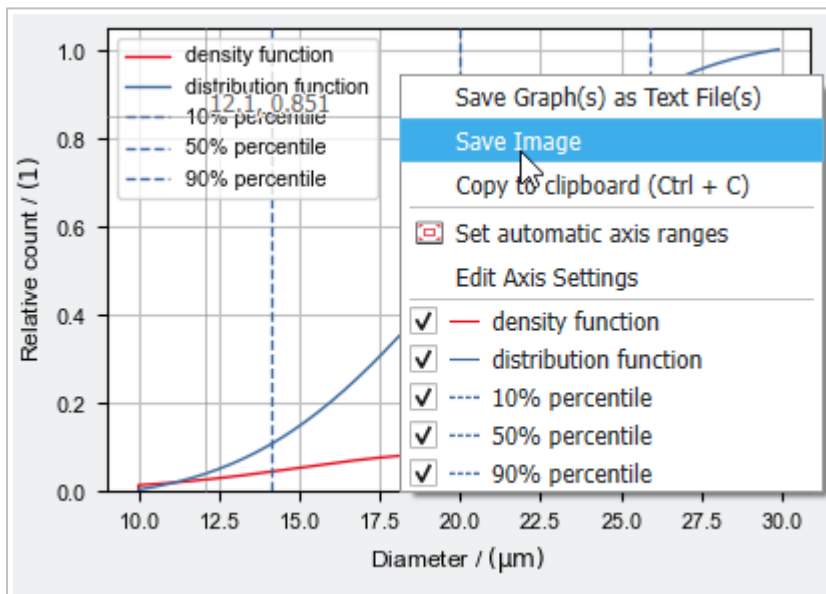
For all distribution options (Gaussian, Probability Distribution and Log-Normal) on the right of the dialog the distribution is visualized in a 2D plot.

The **red** line shows the density distribution defined by Mean Value, Standard Deviation and Distribution Width. It displays how many objects of which diameter will be generated in percent. The **blue** curve shows the cumulative distribution.

The three **dashed blue** lines show the diameter values for 10% percentile, 50% percentile and 90% percentile of the distribution. For example, if the distribution is given for diameters as shown in the screenshot above, on average, 10% of the objects have a diameter smaller than 14 μm (10% percentile), and 90% of the generated objects have a diameter smaller than 26 μm (90% percentile). For further explanations, see the [Wikipedia](#) article.

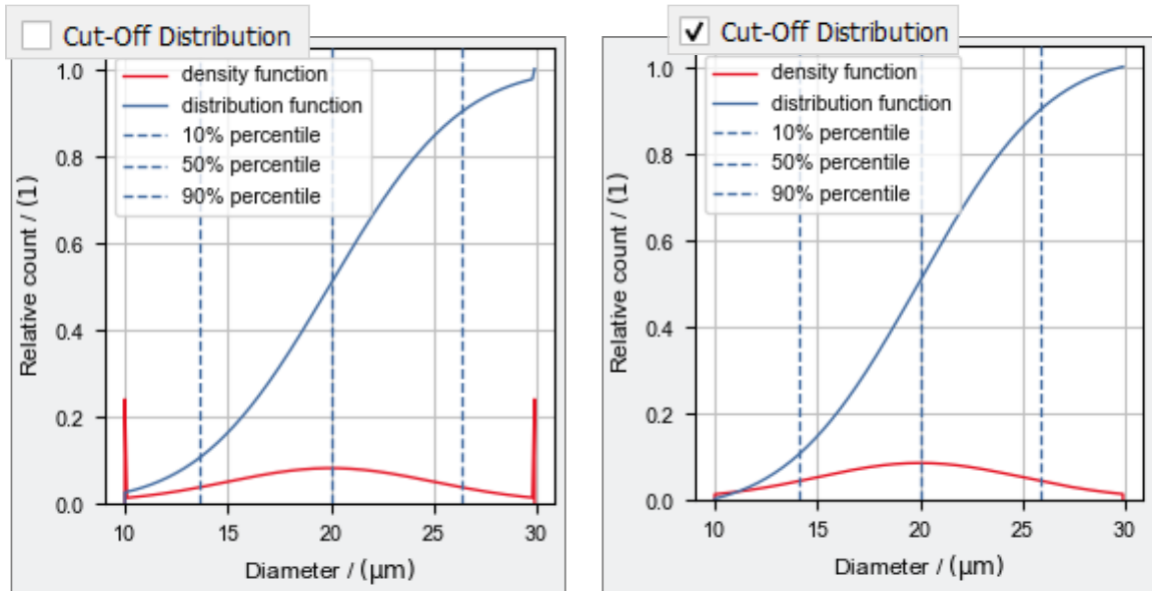
Right-clicking into the plot opens a dialog to **save** the plot or to **Edit the Axis Settings**. Checking or unchecking the checkboxes next to the graph names decides which curves should be displayed.

More information about these options can be found in the [Result Viewer](#) User Guide.

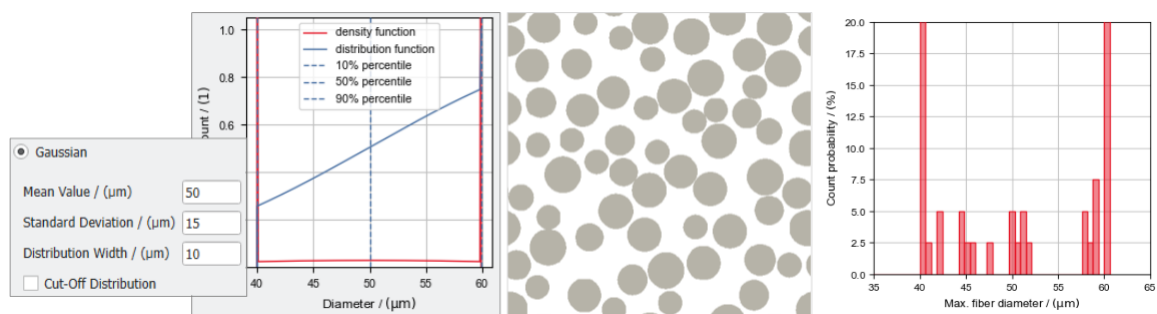


If **Cut-Off Distribution** is checked, the distribution is truncated at the bounds. This means, that all values outside the bounds are dropped and not considered for

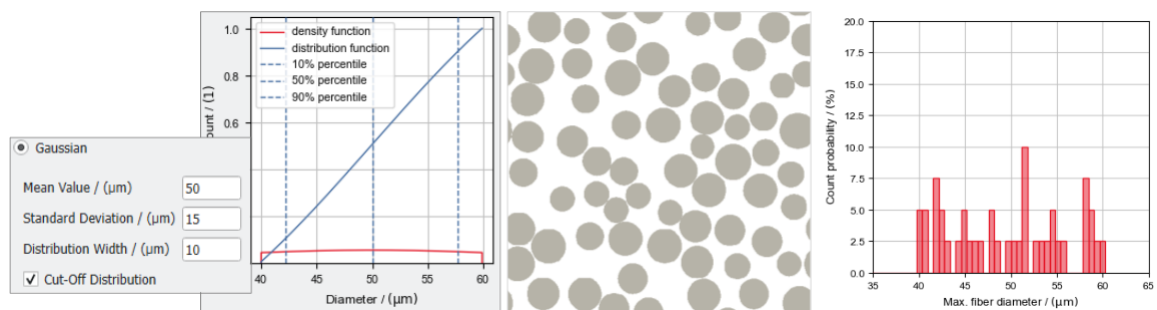
generation. If this option is not checked, then all values that are outside of the bounds are set to be on the distribution bound. Not checking this option leads to an accumulation of values on the bounds.



In the following example, leaving **Cut-Off Distribution** unchecked leads to many objects with diameters of 40 or 60 μm .



In contrast, checking **Cut-Off Distribution** leads to more grains with diameter of 50 μm .



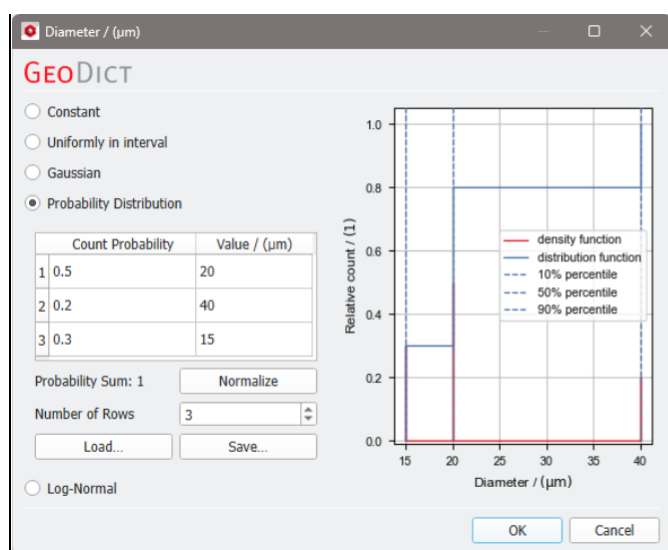
Further details on Gaussian distributions can be found, e.g., on [Wikipedia](https://en.wikipedia.org/wiki/Normal_distribution) on Normal (or Gaussian) distributions.

✓ Probability Distribution

The **Probability Distribution** table allows to enter user-defined probability distributions. The **Number of Rows** can be increased or decreased to enter as many value pairs as desired. The **Value** corresponds to the chosen property, e.g., diameter, length, or angle. The **Count Probability** of the values must lay between 0 and 1 and their sum must be equal to 1.

Especially for large tables, it is useful to observe the value of **Probability Sum**, i.e., the sum of the count probabilities. When the **Probability Sum** is not equal to 1, click the **Normalize** button to automatically round the **Count Probability** values.

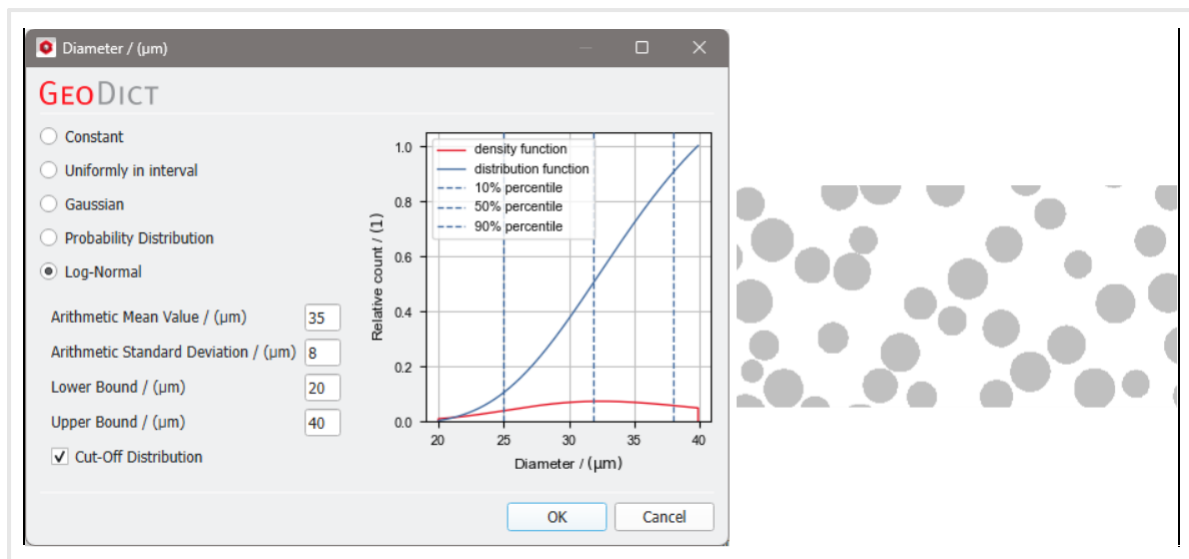
The buttons **Load** and **Save** allow loading a previous probability distribution and saving the current one for later use.



✓ Log-Normal

The **Log-Normal** distribution describes the situation in which the logarithm of the diameter values follows a normal distribution.

The diameter values group around the entered **Arithmetic Mean Value** and scatter according to the entered **Arithmetic Standard Deviation**. The values in **Lower Bound** and **Upper Bound** restrict the possible values that the random diameters can take to the given interval.



Object Overlap

The **Object Overlap** tab contains options dealing with how to define the Material ID in locations where materials in the structure overlap. The overlap locations may exhibit other properties than those of the original materials.

	Material ID 1	Material ID 2	Overlap Material ID
1	01 Glass (Solid)	01 Glass (Solid)	01 Glass (Solid)

✓ Material ID Mode

Through the **Material ID Mode**, select between applying the Material ID based on the materials or the types of objects present in the structure.

✓ Resolve Overlap

If **Resolve Overlap** is checked, the overlap of objects is not assigned to a new Material

ID. Instead, the water-shed algorithm is used to decide which of the overlap voxels belongs to which object in a post-processing step. Thus, each overlap voxel is assigned to one specific object. This option needs more memory and a longer run-time.

In detail, the **Resolve Overlap** algorithm starts with computing a distance map for the overlap voxels, i.e., it computes the distance to the next object for each overlap voxel. On this distance map the watershed algorithm is run using all voxels belonging to an object as seeds. There, all voxels contained in the same object have the same Material ID. Thus, the overlap area is filled with the object IDs according to the distance map.

To mark the contact voxels between the objects with a separate Material ID, select **Mark Contact Voxels** and choose a **Contact Material** from the **Material Database**.

The voxels, where two or more objects IDs meet, are marked as contact voxels, by reassigning them with a new Material ID. Thus, the layer of contact voxels always has a thickness of two voxels.

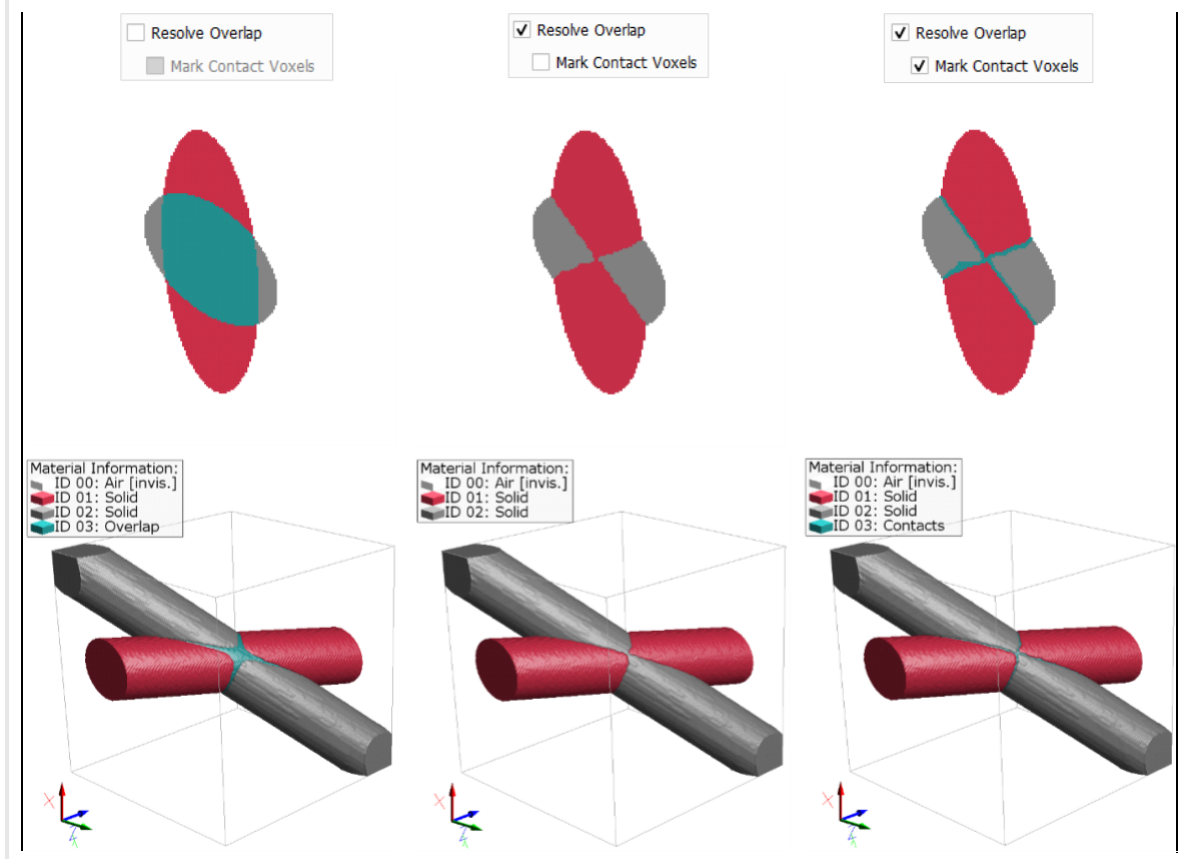
☒ **Resolve Overlap**

☒ **Mark Contact Voxels**

Contact Material (ID 03)

Contact (Solid)...

In the following observe the resulting Material IDs for the overlap for not resolved, resolved and resolved overlap with marked contact voxels, while all other settings are kept the same.



✓ Overlap Rules and Default Overlap Material

Default Overlap Material controls the material assigned to the regions where objects of the generated structure overlap and is only available if [Resolve Overlap](#)⁸⁷ is disabled. The Material ID of these regions is chosen by default as the next available Material ID. The material can be changed by clicking on the button.

Overlap rules can be set to control how the overlap between Material IDs should be handled in the structure. You can set up to 100 rules by selecting a number in the box for **Number of Overlap Rules**, and then define these rules in the panel below.

The materials shown in the panel (as buttons or pull-down menu) correspond to the materials selected under the **Object Options** tab.

For example, you simulate a structure made of plastic fibers that melt together using a negative **isolation distance** as a **Generation and Overlap Mode** under the **Create Options** tab. Then, you can set up a rule that defines what happens with the Material ID at the melting location.

In the example shown below, three rules have been defined: The overlap of objects with Material ID 1 (dark red) will be assigned to ID 3 (turquoise). The overlap of objects with Material ID 2 (gray) will be assigned to ID 4 (blue) and the overlap of ID 1 and ID 2 will be assigned to ID 5 (purple). For all other possible overlap cases, the **Default Overlap Material ID** is applied.

Number of Overlap Rules

	Material ID 1	Material ID 2	Overlap Material ID
1	01 Glass (Solid) ▾	01 Glass (Solid) ▾	03 Glass (Solid) ▾
2	02 Glass (Solid) ▾	02 Glass (Solid) ▾	04 Solid ▾
3	01 Glass (Solid) ▾	02 Glass (Solid) ▾	05 Solid ▾

✓ Overlap Results

Note, that the results for volume in the resulting report do not change for different overlap rules, as the values are computed before the post-processing is applied.

In the three examples given for **Resolve Overlap**, the **Absolute object distribution** is shown below.

Absolute object distribution:

	Count	Volume / (%)	Grammage / (g/m ²)	Density / (g/cm ³)	Weight / (%)
Total	realized: 2 target: 2 error: 0.00	realized: 11.09 target: --- error: ---	realized: --- target: --- error: ---	realized: --- target: --- error: ---	realized: --- target: --- error: ---
Object type 1	realized: 1 target: 1 error: 0.00	realized: 4.42 target: --- error: ---	realized: --- target: --- error: ---	realized: --- target: --- error: ---	realized: --- target: --- error: ---
Object type 2	realized: 1 target: 1 error: 0.00	realized: 6.68 target: --- error: ---	realized: --- target: --- error: ---	realized: --- target: --- error: ---	realized: --- target: --- error: ---

For the volume percentages of the final structure, refer to the **Statistics** in the left of the GeoDict main window. Either just hover over the statistics bar or unfold the Statistics section in the project status panel below.

Here, the volume statistics are shown for the example with default overlap rules. The red fiber has 3.55% of the volume, the gray fiber has 5.81% and the overlap 1.73%.

In the result file the overlap volume is proportionally added to the volume of the overlapping fibers. Here, the red fiber obtains $3.55\% + (1.73/2)\% = 4.415\%$. Rounded, this results in the 4.42% shown in the report.

88.9

C:/User Guide

Structure (200x200x200, 1 µm)

GAD Objects (2)

Statistics

3D

GAD Objects : 2

Material IDs

00 88.91 % (7112422 Voxel)

01 3.55 % (284224 Voxel)

02 5.81 % (465160 Voxel)

03 1.73 % (138194 Voxel)

Statistics for 3D Geometry

GAD Objects 3D: 2

	Volume %	Voxel Number
Material ID00	88.91	7112422
Material ID01	3.553	284224
Material ID02	5.815	465160
Material ID03	1.727	138194
Porosity	88.91	7112422
Air	88.91	7112422
Solid Volume	11.09	887578
Manual 1	3.553	284224
Manual 2	5.815	465160
Manual 3	1.727	138194



Result Options

The generated structure is always saved as a **GeoDict structure file (*.gdt)** (GeoDict binary data). The file is placed in an automatically created result folder inside the chosen project folder (**File** → **Choose Project Folder...** in the menu bar).

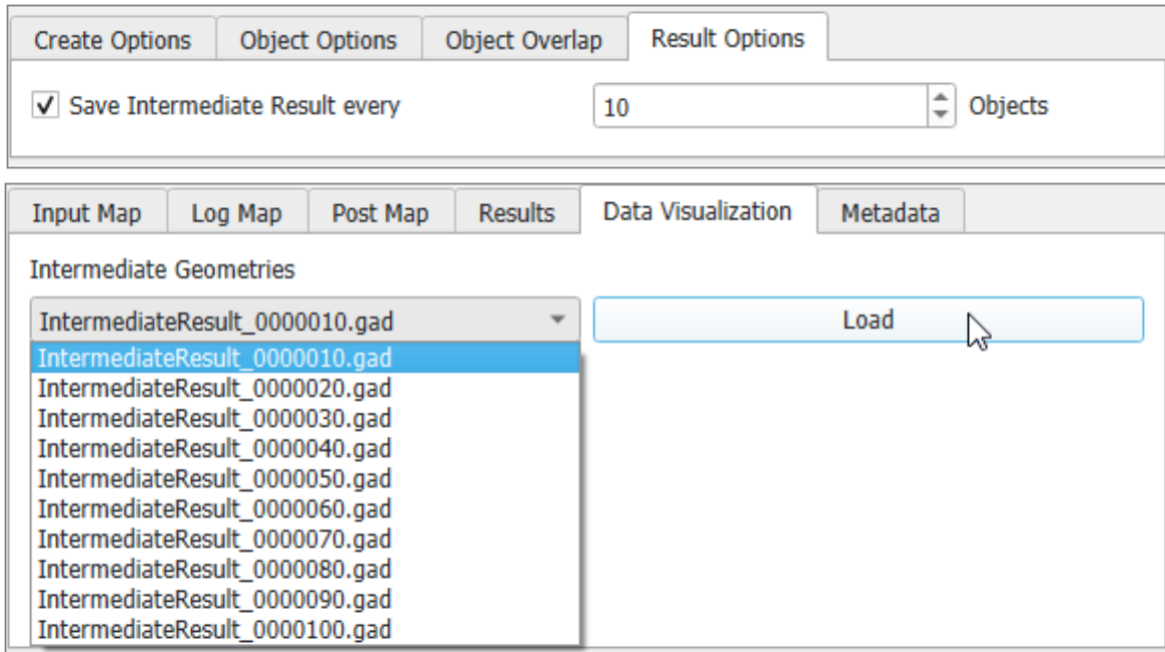
The result file as well as the result folder take the name entered as **Result File Name (*.gdr)** at the top of the dialog.

An additional option to save the generated structure data is to check **Save Intermediate Result every** and enter a number of **Objects** in the box. As objects are added to the structure during the generation, an intermediate result file is saved each time the number of placed

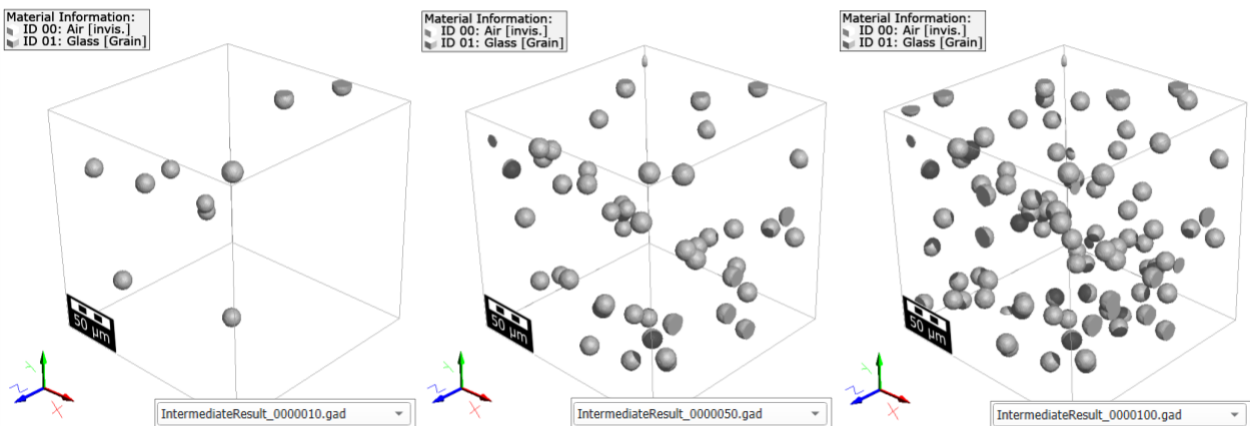
objects reaches a multiple of the entered value.

This option may be interesting when studying the properties of a series of structures with increasing density.

After running the generation, the intermediate geometries can be found as ***.gad** analytic files in the result folder and can be loaded directly from the **Result Viewer** of the *.gdr result file.



Below find an example for the creating 100 spheres. Observe how more and more objects are added.



1.1.2 Results

The generated structure is shown in the visualization area. Learn more about visualization in GeoDict in the **Visualization** chapter.

The result file is automatically opened in the Result Viewer and shows structure statistics in the **Results-Report** and **Results-Plot** tabs. Additionally, it offers 3D **Data Visualization** options depending on the generation settings. Find more information on GeoDict result files in the **Result Viewer** chapter.

Results

✓ Report

The first two tables show the **Absolute** and **Relative object distribution** for all object types.

Input Map	Log Map	Post Map	Results	Data Visualization	Metadata
Report	Plots	Map			
Absolute object distribution:					
	Count	Volume / (%)	Grammage / (g/m ²)	Density / (g/cm ³)	Weight / (%)
Total	realized: 1794 target: --- error: ---	realized: 34.99 target: 35.00 error: -0.01	realized: --- target: --- error: ---	realized: --- target: --- error: ---	realized: --- target: --- error: ---
Object type 1	realized: 992 target: --- error: ---	realized: 17.47 target: 17.50 error: -0.03	realized: --- target: --- error: ---	realized: --- target: --- error: ---	realized: --- target: --- error: ---
Object type 2	realized: 801 target: --- error: ---	realized: 17.52 target: 17.50 error: 0.02	realized: --- target: --- error: ---	realized: --- target: --- error: ---	realized: --- target: --- error: ---
Stopping criterion error: -0.016 %					
Relative object distribution:					
	Count / (%)	Volume / (%)	Weight / (%)		
Object type 1	realized: 55.35 target: --- error: ---	realized: 49.93 target: 50.00 error: -0.14%	realized: --- target: --- error: ---		
Object type 2	realized: 44.65 target: --- error: ---	realized: 50.07 target: 50.00 error: 0.14%	realized: --- target: --- error: ---		
Maximal probability error: 0.14 %					

Afterwards follows a section regarding the overlap between different object types.

Overlap Information:

Overlap of objects of different type: 3.94526 %

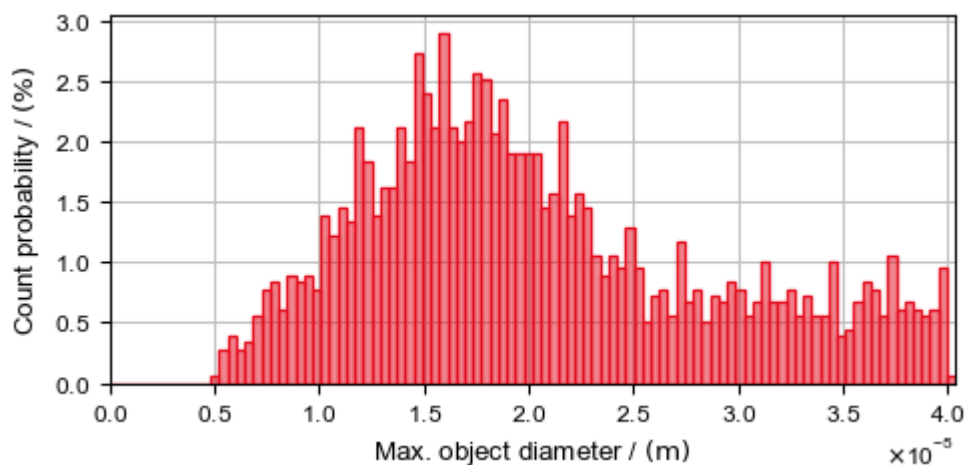
(This overlap may be handled in the geometry post-processing, by the specified overlap rules or by resolve overlap. Both options may change the object type volume fractions.)

Then, the realized, the target, and the error direction tensors for all object types are given. Find below different examples of the direction tensors with isotropic orientation, anisotropy parameters, or orientation tensors.

Direction-tensor object type 1:	Direction-tensor object type 1:	Direction-tensor object type 1:																																																																																	
Anisotropy 1: Target 1.000 Anisotropy 2: Target 1.000 Realized direction tensor: <table> <tr><td>0.3320</td><td>0.0036</td><td>0.0084</td></tr> <tr><td>-</td><td>0.3338</td><td>-0.0036</td></tr> <tr><td>-</td><td>-</td><td>0.3342</td></tr> </table> Target direction tensor: <table> <tr><td>0.3333</td><td>0.0000</td><td>0.0000</td></tr> <tr><td>-</td><td>0.3333</td><td>0.0000</td></tr> <tr><td>-</td><td>-</td><td>0.3333</td></tr> </table> Error tensor: <table> <tr><td>-0.14%</td><td>0.36%</td><td>0.84%</td></tr> <tr><td>-</td><td>0.05%</td><td>-0.36%</td></tr> <tr><td>-</td><td>-</td><td>0.09%</td></tr> </table>	0.3320	0.0036	0.0084	-	0.3338	-0.0036	-	-	0.3342	0.3333	0.0000	0.0000	-	0.3333	0.0000	-	-	0.3333	-0.14%	0.36%	0.84%	-	0.05%	-0.36%	-	-	0.09%	Anisotropy 1: Target 100.000 Anisotropy 2: Target 1.000 Realized direction tensor: <table> <tr><td>0.5026</td><td>-0.0276</td><td>-0.0003</td></tr> <tr><td>-</td><td>0.4970</td><td>0.0000</td></tr> <tr><td>-</td><td>-</td><td>0.0004</td></tr> </table> Target direction tensor: <table> <tr><td>0.4998</td><td>0.0000</td><td>0.0000</td></tr> <tr><td>-</td><td>0.4998</td><td>0.0000</td></tr> <tr><td>-</td><td>-</td><td>0.0004</td></tr> </table> Error tensor: <table> <tr><td>0.28%</td><td>-2.76%</td><td>-0.03%</td></tr> <tr><td>-</td><td>-0.28%</td><td>0.00%</td></tr> <tr><td>-</td><td>-</td><td>0.00%</td></tr> </table>	0.5026	-0.0276	-0.0003	-	0.4970	0.0000	-	-	0.0004	0.4998	0.0000	0.0000	-	0.4998	0.0000	-	-	0.0004	0.28%	-2.76%	-0.03%	-	-0.28%	0.00%	-	-	0.00%	Realized direction tensor: <table> <tr><td>0.8080</td><td>0.0029</td><td>-0.0074</td></tr> <tr><td>-</td><td>0.0934</td><td>0.0000</td></tr> <tr><td>-</td><td>-</td><td>0.0986</td></tr> </table> Target direction tensor: <table> <tr><td>0.8000</td><td>0.0000</td><td>0.0000</td></tr> <tr><td>-</td><td>0.1000</td><td>0.0000</td></tr> <tr><td>-</td><td>-</td><td>0.1000</td></tr> </table> Error tensor: <table> <tr><td>0.80%</td><td>0.29%</td><td>-0.74%</td></tr> <tr><td>-</td><td>-0.66%</td><td>0.00%</td></tr> <tr><td>-</td><td>-</td><td>-0.14%</td></tr> </table>	0.8080	0.0029	-0.0074	-	0.0934	0.0000	-	-	0.0986	0.8000	0.0000	0.0000	-	0.1000	0.0000	-	-	0.1000	0.80%	0.29%	-0.74%	-	-0.66%	0.00%	-	-	-0.14%
0.3320	0.0036	0.0084																																																																																	
-	0.3338	-0.0036																																																																																	
-	-	0.3342																																																																																	
0.3333	0.0000	0.0000																																																																																	
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-	-	0.3333																																																																																	
-0.14%	0.36%	0.84%																																																																																	
-	0.05%	-0.36%																																																																																	
-	-	0.09%																																																																																	
0.5026	-0.0276	-0.0003																																																																																	
-	0.4970	0.0000																																																																																	
-	-	0.0004																																																																																	
0.4998	0.0000	0.0000																																																																																	
-	0.4998	0.0000																																																																																	
-	-	0.0004																																																																																	
0.28%	-2.76%	-0.03%																																																																																	
-	-0.28%	0.00%																																																																																	
-	-	0.00%																																																																																	
0.8080	0.0029	-0.0074																																																																																	
-	0.0934	0.0000																																																																																	
-	-	0.0986																																																																																	
0.8000	0.0000	0.0000																																																																																	
-	0.1000	0.0000																																																																																	
-	-	0.1000																																																																																	
0.80%	0.29%	-0.74%																																																																																	
-	-0.66%	0.00%																																																																																	
-	-	-0.14%																																																																																	

✓ Plots

A plot showing the objects' maximum diameter distribution is shown.

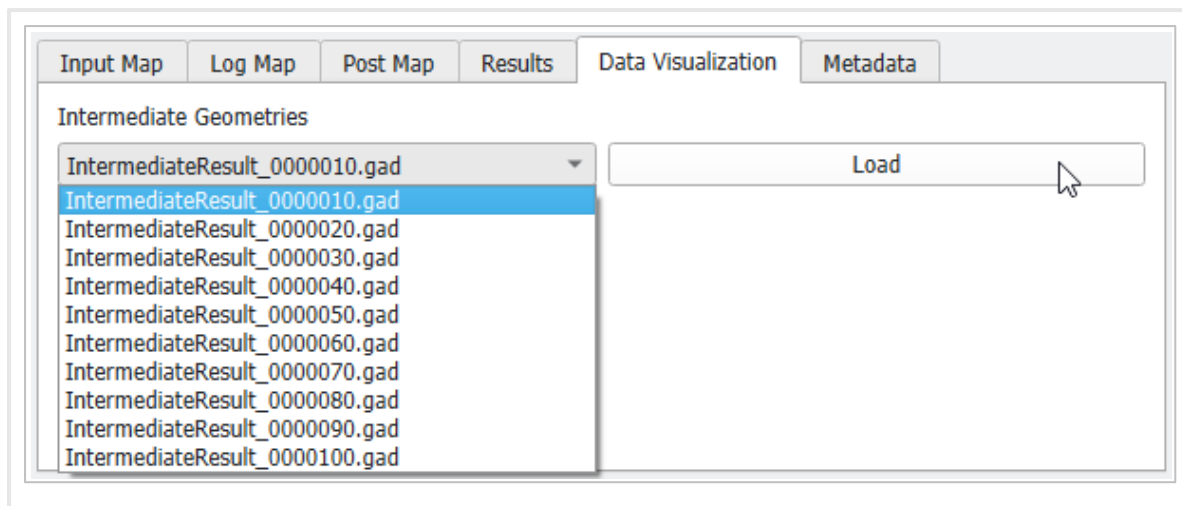


Data Visualization

Depending on the chosen parameters under the **Data Visualization** tab the following results can be visualized in 3D.

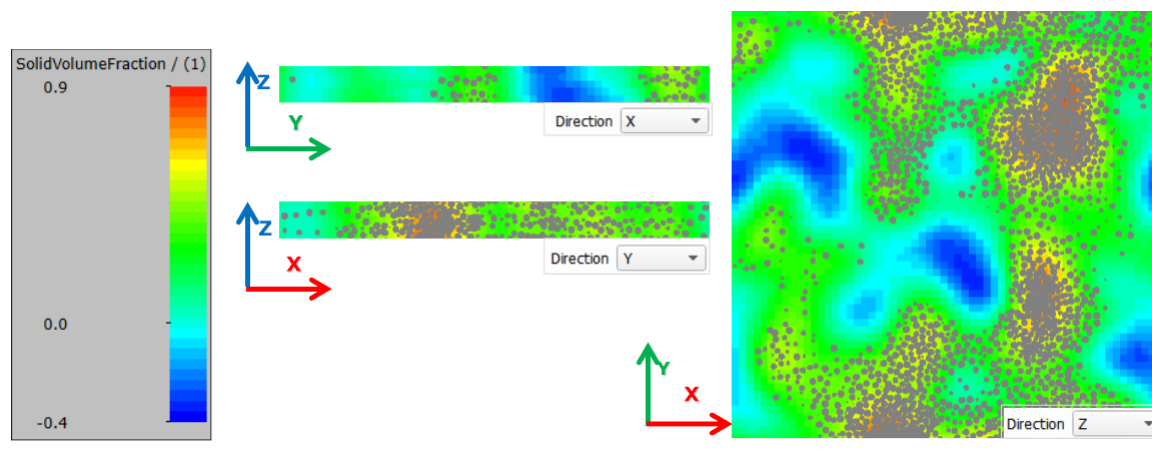
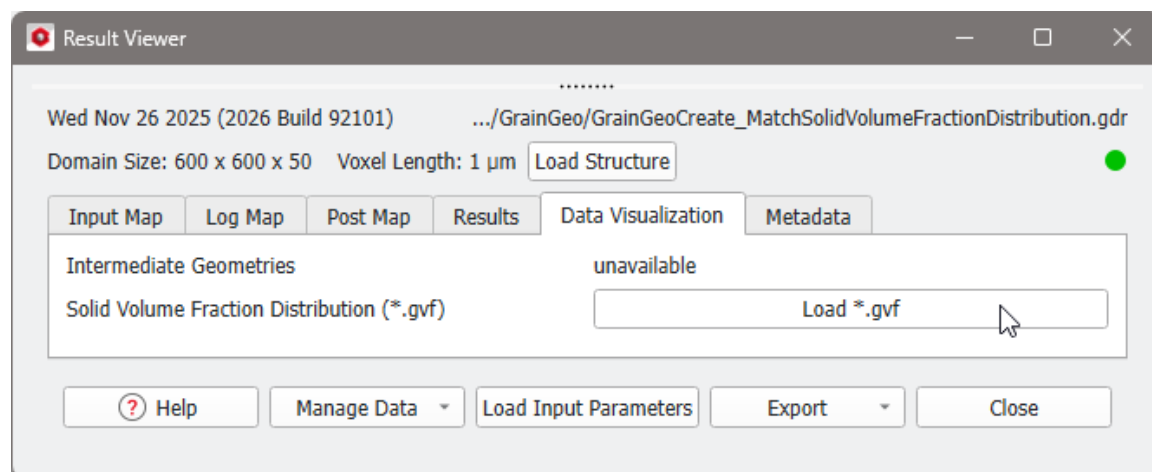
✓ Intermediate Geometries

When selecting **Save Intermediate Results every # Objects** under the **Result Options** tab, you can open the intermediate geometry files (*.gad) after selecting them in the pull-down menu.



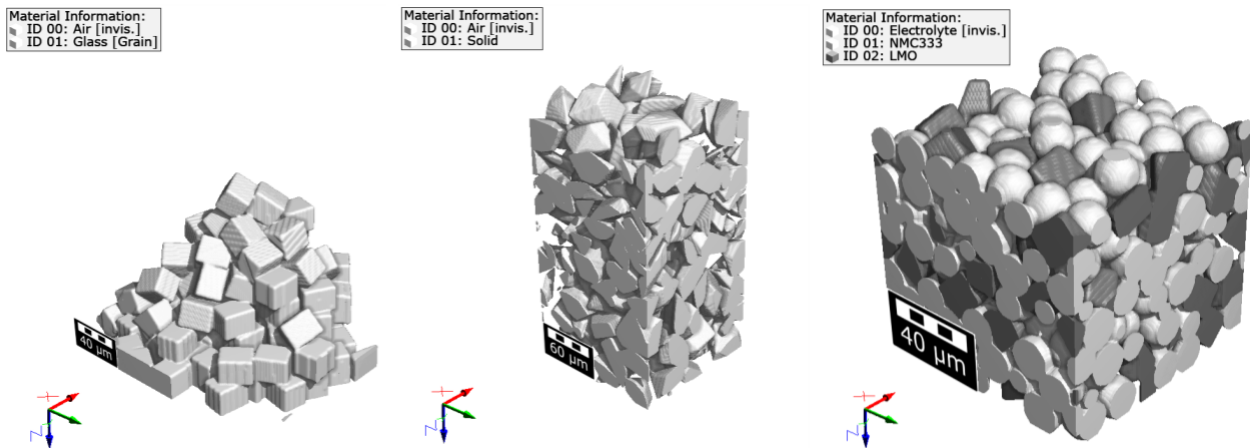
✓ Solid Volume Fraction Distribution

If **Match Solid Volume Fraction Distribution** is checked in the [Generation and Overlap Mode](#) panel under the **Create Options** tab, the volume distribution field (*.gvf) file is saved. Click **Load *.gvf** to load the volume field to the visualization area. Learn more about volume field visualization in the **Visualization** User Guide.



1.2 Pile Grains

With **Pile Grains** simulate grains falling, rotating, and finally settling to create a piled granular structure. The objects either fall from the top or from their initial position in an existing structure. The grains can be from various shapes and sizes.



The Pile Grains command:

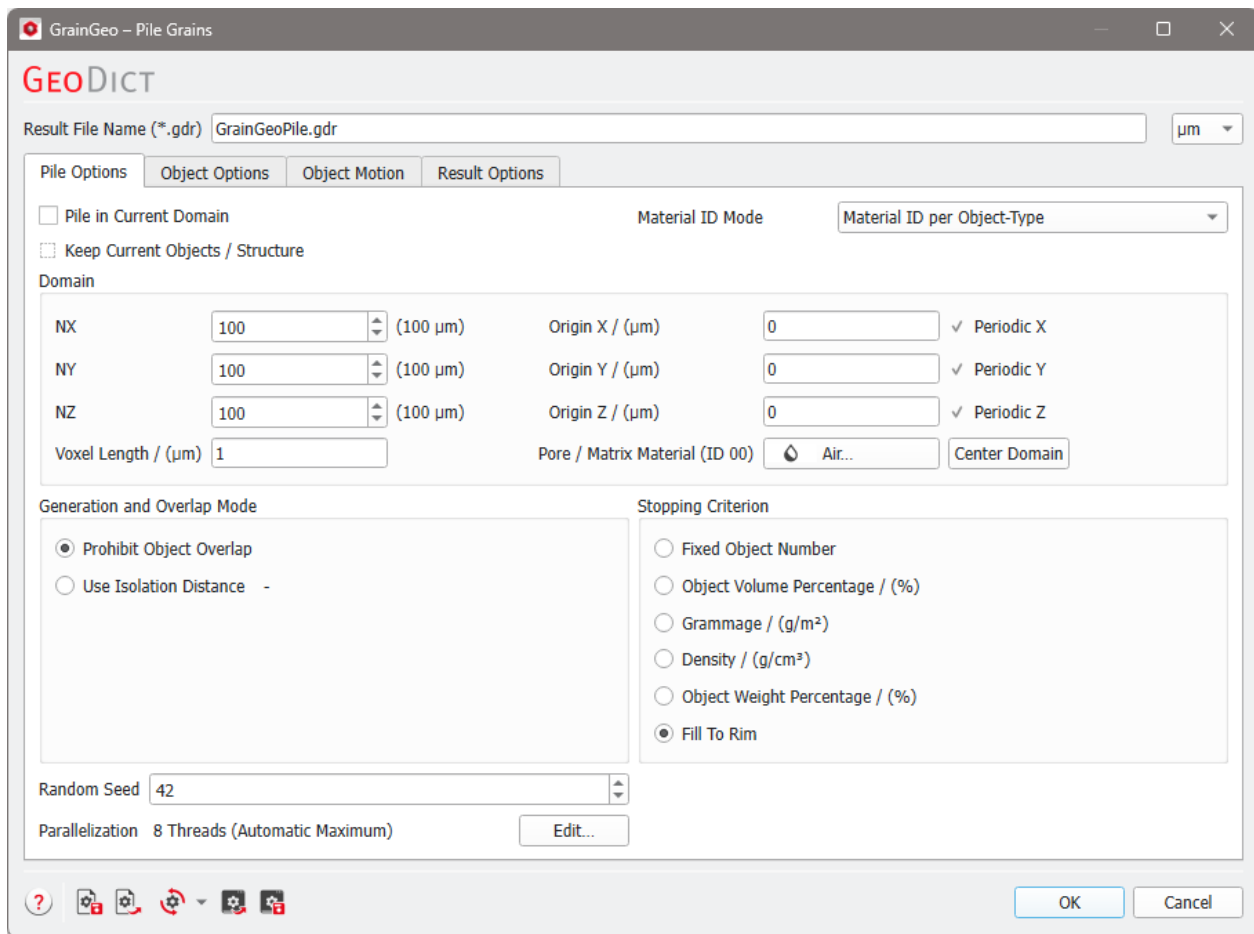
- [Options](#)⁹⁵
Set the parameters for your piling process.
- [Results](#)¹¹⁸
Inspect the result file in the Result Viewer.

1.2.1 Options

At the top left of the dialog, the name for the file containing the generation results can be entered in the **Result File Name (*.gdr)** box. The default name can be kept, or a new name can be chosen, fitting the current project.

The result files are saved in the chosen project folder (**File** → **Choose Project Folder**, in the **Menu bar**). If a GeoDict result file (*.gdr) with the given name already exists in the project folder, a warning message is shown at the start of the creation process. You can either decide to rename the chosen file name to a new one, to cancel the generation process, to overwrite or to back up the old file. When nothing is selected, GeoDict uses the **Back-Up** option after a waiting time.

The available units (m, cm, mm, μm, nm and Inch) are selectable from the pull-down menu at the top right of the dialog. When the units are changed, the entered values are adjusted automatically.



The parameters are organized into tabs:

- [Pile Options](#)^[97]
Determine physical properties of the resulting structure model such as size, resolution, overlapping mode, and object volume percentage.
- [Object Options](#)^[108]
Define the geometrical properties of individual object types such as cross-section, length, and orientation. Up to 254 different object types can be used in one structure.
- [Object Motion](#)^[109]
Control the way the objects are piled. This is done by defining, e.g., different step parameters and the initial object position.
- [Result Options](#)^[117]
Determine if intermediate geometries are saved.

Different Pile Grains Presets

In the bottom of the dialog find several helpful options.



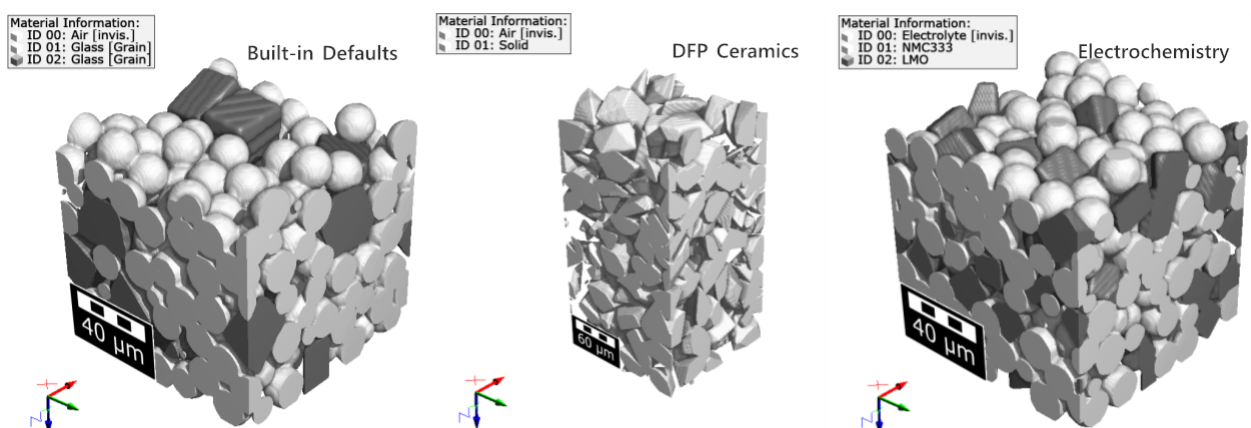
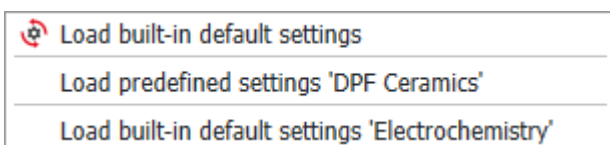
- ? Opens the corresponding User Guide section.
- Save icon Saves the settings to a GeoDict settings file (*.gps).
- Load icon Loads the settings from a GeoDict settings file (*.gps) or a GeoDict result file (*.gdr).
- Reset icon Resets all parameter settings to the built-in default settings.
- Reset icon Resets all parameter settings to the saved start-up settings.
- Save icon Saves the current parameter settings as start-up settings.

Each option is explained by a tooltip which appears when resting the mouse over the icon.

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

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

In **Pile Grains** find the presets **Electrochemistry** and **DPF Ceramics**. Choose the presets and inspect the entered parameters in the different tabs if they are a better base for your applications.



Pile Options

Determine physical properties of the resulting structure model such as size, resolution, overlapping mode, and object volume percentage.

The parameters defining the general properties of the granular structure are entered under the **Pile Options** tab. They are grouped into **Domain**, **Generation and Overlap Mode**, and

Stopping Criterion panels. Additionally, five or six single options, depending on the chosen Stopping Criterion, are available in two groups: the **Structure Options** at the top and the **General Options** at the bottom of the dialog.

The screenshot shows the 'Pile Options' tab of the GrainGeo dialog. It includes checkboxes for 'Pile in Current Domain' and 'Keep Current Objects / Structure'. The 'Material ID Mode' is set to 'Material ID per Object-Type'. The 'Domain' section has input fields for NX, NY, and NZ (all set to 100 μm), Voxel Length (1 μm), and Origin X, Y, Z (all set to 0 μm). The 'Periodic' checkboxes for X, Y, and Z are all checked. The 'Generation and Overlap Mode' section has 'Prohibit Object Overlap' selected. The 'Stopping Criterion' section has 'Fill To Rim' selected. The 'General Options' section shows 'Random Seed' as 42 and 'Parallelization' as 8 Threads (Automatic Maximum). An 'Edit...' button is at the bottom right.

The parameters are organized in the following groups:

- [Structure Options](#)^[98]
Pile in the current domain with or without keeping the current structure and define the Material ID Mode.
- [Domain](#)^[100]
Define the domain parameters, such as resolution and matrix material.
- [Generation and Overlap Mode](#)^[104]
Decide about prohibiting overlap or defining an isolation distance.
- [Stopping Criterion](#)^[104]
Define according to which criteria the piling of objects should be stopped.
- [General Options](#)^[106]
Define parallelization, temperature, and random seed for the piling process.

Structure Options

The following **Structure Options** are available:

- piling in the current domain without keeping the current objects / structure,
- piling in the current domain keeping the current objects / structure, and
- defining how the Material IDs should be set.

☐ Pile in Current Domain

Material ID Mode

Material ID per Object-Type

☐ Keep Current Objects / Structure

Pile in Current Domain and Keep Current Objects / Structure

When checking **Pile in Current Domain**, the structure currently in memory is used in combination with the newly piled structure.

Note that the domain parameters, grouped under the **Domain** panel, cannot be modified when the **Pile in Current Domain** box is checked, because they are taken from the structure already in memory.

☒ Pile in Current Domain

Material ID Mode

Material ID per Object-Type

☐ Keep Current Objects / Structure

Domain

NX	500	(500 μm)	Origin X / (μm)	0	✓ Periodic X
NY	500	(500 μm)	Origin Y / (μm)	0	✓ Periodic Y
NZ	400	(400 μm)	Origin Z / (μm)	0	✓ Periodic Z
Voxel Length / (μm) 1			Pore / Matrix Material (ID 00) Air		

✓ Example

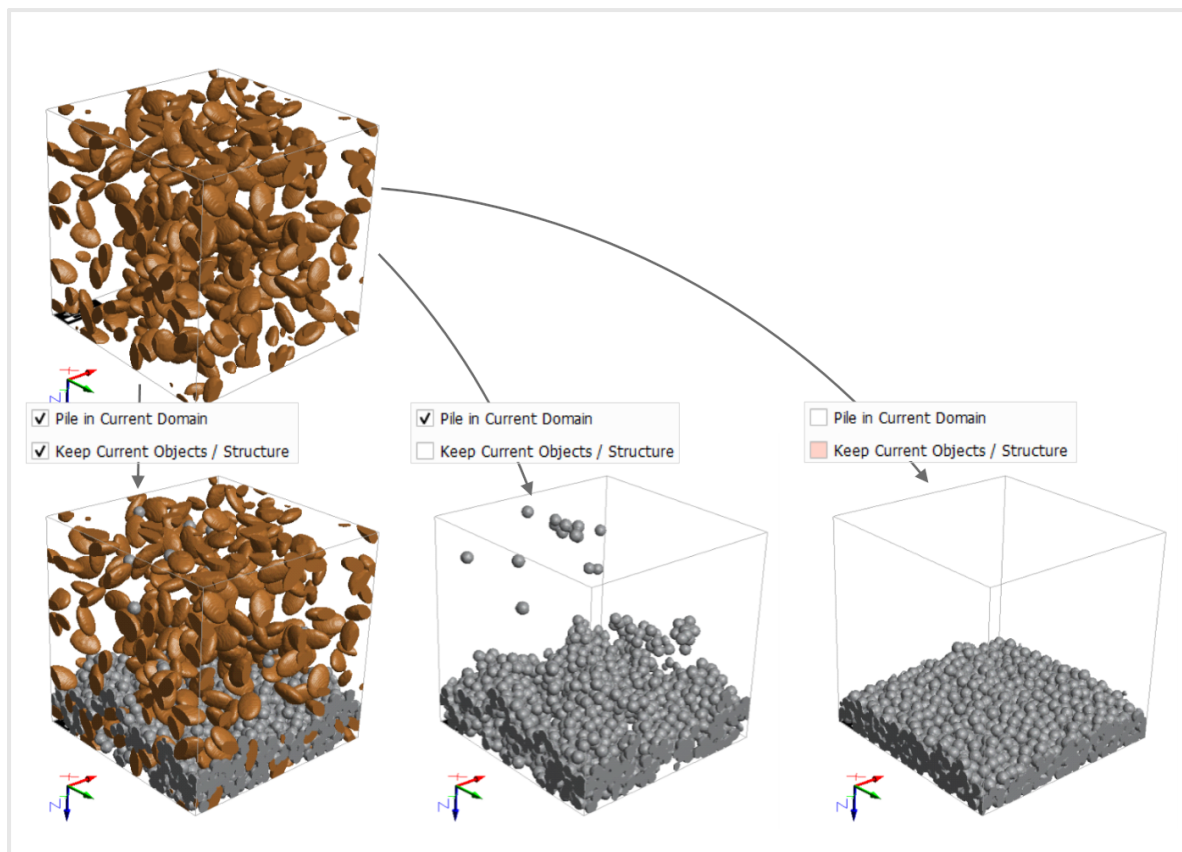
Observe the effect that checking or leaving un-checked **Pile in Current Domain** and **Keep Current Objects / Structure** has on the generation of a piled granular structure.

A structure composed of ellipsoids is already in memory when spheres fall in Z-direction.

When **Pile in Current Domain** is chosen, the new elements (gray) fall on the structure already in memory (copper).

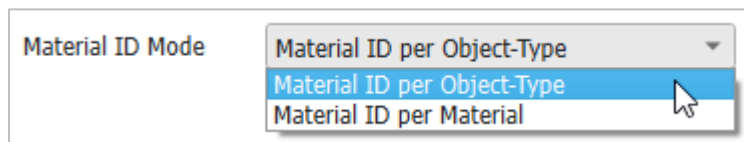
With the **Keep Current Objects / Structure** checkbox, you can decide if the copper structure is kept or deleted after piling.

When **Pile in Current Domain** is not checked, the copper structure is not considered at all and the steel spheres fall all the way to the bottom of the domain.



Material ID Mode

The **Material ID Mode** pull-down menu allows selecting between applying the Material ID based on the materials or the types of objects present in the generated structure.



Assigning a **Material ID** is part of the GeoDict Material Database concept, in which objects in the structure are ascribed to an individual material (e.g., glass, cellulose, PET) with specific physical properties.

If selecting **Material ID per Object-Type**, every object type selected under the **Object Options** tab is assigned to a different Material ID. Otherwise, the chosen material defines the Material ID. Consider for example four object types are chosen, where two of them should be of material cellulose and two should be manual. Then, with **Material ID per Material** selected, the resulting structure consists of only two solid Material IDs.

Domain

The **Domain** panel contains the parameters defining the structure size (**NX**, **NY**, and **NZ**) in combination with the resolution (**Voxel Length**), as well as the **Origin** parameters, the **Periodicity** checkboxes, the **Center Domain** button, and the **Pore / Matrix Material** pull-down

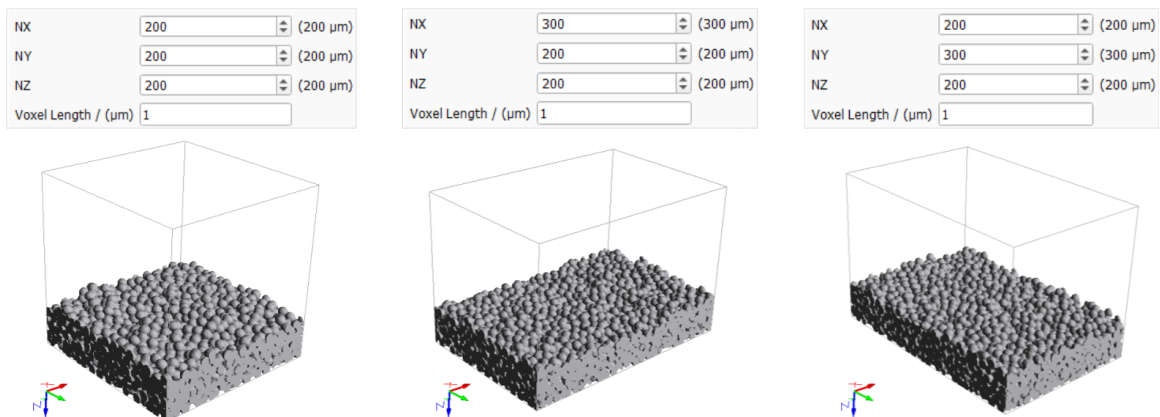
menu. The periodicity boxes are always checked for **Pile**, because the objects are always piled periodically.

Domain					
NX	100	(100 μm)	Origin X / (μm)	0	✓ Periodic X
NY	100	(100 μm)	Origin Y / (μm)	0	✓ Periodic Y
NZ	100	(100 μm)	Origin Z / (μm)	0	✓ Periodic Z
Voxel Length / (μm)	1				
Pore / Matrix Material (ID 00)			Air... Center Domain		

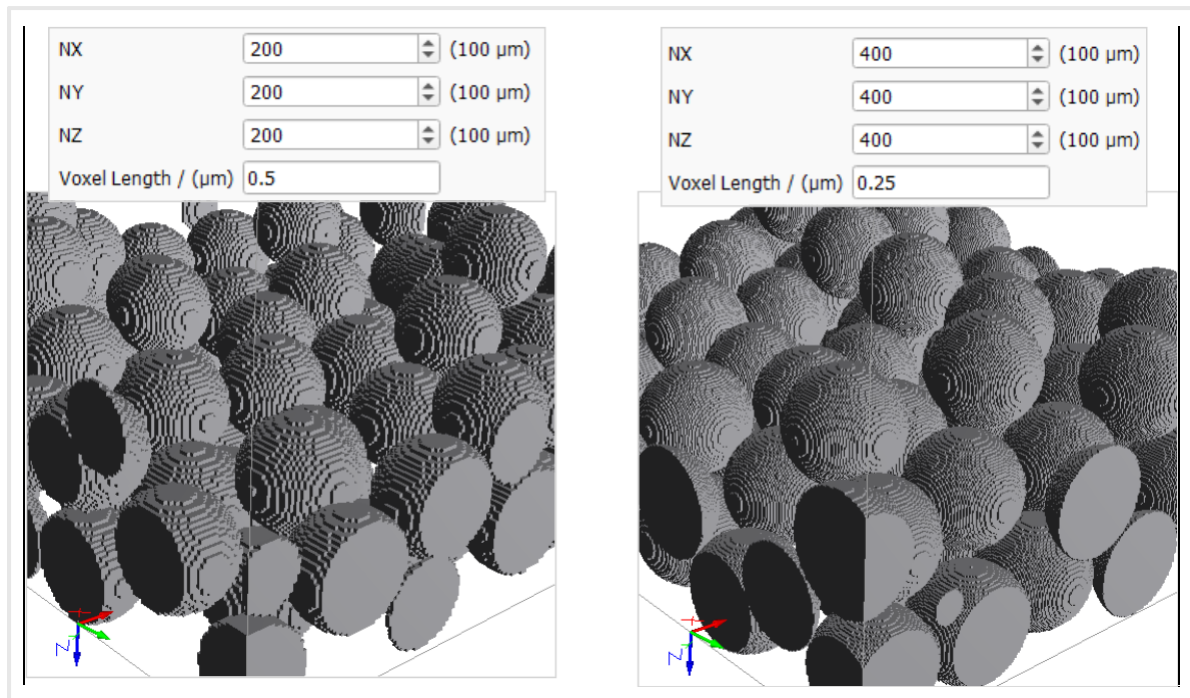
✓ NX, NY, NZ, and Voxel Length

The internal representation of a structure in GeoDict consists of rectangular 3D arrays of equally sized boxes, hereafter called volume elements or **voxels**. **NX**, **NY**, and **NZ** are the number (N) of voxels in X, Y, and Z directions.

The **Voxel Length** is the size of one voxel in the chosen units. Varying the values for **NX**, **NY**, and **NZ** has the effect of changing the size of the piled structure in the given direction. Low values for voxel length in combination with high values for **NX**, **NY**, and **NZ** result in a higher resolution, but also in a higher computational time. After setting the values of **NX**, **NY**, **NZ**, and **Voxel Length**, the physical structure size is automatically displayed in the chosen units.

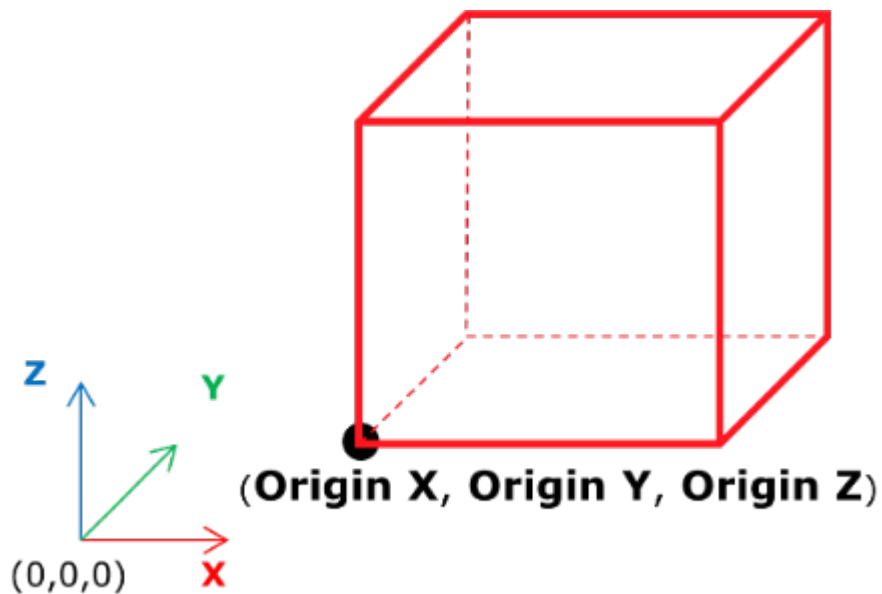


Observe how keeping the structure size constant ($100 \times 100 \times 100 \mu\text{m}^3$) while decreasing the **Voxel Length** from $0.5 \mu\text{m}$ to $0.25 \mu\text{m}$ has the effect of refining the spheres in the pile by increasing the resolution. Since the voxel length has decreased to half, the size of the structure is kept by doubling the **NX**, **NY**, and **NZ** values from 200 to 400.

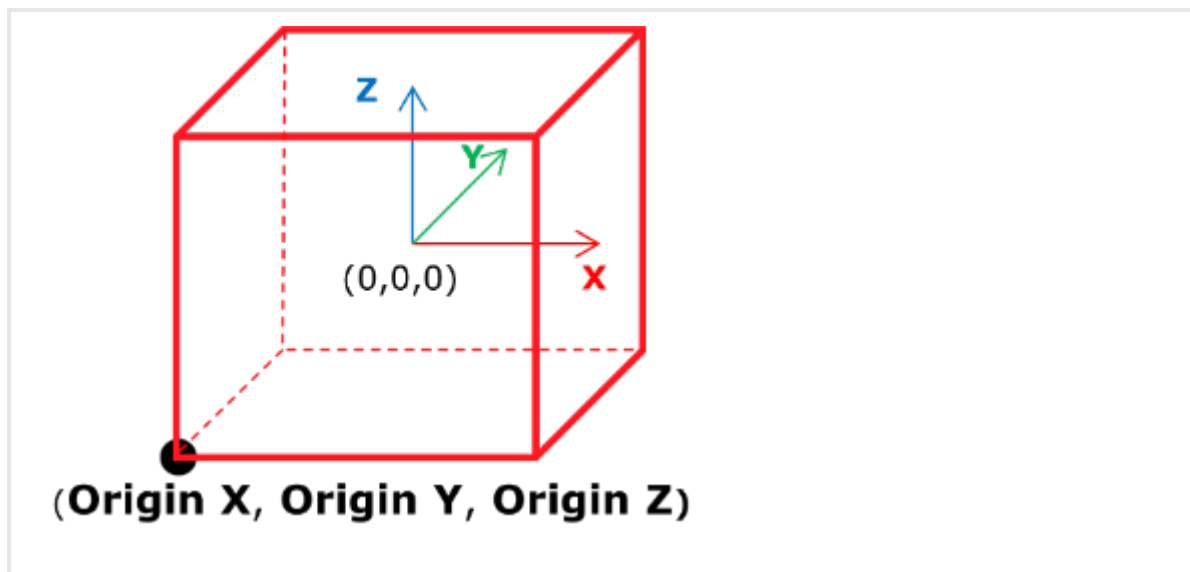


✓ Origin X, Origin Y, Origin Z, and Center Domain

The **Origin X**, **Origin Y**, and **Origin Z** parameters, together with the **Center Domain** button, determine the placement of the structure in the physical space. Zero values for Origin X, Origin Y, and Origin Z mean that the point with (0, 0, 0) coordinates is located at the lower left corner of the structure.



When clicking the **Center Domain** button, the (0, 0, 0)-point is set to the center of the structure as shown below.



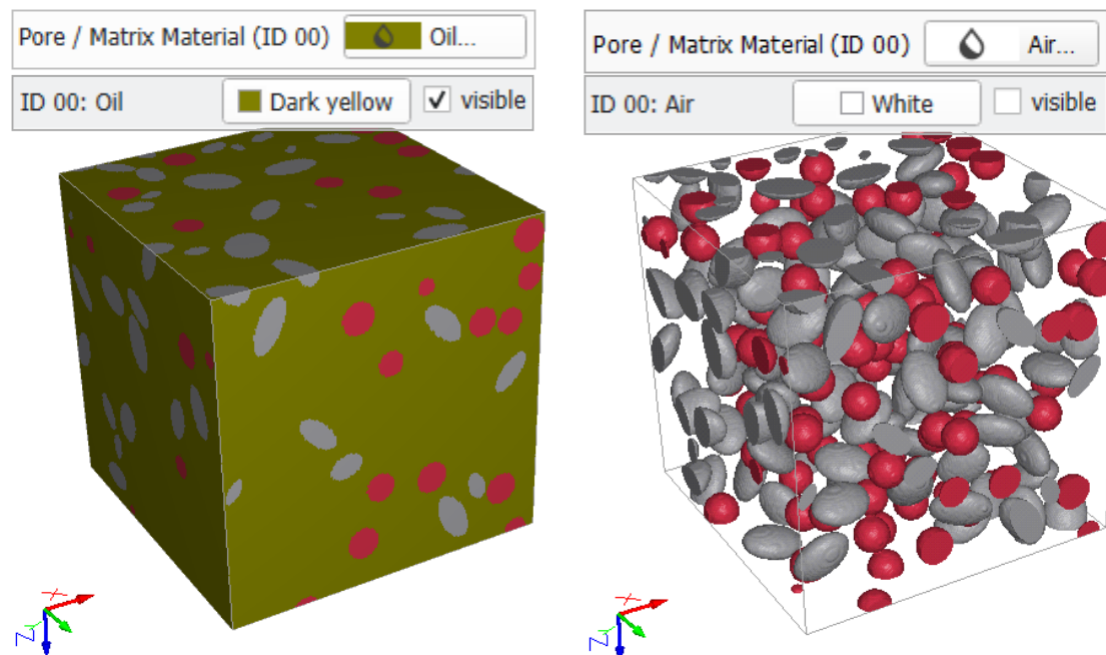
✓ Periodic X, Periodic Y, and Periodic Z

For **GrainGeo Pile** periodicity is always applied in all three directions. To learn more about periodicity refer to the [Domain](#)^[14] chapter of the **Create** parameters

✓ Pore / Matrix Material

Choose the material of the pore space or the matrix around the objects from the pull-down menu.

When the material is chosen to be **Pore**, the objects are embedded in empty pore space. Otherwise, the material filling the matrix can be chosen to be a **Solid**, **Porous** medium, or **Fluid** in which the objects are embedded.

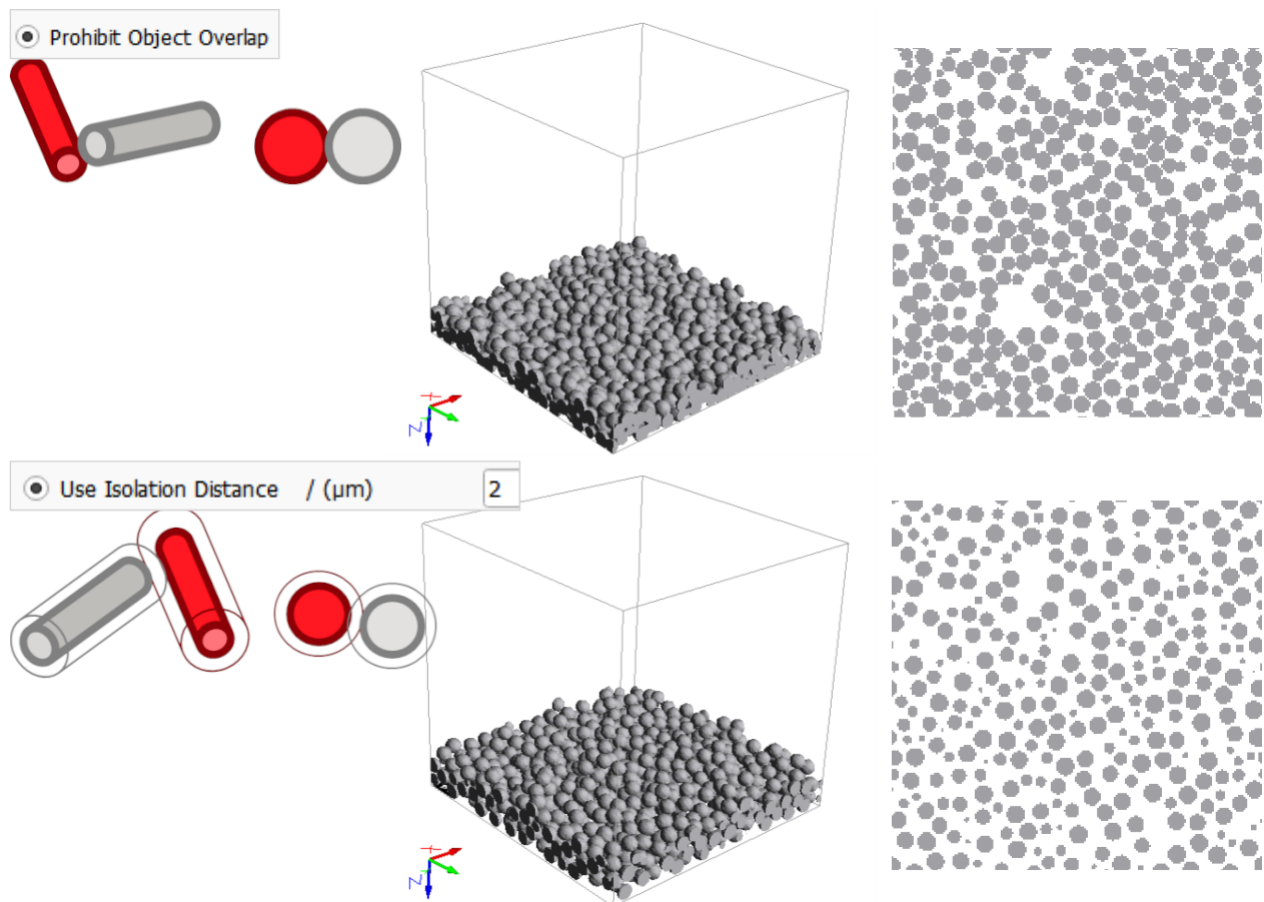


Generation and Overlap Mode

The options in the **Generation and Overlap Mode** panel control the relative position among objects (or with the structure currently in memory).



Objects may touch (but not overlap) when **Prohibit Objects Overlap** is selected. Objects may not touch when **Use Isolation Distance** is selected, and a positive value is entered. Then, all objects have at least this preset distance. The choice of **Use Isolation Distance** may lead to long computation times for large structures. In contrast to **Create Grains**, negative values for the **Isolation Distance** are not allowed.



Stopping Criterion

The parameters in the **Stopping Criterion** panel control the criteria which stop the piling process. The analysis of the results file (GDR file) shows any disparity between the achieved result values and the desired ones.

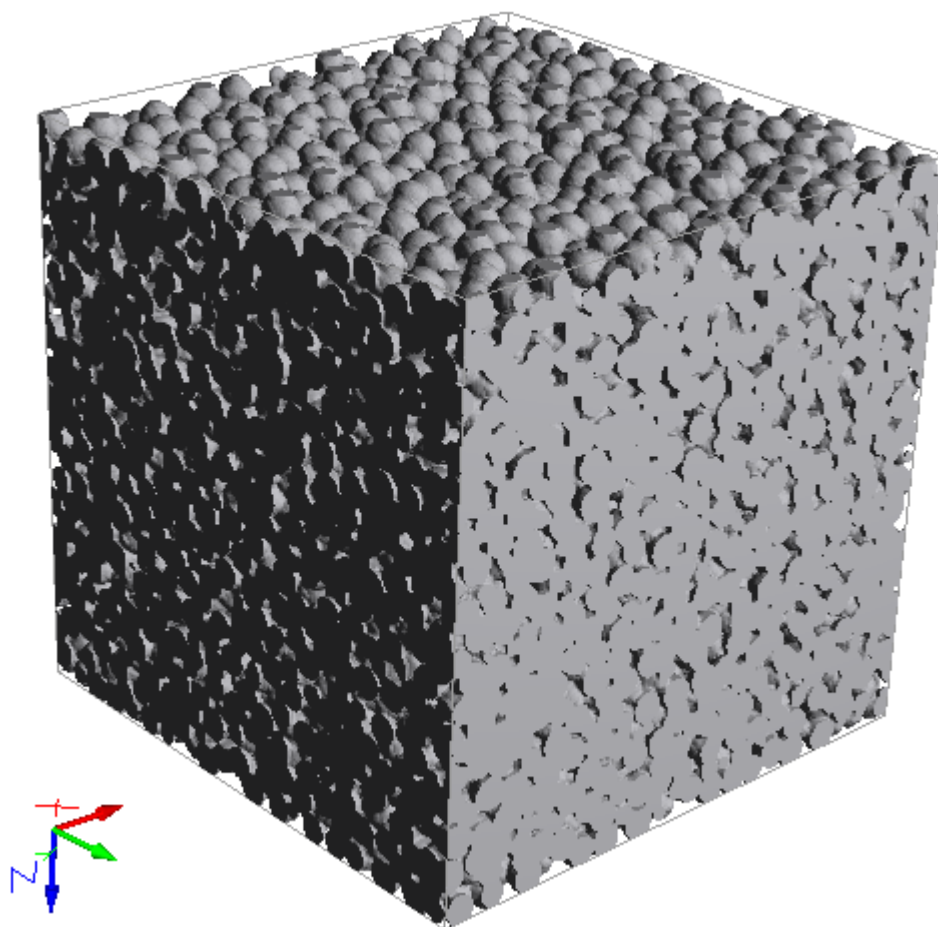
Besides the same options available for [Create Grains](#)³⁰, it is also possible to choose **Fill to Rim**.

Stopping Criterion

- ☐ Fixed Object Number
- ☐ Object Volume Percentage / (%)
- ☐ Grammage / (g/m²)
- ☐ Density / (g/cm³)
- ☐ Object Weight Percentage / (%)
- ☒ Fill To Rim

Fill To Rim

Fill to Rim continues the piling process until the objects reach the top of the bounding box in the Z-direction.



General Options

Define the general parameters temperature, random seed and parallelization.

Random Seed	42	Temperature	20	°C
Parallelization	8 Threads (Automatic Maximum) Edit...			

Temperature

When **Grammage** (or **Density** or **Object Weight Percentage**) is chosen as **Stopping Criterion**, a temperature can be entered. The temperature is considered for materials with temperature dependent density.

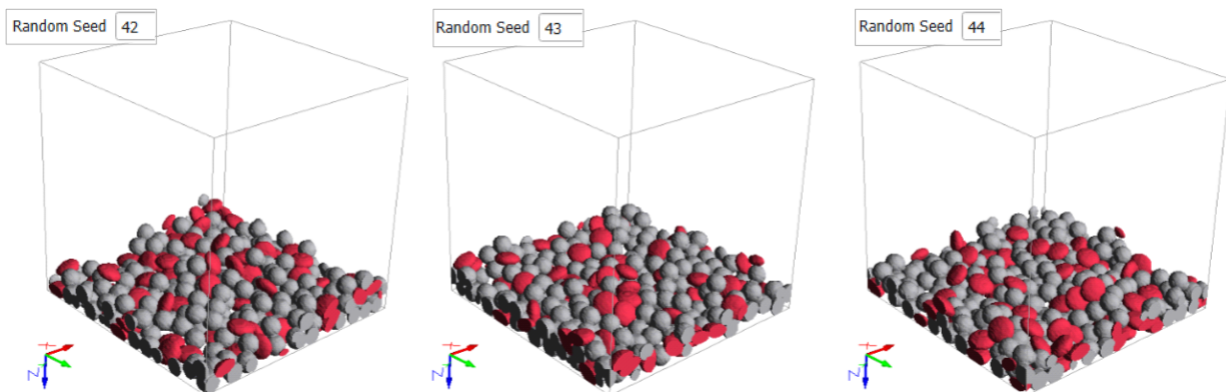
Choose the temperature in Kelvin, Celsius, or Fahrenheit.

Temperature	20	°C
		K <input checked="" type="text" value="°C"/> °F

Random Seed

Random Seed initializes the random number generator behind the structure generator. Changing its value produces different sequences of random numbers and hence, different realizations of the specified structure. If all settings are equal, generating with the same **Random Seed** value produces exactly the same structure, as shown by the **Structure ID** number in the Status section. The **Random Seed** is a non-negative integer number, it increases automatically with every generation run.

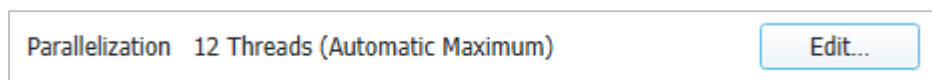
Varying the **Random Seed** allows generating different samples of the same structure for a series of experiments. In the following examples, all parameters are unchanged while the random seed is modified with every generation run.



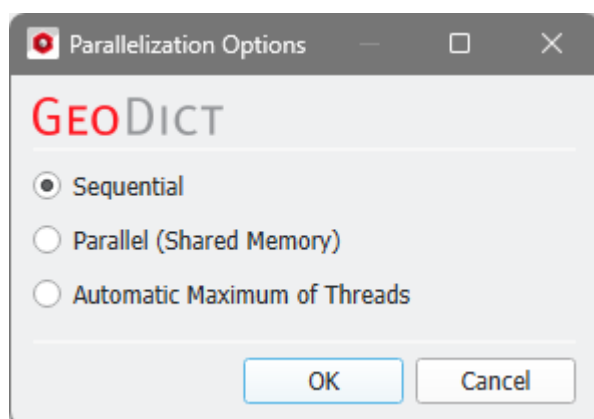
Parallelization

Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

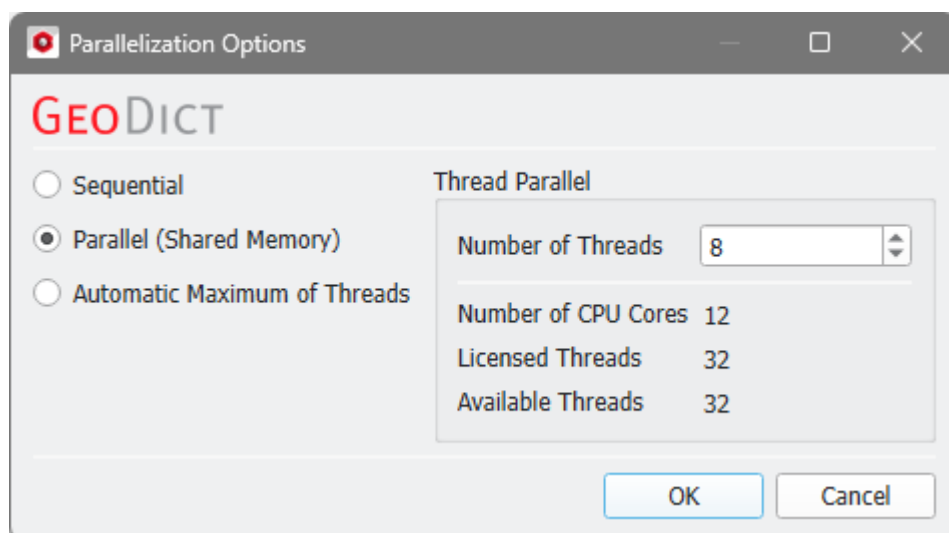
The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.



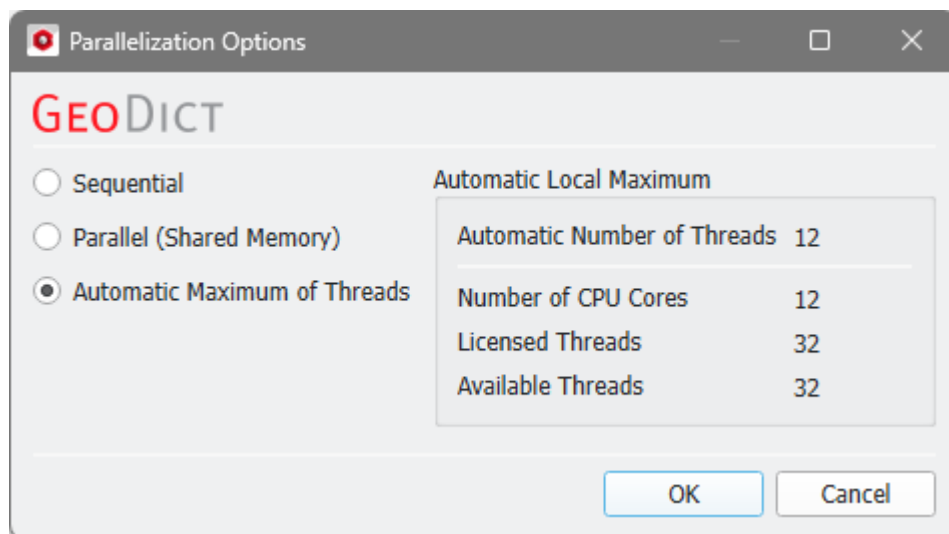
Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.

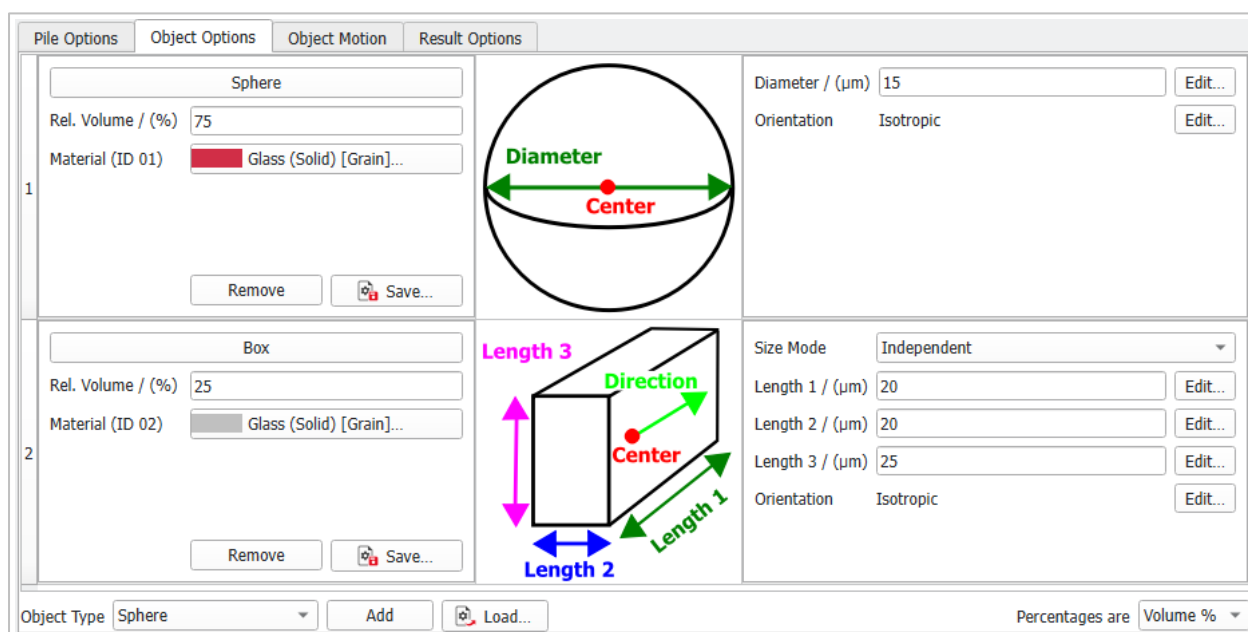


The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.

Object Options

Define the geometrical properties of individual object type. All object options listed here can be separately set for each object type. Up to 254 different object types may be added to the same structure. The object types and their parameters are very similar to those defined for [Create Grains](#)^[37]. But the center position of the objects is a result of the piling process and cannot be specified.

The objects for the piling are organized and listed in three columns. In the left one define the [Object Type](#)^[38] together with its percentage and material, the center one shows a [scheme of the parameters](#)^[41] of the chosen object type and in the right one you can edit the [object parameters](#)^[48]. In the bottom, find the options to choose additional object types and how the object percentage should be given.



Object Motion

The **Object Motion** parameters control the object's movement and initial position during the piling process, and are grouped into the **Piling Step**, and the **Object Position** panels. The **Pile Mode** can be selected from the pull-down menu.

The screenshot shows the 'Object Motion' panel with the following settings:

- Piling Step**
 - Direction: Z
 - Number of Shifts: 40
 - Maximum Shift Angle / (°): 89
 - Number of Rotations: 20
 - Maximum Rotation Angle / (°): 5
 - ☒ Find Stable Minimum
 - Maximum Check Length / (Voxel): 1
- Pile Mode**: Object after Object
- Object Position**
 - Initial Object Position: On Inflow Plane
 - Number of Positioning Trials: 100

The parameters are organized in the following groups:

- [Piling Step](#)¹⁰⁹
Define the parameters for the piling algorithm.
- [Pile Mode](#)¹¹³
Define the pile mode and initial object positions.

Piling Step

The object movements during the piling steps are mainly defined by the falling **Direction** and by the automatic finding of the stable minimum (**Find Stable Minimum**).

When the result is unsatisfactory, additional parameters can be used to refine it (**Number of Shifts**, **Maximum Shift Angle**, **Number of Rotations** per shift and **Maximum Rotation Angle**).

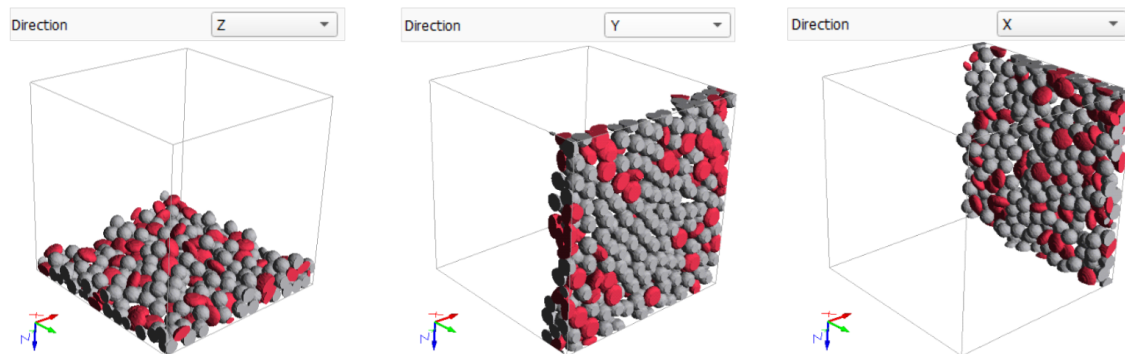
The screenshot shows the 'Piling Step' panel with the following settings:

- Direction: Z
- Number of Shifts: 40
- Maximum Shift Angle / (°): 89
- Number of Rotations: 20
- Maximum Rotation Angle / (°): 5
- ☒ Find Stable Minimum
- Maximum Check Length / (Voxel): 1

The option to find the stable minimum is not available when all objects fall at the same time ([Pile Mode → All Objects at Once](#)¹¹³).

✓ Direction

The **Direction** in which the piling process happens can be chosen from the pull-down menu. For all three axes, the objects fall towards the positive direction (X+, Y+, or Z+). Observe the piling of objects with **On Inflow Plane Center** as initial object position, falling from all three directions.



✓ Number of Shifts, Maximum Shift Angle, Number of Rotations, Maximum Rotation Angle

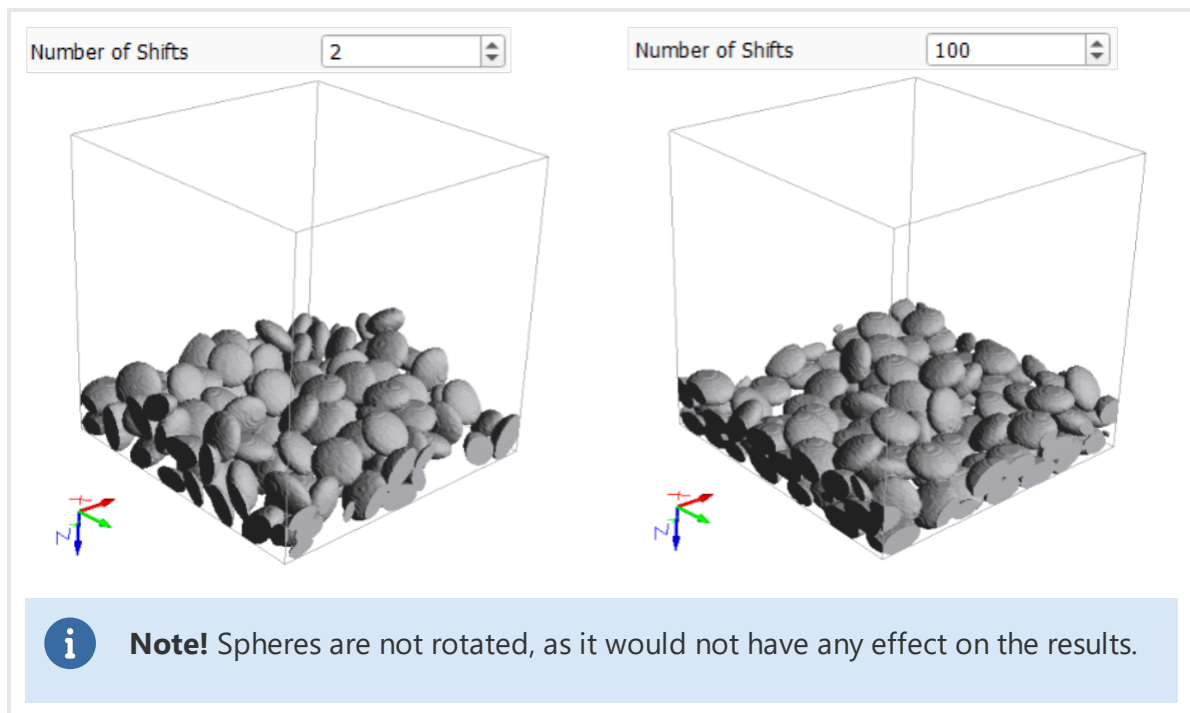
Throughout the piling process, the objects fall and roll to their final location in the structure. After the fall, i.e., after hitting an obstacle as the bottom domain boundary or another object, the objects shift and rotate as many times as defined by the values for **Number of Shifts** and **Number of Rotations** before they come to rest at the bottom of the structure. Low values for shifts and rotations produce structures with objects that settle earlier compared to larger values of these parameters, resulting in a lower packing density.

In detail, the algorithm for each shift tries the given number of rotations. If a better position is found for the object, lower in the specified direction and without overlapping with other objects, it is used as a new point for the object. Then, the numbers of shift and rotation are reset. The algorithm terminates if no new position is found for the given number of shifts and rotations.

The **Maximum Shift Angle** restricts the angle that the objects can shift with respect to the piling direction. The maximum shift angle must be smaller than 90°.

The **Maximum Rotation Angle** describes the maximum angle the objects can rotate from step to step. The object is rotated around the center defined for the object, which in most cases is the center of mass.

Observe the effect of setting a low or a high **Number of Shifts** value on the final position of objects in the otherwise same structure.

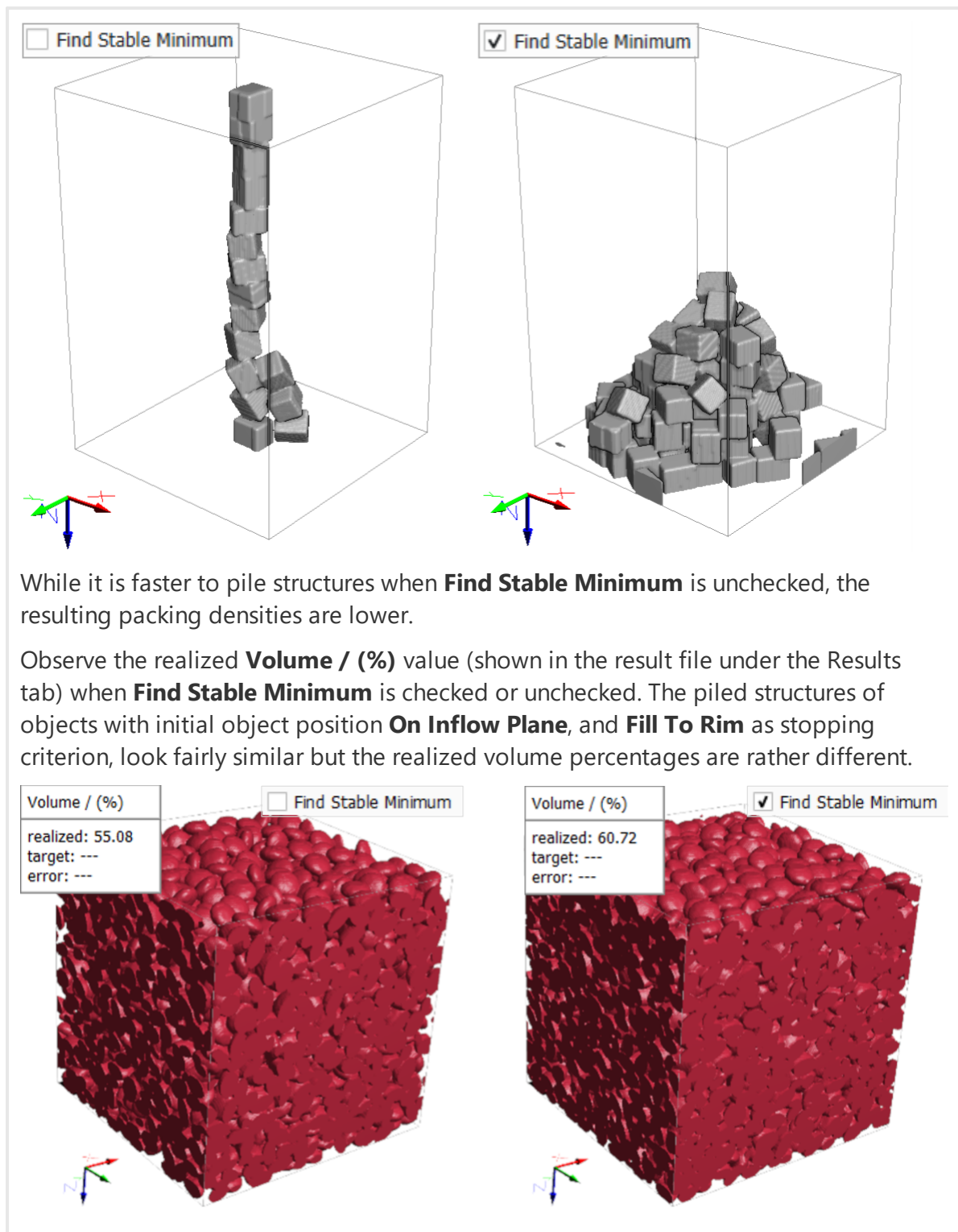


✓ Find Stable Minimum

When checking **Find Stable Minimum**, each object is checked to have a stable state with respect to gravity at the end of the piling process.

When an object cannot be moved further downwards, it is checked if it is possible to move it in the plane perpendicular to the specified direction without obtaining overlap with other objects to find a new position where the potential energy can be further reduced. If not, it has the lowest position possible and is considered as stable.

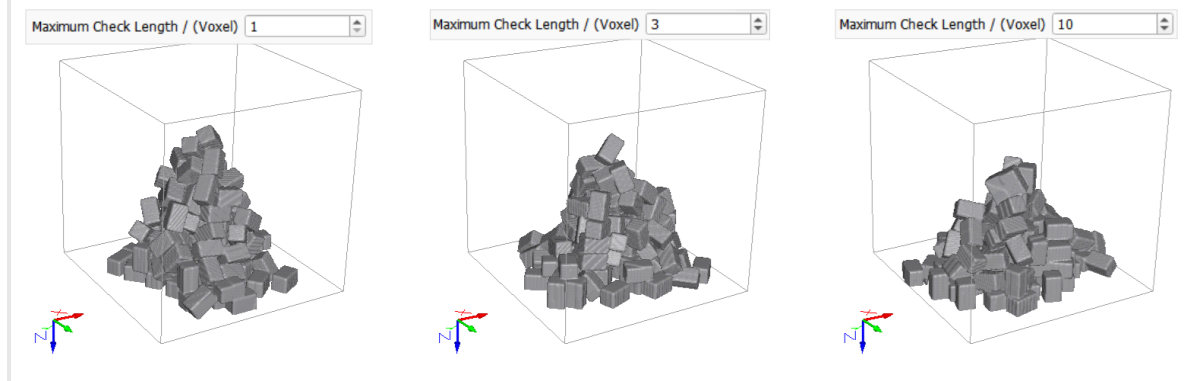
Observe the effect of checking or unchecking **Find Stable Minimum** in the piling 100 objects with initial object position **On Inflow Plane Center**.



✓ Maximum Check Length

The **Maximum Check Length** is a further refinement when finding the stable minimum. For every object, the algorithm checks for an even more stable position around the already reached minimum with a radius defined by the voxel value entered in the field. A higher value increases the stability of the pile.

Observe the effect having checked **Find Stable Minimum**, and then entering increasing values of **Maximum Check Length** (1, 3, and 10) in the piling of 100 boxes with [initial object position](#)¹¹³ **On Inflow Plane Center**.



Pile Mode

Define the pile mode and the initial object position.

Pile Mode

Select from the pull-down menu whether the objects should fall one after another (**Object after Object**) or all should fall at once (**All Objects at Once**).

Pile Mode Object after Object	Pile Mode All Objects at Once
Object Position	
Initial Object Position On Inflow Plane	Initial Object Position Objects from gad-File
Number of Positioning Trials 100	Start File (*.gad) Browse...
	Loosen Objects 0
	Lift Objects / (μm) 0

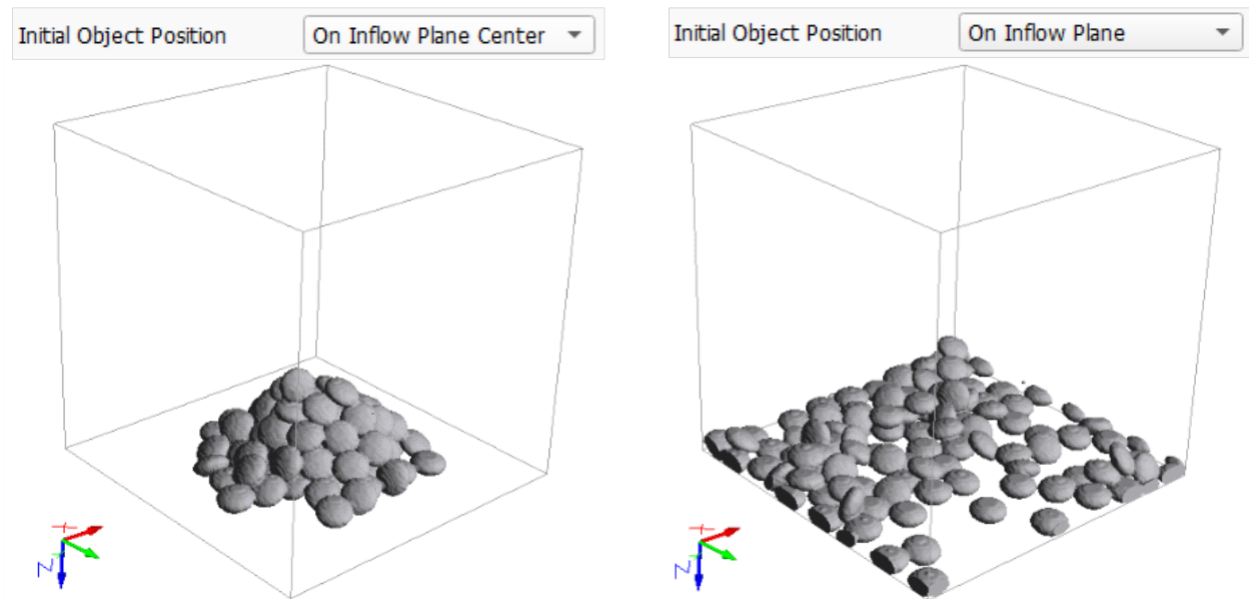
Object Position

When choosing **Object after Object**, the pull-down menu for **Initial Object Position** allows setting the initial position from which the piling objects are set to fall: the whole initial position plane (**On Inflow Plane**), from its center (**On Inflow Plane Center**), or to originate from an existing structure (**Objects from gad-File**). When **All Objects at Once** is selected, the objects must be loaded from a *.gad file.

On Inflow Plane or On Inflow Plane Center

When piling objects **On Inflow Plane** or **On Inflow Plane Center**, the **Number of Positioning Trials** can be adjusted at the cost of additional runtime to increase the quality of the piled

structure.



Objects from gad-File

When piling from an existing *.gad file, the objects are taken from that file. Thus, no objects (and their geometry parameters) need to be selected through the **piling Options** tab. Clicking **Browse**, a structure saved in GAD format can be selected as the origin of the objects.



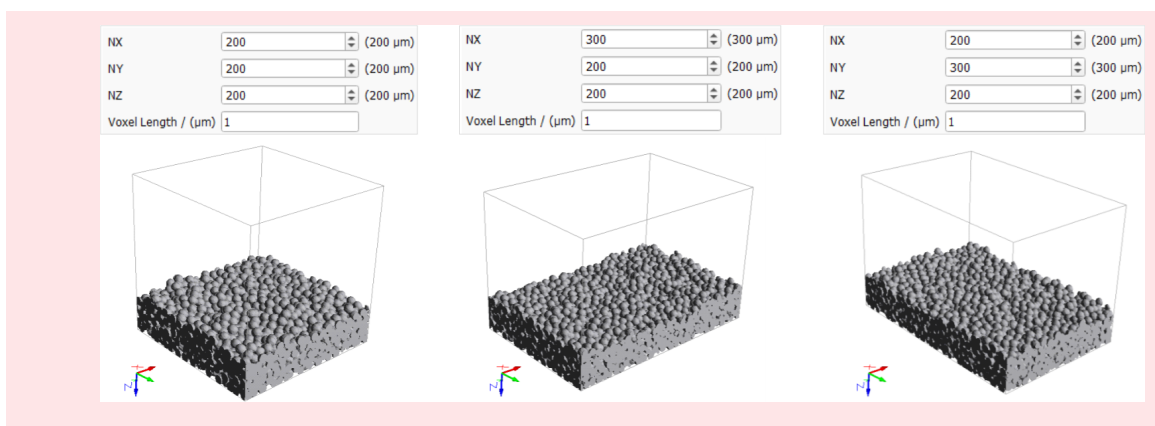
Important! Structures in GAD format to be used for piling must conform to certain requirements (no overlapping, periodicity, no objects crossing bottom plate) and should be generated for later piling with these requirements in mind. Overlap can be removed after generation using **GadGeo** → **Remove Object Overlap**, as explained in the GadGeo chapter.

✓ Requirements for objects from gad file

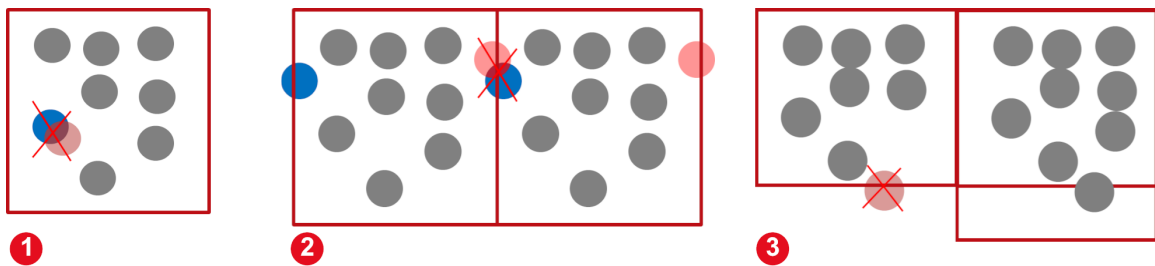


Important! Before piling, the domain size in all three directions under the **Pile Options** tab must be set to at least the size of the gad file.

For example:



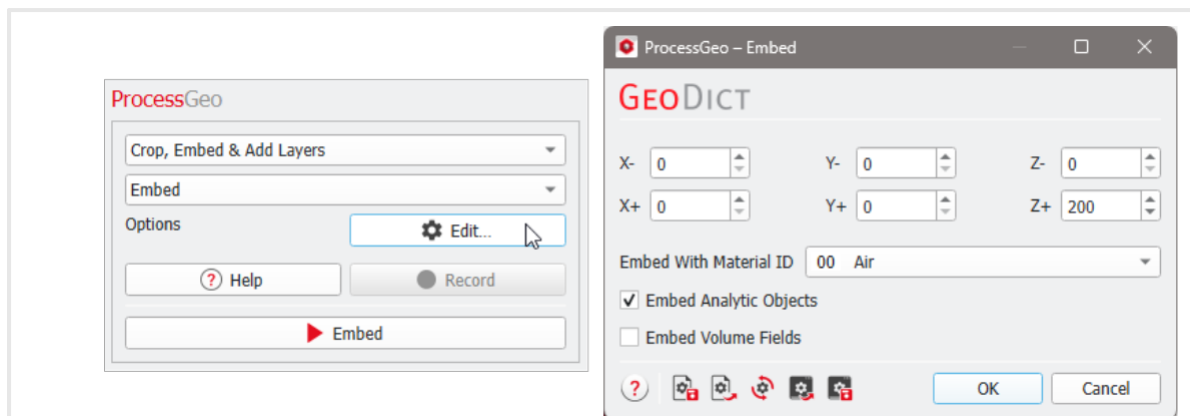
Assuming the Z-direction to be the piling direction, and downwards to be the positive direction (Z+), the following situations have to be considered:



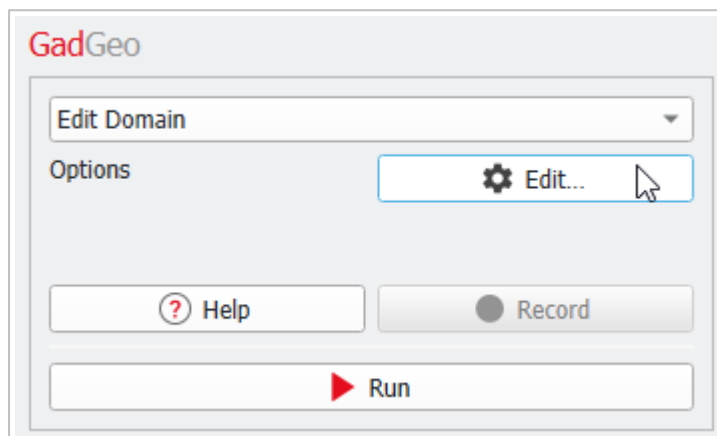
1. Touching, but not overlapping, is allowed for piling. The initial structure must be generated without overlapping. For example, by selecting Remove Overlap when generating with Create (or other GeoDict structure generators).
2. Periodicity is needed in the X and Y directions for piling, to avoid undesired intersections at the edge of the structure. The initial GAD file must be generated to be periodic (in all directions).
3. No objects are allowed to drop off the bottom of the structure. When this happens, the dimensions of the initial *.gad file must be processed to include the extruding object.

The dimensions of the initial *.gad file can be changed by adding enough empty voxels in Z+ direction. The number of voxels to be added depends on how far objects overlap the original domain in Z-direction. Two different possibilities are available for this task:

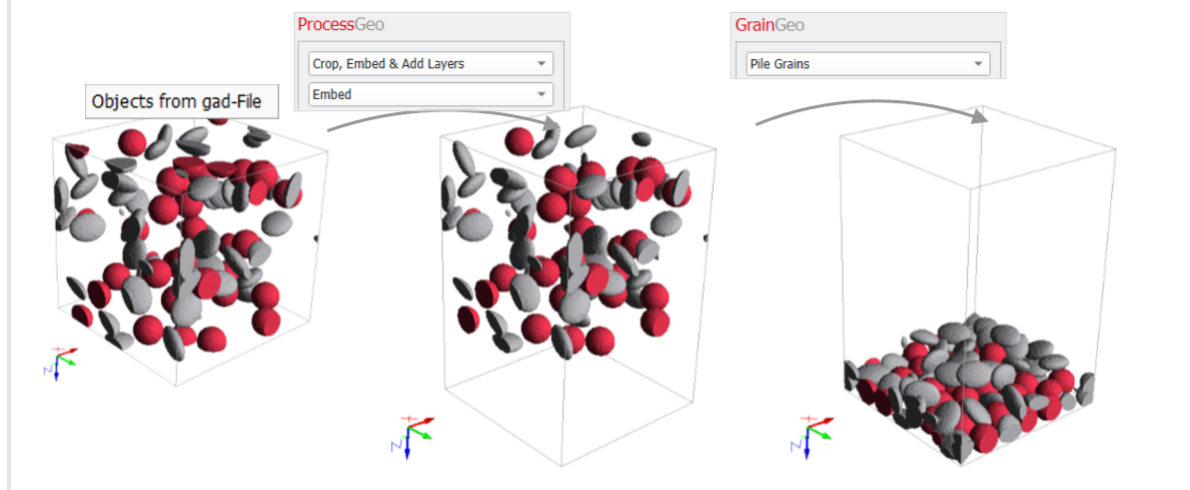
1. **Model** → **ProcessGeo** → **Embed** and check **Embed Analytic Objects**. This explicitly adds voxels in the specified direction. For more information refer to the ProcessGeo chapter.



2. **Model** → **GadGeo** → **Edit Domain**. This changes the domain size as defined. For more information refer to the GadGeo chapter.



Example:



✓ Parameters for objects from gad file

Before the piling process starts from a structure in GAD-format, the initial position of the contained objects can be slightly changed by two parameters.

Loosen Objects	0
Lift Objects / (μm)	0

The distance between the objects in the piling direction can be enlarged by the factor entered in **Loosen Objects**.

Additionally, all objects can be lifted by the distance entered in **Lift Objects**. For example, these parameters can be used to generate structures similar to those from sieving processes combined with additional shaking.

Result Options

The generated structure is always saved as a **GeoDict structure file (*.gdt)** (GeoDict binary data). The file is placed in an automatically created result folder inside the chosen project folder (**File** → **Choose Project Folder...** in the menu bar).

The result file as well as the result folder take the name entered as **Result File Name (*.gdr)** at the top of the dialog.

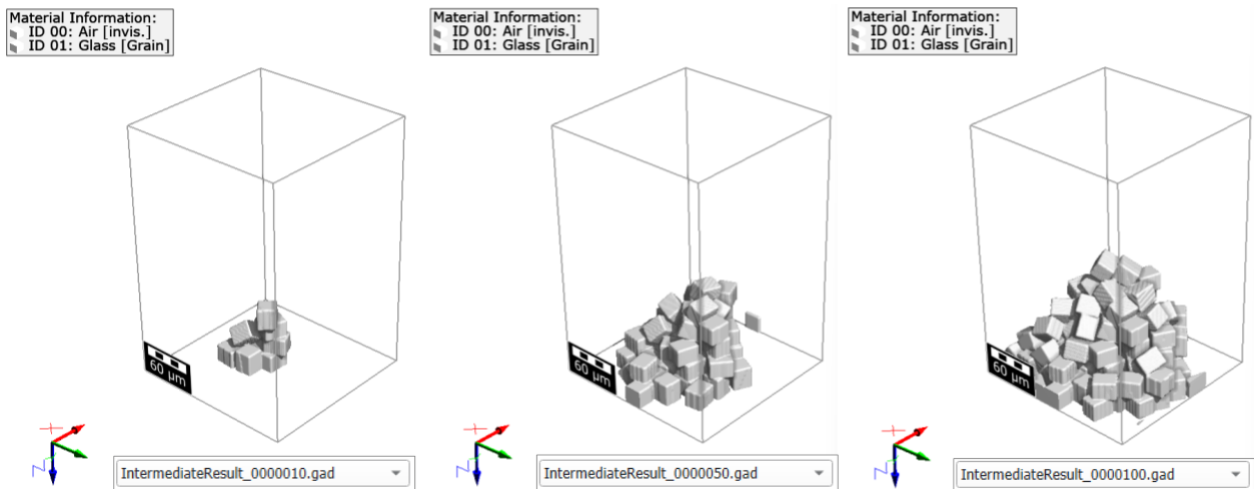
An additional option to save the generated structure data is to check **Save Intermediate Result every** and enter a number of **Objects** in the box. As objects are added to the structure during the generation, an intermediate result file is saved each time the number of placed objects reaches a multiple of the entered value.

This option may be interesting when studying the properties of a series of structures with increasing density.

After running the generation, the intermediate geometries can be found as ***.gad** analytic files in the result folder and can be loaded directly from the **Result Viewer** of the *.gdr result file.

The screenshot shows two parts of the software interface. The top part is the 'Result Options' tab, which has a checkbox labeled 'Save Intermediate Result every' that is checked. Next to it is a text input field containing the number '10', followed by a small up/down arrow icon and the label 'Objects'. The bottom part of the screenshot shows the 'Results' tab of the 'Result Viewer'. It features a list titled 'Intermediate Geometries' containing ten files: 'IntermediateResult_0000010.gad', 'IntermediateResult_0000010.gad', 'IntermediateResult_0000020.gad', 'IntermediateResult_0000030.gad', 'IntermediateResult_0000040.gad', 'IntermediateResult_0000050.gad', 'IntermediateResult_0000060.gad', 'IntermediateResult_0000070.gad', 'IntermediateResult_0000080.gad', 'IntermediateResult_0000090.gad', and 'IntermediateResult_0000100.gad'. The second file in the list is highlighted in blue. To the right of the list is a 'Load' button with a mouse cursor pointing at it.

Below find an example for the piling of 100 boxes from inflow plane center. Observe how more and more objects are added.



1.2.2 Results

The generated structure is shown in the visualization area. Learn more about visualization in GeoDict in the **Visualization** chapter.

The result file is automatically opened in the Result Viewer and shows structure statistics in the **Results-Report** and **Results-Plot** tabs. Additionally, it offers 3D **Data Visualization** options depending on the generation settings. Find more information on GeoDict result files in the **Result Viewer** chapter.

Results -Report

The first two tables show the **Absolute** and **Relative object distribution** for all object types.

Input Map

Log Map

Post Map

Results

Data Visualization

Metadata

Report

Plots

Map

Absolute object distribution:

	Count	Volume / (%)	Grammage / (g/m ²)	Density / (g/cm ³)	Weight / (%)
Total	realized: 1794 target: --- error: ---	realized: 34.99 target: 35.00 error: -0.01	realized: --- target: --- error: ---	realized: --- target: --- error: ---	realized: --- target: --- error: ---
Object type 1	realized: 992 target: --- error: ---	realized: 17.47 target: 17.50 error: -0.03	realized: --- target: --- error: ---	realized: --- target: --- error: ---	realized: --- target: --- error: ---
Object type 2	realized: 801 target: --- error: ---	realized: 17.52 target: 17.50 error: 0.02	realized: --- target: --- error: ---	realized: --- target: --- error: ---	realized: --- target: --- error: ---

Stopping criterion error: -0.016 %

Relative object distribution:

	Count / (%)	Volume / (%)	Weight / (%)
Object type 1	realized: 55.35 target: --- error: ---	realized: 49.93 target: 50.00 error: -0.14%	realized: --- target: --- error: ---
Object type 2	realized: 44.65 target: --- error: ---	realized: 50.07 target: 50.00 error: 0.14%	realized: --- target: --- error: ---

Maximal probability error: 0.14%

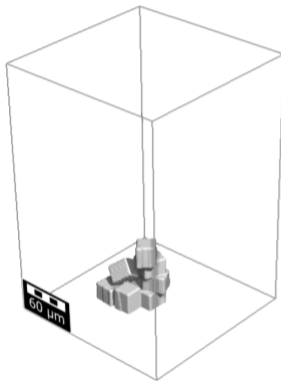
Data Visualization

When selecting **Save Intermediate Results every # Objects** under the **Result Options** tab, you can open the intermediate geometry files (*.gad) after selecting them in the pull-down menu.

Input Map	Log Map	Post Map	Results	Data Visualization	Metadata
Intermediate Geometries					
IntermediateResult_0000010.gad IntermediateResult_0000010.gad IntermediateResult_0000020.gad IntermediateResult_0000030.gad IntermediateResult_0000040.gad IntermediateResult_0000050.gad IntermediateResult_0000060.gad IntermediateResult_0000070.gad IntermediateResult_0000080.gad IntermediateResult_0000090.gad IntermediateResult_0000100.gad				Load	

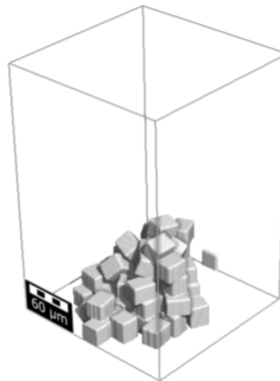
Below find an example for the piling of 100 boxes from inflow plane center. Observe how more and more objects are added.

Material Information:
ID 00: Air [invis.]
ID 01: Glass [Grain]



IntermediateResult_0000010.gad

Material Information:
ID 00: Air [invis.]
ID 01: Glass [Grain]



IntermediateResult_0000050.gad

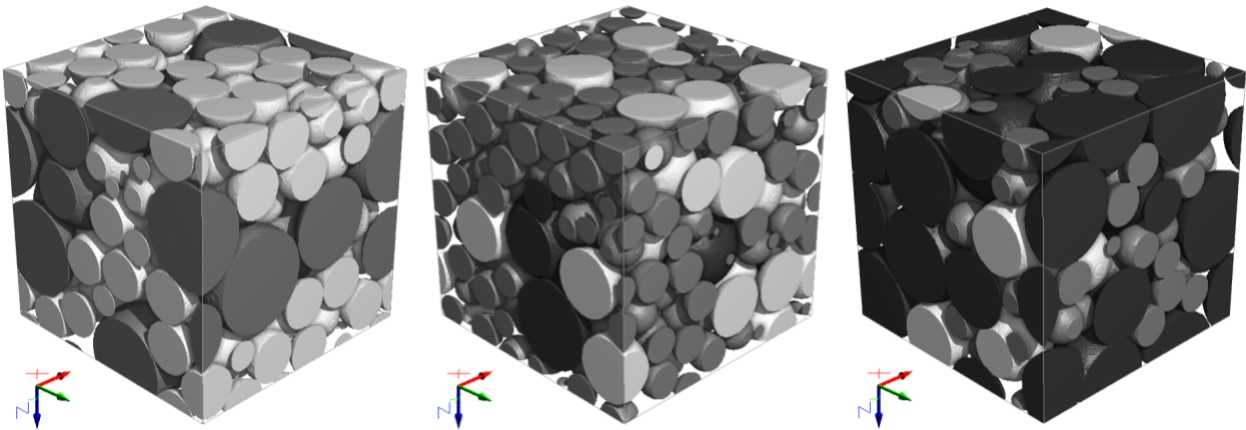
Material Information:
ID 00: Air [invis.]
ID 01: Glass [Grain]



IntermediateResult_0000100.gad

1.3 Pack Analytic Spheres

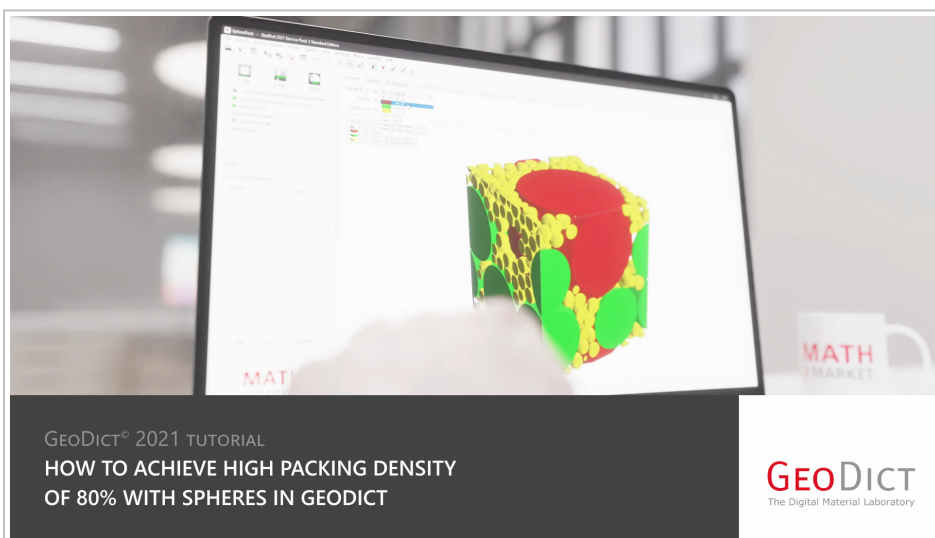
When choosing **Pack Analytic Spheres** from the pull-down menu in the GrainGeo section, densely packed spheres are generated. GeoDict uses a force-biased algorithm to create the dense packing (see [Ohser et al., 2009](#)^[255], and [Mościński, 1989](#)^[255]).



The Pack Analytic Spheres command:

- [Options](#)^[122]
Define the packing parameters.
- [Results](#)^[135]
Statistics about the analytical sphere generation are given in the Result Viewer. Also the generation process can be visualized in 3D.

GeoDict Tutorial: How to achieve high packing density of 80% with spheres in GeoDict



1.3.1 Options

At the top left of the dialog, the name for the file containing the generation results can be entered in the **Result File Name (*.gdr)** box. The default name can be kept, or a new name can be chosen, fitting the current project.

The result files are saved in the chosen project folder (**File** → **Choose Project Folder**, in the **Menu bar**). If a GeoDict result file (*.gdr) with the given name already exists in the project folder, a warning message is shown at the start of the creation process. You can either decide to rename the chosen file name to a new one, to cancel the generation process, to overwrite or to back up the old file. When nothing is selected, GeoDict uses the **Back-Up** option after a waiting time.

The available units (m, mm, and μm) are selectable from the pull-down menu at the top right of the dialog. When the units are changed, the entered values are adjusted automatically.

GrainGeo – Pack Analytic Spheres

GEOdict

Result File Name (*.gdr) μm ▾

Pack Options | Sphere Distribution | Equations & References

Packing Mode Create New Packing ▾

Materials

Material ID Mode Material ID per Material ▾

Pore / Matrix Material (ID 00) Air...

Packing

Random Seed 42 ▴ ▾ Maximum Iterations 1000000 ▴ ▾

Packing Density 0.63 Maximum Run Time / (h) 24

Domain

NX 300 ▴ ▾

NY 300 ▴ ▾

NZ 300 ▴ ▾

Analysis

☐ Save GeoDict Particle Trajectories for Animation of sphere motion (*.gpt File)

☐ Save Two-Point Correlation Information (*.tpc File)

☒ Compute Object Contacts Information Based on Voxel Image

☐ Compute Contacts Number Information Based on Analytic Data

Contact Distance 2 Voxel ▾

Parallelization 8 Threads (Automatic Maximum) Edit...

? OK Cancel

The parameters are organized into tabs:

- [Pack Options](#)¹²³
Enter the general properties of the packed structure.
- [Sphere Distribution](#)¹³⁰
Determine the parameters for the sphere size probability distribution.



	Opens the corresponding User Guide section.
	Saves the settings to a GeoDict settings file (*.gps).
	Loads the settings from a GeoDict settings file (*.gps) or a GeoDict result file (*.gdr).
	Resets all parameter settings to the built-in default settings.
	Resets all parameter settings to the saved start-up settings.
	Saves the current parameter settings as start-up settings.

Each option is explained by a tooltip which appears when resting the mouse over the icon.

Pack Options

The general properties of the packed structure are entered under the **Pack Options** tab. These parameters are grouped into the panels **Packing Mode**, **Domain**, **Materials**, **Packing**, **Analysis**, and **Parallelization**.

Pack Options

Sphere Distribution

Equations & References

Packing Mode

Create New Packing

Materials

Material ID Mode

Material ID per Material

Pore / Matrix Material (ID 00)

Air...

Packing

Random Seed

42

Maximum Iterations

1000000

Packing Density

0.63

Maximum Run Time / (h)

24

Analysis

☐ Save GeoDict Particle Trajectories for Animation of sphere motion (*.gpt File)
 ☐ Save Two-Point Correlation Information (*.tpc File)
 ☒ Compute Object Contacts Information Based on Voxel Image
 ☐ Compute Contacts Number Information Based on Analytic Data

Contact Distance

2

Voxel

Domain

NX

300

NY

300

NZ

300

Parallelization

8 Threads (Automatic Maximum)

Edit...

Packing Mode

From the **Packing Mode** pull-down menu, select to **Create New Packing** or to **Re-Compact Existing Packing**.

✓ Create New Packing

The spheres are packed into a new structure. The available parameters for the generation are listed and explained below for the panels **Materials**, **Packing**, and **Domain**.

Packing Mode

Create New Packing

Materials

Material ID Mode

Material ID per Material

Pore / Matrix Material (ID 00)

Air...

Packing

Random Seed

42

Maximum Iterations

1000000

Packing Density

0.63

Maximum Run Time / (h)

24

Domain

NX

300

NY

300

NZ

300

✓ Re-Compact Existing Packing

Re-Compact Existing Packing is useful when trying to achieve a higher packing density from an already existing packing result.

When choosing this option, the **Materials** panel is missing but some **Packing** and **Domain** parameters under the **Pack Options** tab can be set.

Choosing to re-compact an existing packing enables to Browse and load the GDR result file from a previously run packing process. This GeoDict result file, and corresponding result folder, already include the packing parameters.

Under the [Sphere Distribution](#)¹³⁰ tab, all parameters are directly entered from the selected GDR file and from the corresponding result directory of a previous GrainGeo run. Additionally, you can choose to [Apply Gravity](#)¹³⁴.

The screenshot shows the 'Pack Options' tab in GrainGeo. The 'Packing Mode' dropdown is set to 'Re-Compact Existing Packing'. Below it is a 'Browse' button. The 'Packing' section contains four input fields: 'Random Seed' (42), 'Maximum Iterations' (1000000), 'Packing Density' (0.63), and 'Maximum Run Time / (h)' (24). The 'Domain' section on the right has three vertical sliders for 'NX', 'NY', and 'NZ', all of which are currently set to the value 300.

Domain

In the **Domain** panel, enter the values for **NX**, **NY**, and **NZ**, indicating the number of voxels that the packed structure should have in the X, Y, and Z-direction, respectively.

This is a close-up of the 'Domain' panel. It contains three vertical sliders labeled 'NX', 'NY', and 'NZ'. Each slider has a numerical display showing the value 300 and small up/down arrow buttons on the right side.

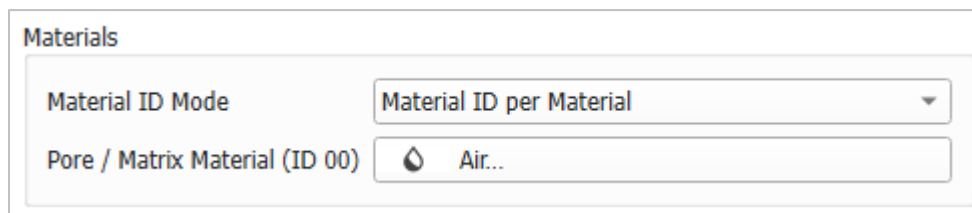
Change NX, NY, and NZ by direct insertion or by clicking the arrow buttons. The voxel length is automatically set according to the needs for the sphere distribution.

When **Re-Compact Existing Packing** is selected, only **NX** can be changed. The values for **NY** and **NZ** and the voxel length are then changed automatically to keep the actual domain size. Entering larger values for **NX** lead to a finer resolution.

Materials

Define the materials in the structure. This is part of the GeoDict Material Database concept, in which objects and pore space in the structure are ascribed to an individual material (e.g., glass, iron, PET, air,...) with specific physical properties.

The panel does not appear when **Re-Compact Existing Packing** is selected. Then, the materials from the existing packing are kept.



The Materials panel contains two main controls:

- Material ID Mode:** A dropdown menu currently set to "Material ID per Material".
- Pore / Matrix Material (ID 00):** A button with a water drop icon and the text "Air...", used to select a material for the pore space.

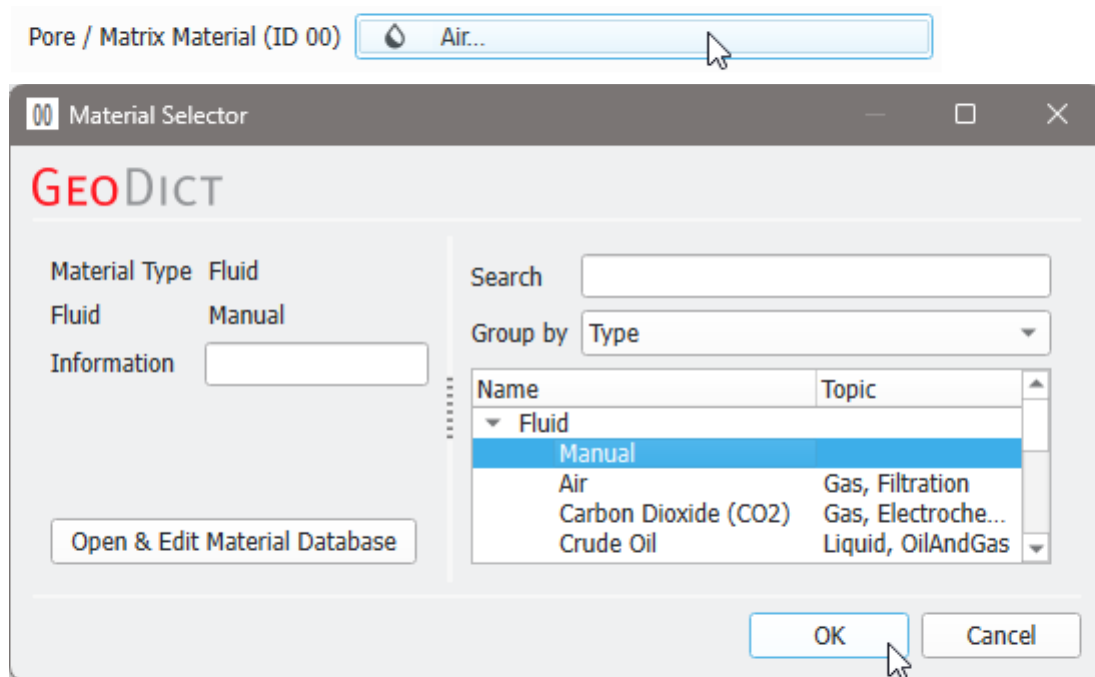
✓ Material ID Mode

The pull-down menu allows selecting between applying the **Material ID** based on the materials or the types of objects present in the packed structure.

By leaving the default **Material ID per Material**, sphere types of the same material (defined in the [Sphere Distribution](#) ¹³⁰ tab) are assigned the same Material ID.

Changing it to **Material ID per Object-Type** allows assigning different Material IDs to the spheres based on their size (diameter) while keeping the same material.

By clicking the button to the right of **Pore / Matrix Material (ID 00)**, it is possible to change the Material ID assigned to the pore space / matrix surrounding the objects in the structure from the default Air (Fluid) to any other material.



The Material Selector dialog box is shown with the following components:

- Title Bar:** "00 Material Selector"
- GEO DICT Logo:** Located at the top left.
- Material Type:** A dropdown menu set to "Fluid".
- Fluid:** A dropdown menu set to "Manual".
- Information:** An empty text input field.
- Search:** An empty search bar.
- Group by:** A dropdown menu set to "Type".
- Material List:** A table with two columns: "Name" and "Topic".

Name	Topic
Fluid	
Manual	
Air	Gas, Filtration
Carbon Dioxide (CO2)	Gas, Electroche...
Crude Oil	Liquid, OilAndGas
- Buttons:** "Open & Edit Material Database", "OK", and "Cancel".

Packing

Define the parameters for the packing algorithm.

Packing

Random Seed	42	Maximum Iterations	1000000
Packing Density	0.63	Maximum Run Time / (h)	24

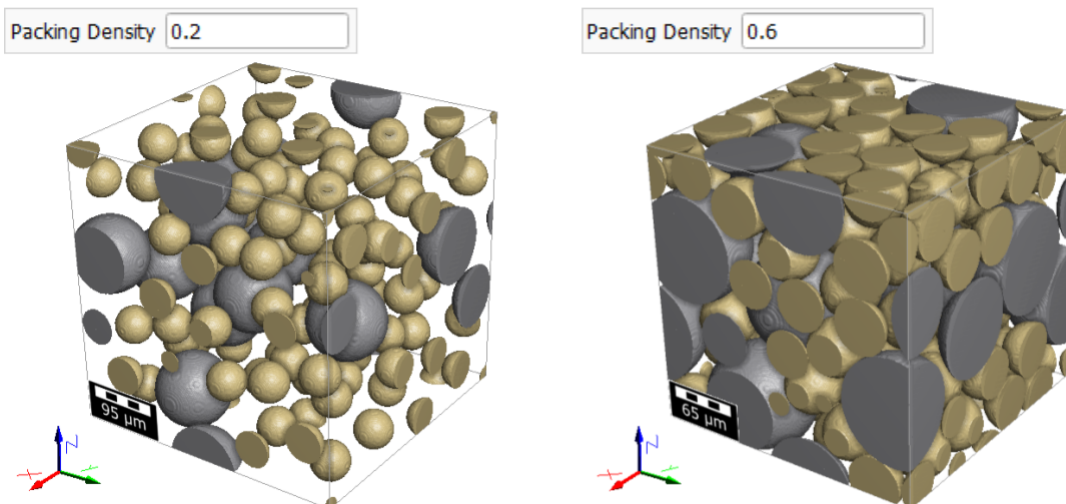
For **Re-Compact Existing Packing** the parameter random seed is not available.

✓ Random Seed

The **Random Seed** is a non-negative integer number that defines the random initial position of the spheres. Changing its value produces different sequences of random numbers and, hence, different realizations of the specified structure. If all settings are equal, generating with the same **Random Seed** value produces exactly the same structure.

✓ Packing Density

For **Packing Density** enter values between 0 and 1 (0% to 100% packing density).



✓ Maximum Iterations

The parameter **Maximum Iterations** allows setting an upper limit to the number of steps for the packing process.

✓ Maximum Run Time

The **Maximum Run Time (h)** permits setting the upper time limit for the packing process.

Analysis

Define which result files should be created and which post-processing should be applied.

Analysis

☐ Save GeoDict Particle Trajectories for Animation of sphere motion (*.gpt File)
☐ Save Two-Point Correlation Information (*.tpc File)
☒ Compute Object Contacts Information Based on Voxel Image
☐ Compute Contacts Number Information Based on Analytic Data

Contact Distance

Voxel ▾

✓ Save GeoDict Particle Trajectories for Animation of sphere motion (*.gpt File)

Checking **Save GeoDict Particle Trajectories for Animation of sphere motion (*.gpt File)** creates a file containing the sphere trajectories during the packing process. The particle trajectory file can be loaded for [visualization](#)^[138]. Since saving the sphere trajectories results in a significant slowing down of the packing process, while the files are opened and trajectories for every sphere are saved, there is no need to select this option unless knowing the trajectories is essential for the project.

✓ Save Two-Point Correlation Information (*.tpc File)

Checking the box **Save Two-Point Correlation Information (*.tpc File)**, creates the two-point correlation file inside the [results folder](#)^[139] in the project folder.

✓ Compute Object Contacts Information Based on Voxel Image

If **Compute Object Contacts Information Based on Voxel Image** is checked, GeoDict counts the number of sphere-to-sphere contacts by checking if a voxel belonging to one sphere is in direct face-to-face contact with a voxel belonging to another sphere. This is reported as [Voxel Contacts](#)^[135] under the **Results - Report** subtab of the **Result Viewer** of the GDR result file, after the packing process has run.

✓ Compute Contacts Number Information Based on Analytical Data

If **Compute Contacts Number Information Based on Analytical Data** is checked, GeoDict counts the number of sphere contacts based on the given **Contact Distance**. Thus, contacts are also found for objects that do not touch but have a distance smaller than the given contact distance. This is reported as [Analytic Contacts](#)^[135] under the **Results - Report** subtab of the **Result Viewer** of the GDR result file, after the packing process has run. The contact distance can be given in Voxel or the unit given in the top right corner of the dialog.

☒ Compute Contacts Number Information Based on Analytic Data

Contact Distance
Voxel ▾

Parallelization

Parallelization
 4 Threads
Edit...

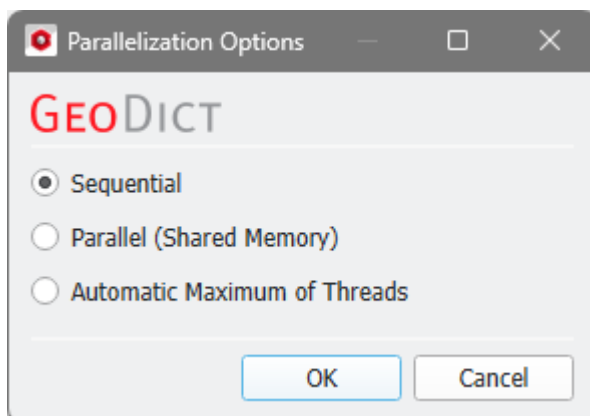
✓ Parallelization Options

Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

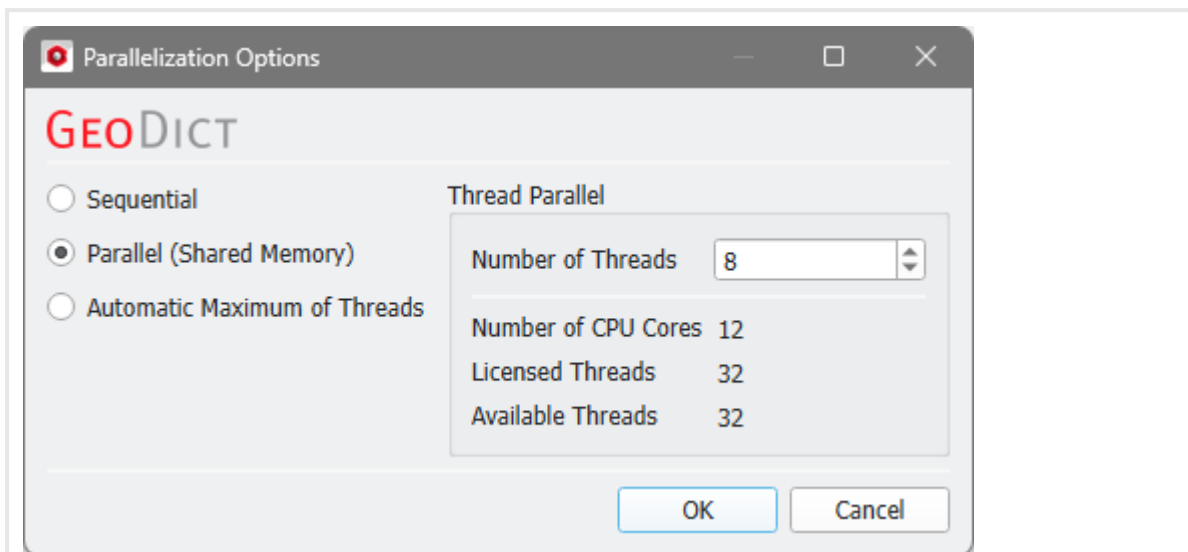
The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.

Parallelization
 12 Threads (Automatic Maximum)
Edit...

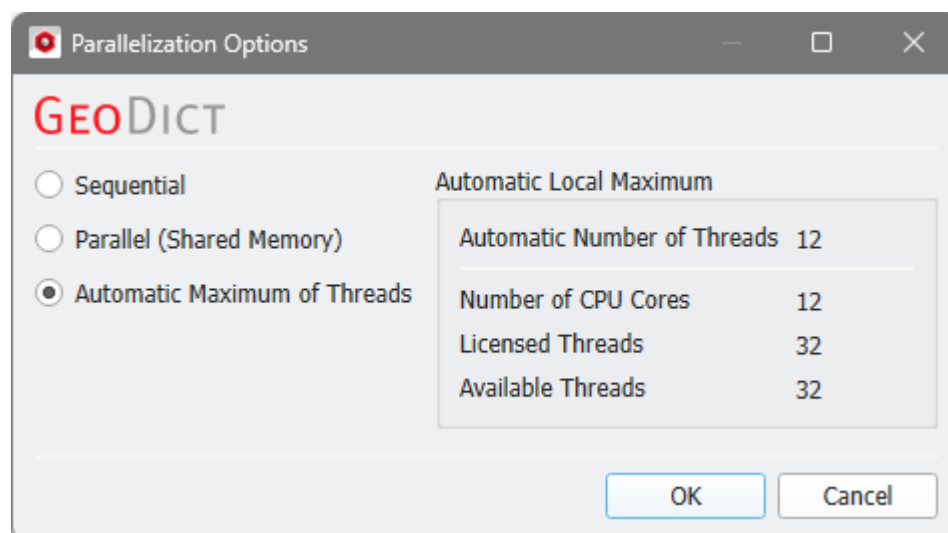
Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.

Sphere Distribution

Define the sphere size distribution.

Pack Options
Sphere Distribution
Equations & References

Probability Mode
Volume Probability

Draw Mode
Compute Sphere Type Numbers

Spheres
100
Suggest Sphere Number

Sphere Types
2

	Probability	Diameter / (μm)	Achieved Distribution	Sphere Number	Material ID	Material
1	0.5	100	0.497175	11	01	 Glass (Solid) [Sphere]...
2	0.5	50	0.502825	89	02	 Nickel (Solid) [Sphere]...

Edit / Paste Distribution Table

☐ Apply Gravity

✓ Probability Mode

With **Count Probability** as the **Probability Mode**, the Probability value in the [distribution table](#)^[132] (first column) refers to the number of spheres of a type.

With **Volume Probability**, it refers to the volume of spheres of a type.

✓ Draw Mode

The **Draw Mode** controls how the number of each sphere type is determined:

- **Draw Spheres:** A random generator sets the type of each sphere in the structure depending on the given probabilities. Thus, the number of spheres of each type depends on the [Random Seed](#)^[126].
- **Compute Sphere Type Numbers:** The number of spheres for each type is computed analytically, based on the probabilities, but without a random generator. The number of spheres of each type is the same for different Random Seeds.

For example, choosing **Count Probability** and **Compute Sphere Type Numbers** and specifying that of 100 spheres, 70% should be 100 μm and 30% should be 50 μm , exactly 70 spheres have a diameter of 100 μm and 30 spheres have a diameter of 50 μm .

Probability Mode:

Draw Mode:

Spheres:

Sphere Types:

	Probability	Diameter / (μm)	Achieved Distribution	Sphere Number	Material ID	Material
1	0.7	100	0.7	70	01	 Glass (Solid) [Sphere]...
2	0.3	50	0.3	30	02	 Nickel (Solid) [Sphere]...

In contrast, selecting **Draw Spheres** determines that for each of the 100 spheres in the example the type is randomly drawn. Thus, each sphere has a 70% probability to have a diameter of 100 μm , and a 30% probability to have a diameter of 50 μm . Therefore, the **Achieved Distribution** of type 1 is dependent on the Random Number, and binomially distributed around an expectation value of 0.7.

Probability Mode:

Draw Mode:

Spheres:

Sphere Types:

	Probability	Diameter / (μm)	Achieved Distribution	Sphere Number	Material ID	Material
1	0.7	100	0.66	66	01	 Glass (Solid) [Sphere]...
2	0.3	50	0.34	34	02	 Nickel (Solid) [Sphere]...

✓ Spheres and Suggest Sphere Number

Enter the number of spheres to be packed.

When working with Volume probability and strongly differing sphere diameters, it might happen that only a very small number of the larger spheres appears in the structure, or that they are completely missing.

By clicking **Suggest Sphere Number** a number of spheres is proposed so that ratios close to the desired probabilities can be reached. Depending on the chosen parameters (for example Volume Probability and strongly differing diameters), the suggested number of spheres might be large.

✓ Sphere Type

Determine the number of different sphere types to be packed. Increasing the number adds rows in the [distribution table](#)^[132] below.

✓ Distribution Table

The distribution table contains the parameters for the different sphere types to be packed. The parameters for up to 255 sphere types can be entered in the table, when selecting **Material ID per Object Type** and up to 1000 when selecting **Material ID per Material** for [material mode](#)¹²⁵.

The table consists of the following columns:

- Enter the **Probability** of the sphere type.
- Enter the **Diameter** of the sphere type in the chosen unit.
- The **Achieved Distribution** is drawn automatically given the previously entered number of spheres, and the values for diameter and probability for the distinct sphere types and shows the achieved ratio of the respective sphere types.
- The **Sphere Number** is also drawn automatically and shows the number of spheres of that type.
- The **Material ID** is chosen automatically counting the sphere types or materials depending on the [material mode](#)¹²⁵.
- Select the **Material** from the GeoDict material database by clicking on it.

	Probability	Diameter / (μm)	Achieved Distribution	Sphere Number	Material ID	Material
1	0.7	100	0.66	66	01	 Glass (Solid) [Sphere]...
2	0.3	50	0.34	34	02	 Nickel (Solid) [Sphere]...

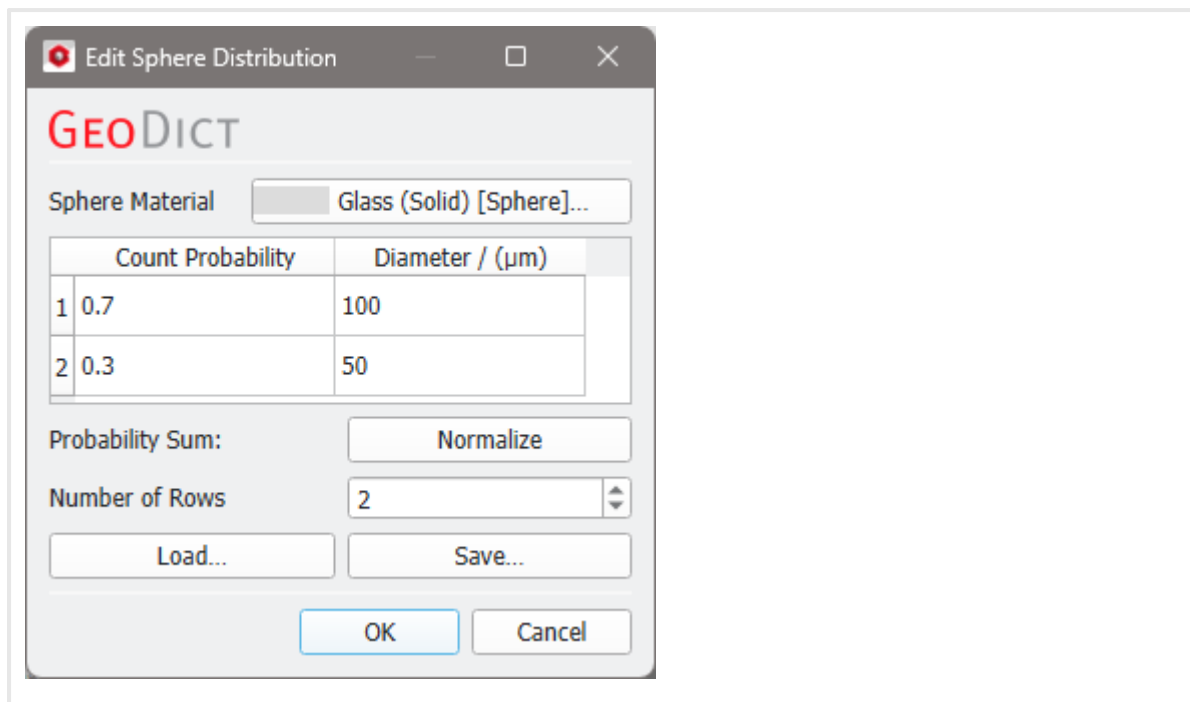
Edit / Paste Distribution Table

Click the **Edit / Paste Distribution Table** button to edit the values for **Diameter** and **Probability** (depending on the choice for probability mode) in the **Edit Sphere Distribution** dialog.

Clicking **Normalize** ensures that the **Probability** values sum up to one.

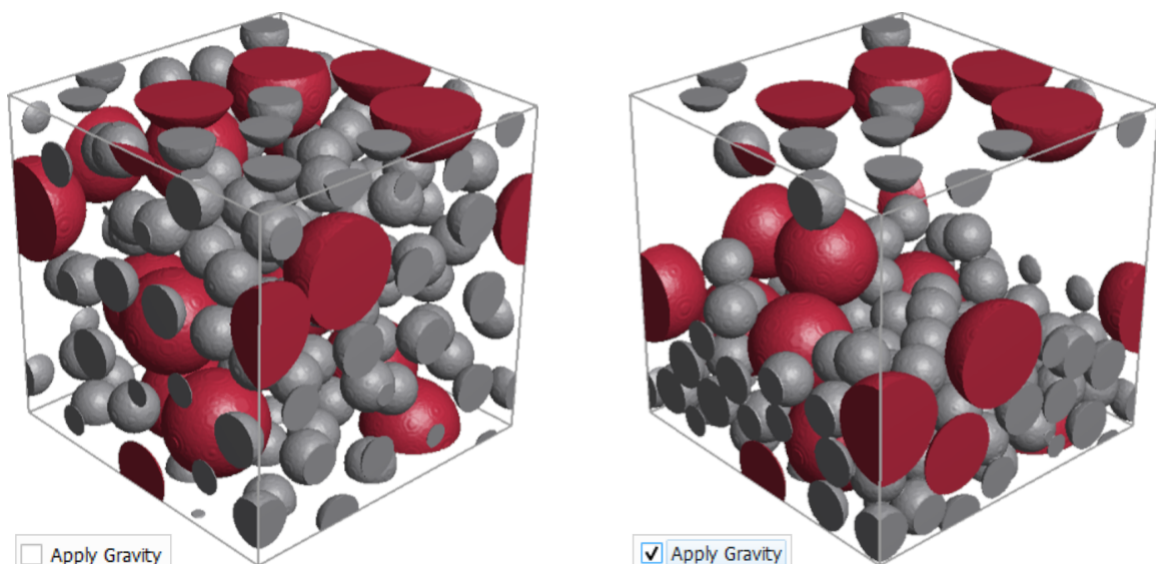
Alternatively, the distribution can be pasted from other software, for example from Microsoft Excel, or it can be loaded from a *.txt-file. With the **Save...** button, the distribution table can be written to a *.txt file.

The given **Sphere Material** is applied to all sphere types. If different materials should be present in the structure, change the according materials afterwards.



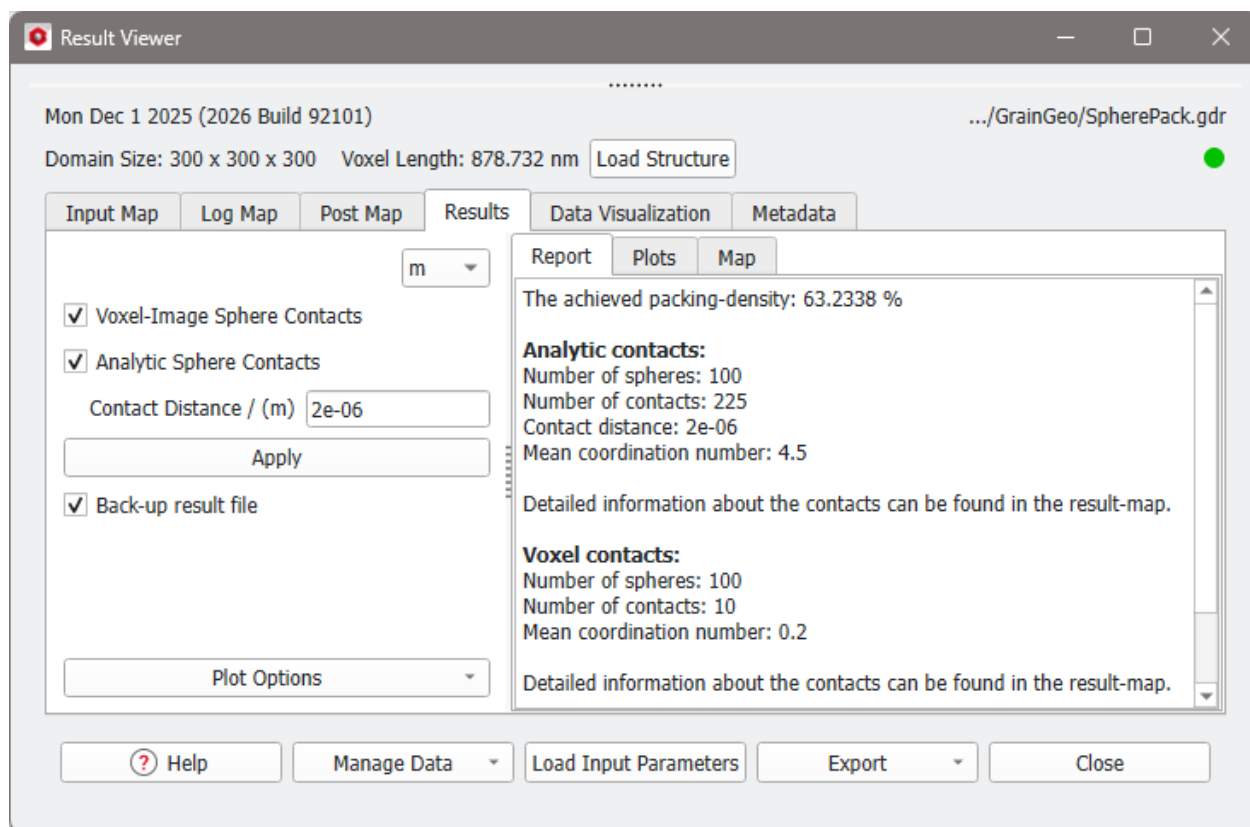
✓ Apply Gravity

Checking **Apply Gravity** includes a simulation of gravitational force on the packed spheres after the packing process, so that the spheres “fall down” in the Z-direction from their positions in the packing. The effect of applying gravity to a packed structure is obvious for low packing density (under 30%). As the domain is always periodic for the packing, the spheres cutting the bottom of the domain reappear in the top. If this is not desired, use ProcessGeo - Crop to crop the top of the domain.



1.3.2 Results

After generating analytic spheres the corresponding GeoDict result file (*.gdr) is opened in the Result Viewer automatically.



Besides the result file, a result folder with the same name is created. In this directory, GrainGeo saves files from the packing or [piling](#)^[141] run in the several formats. Some of these formats are optional and only saved if the corresponding checkbox in the **Analysis** panel of the [Pack Options](#)^[128] or [Pile Options](#)^[141] tab is checked.

Information on the analytic and discretized (voxelized) sphere contacts is internally and automatically saved and appears in the Result Viewer of the result file (*.gdr) under the **Results – Report** and the **Results – Map** subtabs. This includes such information as the contact distance, mean coordination number, the number of contacts, and a list of all sphere contacts.

✓ Report

Under the **Results – Report** tab you can always find the achieved packing density at the top.

Afterward follow the **Analytic contacts** and the **Voxel contacts**, if they were selected in the **Analysis** panel in the [Pack Options](#)^[128] or [Pile Options](#)^[141] tab. They can also be enabled or disabled after the structure generation via the post-[processing panel](#)^[137] on the left.

The **Mean coordination number** is the mean number of neighboring spheres that any sphere touches. It is computed as 2x the total **Number of contacts** divided by the total

Number of spheres. Each contact needs to be counted twice, once for each sphere which participates in this contact.

The screenshot shows a software window with three tabs: 'Report', 'Plots', and 'Map'. The 'Report' tab is active and displays the following information:

The achieved packing-density: 63.2338 %

Analytic contacts:
 Number of spheres: 100
 Number of contacts: 225
 Contact distance: 2e-06
 Mean coordination number: 4.5

Detailed information about the contacts can be found in the result-map.

Voxel contacts:
 Number of spheres: 100
 Number of contacts: 10
 Mean coordination number: 0.2

Detailed information about the contacts can be found in the result-map.

Total runtime: 00:00:27, Total memory usage: 1.167 GiB

✓ Result Map

In the **Results – Map** subtab, detailed information about each contact can be found:

- Under the **AnalyticContacts** key, the index numbers of the two objects that are in contact with each other are shown.
- Under the **VoxelContacts** key, the index numbers of the two objects that are in contact with each other, and the number of contacting voxel faces of each contact is shown.

Input Map

Log Map

Post Map

Results

Data Visualization

Metadata

Report

Plots

Map

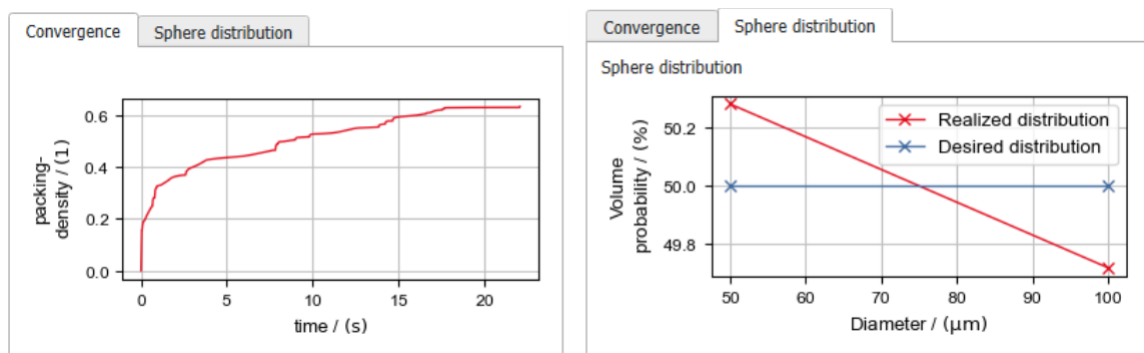
Key	Unit	Value
VoxelLength	m	8.787316322e-07
PackingDensity	1	0.632338
NumberOfSpheres		11, 89
Diameter		0.0001, 5e-05
▶ AdditionalFiles		
▼ AnalyticContacts		
▼ Contacts		
Object1		1, 1, 1, 1, 1, 1, 1, 1, 2, 2, 2, 2, 2, 2, 2, 2, 2, 2, 3, 3, 3, 3, 3, 3, 3, ...
Object2		3, 6, 9, 23, 27, 44, 65, 94, 4, 9, 10, 11, 20, 30, 65, 66, 67, 68, 73, 77, 99, 6, 11, 19, ...
ContactDistance		2e-06
NumberOfObjects		100
NumberOfContacts		225
MeanCoordinationNumber		4.5
▼ VoxelContacts		
▼ Contacts		
Object1		1, 1, 1, 3, 3, 4, 6, 8, 9, 10
Object2		3, 65, 94, 6, 11, 65, 10, 10, 38, 11
ContactFaces		63, 59, 1, 7, 26, 59, 8, 20, 3, 21
NumberOfObjects		100
NumberOfContacts		10
TotalContactFaces		267
MeanCoordinationNumber		0.2

✓ Plots

Under the **Results - Plots** tab two plots can be found.

The **Convergence** plot shows the packing density achieved by the algorithm over time.

The **Sphere distribution** tab compares the realized distribution with the desired distribution entered in the [Sphere Distribution](#) ¹³⁰ tab.



✓ Post-Processing Panel

In the post-processing panel on the left, decide if the **Voxel-Image Sphere Contacts** and the **Analytic Sphere Contacts** should be shown or not. For analytic sphere contacts additionally, the **Contact Distance** must be given in the selected unit.

The post-processing is applied after clicking **Apply**. This changes the result file, but if **Back-up result file** is checked, the original result file is backed up in the result folder as described in the Result Viewer User Guide.

If [Compute Contacts Number Information Based on Analytic Data](#)^[128] is checked, GeoDict counts the number of sphere-to-sphere contacts by checking if the distance between the center points of the spheres is large enough. For numerical reasons, it is highly unlikely that two spheres will exactly touch each other. Rather, there will always be a small distance between them.

For example, with a given **Contact Distance** of 0.5 μm , a sphere of diameter 20 μm is defined to be in contact with a sphere of diameter 10 μm , if the distance between their center points is less than 15.5 μm .

The chosen **Contact Distance** can be changed during post-processing. Smaller contact distances lead to less contacts found.

The image displays two screenshots of the GrainGeo software interface, specifically the 'Results' tab. The top screenshot shows the 'Contact Distance / (m)' set to 2e-06, resulting in 225 contacts. The bottom screenshot shows the 'Contact Distance / (m)' set to 1e-06, resulting in 33 contacts. Both screenshots show a 'Report' panel with packing density and contact statistics.

Top Screenshot (Contact Distance: 2e-06):

- ☐ Voxel-Image Sphere Contacts
- ☒ Analytic Sphere Contacts
- Contact Distance / (m) 2e-06
- Apply
- ☒ Back-up result file
- Plot Options
- Report: The achieved packing-density: 63.2338 %
- Analytic contacts:**
 - Number of spheres: 100
 - Number of contacts: 225
 - Contact distance: 2e-06
 - Mean coordination number: 4.5
- Detailed information about the contacts can be found in the result-map.

Bottom Screenshot (Contact Distance: 1e-06):

- ☐ Voxel-Image Sphere Contacts
- ☒ Analytic Sphere Contacts
- Contact Distance / (m) 1e-06
- Apply
- ☒ Back-up result file
- Plot Options
- Report: The achieved packing-density: 63.2338 %
- Analytic contacts:**
 - Number of spheres: 100
 - Number of contacts: 33
 - Contact distance: 1e-06
 - Mean coordination number: 0.66
- Detailed information about the contacts can be found in the result-map.

✓ Data Visualization

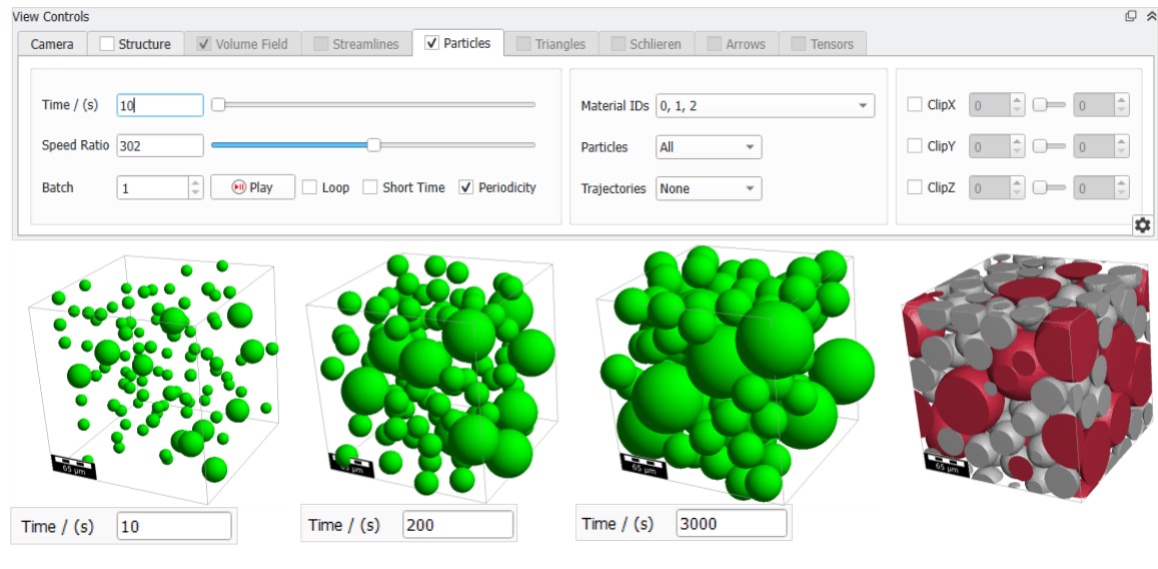
If **Save GeoDict Particle Trajectories for Animation of sphere motion** was checked in the [Analysis](#)^[128] panel, in the Result Viewer under the **Data Visualization** tab the particles and their trajectories can be loaded.

The image displays a screenshot of the GrainGeo software interface, specifically the 'Data Visualization' tab. It shows the file paths for the final particle position and the particle trajectory files, and a button to load the particles.

Data Visualization Tab:

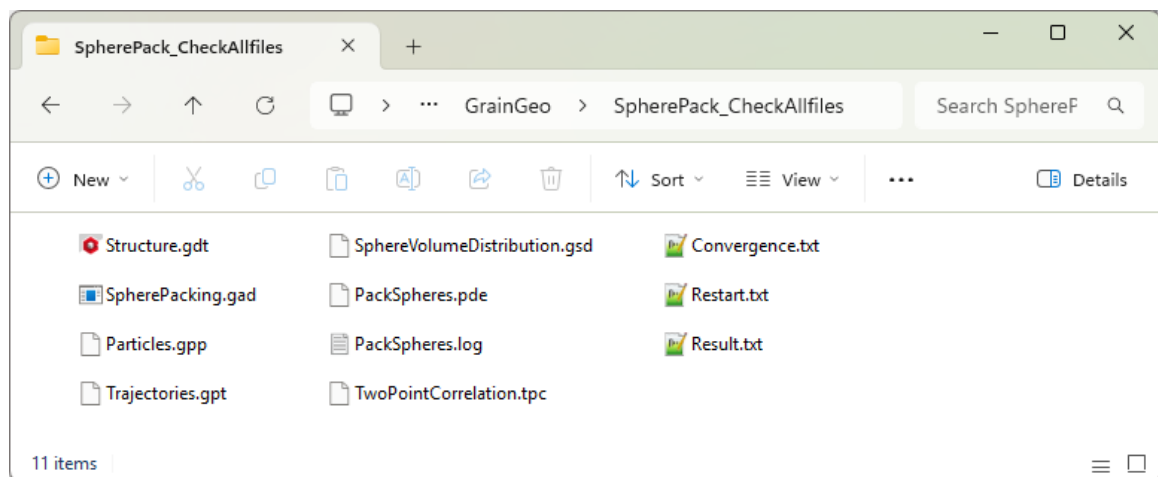
- Final particle position file: Particles.gpp
- Particle trajectory file: Trajectories.gpt
- Load Particles

In the **View Controls** uncheck **Structure** and go to the **Particles** tab to visualize the particles movement during the packing process until they reach their final position by clicking **Play** or moving the slider for **Time**. Learn more about particle visualization settings in the Visualization User Guide.



✓ Result Folder

The result folder contains the following files:

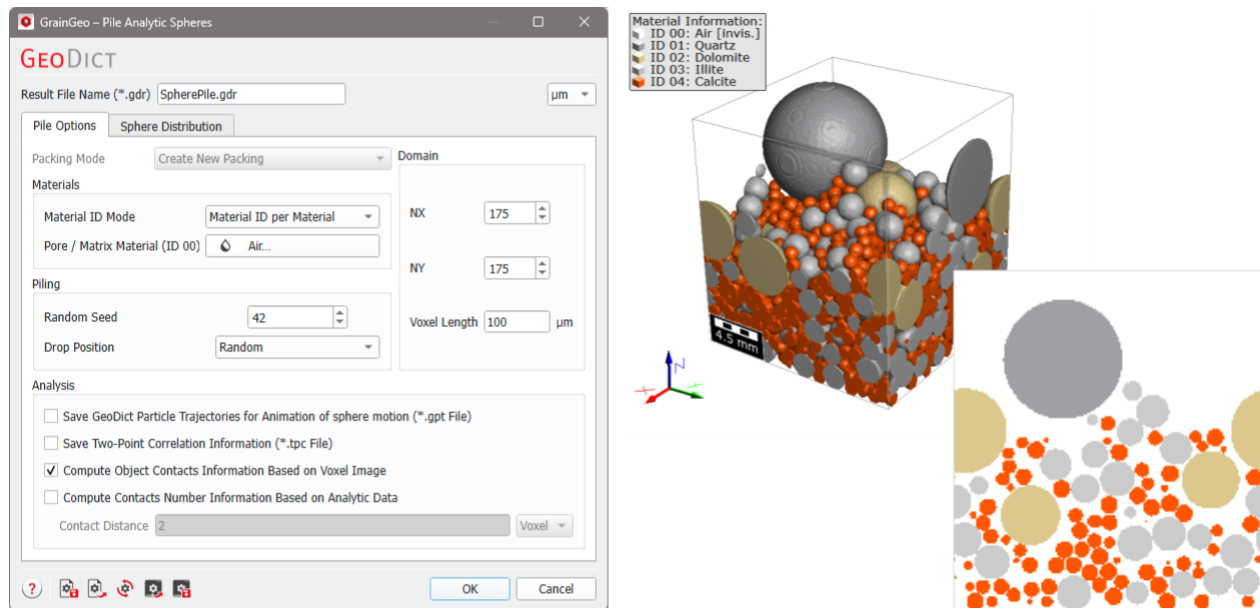


- **Structure.gdt** file containing the GeoDict 3D voxelized geometry and the analytic data of the object packing.
- **SpherePacking.gad** (GeoDict analytic data) files contain the analytic data about the geometry of the object packing, such as object Material ID, object type, object position, and (sphere) diameter.
- optionally saved results (choose to save them in the [Analysis](#)^[128] panel)

- **Trajectories.gpt** (GeoDict **p**article **t**rajectory) files contain a record of the movement of the spheres during the packing (or piling). This file can be used to [visualize](#)¹³⁸ the packing process.
- **Particles.gpp** (GeoDict **p**article **p**osition) files contain information on the position of the spheres after the packing (or piling).
- **TwoPointCorrelation.tpc** (two-**p**oint **c**orrelation) file contains a list with the distances between all spheres.
- **Convergence.txt** relates the convergence at a given time with a certain packing-density.
- **Restart.txt** contains information about the sphere distribution parameters to re-start the packing process.
- **Result.txt** contains the achieved packing density, which is set to zero for the piling process.
- **PackSpheres.log** contains the chronological record of the packing process.
- **PackSpheres.pde** is a parameter file that contains the input data for the external packing code.
- **SphereVolumeDistribution.gsd** (GeoDict **s**phere **d**istribution) contains the diameter, probability and number of each distinct sphere type, which can also be found in the Map tab of the Result Viewer.

1.4 Pile Analytic Spheres

Use **Pile Analytic Spheres** to pile analytical spheres in Z-direction.



The parameters for the piling are organized in the [Pile Options](#)^[123] and [Sphere Distribution](#)^[130] tabs.

Many of the **Pile Options** to pile analytic spheres are similar to the options shown for [Pack Analytic Spheres](#)^[122].

The options are the same for:

- the [Units](#)^[122] and [Result File Name](#)^[122] above the different tabs,
- the [Materials](#)^[125] and the [Analysis](#)^[128] panel under the Pile Options tab,
- the [Sphere Distribution](#)^[130] tab is identical, except, that for pile analytic spheres, there is no option to apply gravity, because the piling process already applies gravity.

The [results](#)^[135] are also very similar to those from sphere packing.

In the following the **Domain** and **Piling** panels are described, which are different or not available for the sphere packing.

✓ Domain

The **Domain** value for **NX** and **NY** can be chosen by direct insertion or by clicking the arrow buttons, to indicate the number (N) of voxels in X- and Y-direction.

Domain

NX
175

NY
175

Voxel Length
100
μm

Since the spheres fall in Z-direction, the size value for Z is determined by the height of the pile of spheres and depending on the number of spheres to be piled.

In the Voxel Length box, enter the length of the voxels in the selected units.

✓ Piling

In the **Piling** panel, the **Drop Position** from **Center** or **Random** can be selected from the pull-down menu.

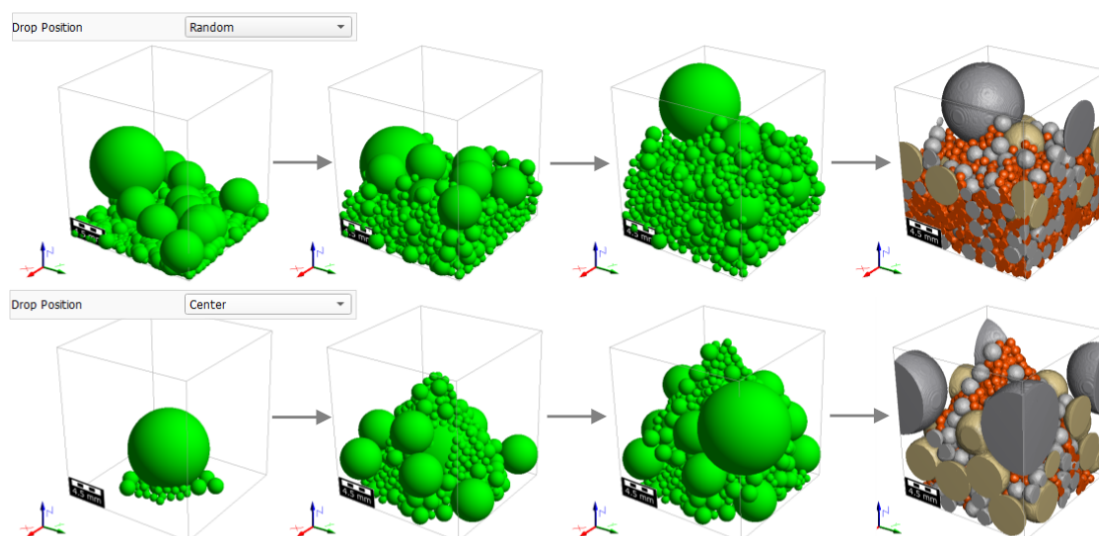
Piling

Random Seed
42

Drop Position
Random

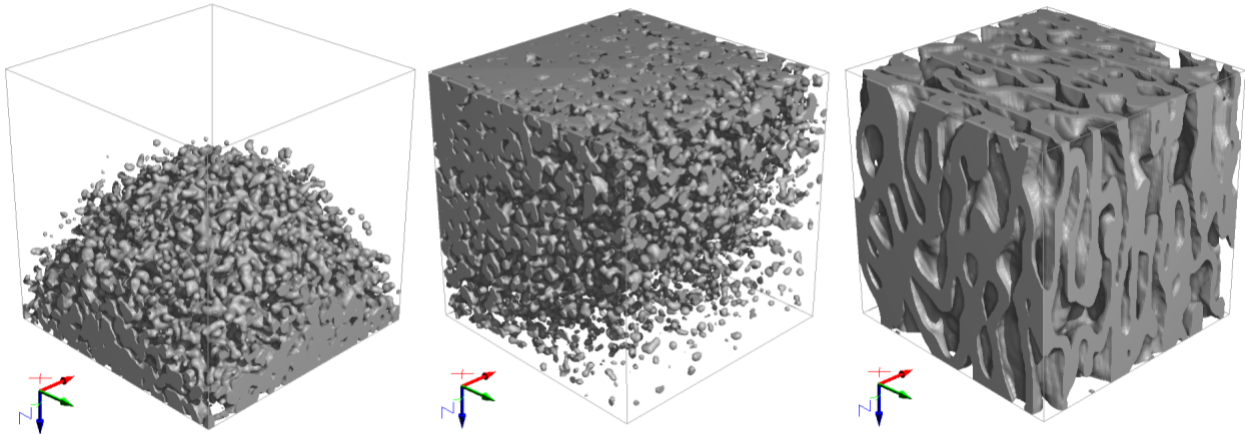
When selecting **Center**, the spheres are dropped from the center of the X-Y plane, instead of being dropped from any random position on the plane.

In the example below observe how the spheres are placed after another for random and center drop position. The visualization is done with particles as explained in the [Results](#) ¹³⁸ section.



1.5 Stochastic Field Thresholding

Choose **Stochastic Field Thresholding** to create structures by generating and segmenting stochastic fields according to selected threshold criteria (see also [Hyman et al., 2014](#)^[255] and [García-Ojalvo et al., 1999](#)^[255]). The generated structure consists of two materials: a solid material and a surrounding pore / matrix material.



The Stochastic Field Thresholding command:

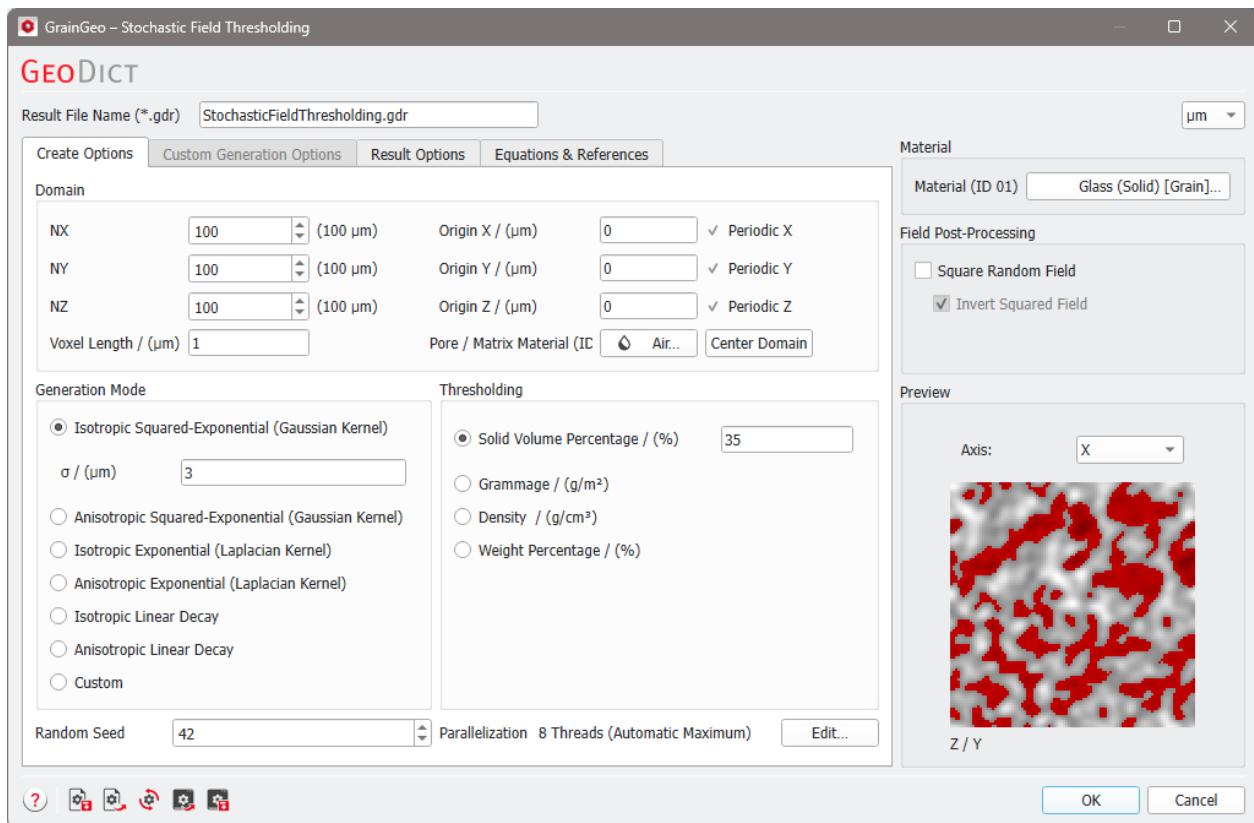
- [Options](#)^[143]
Define the parameters for the stochastic field generation and the thresholding.
- [Results](#)^[163]
View the results.

1.5.1 Options

At the top left of the dialog, the name for the file containing the generation results can be entered in the **Result File Name (*.gdr)** box. The default name can be kept, or a new name can be chosen, fitting the current project.

The result files are saved in the chosen project folder (**File** → **Choose Project Folder**, in the **Menu bar**). If a GeoDict result file (*.gdr) with the given name already exists in the project folder, a warning message is shown at the start of the creation process. You can either decide to rename the chosen file name to a new one, to cancel the generation process, to overwrite or to back up the old file. When nothing is selected, GeoDict uses the **Back-Up** option after a waiting time.

The available units (m, cm, mm, μm , nm and Inch) are selectable from the pull-down menu at the top right of the dialog. When the units are changed, the entered values are adjusted automatically.



The parameters are organized in the following tabs:

- [Material and Preview](#)¹⁴⁵
Determine the material, apply field post-processing, and observe a preview visualizing the current settings.
- [Create Options](#)¹⁴⁶
Determine general properties of the resulting structure, such as size, position, resolution, and solid volume percentage.
- [Custom Generation Options](#)¹⁵⁶
Choose individual combinations of stochastic fields to create a custom random field.
- [Result Options](#)¹⁶³
Determine if the random field should be saved in the result folder.



- Opens the corresponding User Guide section.
- Saves the settings to a GeoDict settings file (*.gps).
- Loads the settings from a GeoDict settings file (*.gps) or a GeoDict result file (*.gdr).
- Resets all parameter settings to the built-in default settings.
- Resets all parameter settings to the saved start-up settings.



Saves the current parameter settings as start-up settings.

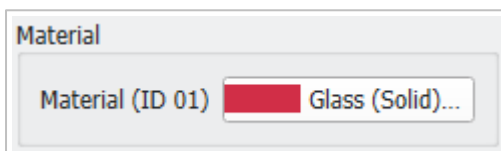
Each option is explained by a tooltip which appears when resting the mouse over the icon.

Material and Preview

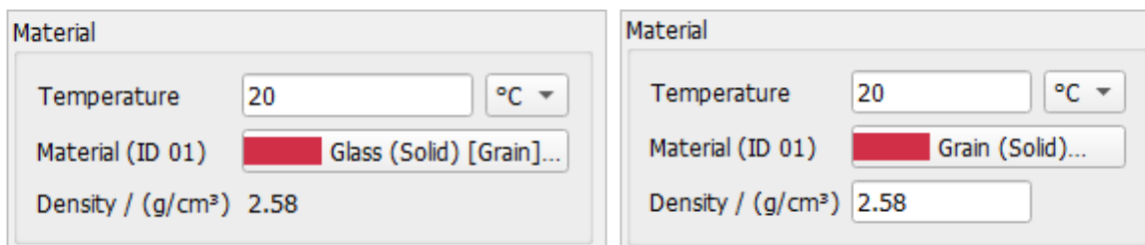
Determine the material and observe a preview visualizing the current settings entered in the [Create Options](#)^[146] and [Custom Generation Options](#)^[156] tabs.

Material

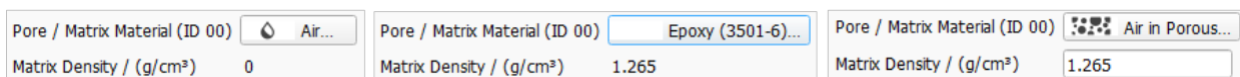
The generated structure consists of two materials: a solid material and a surrounding pore / matrix material. In the **Material** panel select the **Material (ID 01)** for the solid material from the material database.



If **Grammage**, **Density**, or **Weight Percentage** are selected for [thresholding](#)^[153], also the **Temperature** can be edited. The temperature unit can be chosen as K, °C, or °F. If **Manual** is chosen as material a **Density** must be entered.



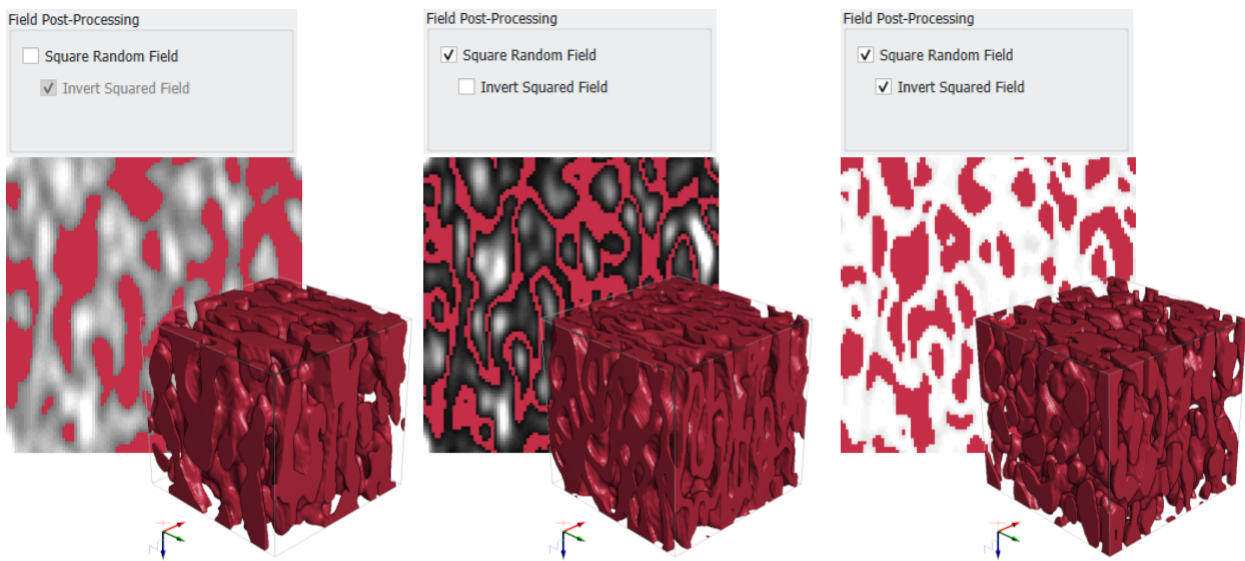
The **Pore / Matrix Material (ID 00)** is defined in the **Domain** panel. The material filling the pore space can be Solid, Porous, or Fluid. For a porous matrix material, a density can be entered, if grammage, density, or weight percentage are chosen for [thresholding](#)^[153].



Field Post-Processing

Check **Square Random Field** to square the random field equation before thresholding. This breaks the symmetry of the random field.

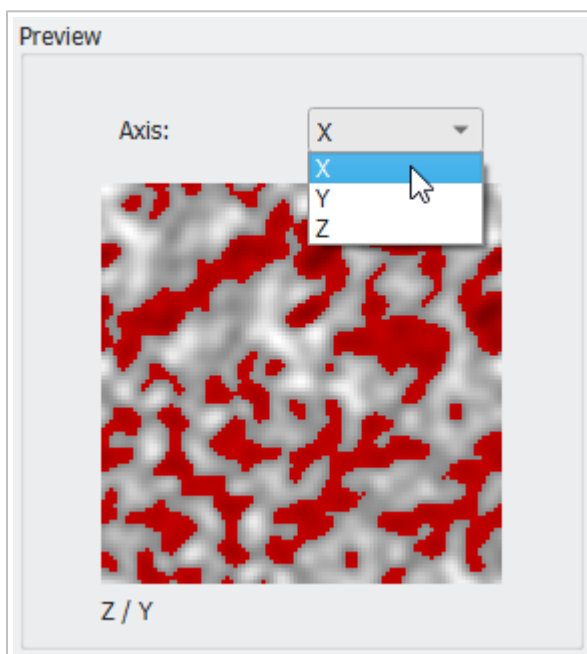
When additionally checking **Invert Squared Field**, the field and thus, the resulting structure are inverted.



Preview

In the bottom right of the **Stochastic Field Thresholding** dialog a preview of the generated random field (gray values) and the segmentation result (red for Material ID 01) is displayed.

The preview is automatically updated when changing the values for the **Domain**, **Generation Mode**, and **Thresholding** parameters. The view direction can be selected from the pull-down menu for **Axis**.



Create Options

The parameters defining the general properties of the granular structure are entered under the **Create Options** tab. They are grouped into the [Domain](#)¹⁴⁷, [Generation Mode](#)¹⁴⁸, and

[Thresholding](#)¹⁵³ panels. Additionally the options [Random Seed and Parallelization](#)¹⁵⁴ are available.

The parameters are organized in the following groups:

- [Domain](#)¹⁴⁷
Define the domain parameters, such as resolution, origin, and matrix material.
- [Generation Mode](#)¹⁴⁸
Define the parameters of the stochastic field.
- [Thresholding](#)¹⁵³
Define the parameters to threshold the generated stochastic field.
- [General Options](#)¹⁵⁴
Define the random seed and the number of parallel threads used for the structure generation.

Domain

The **Domain** panel contains the parameters defining the structure size (**NX**, **NY**, and **NZ**) in combination with the resolution (**Voxel Length**), as well as the **Origin** parameters and **Center Domain**.

These options are the same as for the [GrainGeo Create Options](#)¹¹.

Domain

NX
(100 μm)

Origin X / (mm)
✓ Periodic X

NY
(100 μm)

Origin Y / (mm)
✓ Periodic Y

NZ
(100 μm)

Origin Z / (mm)
✓ Periodic Z

Voxel Length / (mm)

Pore / Matrix Material (ID 00)

In general, the structure is periodic. Only if the parameters define a domain smaller than the chosen correlation length(s), periodicity cannot be achieved. That is because a bigger structure is generated and cropped to the desired size. In that case, warning messages appear in the result viewer for the affected directions. The runtime and memory requirements increase, corresponding to the needed domain size.

Input Map
Log Map
Post Map
Results
Data Visualization
Metadata

Report
Map

Reached SVF: 35.2%

Warning:
The created structure is not periodic in x-direction as the domain size is too small for the chosen correlation length(s).
The created structure is not periodic in y-direction as the domain size is too small for the chosen correlation length(s).
The created structure is not periodic in z-direction as the domain size is too small for the chosen correlation length(s).
In this case a larger structure is created and cut to the requested size.

Generation Mode

The options in the **Generation Mode** panel control the distribution used for the stochastic field which is segmented to obtain the final structure. It is possible to choose **Isotropic Squared-Exponential (Gaussian Kernel)**, **Anisotropic Squared-Exponential (Gaussian Kernel)**, **Isotropic Exponential (Laplacian Kernel)**, **Anisotropic Exponential (Laplacian Kernel)**, **Isotropic Linear Decay**, **Anisotropic Linear Decay**, or a **Custom** random field.

Generation Mode

☐ Isotropic Squared-Exponential (Gaussian Kernel)
☒ Anisotropic Squared-Exponential (Gaussian Kernel)

σ_X / (mm)

σ_Y / (mm)

σ_Z / (mm)

☐ Isotropic Exponential (Laplacian Kernel)
☐ Anisotropic Exponential (Laplacian Kernel)
☐ Isotropic Linear Decay
☐ Anisotropic Linear Decay
☐ Custom

✓ **Isotropic Squared-Exponential (Gaussian Kernel)**

An **Isotropic Squared-Exponential (Gaussian Kernel)** random field is used to create the structure. Enter the **Correlation Length** σ to define the standard deviation of the used **Gauss** kernel. With higher values the features of the generated structure become larger.

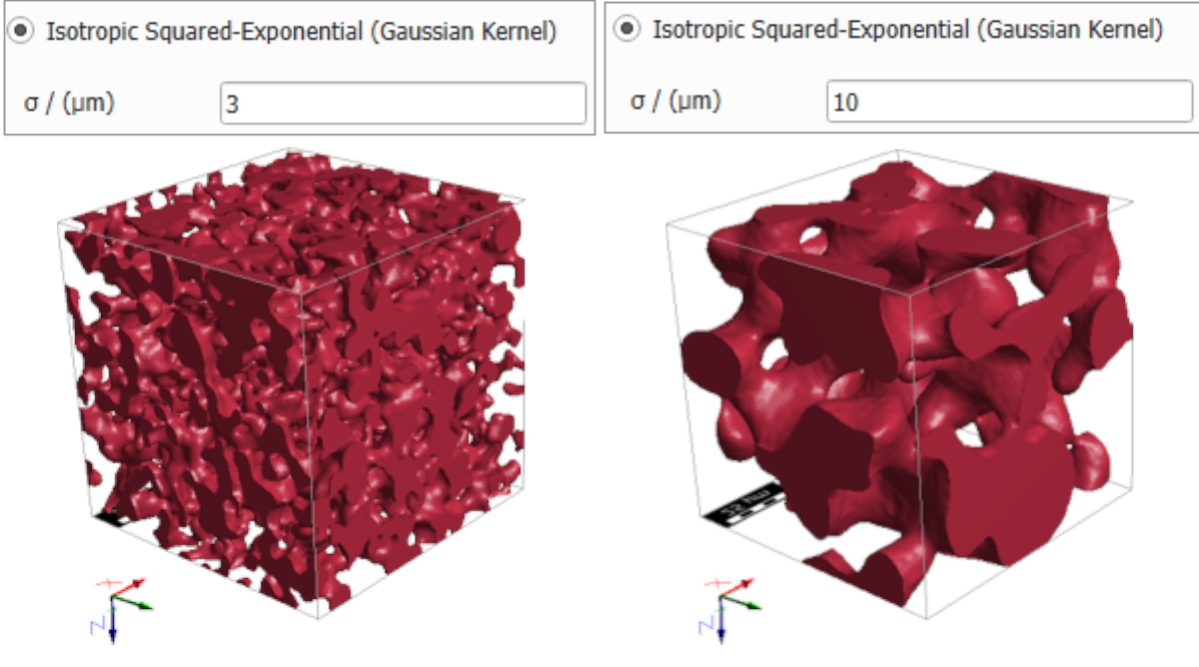
For the Gaussian Kernel the following equation applies:

$$F(x, y, z) = \exp\left(-\frac{1}{2}\left(\frac{x^2 + y^2 + z^2}{\sigma^2}\right)\right)$$

(6) Isotropic
Gaussian
Kernel

where σ is the correlation length.

In the following example observe how the feature size changes for two different correlation lengths, while all other parameters are kept the same.



✓ Anisotropic Squared-Exponential (Gaussian Kernel)

A **Gaussian** random field is used to create the structure. Enter the **Correlation Length** for X-direction σ_X , Y-direction σ_Y , and Z-direction σ_Z . These values define the standard deviations in each main axis of the used Gaussian kernel. Higher values lead to larger pores. If the same value is entered for all three directions, it is the same as **Isotropic Squared-Exponential**.

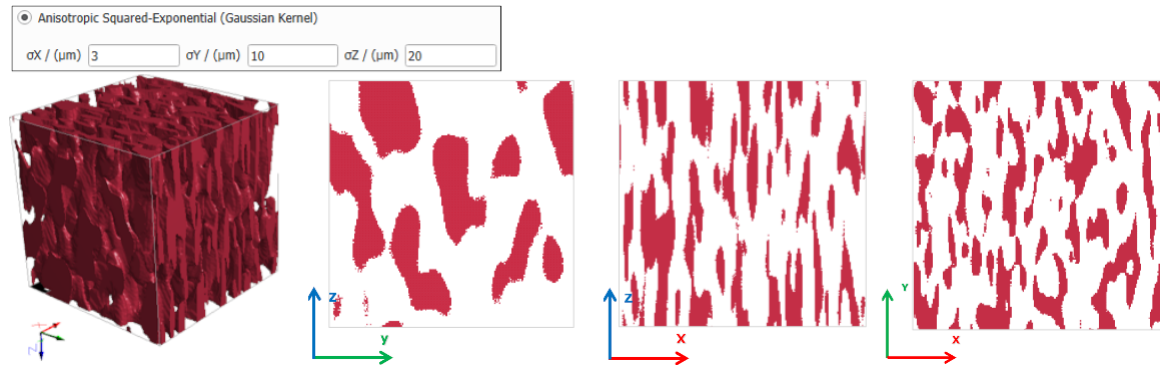
For the Gaussian Kernel the following equation applies:

$$F(x, y, z) = \exp\left(-\frac{1}{2}\left(\frac{x^2}{\sigma_x^2} + \frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2}\right)\right)$$

(7)
Anisotropic
Gaussian
Kernel

where σ is the correlation length in the respective direction.

In the following example, the values 3, 10 and 20 are used for σ_X , σ_Y , and σ_Z , respectively. Observe the different feature shapes for the different view directions.



✓ Isotropic Exponential (Laplacian Kernel)

An **Isotropic Exponential (Laplacian Kernel)** random field is used to create the structure. Enter the **Correlation Length** σ to define the standard deviation of the used **Laplacian Kernel**. With higher values the features of the generated structure become larger.

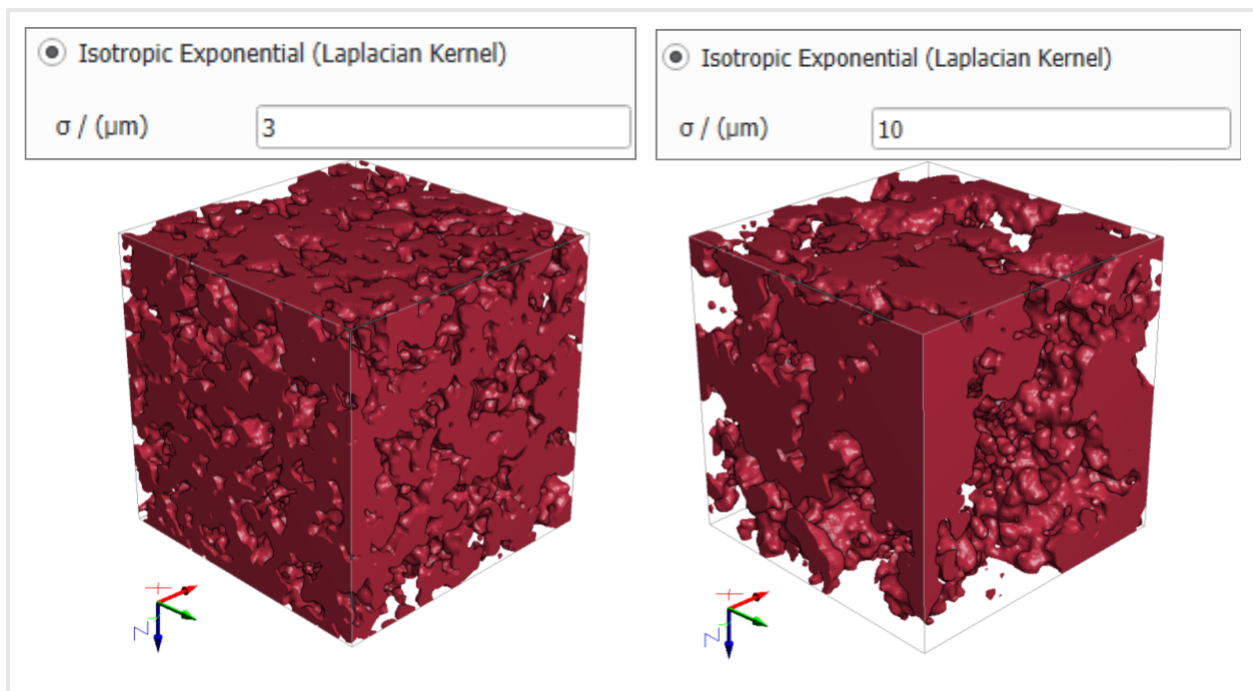
For a Laplacian Kernel the following equation applies:

$$F(x, y, z) = \exp\left(-\sqrt{\frac{x^2 + y^2 + z^2}{\sigma^2}}\right)$$

(8) Isotropic
Laplacian
Kernel

where σ is the correlation length.

In the following example observe how the feature size changes for two different correlation lengths, while all other parameters are kept the same.



✓ Anisotropic Exponential (Laplacian Kernel)

An **Laplacian** random field is used to create the structure. Enter the **Correlation Length** for X-direction σX , Y-direction σY , and Z-direction σZ . These values define the standard deviations in each main axis of the used Laplacian kernel. Higher values lead to larger pores. If the same value is entered for all three directions, it is the same as **Isotropic Exponential**.

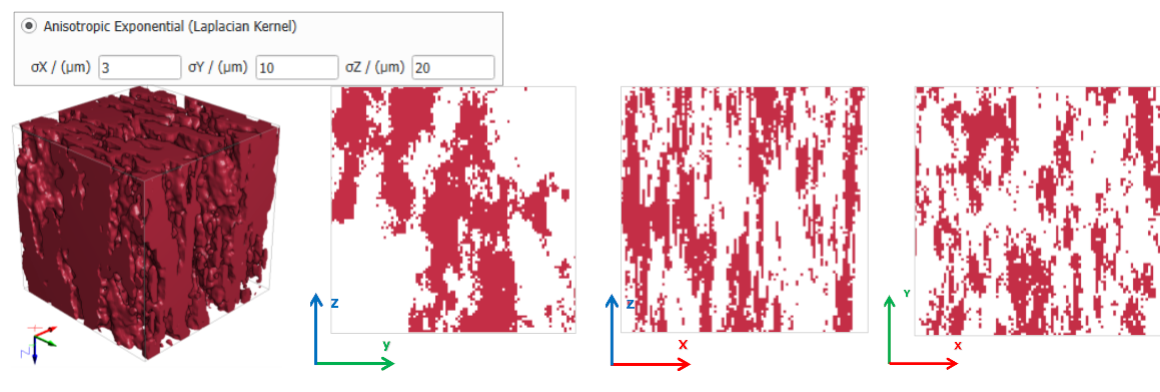
For a Laplacian Kernel the following equation applies:

$$F(x, y, z) = \exp\left(-\sqrt{\frac{x^2}{\sigma_x^2} + \frac{y^2}{\sigma_y^2} + \frac{z^2}{\sigma_z^2}}\right) \quad (9)$$

Anisotropic
Laplacian
Kernel

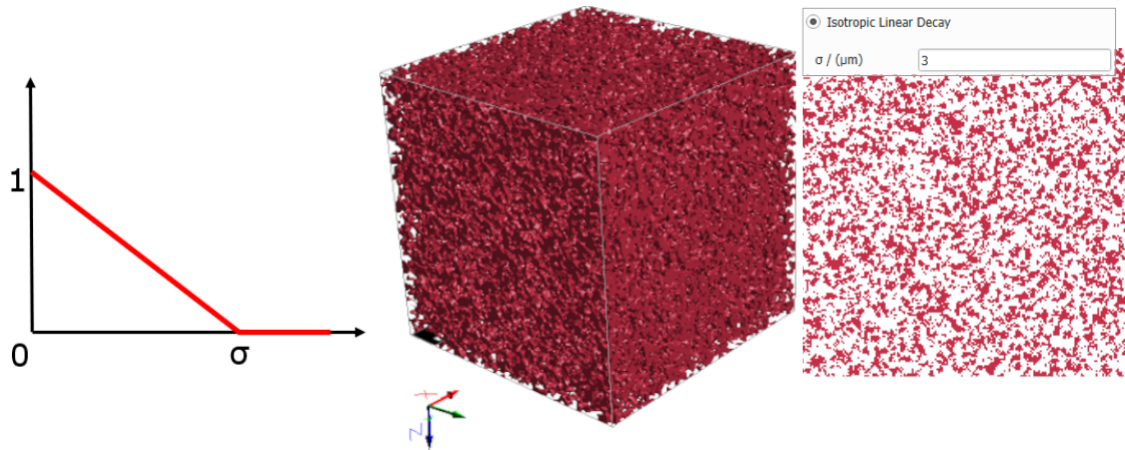
where σ is the correlation length in the respective direction.

In the following example, the values 3, 10 and 20 are used for σX , σY , and σZ , respectively. Observe the different feature shapes for the different view directions.



✓ Isotropic Linear Decay

If **Isotropic Linear Decay** is selected, a linear decreasing correlation function is used to create the stochastic field. It starts in 0 with the value 1. The correlation function reaches 0 in σ and stays 0 for larger values. Thus, the gradient is $-\frac{1}{\sigma}$ between 0 and sigma and 0 for larger values.

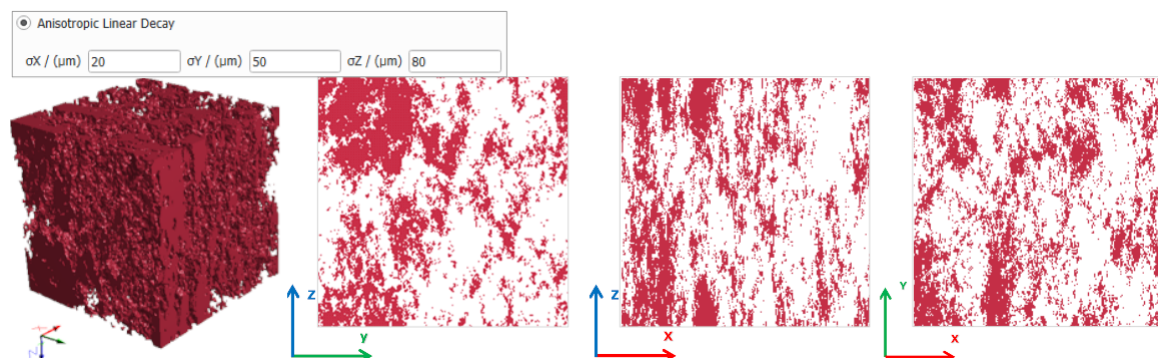


With higher values the features of the generated structure become larger. It can be necessary to post-process the results with **ProcessGeo Cleanse**.

✓ Anisotropic Linear Decay

If **Anisotropic Linear Decay** is selected, different linear decreasing correlation functions are used for X-, Y-, and Z-direction to create the stochastic field. They are defined as described for the isotropic case above. Enter σ_X , σ_Y , and σ_Z to determine the corresponding gradients: $-\frac{1}{\sigma_X}$, $-\frac{1}{\sigma_Y}$, and $-\frac{1}{\sigma_Z}$. Higher values lead to larger features. It can be necessary to post-process the results with **ProcessGeo Cleanse**.

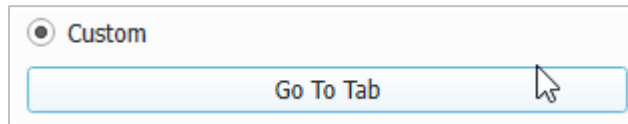
In this example, observe the differences in the three view directions.



✓ Custom

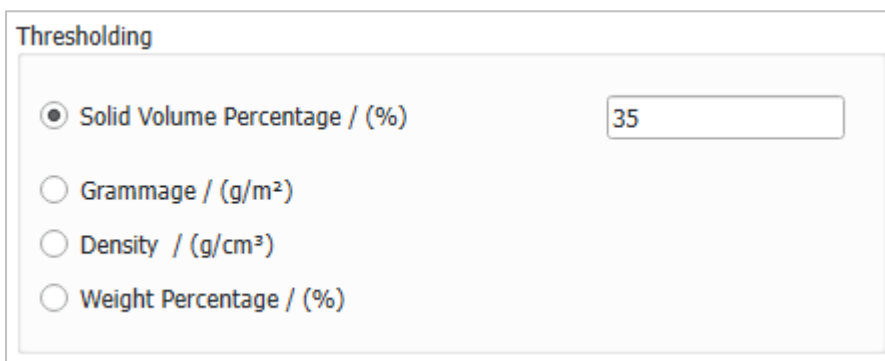
A **Custom** stochastic field is created and segmented to generate the structure.

If checked, the tab [Custom Generation Options](#)¹⁵⁶ becomes available. Combine the different random field and gradient options in the **Custom Generation Options** tab. This tab can also be reached by clicking **Go To Tab** in the **Generation Mode** panel. In addition to linear and Gaussian random fields also linear gradient, sphere gradient and membrane gradient are available.



Thresholding

The parameters in the **Thresholding** panel of the **Stochastic Field Thresholding** dialog define the criteria for the segmentation threshold applied to the generated stochastic field to obtain the structure. The available parameters are **Solid Volume Percentage / (%)**, **Grammage / (g/m²)**, **Density / (g/cm³)** and **Weight Percentage / (%)**.



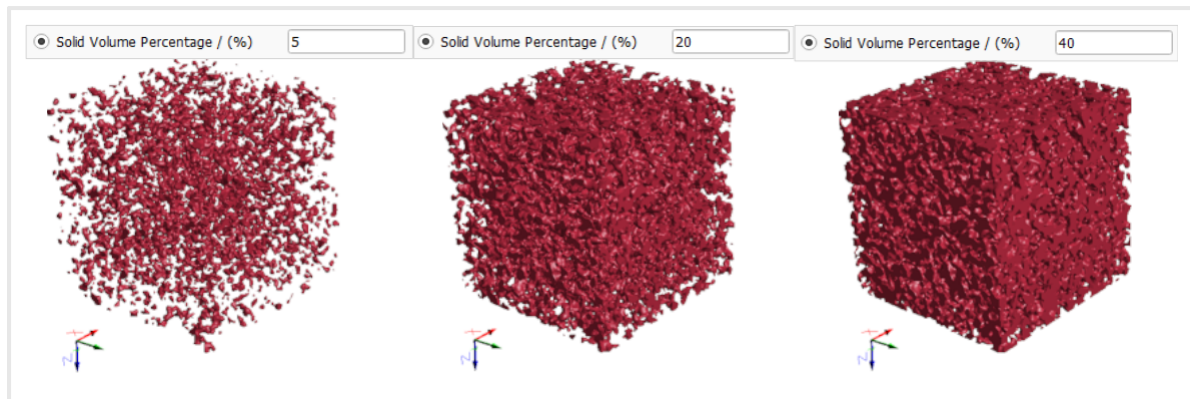
When **Grammage**, **Density**, or **Weight Percentage** are chosen as stopping criterion, the temperature must be set as additional parameter in the [Material](#)¹⁴⁵ panel. The density of the constituent materials will be set with respect to the chosen temperature based on the Material Database.

When choosing **Solid Volume Percentage**, the **Temperature** parameter is not available.

✓ Solid Volume Percentage

Solid Volume Percentage (SVP) determines the fraction of the total volume in percent that the structure should have. Accepted values range from 0% to 100%.

For example, a structure with a **Solid Volume Percentage** of 40 consists of 40% solid and 60% void space. Porosity is defined as $(1 - \text{SVP}/100)$. The threshold to segment the stochastic field is chosen to match the given SVP. Observe the difference in a structure when varying the solid volume percentage from 5%, to 20%, and finally to 40%, while all other parameters are left unchanged.



✓ Grammage

The **Grammage / (g/m²)** determines the mass per unit area (in the XY-Plane) of the resulting structure. When **Grammage** is chosen as stopping criterion, the **Density / (g/cm³)** of the **Bulk Material** must be defined in the [Material](#)^[145] panel and the temperature must be set.

✓ Density

The **Density / (g/cm³)** of the resulting structure depends on the density of the chosen [materials](#)^[145]. It cannot be set smaller than the lowest occurring density or larger than the highest occurring density.

✓ Weight Percentage

The **Weight Percentage** determines the weight of the created object in relation to the weight of the whole structure (including the pore material). Choosing this option only makes sense when the density of the **Pore / Matrix Material** is greater than zero. Otherwise, the domain will stay empty. See [Material and Preview](#)^[145] for more information.

General Options

Define general options for the structure generation.

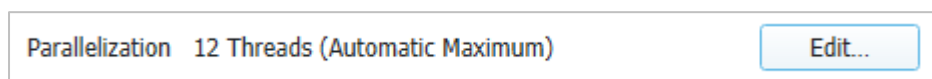
Random Seed

Random Seed initializes the random number generator behind the stochastic field generator. Changing its value produces different sequences of random numbers and hence, different realizations of the specified structure. If all settings are equal, generating with the same **Random Seed** value produces an identical structure. **Random Seed** must be a non-negative integer number.

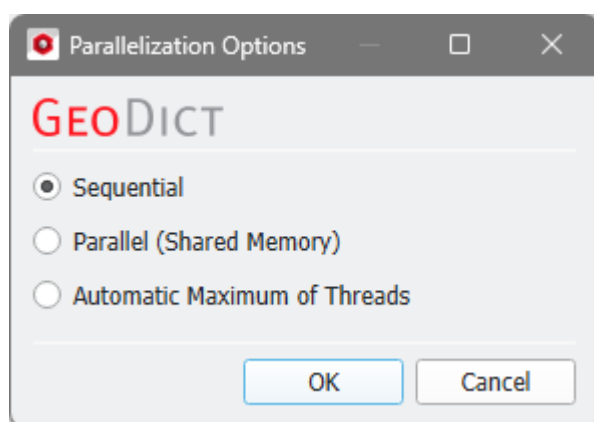
Parallelization

Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

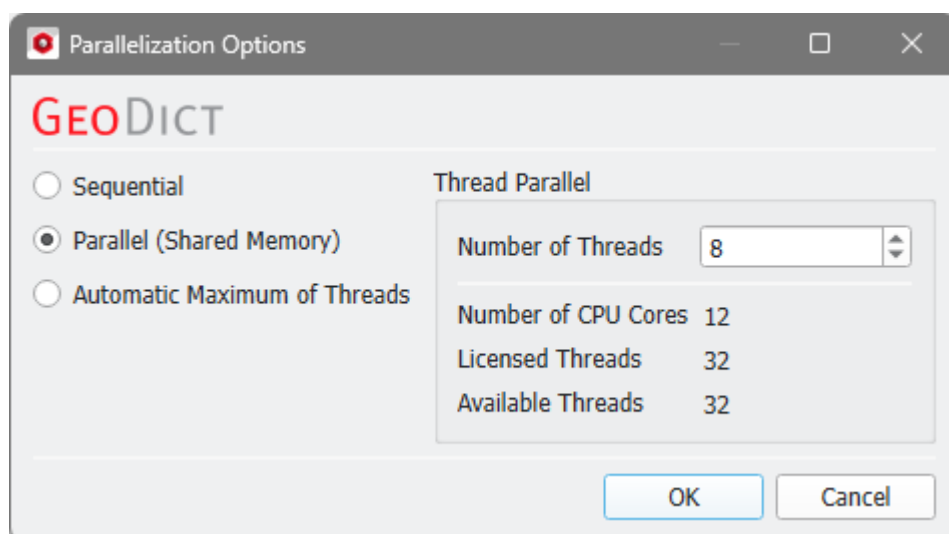
The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.



Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.

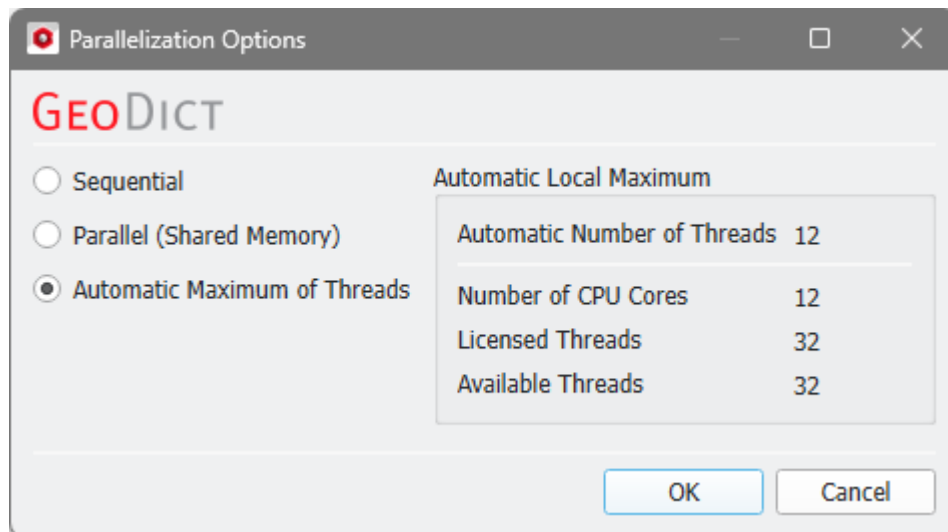


When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel

processes.



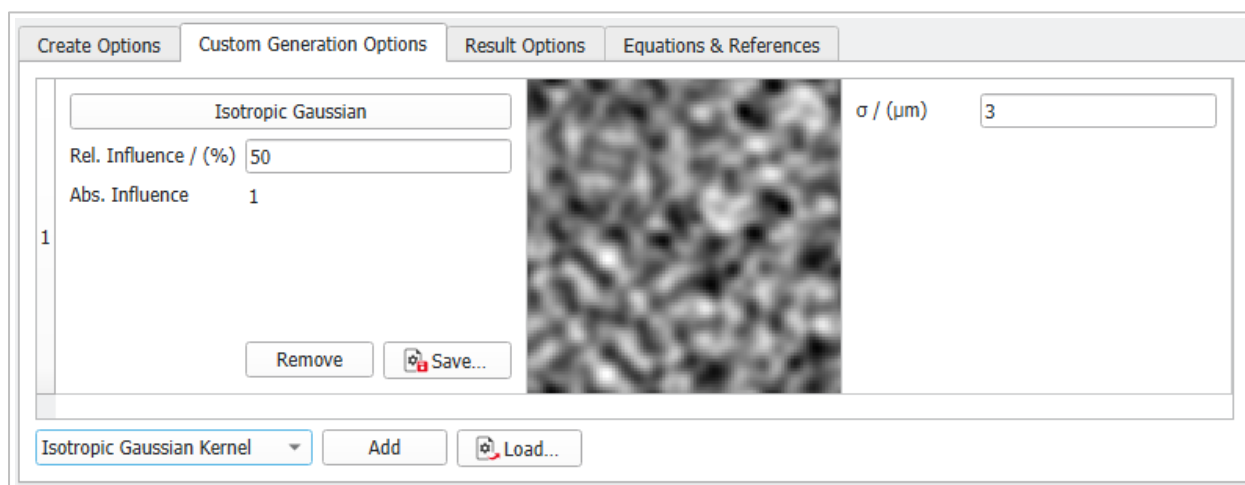
The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.

Custom Generation Options

The stochastic field and gradient types available for the generation are organized and listed in panels. For all objects, the left column of the panel contains the **Component Type** name, the **Relative Influence** and the **Absolute Influence**. The absolute influence is computed automatically from the corresponding relative influence.

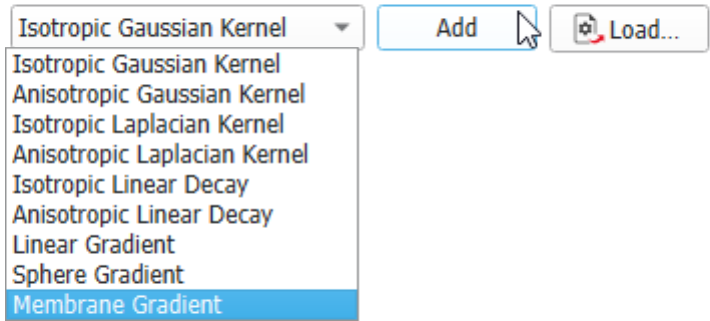
The resulting combined random field is the weighted sum of all components, where the weights depend on the **Relative Influence**.

The middle column shows a preview of the defined field or gradient. In the right column, the stochastic parameters of the components can be entered. These parameters include correlation length, direction vector and perpendicular axis.



Components

Isotropic Gaussian Kernel is the default **Component**. The **Random Field** and **Gradient Components** are selected from the pull-down menu at the lower left of the **Custom Generation Options** tab and clicking **Add**.



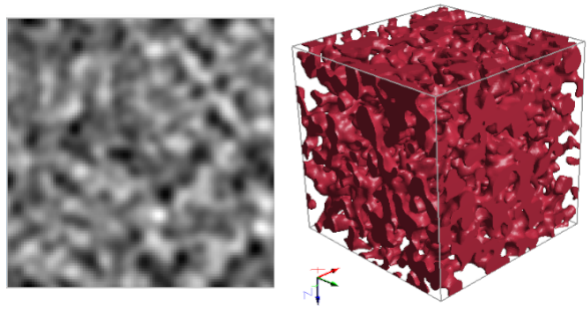
Components can be discarded again when clicking **Remove** in the left panel or can be saved as predefined component using the **Save...** button. Previously saved components with individually defined parameters can be loaded via the **Load...** button.

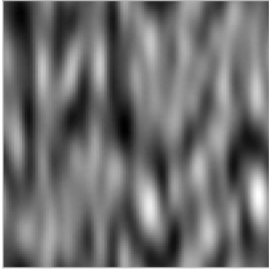
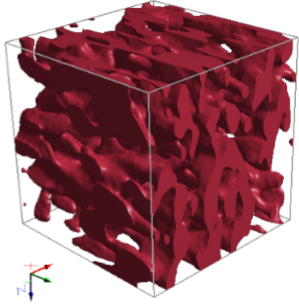
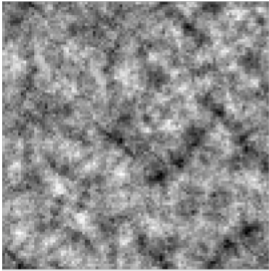
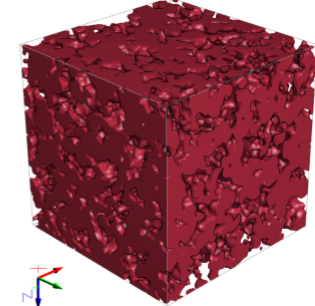
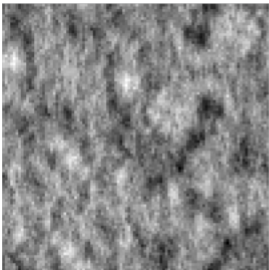
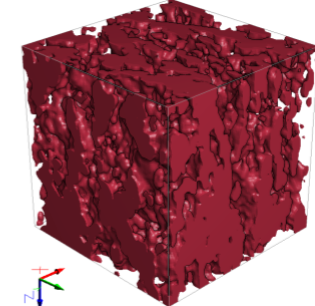
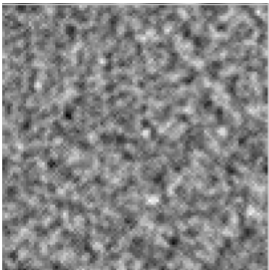
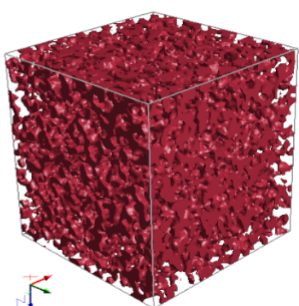
Component Topics

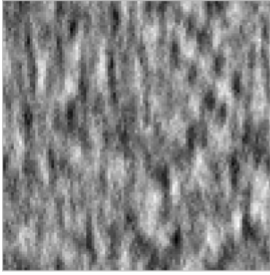
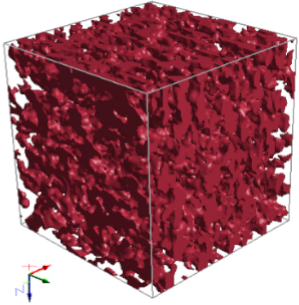
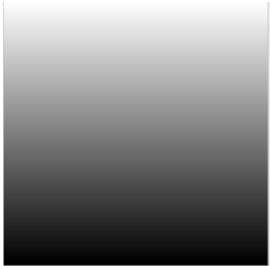
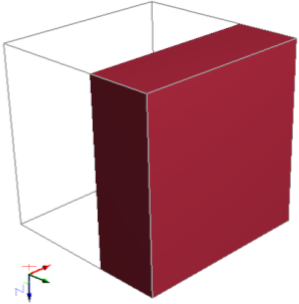
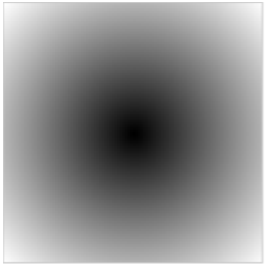
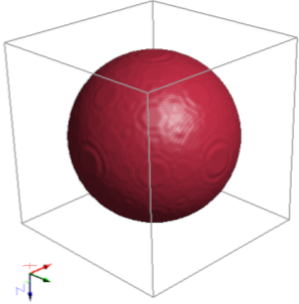
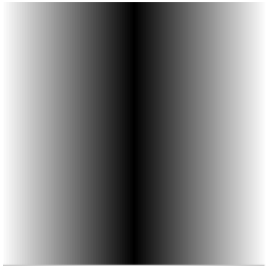
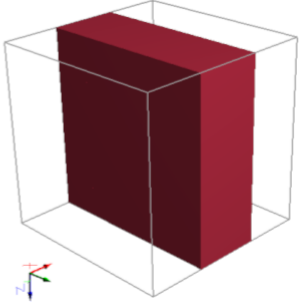
- [Component Overview](#)¹⁵⁷
View examples of all available components.
- [Component Parameters](#)¹⁵⁹
Descriptions of all component parameters and combination examples.

Component Overview

The following table summarizes the components that can be used with GrainGeo **Stochastic Field Thresholding** commands:

Field type	Stochastic field and Example
Isotropic Gaussian Kernel	

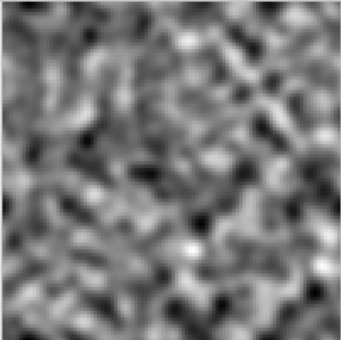
Field type	Stochastic field and Example
Anisotropic Gaussian Kernel	 
Isotropic Laplacian Kernel (Isotropic Exponential)	 
Anisotropic Laplacian Kernel (Anisotropic Exponential)	 
Isotropic Linear Decay	 

Field type	Stochastic field and Example	
Anisotropic Linear Decay		
Linear Gradient		
Sphere Gradient		
Membrane Gradient		

Component Parameters

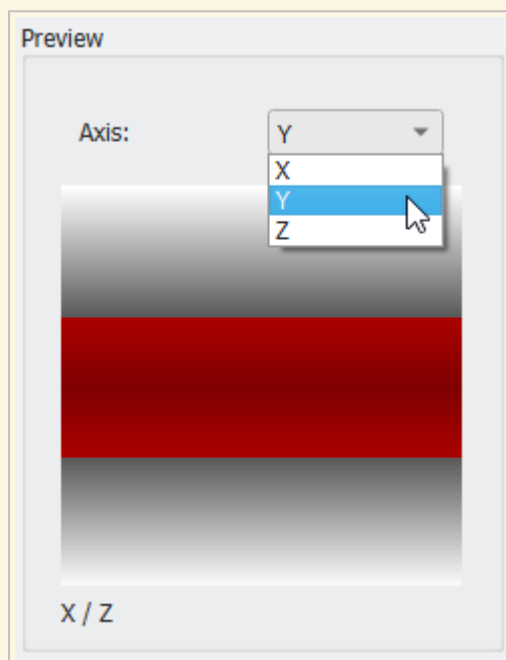
In the left find the name of the field type and the influence on the field generation when combining different field types. This is explained in more detail [below](#).

In the center column, a preview of the field type is shown and in the right column the field type parameters are defined. In the following they are explained for the different field types.

Anisotropic Gaussian Rel. Influence / (%) 50 Abs. Influence 0.5 Remove Save...			σ_X / (mm) 0.003 σ_Y / (mm) 0.003 σ_Z / (mm) 0.003
---	--	--	--



Know how! Depending on the entered parameters, it might be necessary to change the preview direction in the [Preview](#)^[146] panel on the bottom right of the dialog to see a preview of the generated field.



✓ Isotropic and Anisotropic random fields

For [Isotropic Gaussian Kernel](#)^[148], [Anisotropic Gaussian Kernel](#)^[149], [Isotropic Exponential](#)^[150], [Anisotropic Exponential](#)^[151], [Isotropic Linear Decay](#)^[152], and [Anisotropic Linear Decay](#)^[152], the parameters in the right column are the same as described for **Generation Mode**.

✓ Linear Gradient

For **Linear Gradient**, enter the desired direction vector of the gradient.

For the default (0,-1,0) the field starts with black in the bottom and smoothly becomes lighter in Y-direction.

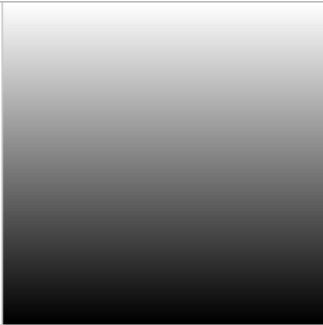
Linear Gradient

Rel. Influence / (%)50

Abs. Influence0.25

Remove

Save...



X0

Y-1

Z0

✓ Sphere Gradient

No parameters can be entered for Sphere Gradient.

The gradient always starts black in the center of the domain and becomes smoothly lighter towards the borders, resulting in a sphere after thresholding, if no other components are selected.

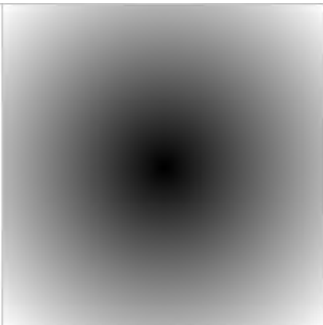
Sphere Gradient

Rel. Influence / (%)50

Abs. Influence0.25

Remove

Save...



✓ Membrane Gradient

For **Membrane Gradient**, select the axis perpendicular to the membrane from the pull-down menu. If, for example, X is chosen, the gradient starts as a black plane perpendicular to the X-axis in the center of the structure.

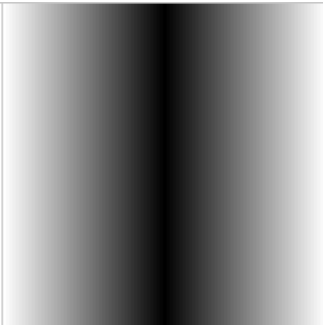
Membrane Gradient

Rel. Influence / (%)50

Abs. Influence0.25

Remove

Save...



X

X

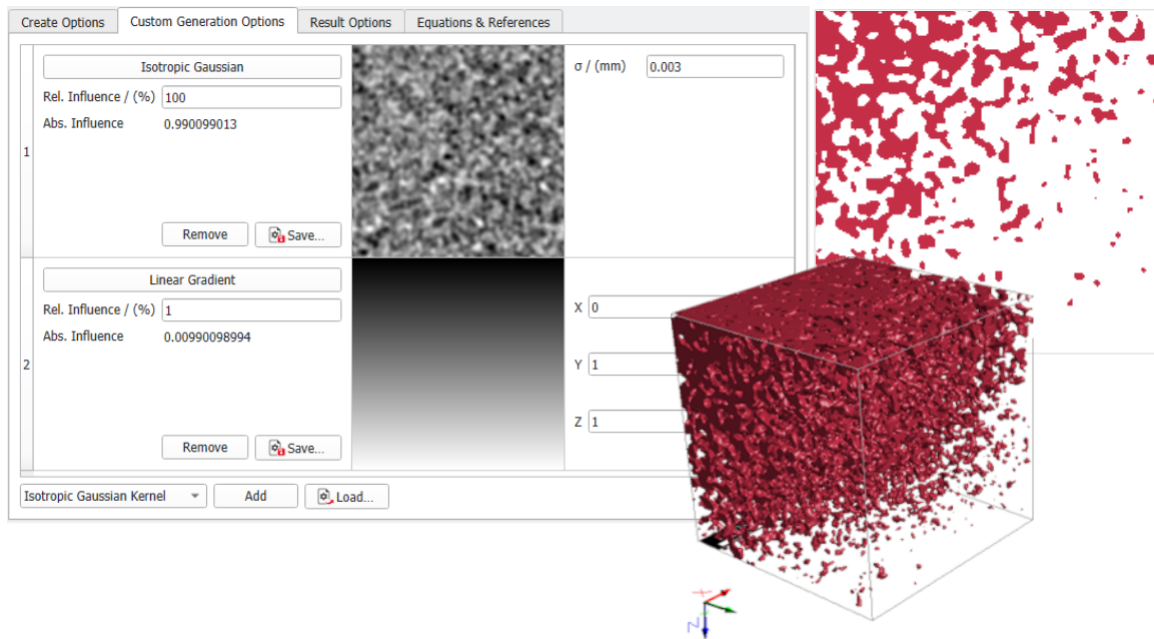
Y

Z

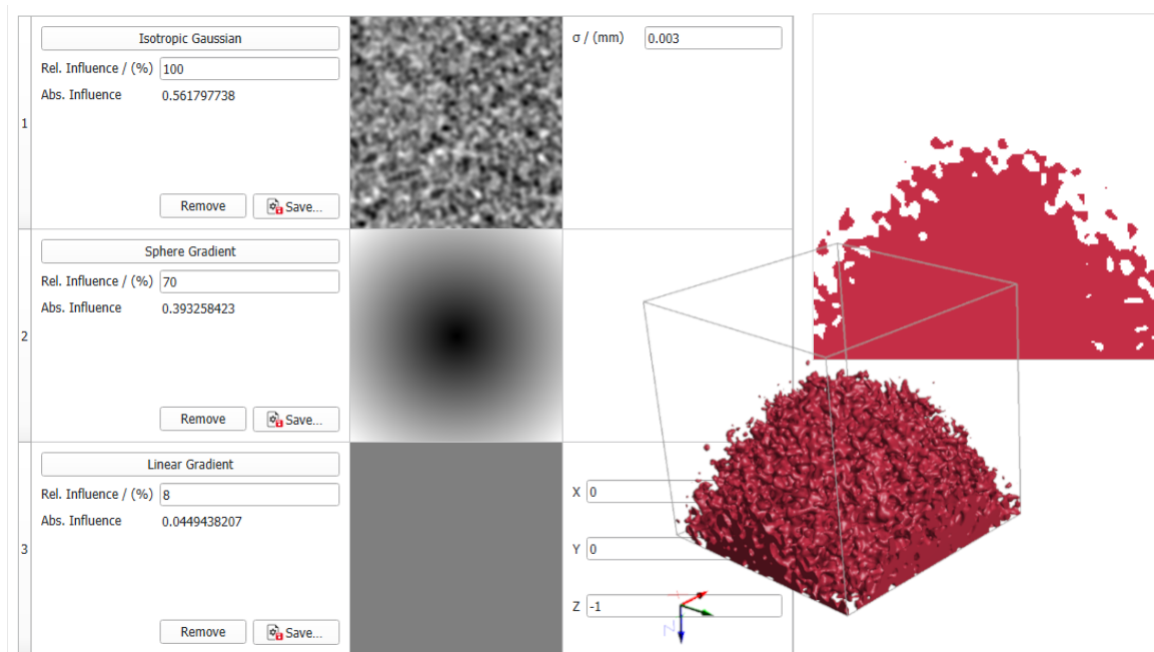
✓ Combine components

Using more than one component, the resulting combined random field is the weighted sum of all components, where the weights depend on the **Relative Influence**.

In this example, a combination of **Isotropic Gaussian Kernel** and **Linear Gradient** was selected. With **Rel. Influence** of 100 for the **Isotropic Gaussian** field and 1 for the **Linear Gradient**, observe, how the density of the structure differs according to the entered gradient vector (0,1,1).



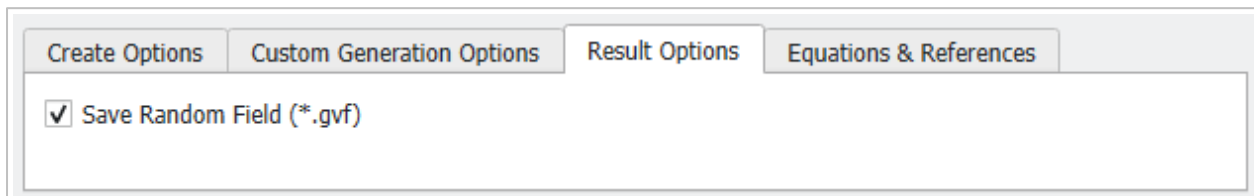
In the next example, a combination of **Isotropic Gaussian Kernel**, **Linear Gradient**, and **Sphere Gradient** was selected. With rel. influence of 100 for the **Isotropic Gaussian Kernel** field, 8 for the **Linear Gradient** and 70 for the **Sphere Gradient**, the structure forms a hill with a rough surface.



Result Options

GrainGeo always saves the generated structure as a GeoDict structure file (Structure.gdt). The file is placed in an automatically created result folder inside the chosen project folder (**File** → **Choose Project Folder...** in the menu bar).

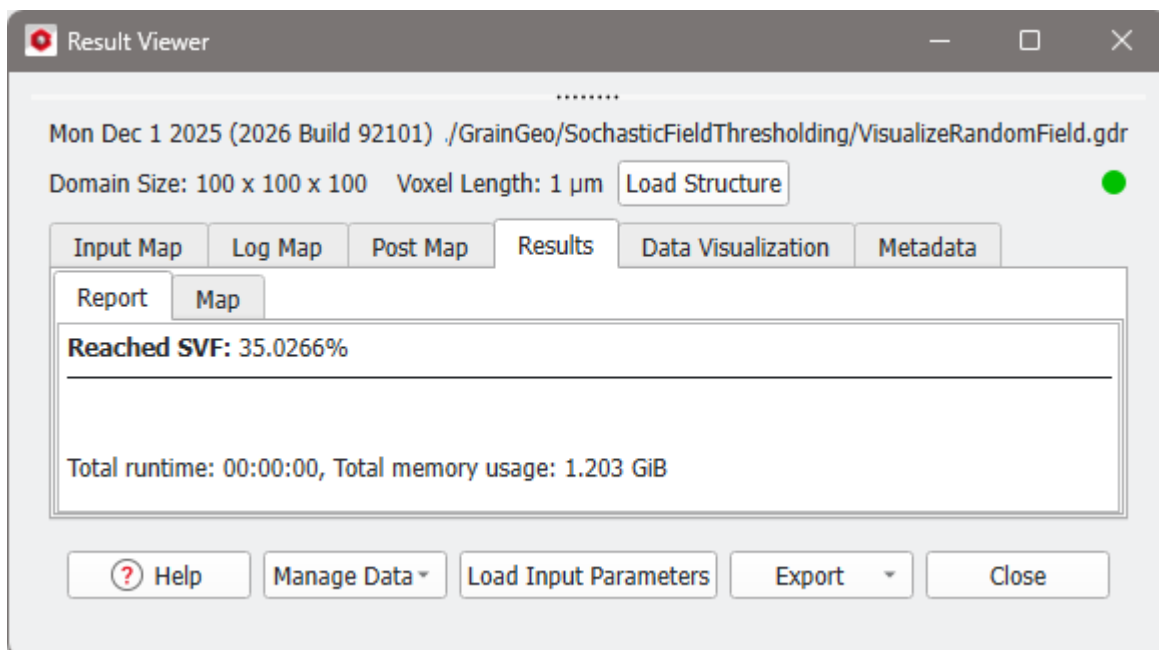
An additional option to save generation data, is to check **Save Random Field (*.gvf)** to also save the generated stochastic field in the result folder.



This random field can also be loaded from the result file in the [Result Viewer](#)¹⁶³.

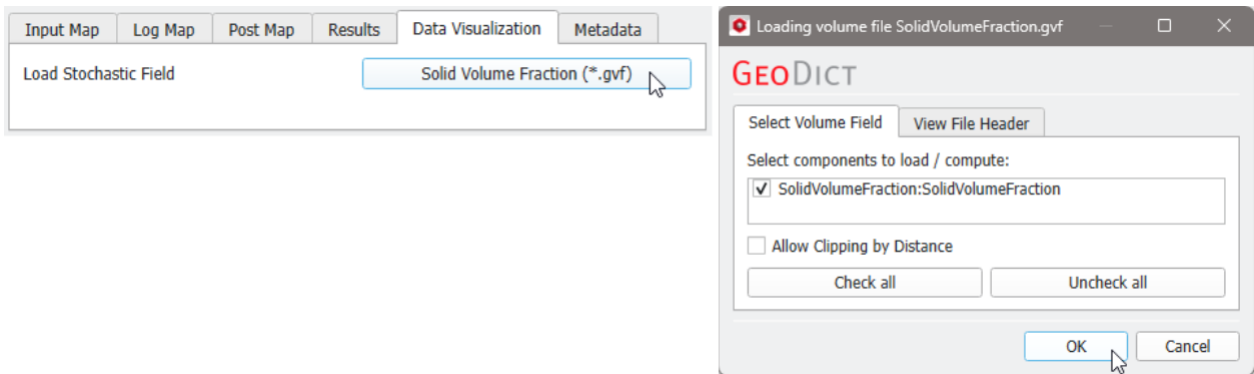
1.5.2 Results

After thresholding a stochastic field the corresponding GeoDict result file (*.gdr) is opened in the Result Viewer automatically.

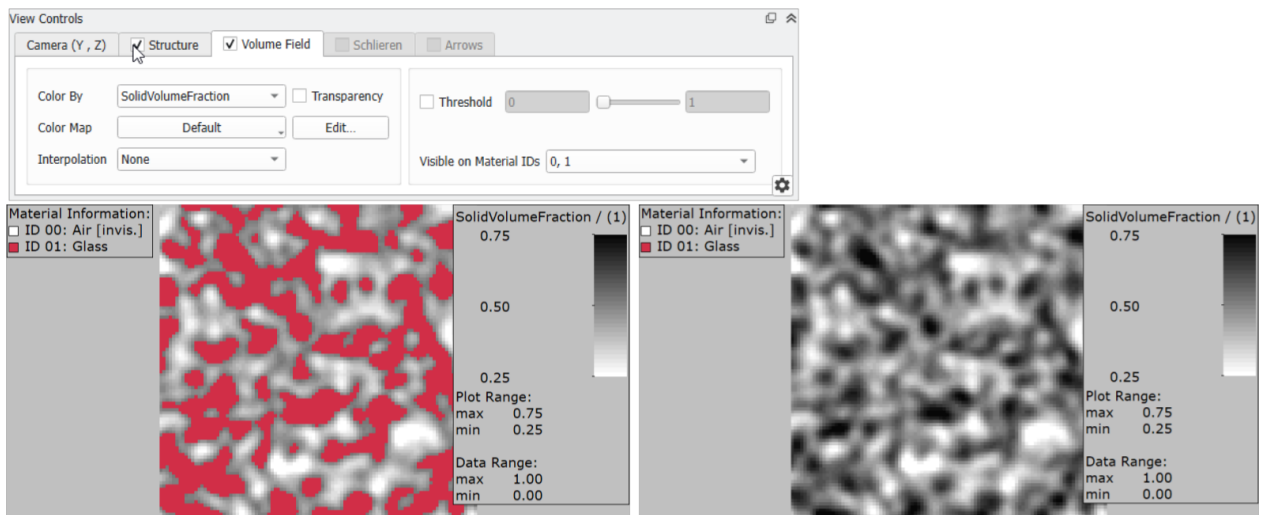


The **Report** tab of the result file only shows the reached solid volume fraction.

From the **Data Visualization** tab, the generated stochastic field can be loaded if **Save Random Field (*.gvf)** was checked in the [Result Options](#)¹⁶³. Click **Solid Volume Fraction (*.gvf)** and in the opening dialog click **OK**.



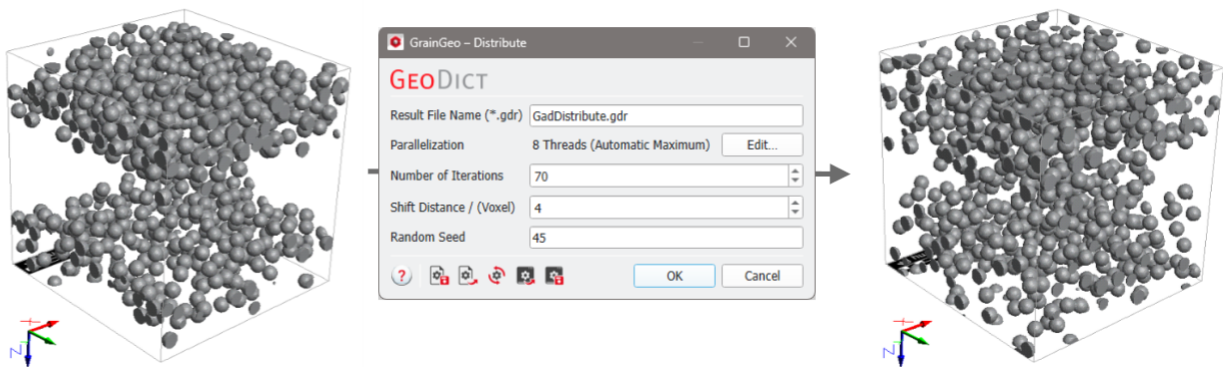
The visualization of the structure can be turned off by unchecking the **Structure** tab in the visualization panel above of the visualization area in the GeoDict GUI. To learn more about the GeoDict visualization settings, e.g., how to change the color of the volume field, see the Visualization User Guide.



1.6 Distribute

When **Distribute** is selected from the pull-down menu in the **GrainGeo** section, the objects are uniformly spread throughout the structure. Only structures that contain analytic information (GAD objects) can be used for the distribution of objects.

Observe the process of distributing spheres in a 200 x 200 x 200 structure, periodic in all directions, generated with **GrainGeo Create** with a Voxel Length of 1 μm . The grain's centers follow a density distribution, which results in a layered structure.



Clicking the **Options' Edit...** button opens the **Distribute Options** dialog.

When the desired parameters have been entered in the **Distribute Options** dialog, clicking **OK** closes the dialog and returns to the **GrainGeo** section.

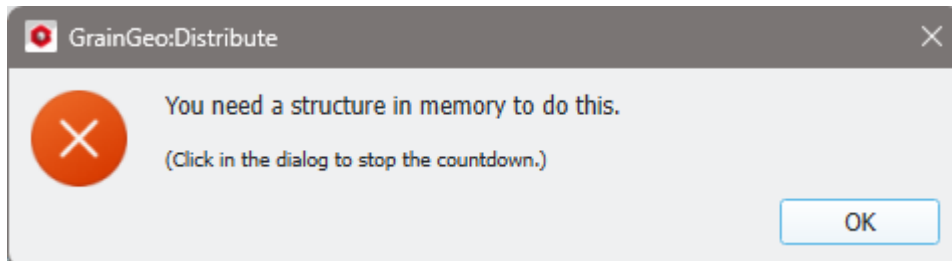
Clicking **Generate** starts the distribution process.

✓ Preparations and Requirements

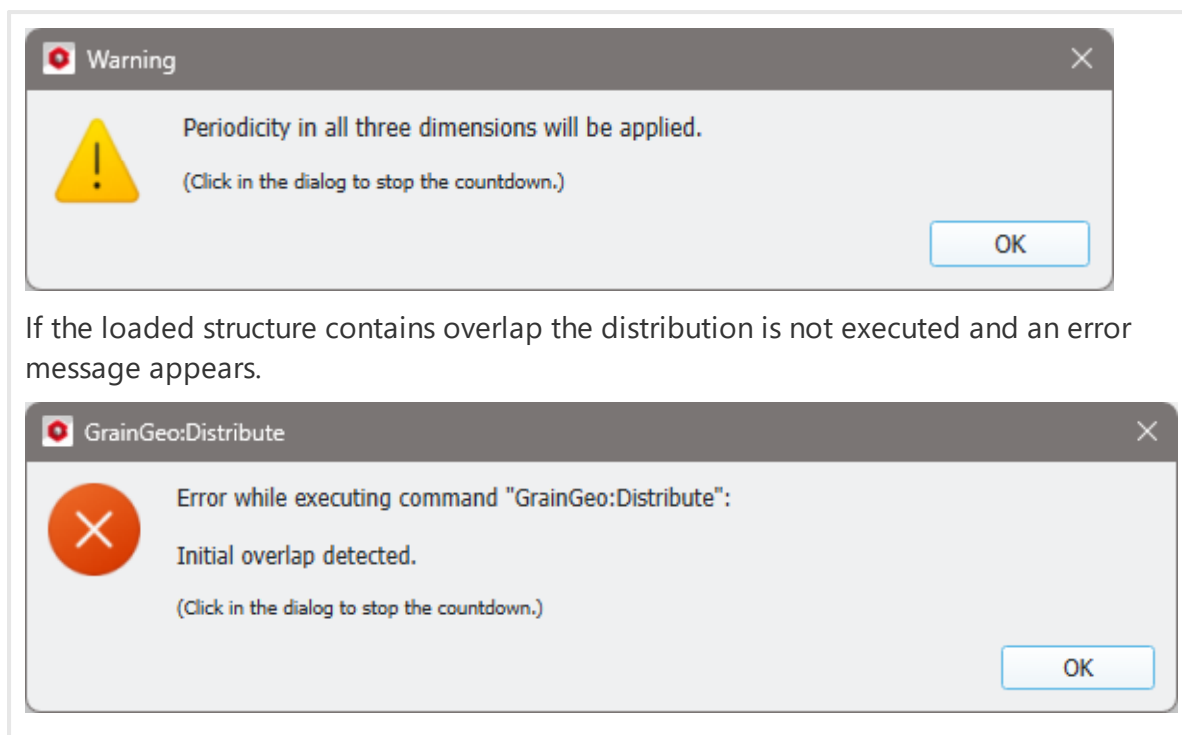
A granular structure containing GAD information has to be in memory.

To use this feature, the domain must be periodic, and the objects are not allowed to overlap. **Distribute** allows to create a homogeneous structure even for structures created with **Pile** where boundary effects occur in the pile direction.

Without a structure in memory, clicking **Generate** results in an error message.



When the structure in the selected file is not periodic, an information message appears indicating that periodicity will be applied in all three directions and the loaded structure will be treated as periodic. The GAD objects are still distributed.



If the loaded structure contains overlap the distribution is not executed and an error message appears.

Distribute Parameters

In the **Distribute Options** dialog, **Number of Iterations**, **Shift Distance**, and **Random Seed** specify the distribution process.

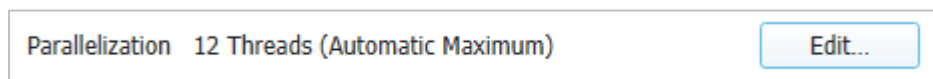
✓ Result File Name

At the top, the name for the file and folder containing the generation results can be entered in the **Result File Name (*.gdr)** box. The default name can be kept, or a new name can be chosen fitting the current project. The result file is shown after the distribution process is finished. The result file does only contain the usual information about input parameters and runtime. The resulting structure is saved in the corresponding result folder.

✓ Parallelization

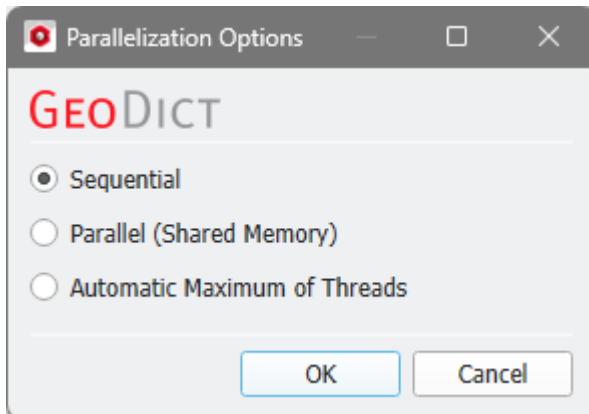
Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.

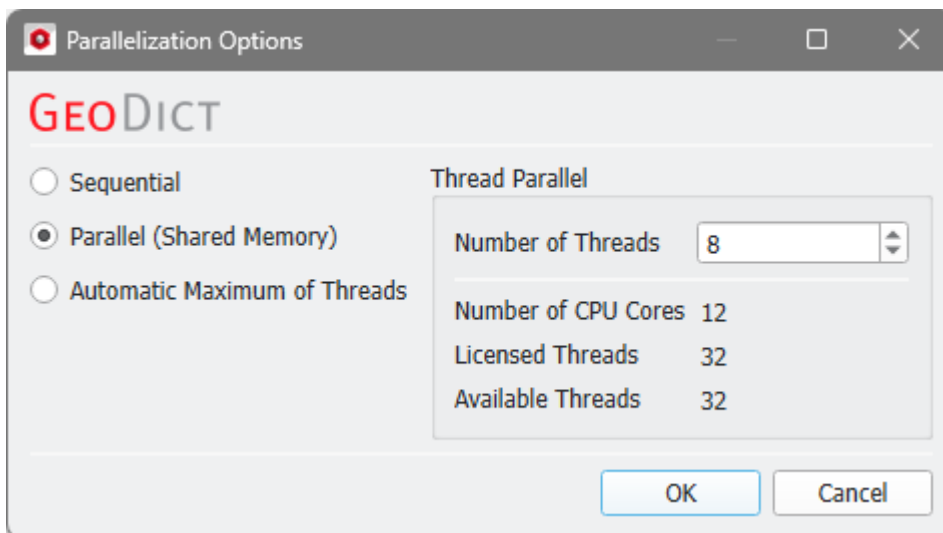


Selecting **Sequential** will not apply parallelization and only one thread is used for the

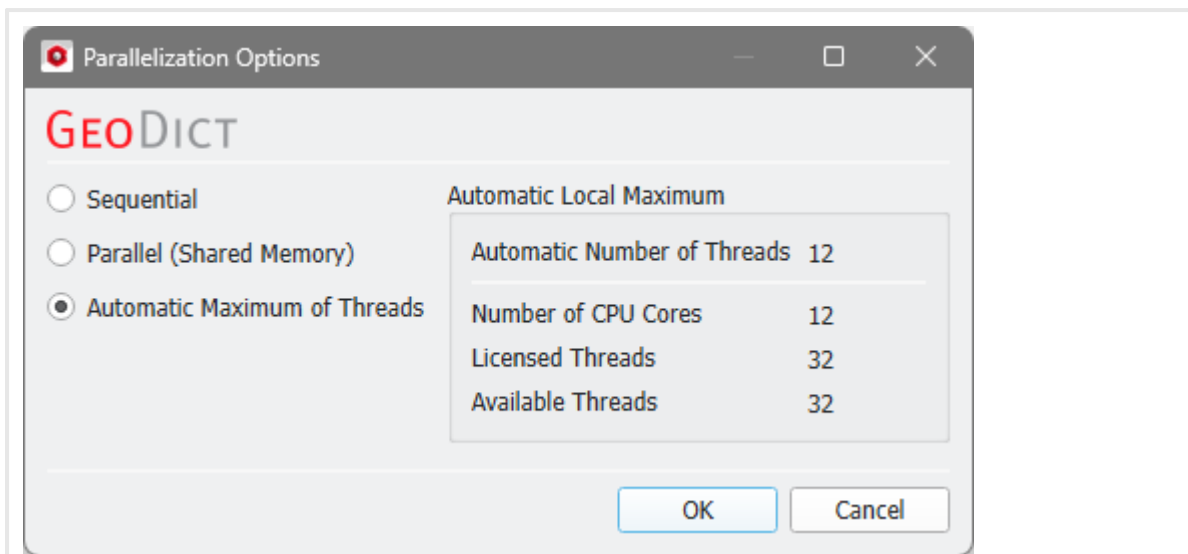
computation.



When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



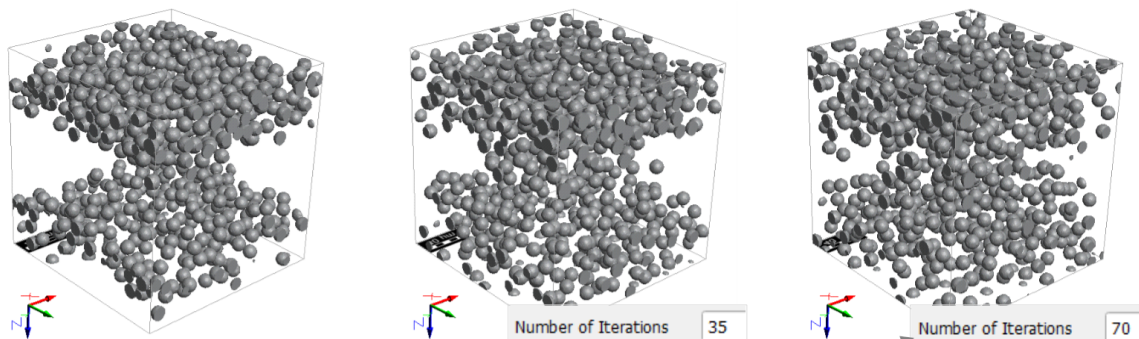
If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



The **Automatic Local Maximum** of processes is automatically selected, which is the minimum of **Number of CPU Cores**, **Licensed Threads**, and **Available Threads**.

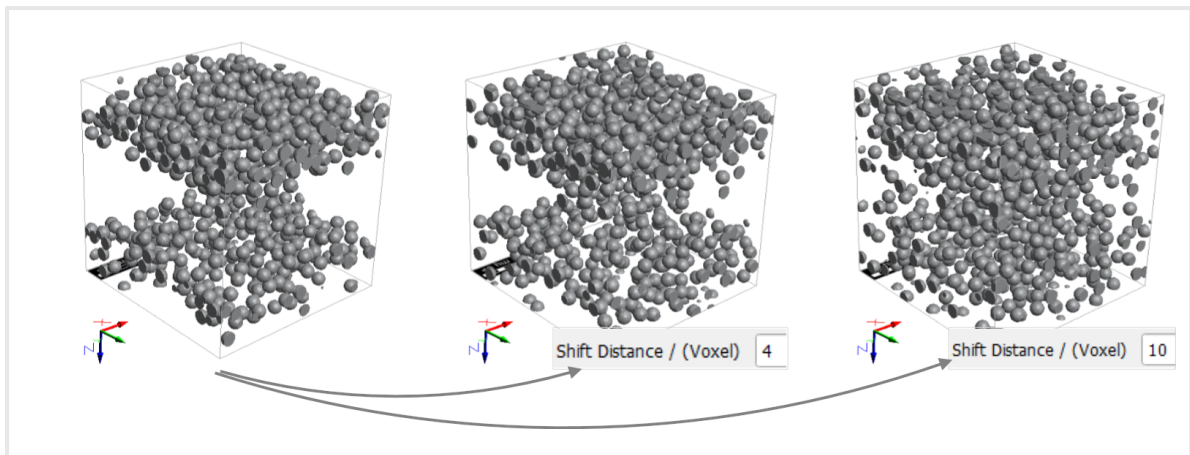
✓ Number of Iterations

The **Number of Iterations** determines how many distribution steps are done. More distribution steps lead to a wider distribution of the objects, which is getting closer to a uniform distribution.



✓ Shift Distance

The **Shift Distance** determines the maximal object movement during a single iteration. Large shift distances lead to more computational time per iteration. Observe the effect of increasing the shift distance from 1 to 4 and then to 10, while the number of iterations is kept at 35.

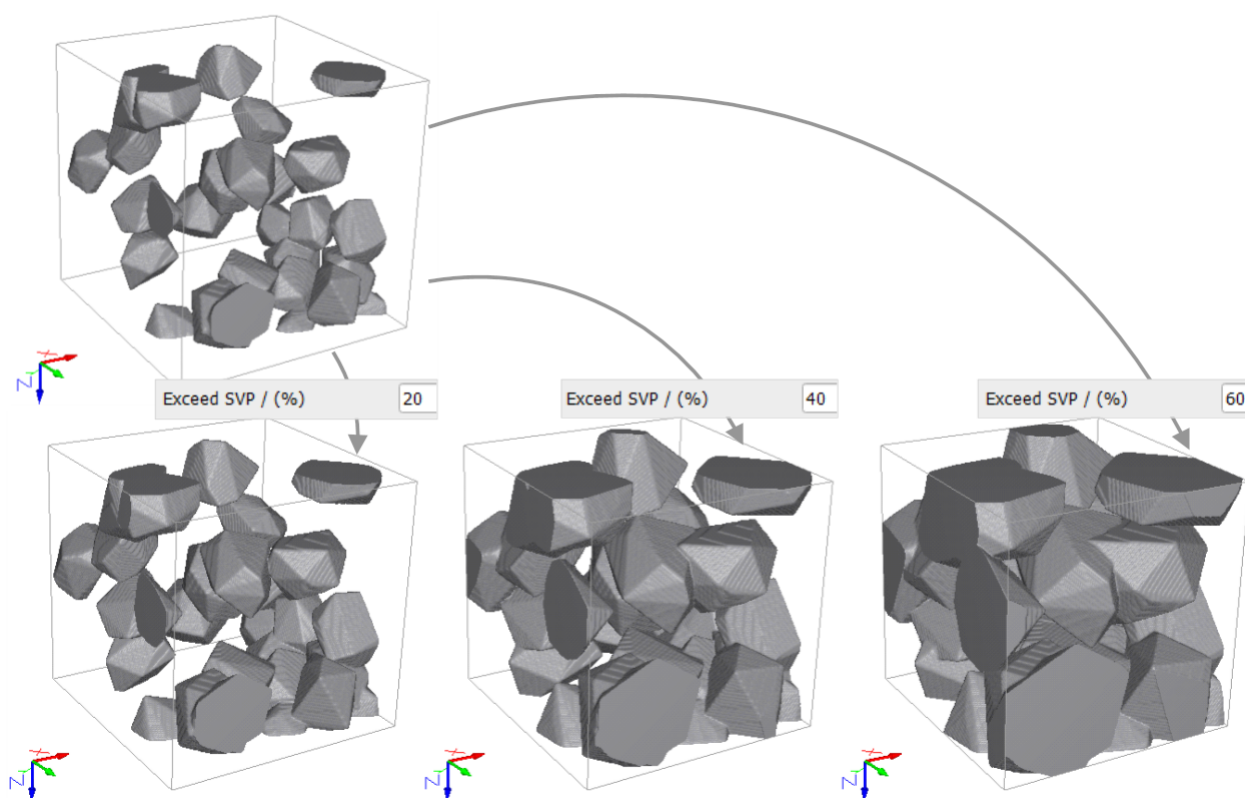


✓ Random Seed

Random Seed initializes the random number generator behind the object distribution. Changing its value produces different sequences of random numbers and hence, different realizations of the distribution. If all settings are equal, distributing the same initial structure with the same **Random Seed** value produces exactly the same structure. The **Random Seed** is a non-negative integer number, it increases automatically with every generation run.

1.7 Sinter & Crystallization

With **Sinter & Crystallization**, virtually sintered and crystallized structures can be generated from GeoDict analytic structures (GAD format). The structure is virtually compressed until a desired parameter is reached (**Sinter Mode**). The voxel size in the structure decreases, while the number of voxels in the structure remains constant. Grains are deformed at their touching points and an **Interface Material** can be added.



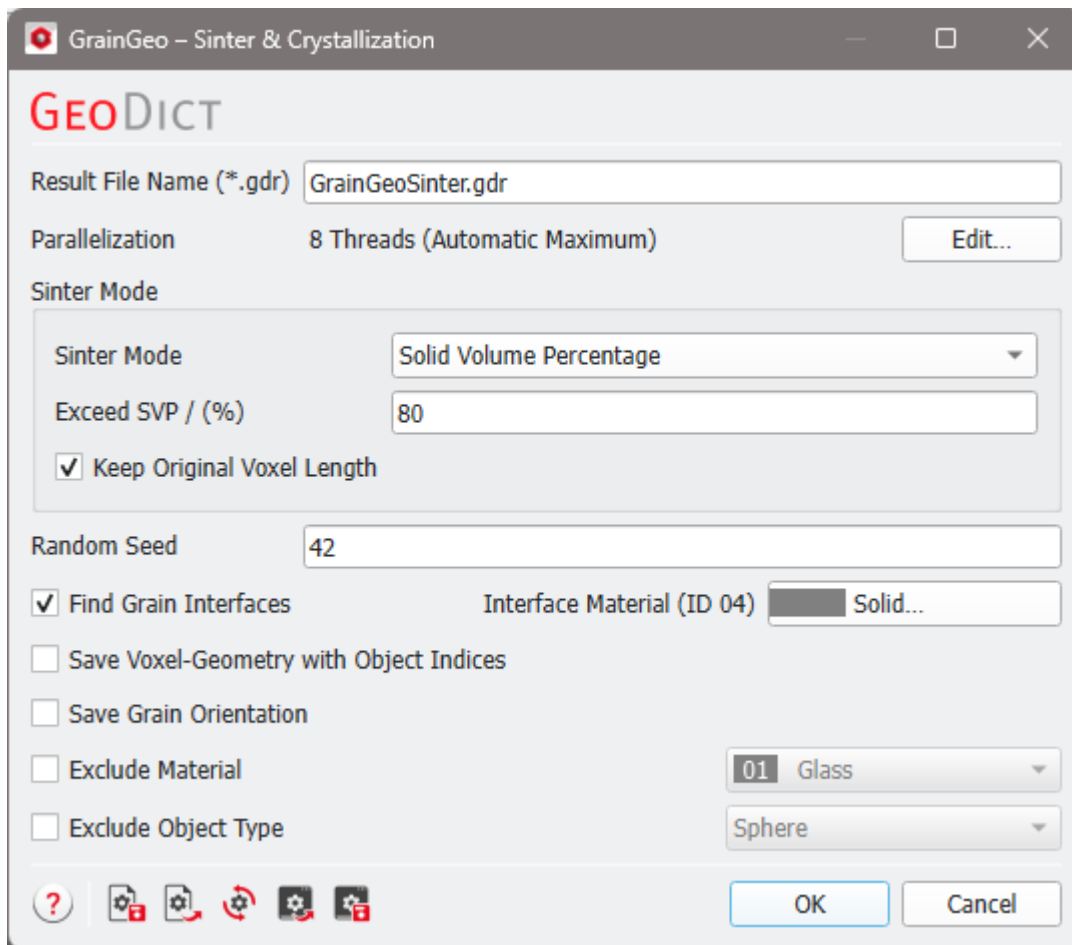
The Sinter & Crystallization command:

- [Options](#)¹⁷⁰
Define the parameters for the sintering process.
- [Results](#)¹⁷⁷
View the results in the Result Viewer.

1.7.1 Options

Clicking the Options' **Edit...** button opens the **Sinter & Crystallization** options dialog to enter the desired parameters. Clicking **OK** closes the dialog and returns to the GrainGeo section. Clicking **Generate** starts the sintering process.

A structure containing GAD information must be in memory.



General Parameters

Result File Name (*.gdr)

Parallelization 8 Threads (Automatic Maximum)

✓ Result File Name

At the top of the **Sinter & Crystallization** dialog, the name for the files containing the generation results can be entered in the **Result File Name (*.gdr)** box. The default name can be kept, or a new name can be chosen fitting the current project.

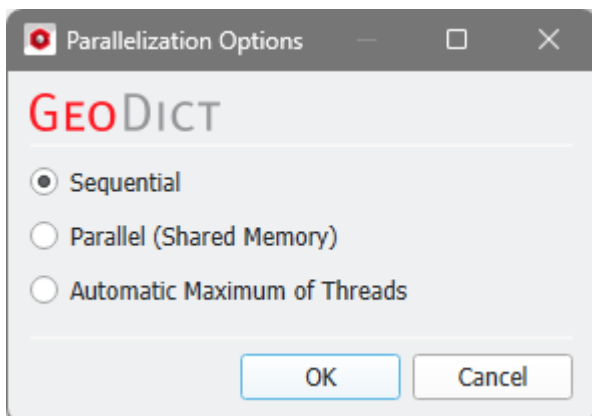
✓ Parallelization

Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

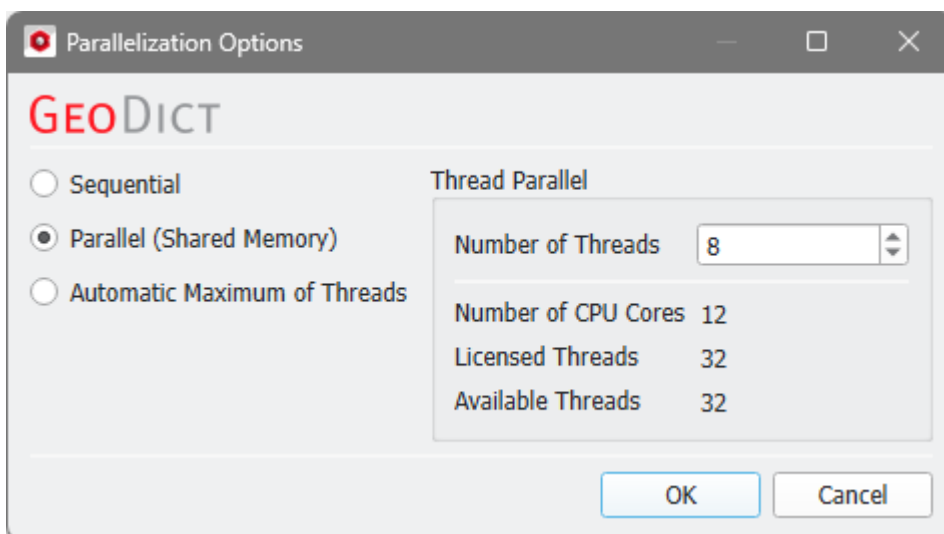
The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.

Parallelization 12 Threads (Automatic Maximum) Edit...

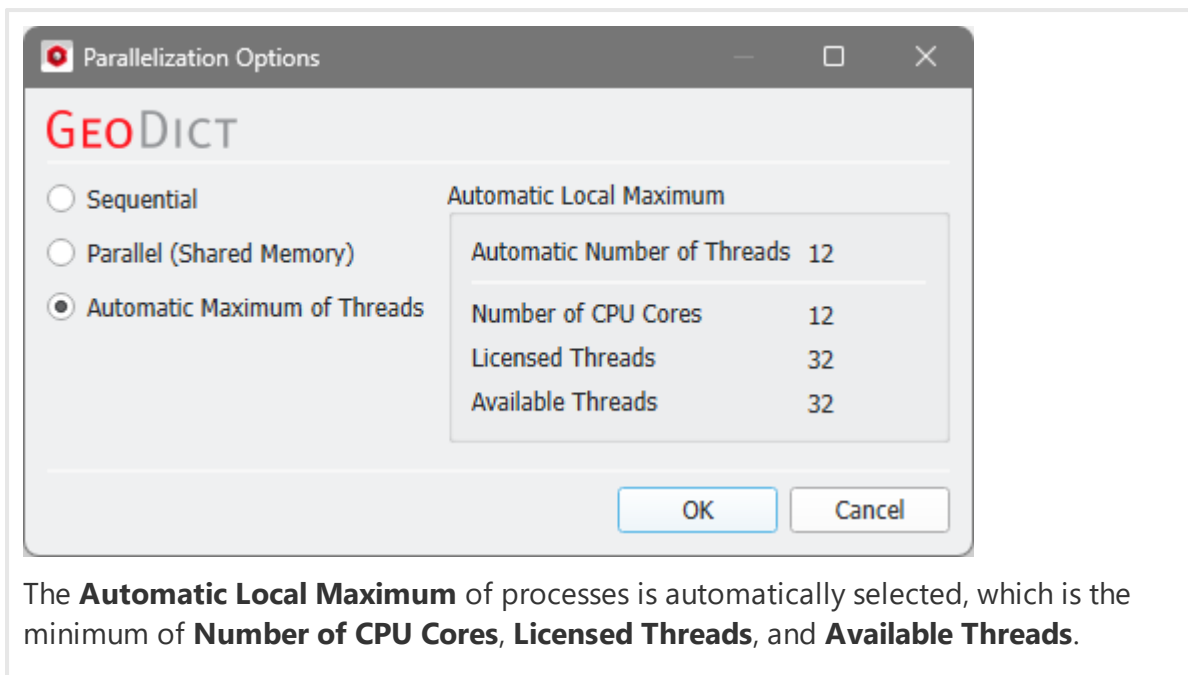
Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



Sinter Mode

In the **Sinter Mode** panel, several parameters can be entered to control the sintering process.

Two different stopping criteria for the sintering process can be selected from the **Sinter Mode** pull-down menu:

- **Solid Volume Percentage:** The sintering process continues until the desired Solid Volume Percentage is exceeded (**Exceed SVP**). For this mode, you can decide to keep the original voxel length.
- **Shrinkage** defines the percentage by which the structure is contracted in each direction.

Sinter Mode

Sinter Mode Solid Volume Percentage

Exceed SVP / (%) 80

☒ Keep Original Voxel Length

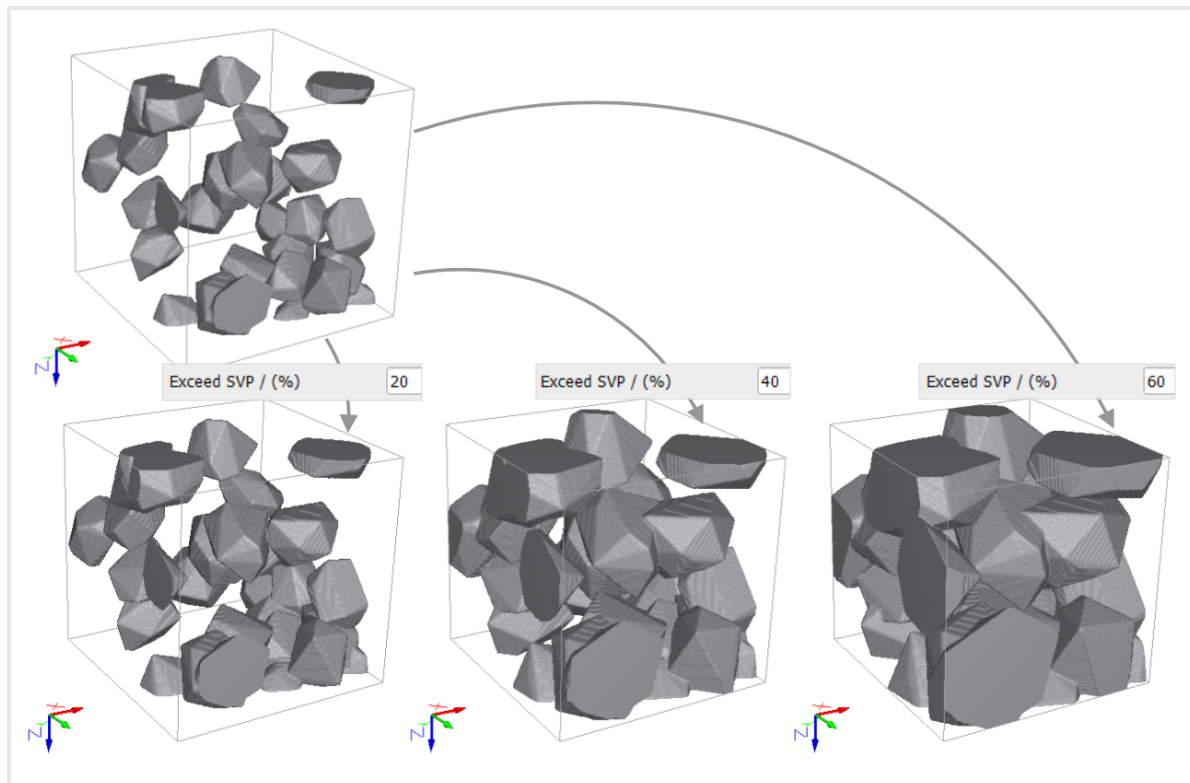
Sinter Mode

Sinter Mode Shrinkage

Shrinkage / (%) 20

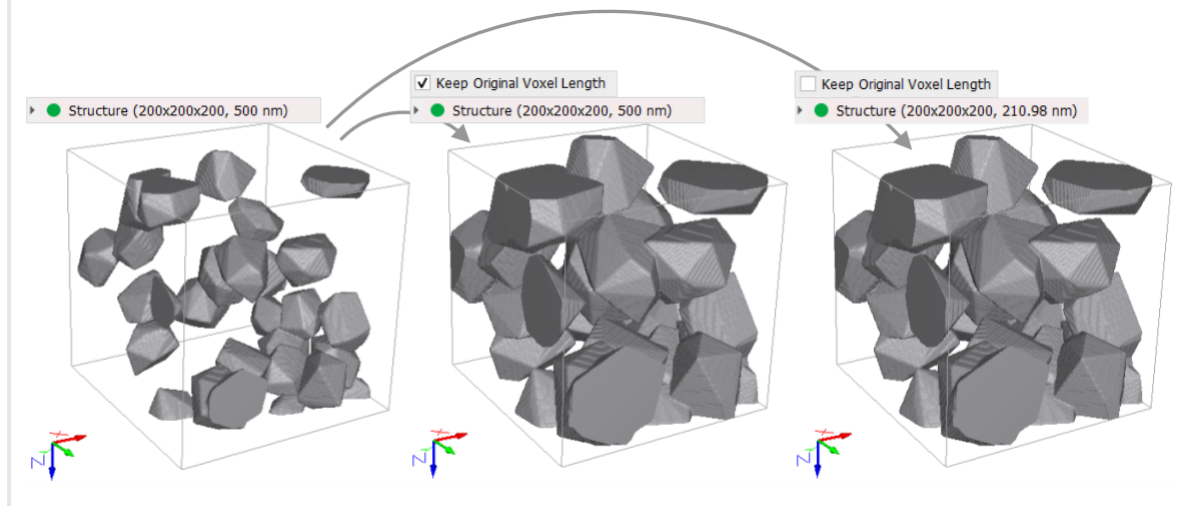
✓ Example for Exceed SVP

Observe the effect of increasing **Exceed SVP** from 20%, to 40% and then to 60%, when a structure made of convex polyhedrons is sintered.



✓ Keep Original Voxel Length

By default, the structure's original voxel length is kept (**Keep Original Voxel Length**), which enlarges the solids. Unchecking this option decreases the voxel length, while the number of voxels remains constant.



Specify Sintering

Specify which materials or object types should be sintered and if grain interfaces should be found or not.

Random Seed

☒ Find Grain Interfaces Interface Material (ID 04)

☐ Save Voxel-Geometry with Object Indices

☐ Save Grain Orientation

☐ Exclude Material

☐ Exclude Object Type

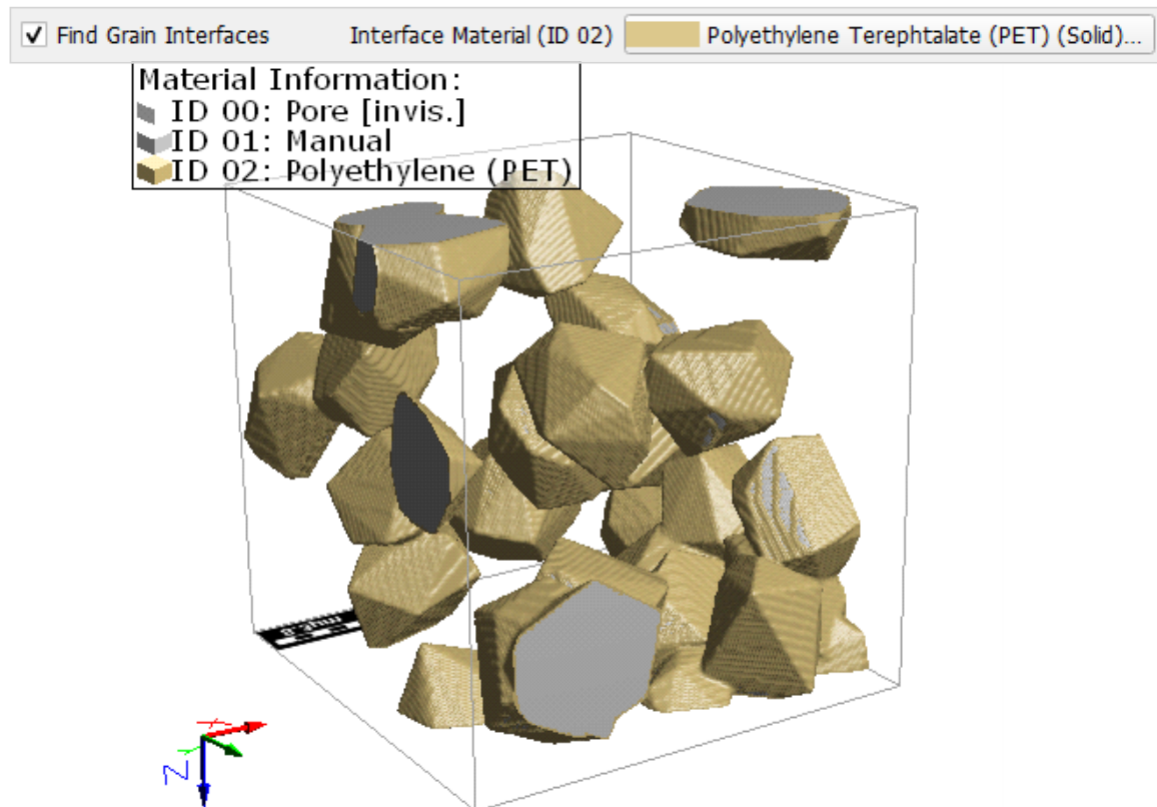
✓ Random Seed

Random Seed is a simulation parameter controlling the sequence in which objects are sintered. Thus, different random seeds lead to slightly different sintered structures. The random seed increases automatically with every sintering process.

✓ Find Grain Interfaces

If **Find Grain Interfaces** is checked, the **Interface Material** of the sintered objects can be chosen from the GeoDict material database by clicking the button.

This results into a different material ID being assigned to the entire grain surface, including the interfaces with other objects. For example, later mechanical properties can be applied just to the grain interfaces for deformation or other elastic properties simulations with the ElastoDict module.



✓ Save Voxel-Geometry with Object Indices

To save index image of the sintered grains in *.g32 format, check **Save Voxel-Geometry with Object Indices**. This file can be used, together with the structure, to track objects while computing, e.g., elastic properties with transversal isotropic or orthotropic constituent materials laws with the ElastoDict module.

If selected, the 3D result file can be loaded from the Result Viewer (**Load (*.g32)**).

Input Map	Log Map	Post Map	Results	Data Visualization	Metadata
Basis Geometry (*.gad)			Load *.gad		
Load Object Indices Image (*.g32)			Load (*.g32)		
Load Object Orientation File (*.gof)			Load (*.gof)		

✓ Save Grain Orientation

To save the available information about the sintered grains in *.gof format, check **Save Grain Orientation**. This file can be used, together with the structure, to compute, e.g., elastic properties with transversal isotropic or orthotropic constituent materials laws with the ElastoDict module.

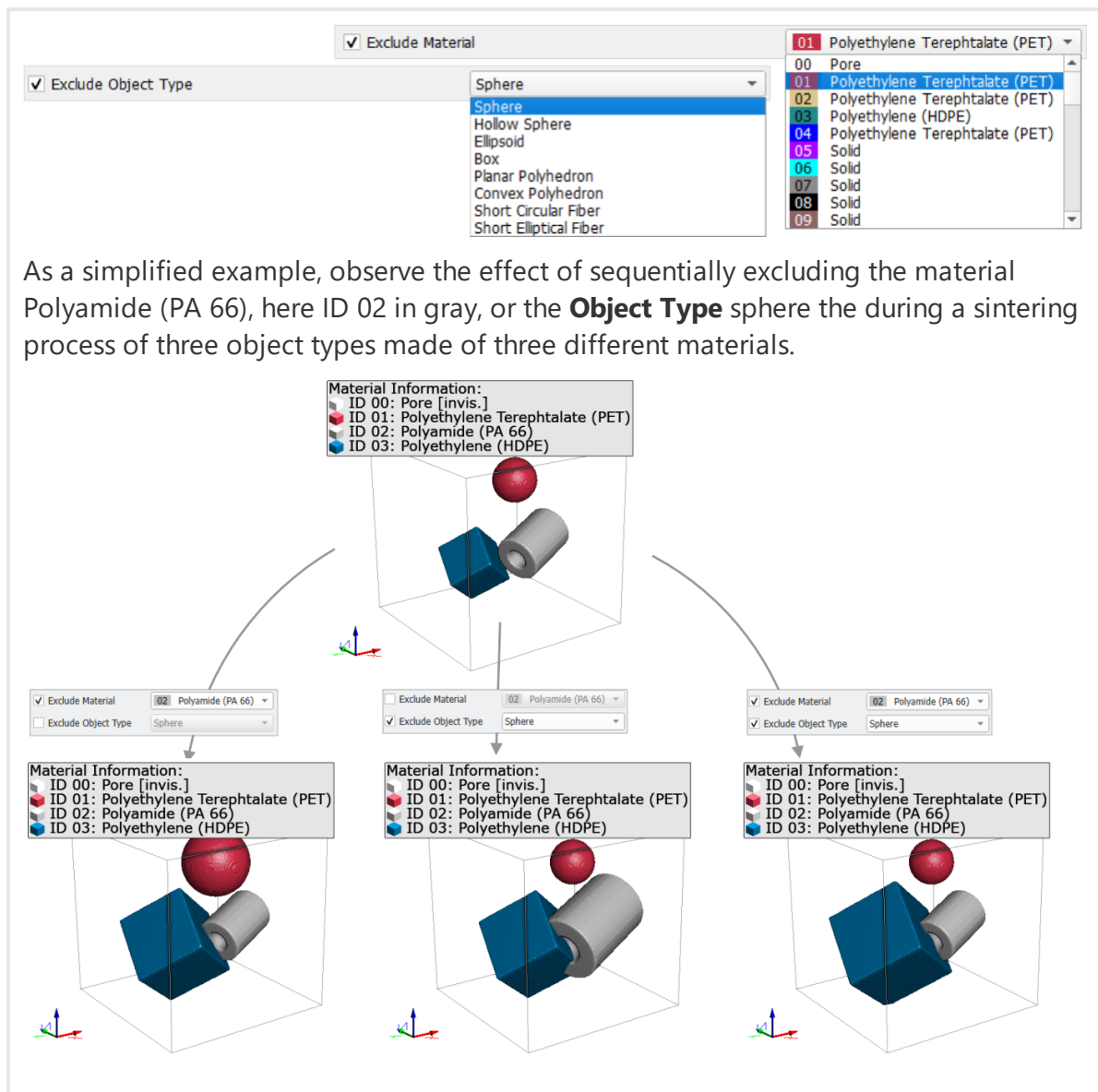
If selected, the 3D result file can be loaded from the Result Viewer (**Load (*.gof)**).

Input Map	Log Map	Post Map	Results	Data Visualization	Metadata
Basis Geometry (*.gad)			Load *.gad		
Load Object Indices Image (*.g32)			Load (*.g32)		
Load Object Orientation File (*.gof)			Load (*.gof)		

✓ Exclude Material and Exclude Object Type

One object Material ID and/or one object type per structure can be excluded from the sintering process when checking **Exclude Material** or **Exclude Object Type** and choosing the Material ID or the object type name from the pull-down menus.

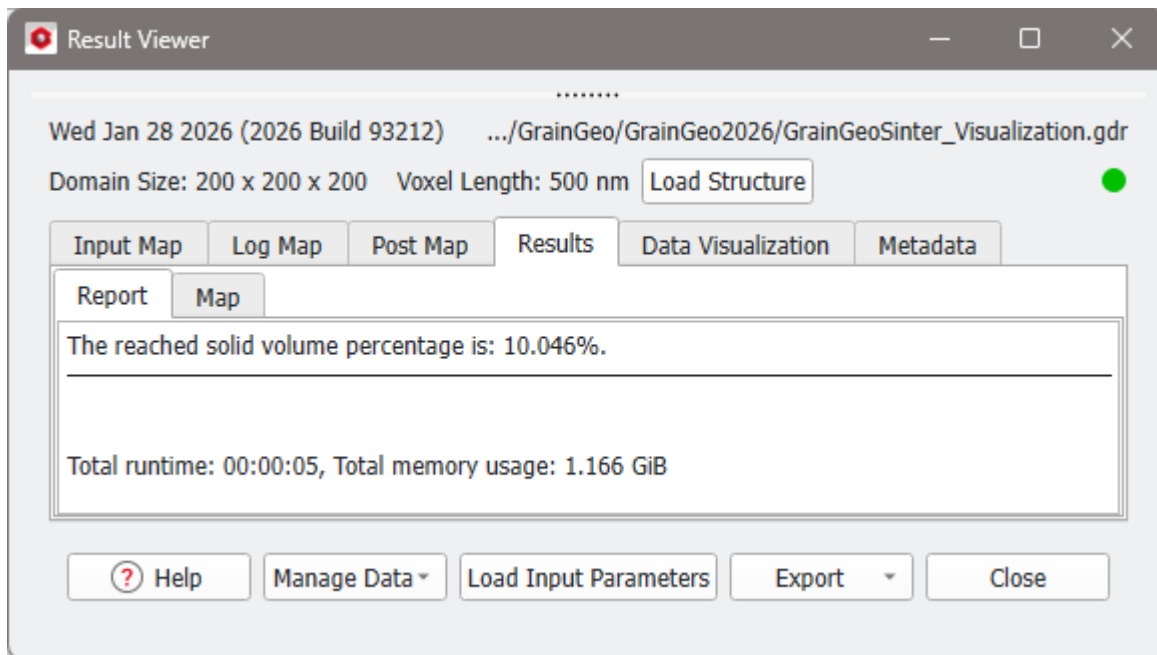
Exclude Material and **Exclude Object Type** can be simultaneously selected to exclude objects, that have a certain type or a certain material. For example, exclude all objects with Material ID 01 and additionally all spheres.



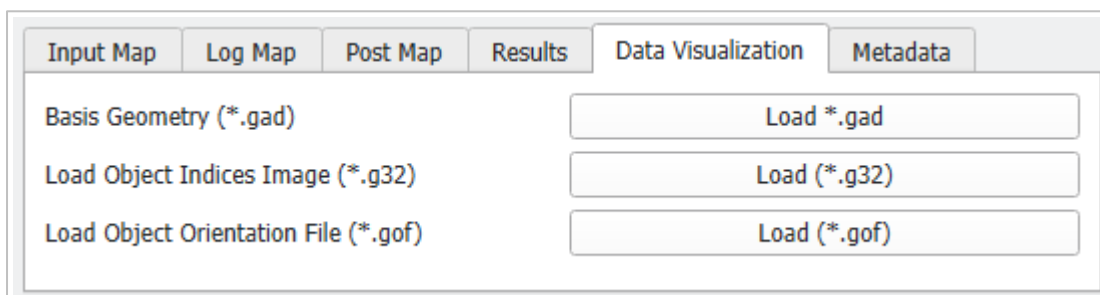
1.7.2 Results

The sintered structure is shown in the visualization area. Learn more about visualization in GeoDict in the **Visualization** User Guide.

The result file is automatically opened in the Result Viewer and shows the reached solid volume percentage in the **Results - Report** tab. Additionally, it offers 3D **Data Visualization** options depending on the generation settings. Find more information on GeoDict result files in the **Result Viewer** User Guide.



From the **Data Visualization** tab several files can be loaded.



It is always possible to load the original structure before sintering by clicking **Load *.gad**.

If **Save Voxel-Geometry with Object Indices** was selected in the [Options](#)^[176] dialog, you can load the object indices image by clicking **Load (*.g32)**.

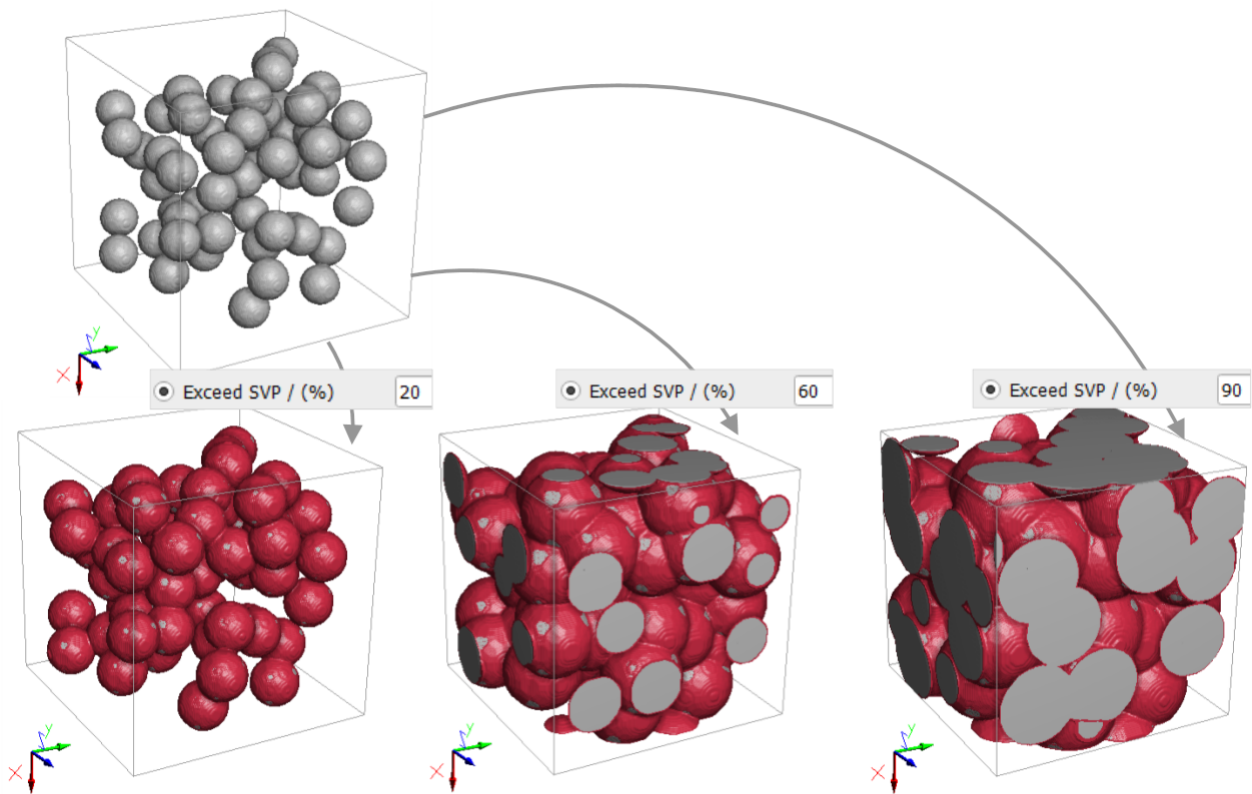
If **Save Grain Orientation** was selected in the [Options](#)^[176] dialog, you can load the object orientation image by clicking **Load (*.gof)**.

These two files can be used, together with the structure, to compute, e.g., elastic properties with transversal isotropic or orthotropic constituent materials laws with the ElastoDict module.

1.8 Grow Sediment

With **Grow Sediment** layers of a new material (**Interface Material**) are added to the original structure.

Sediments can only be grown on structures that contain analytic information (GAD format).



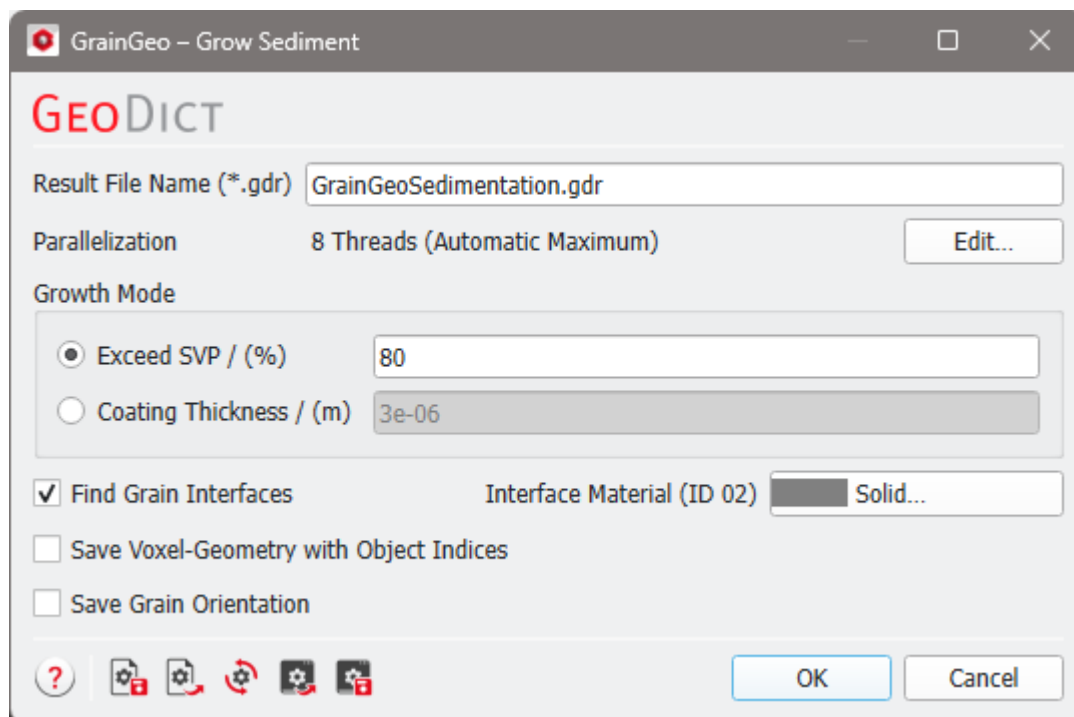
The Grow Sediment command:

- [Options](#)¹⁷⁹
Define the parameters for the sediment growth.
- [Results](#)¹⁸⁵
View the results in the Result Viewer.

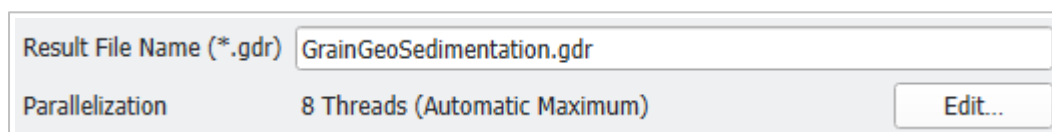
1.8.1 Options

Clicking the Options' **Edit...** button opens the **Grow Sediment** options dialog to enter the desired parameters. Clicking **OK** closes the dialog and returns to the GrainGeo section. Clicking **Generate** starts the process of growing sediments on the structure.

A structure containing GAD information must be in memory.



General Parameters



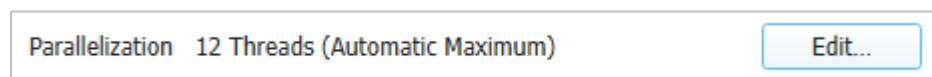
✓ Result File Name

At the top of the **Grow Sediment** dialog, the name for the files containing the generation results can be entered in the **Result File Name (*.gdr)** box. The default name can be kept, or a new name can be chosen fitting the current project.

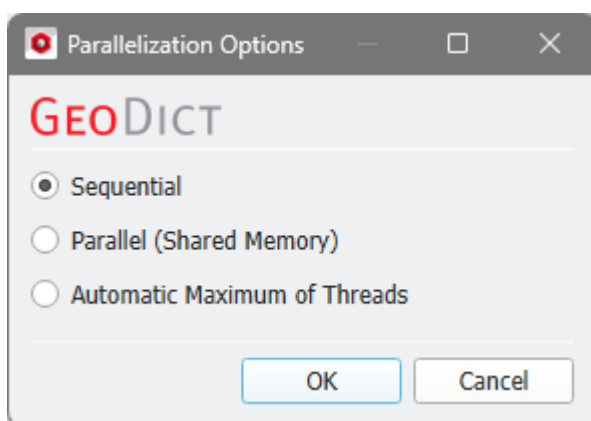
✓ Parallelization

Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

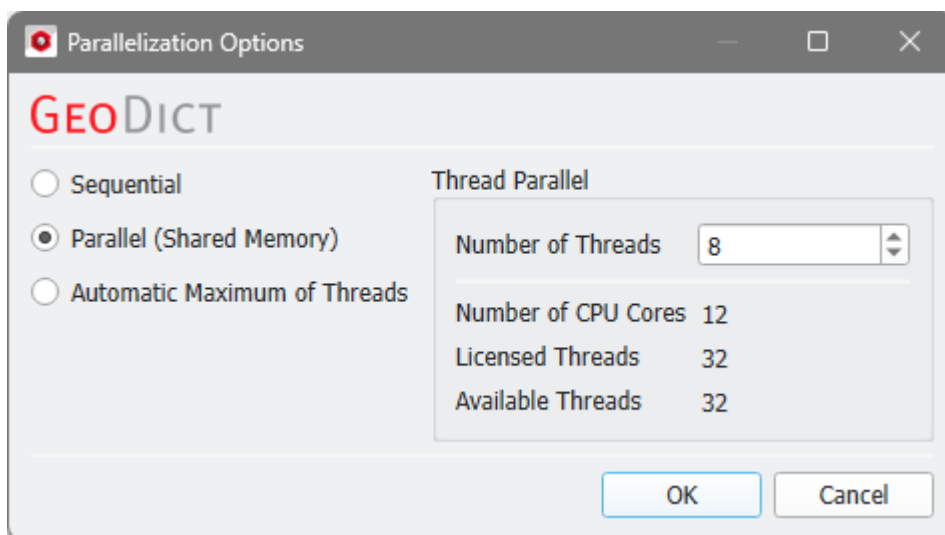
The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.



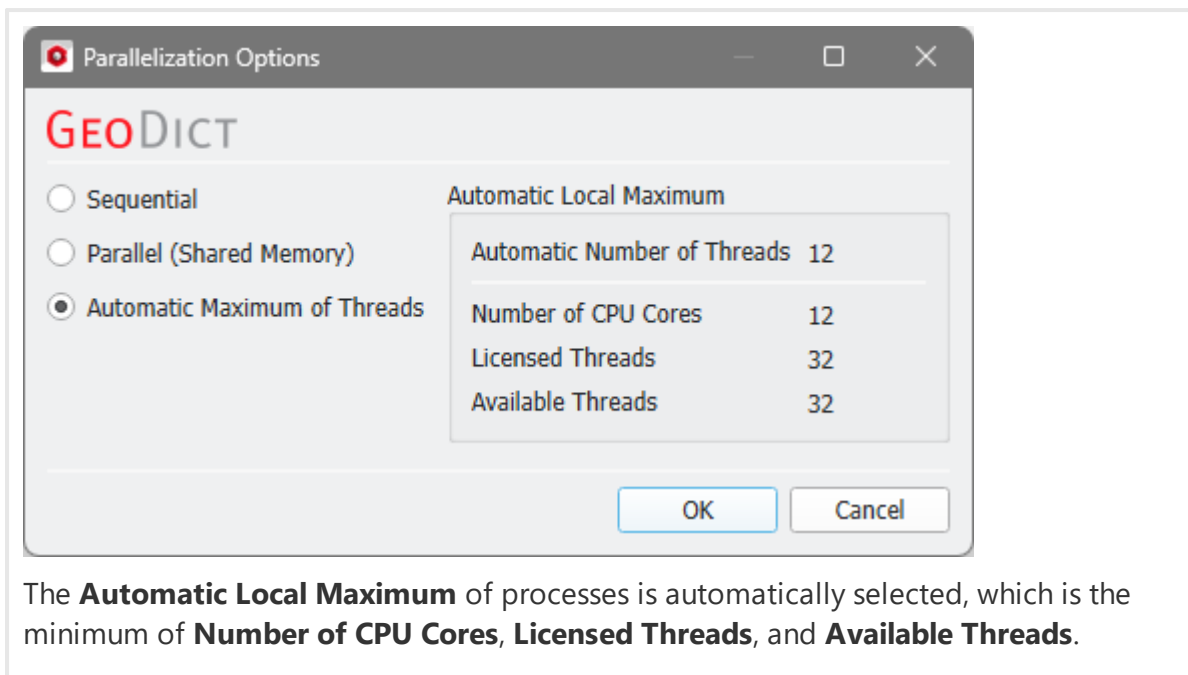
Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



Growth Mode

The amount of the added sediment material on the structure can be controlled either by volume percentage (**Exceed SVP**) or by the **Coating Thickness**.

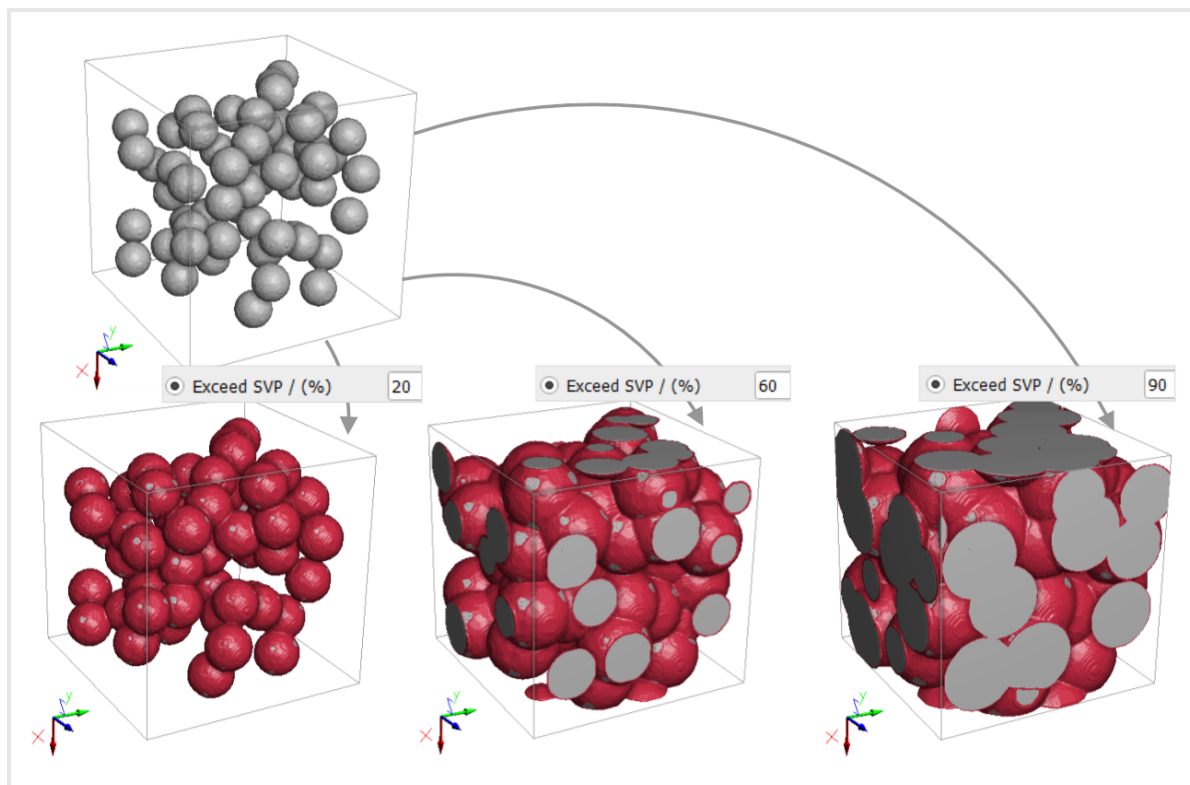
Growth Mode

☒ Exceed SVP / (%)

☐ Coating Thickness / (m)

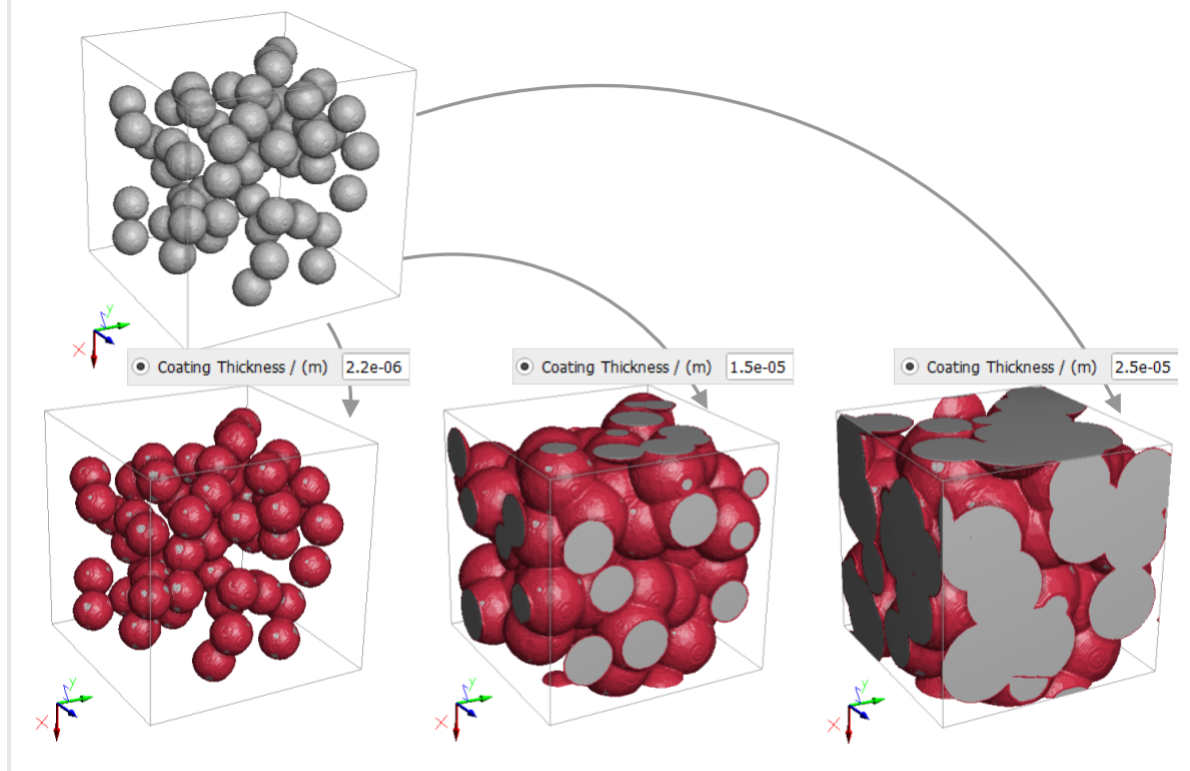
✓ Exceed SVP

Observe the effect of increasing **Exceed SVP' / (%)** from 20%, to 60% and then to 90%, when growing sediments on a structure made of spheres.



✓ Coating Thickness

Observe the effect when selecting the **Coating Thickness** to be $2.2\text{e-}06\text{ m}$ ($2.2\text{ }\mu\text{m}$), $1.5\text{e-}05\text{ m}$ ($15\text{ }\mu\text{m}$), and $2.5\text{e-}05\text{ m}$ ($25\text{ }\mu\text{m}$).



Specify Growing Sediment

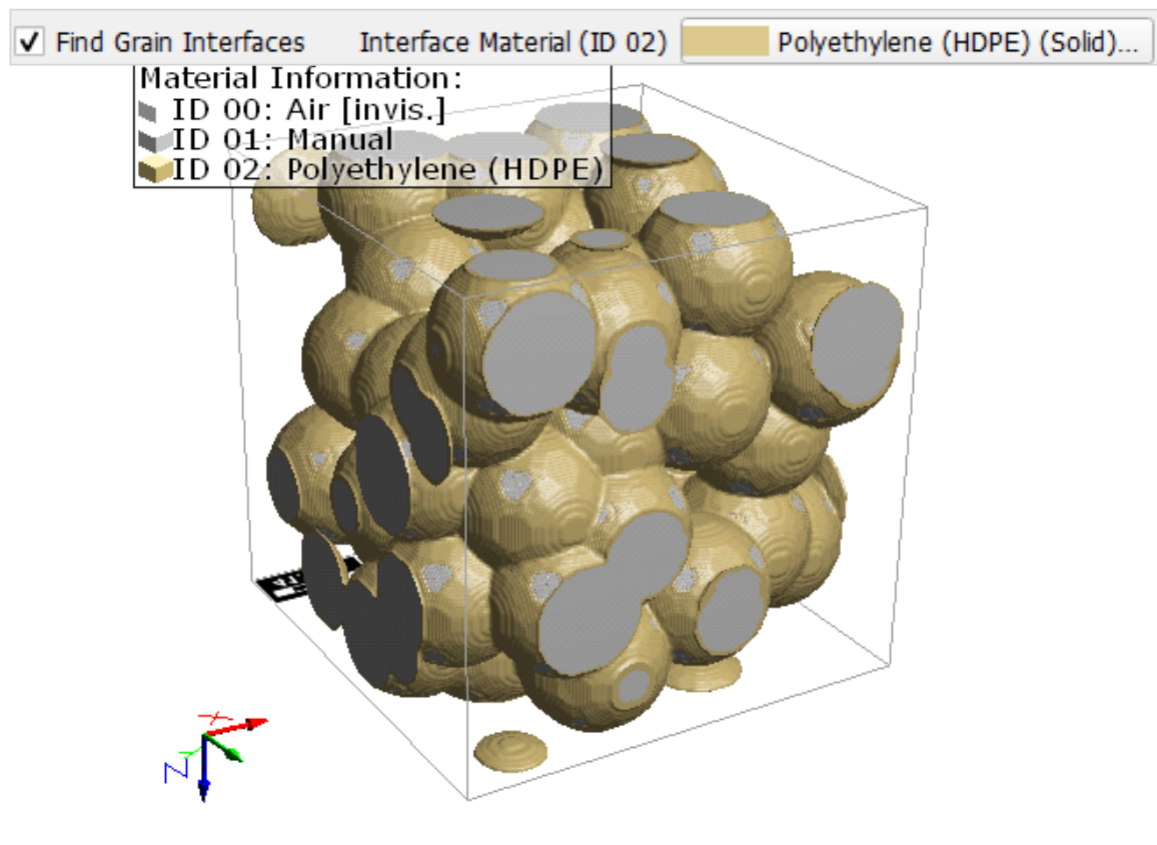
Specify the **Interface Material** and whether to **Save Voxel-Geometry with Object Indices** and to **Save Grain Orientation**.

☒ Find Grain Interfaces Interface Material (ID 02) Solid...
☐ Save Voxel-Geometry with Object Indices
☐ Save Grain Orientation

✓ Find Grain Interfaces

If **Find Grain Interfaces** is checked, the **Interface Material** of the sintered objects can be chosen from the GeoDict material database by clicking the button.

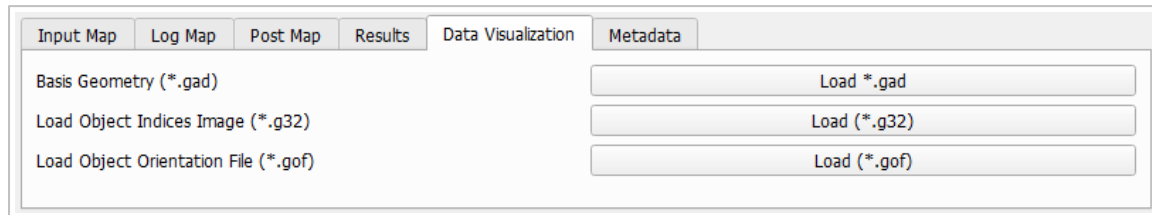
This results into a different material ID being assigned to the entire grain surface, including the interfaces with other objects.



✓ Save Options

As mentioned for the [Sinter & Crystallization](#) ¹⁷⁶ feature, the geometry information can be saved as binary in *.g32 format by checking **Save Voxel-Geometry with Object Indices**.

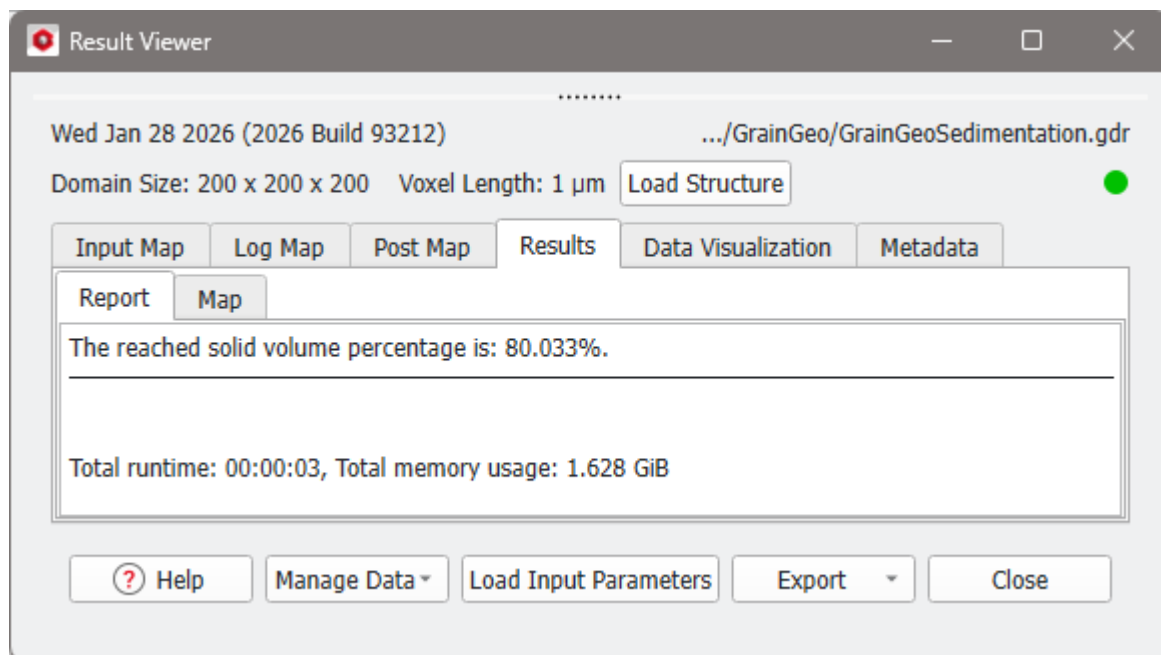
The grain orientation can be saved as *.gof file by checking **Save Grain Orientation**. Load the resulting data from the **Data Visualization** tab in the **Result Viewer**.



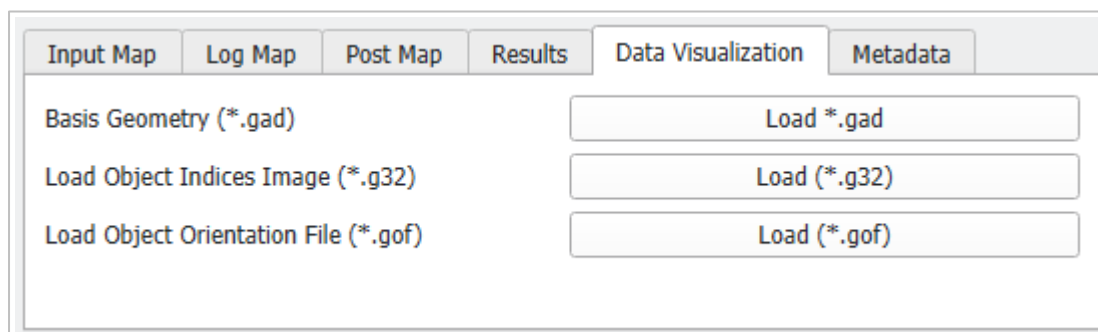
1.8.2 Results

The structure with grown sediment is shown in the visualization area. Learn more about visualization in GeoDict in the **Visualization** User Guide.

The result file is automatically opened in the Result Viewer and shows the reached solid volume percentage in the **Results - Report** tab. Additionally, it offers 3D **Data Visualization** options depending on the generation settings. Find more information on GeoDict result files in the **Result Viewer** User Guide.



From the **Data Visualization** tab several files can be loaded.



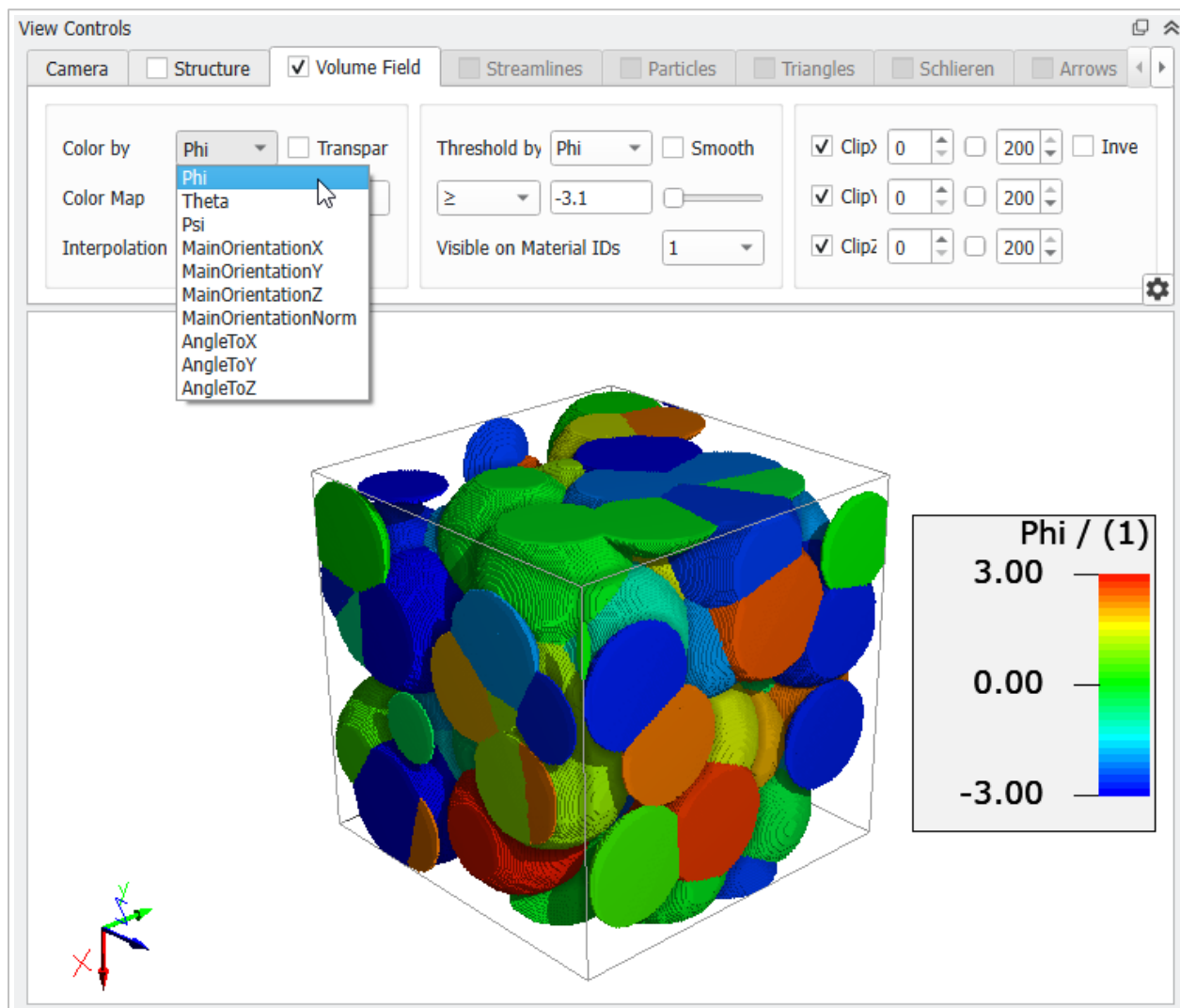
It is always possible to load the original structure before growing sediment by clicking **Load *.gad**.

If **Save Voxel-Geometry with Object Indices** was selected in the [Options](#)¹⁸⁴ dialog, you can load the object indices image by clicking **Load (*.g32)**.

If **Save Grain Orientation** was selected in the [Options](#)¹⁸⁴ dialog, you can load the object orientation image by clicking **Load (*.gof)**.

These two files can be used, together with the structure, to compute, e.g., elastic properties with transversal isotropic or orthotropic constituent materials laws with the ElastoDict module.

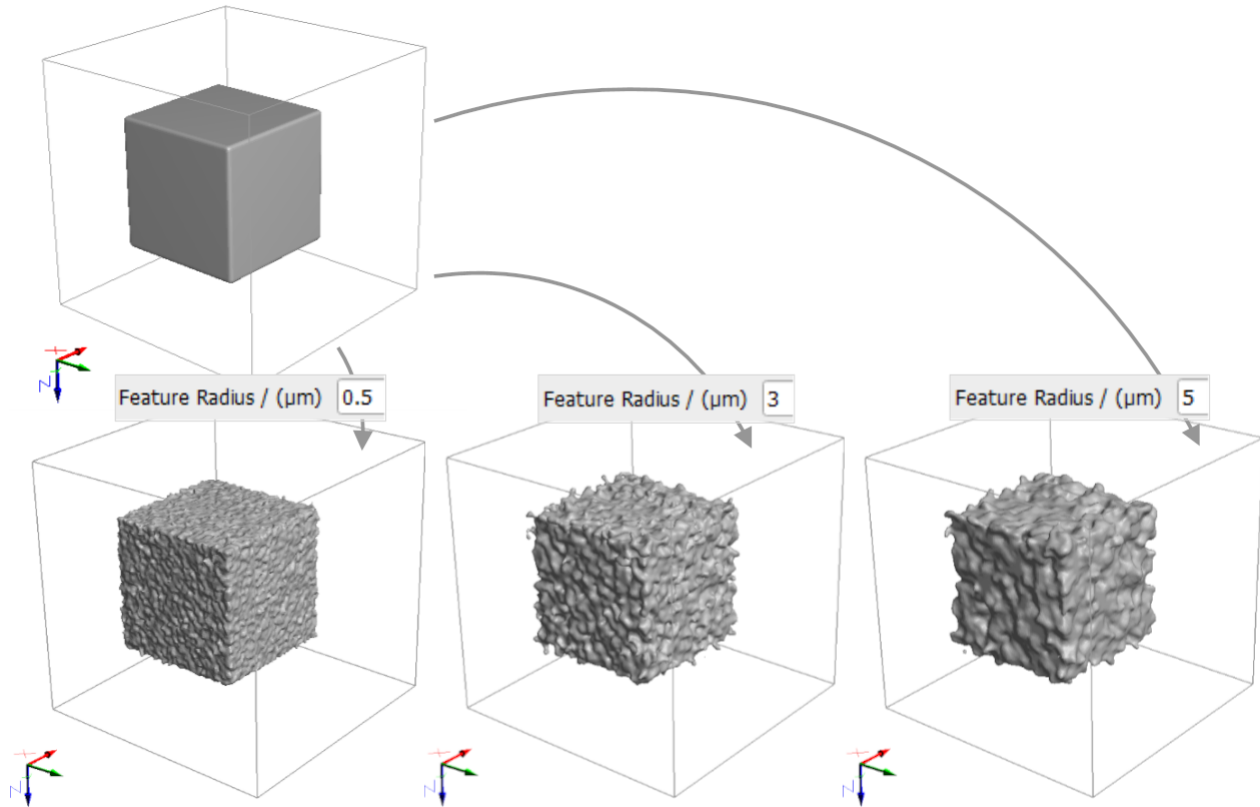
Below an example for an orientation image is shown.



Find more information about visualization of volume fields in the Visualization User Guide.

1.9 Roughen Surface

With **Roughen Surface**, the structure's surface is roughened. The structure to be roughened must already be in memory.



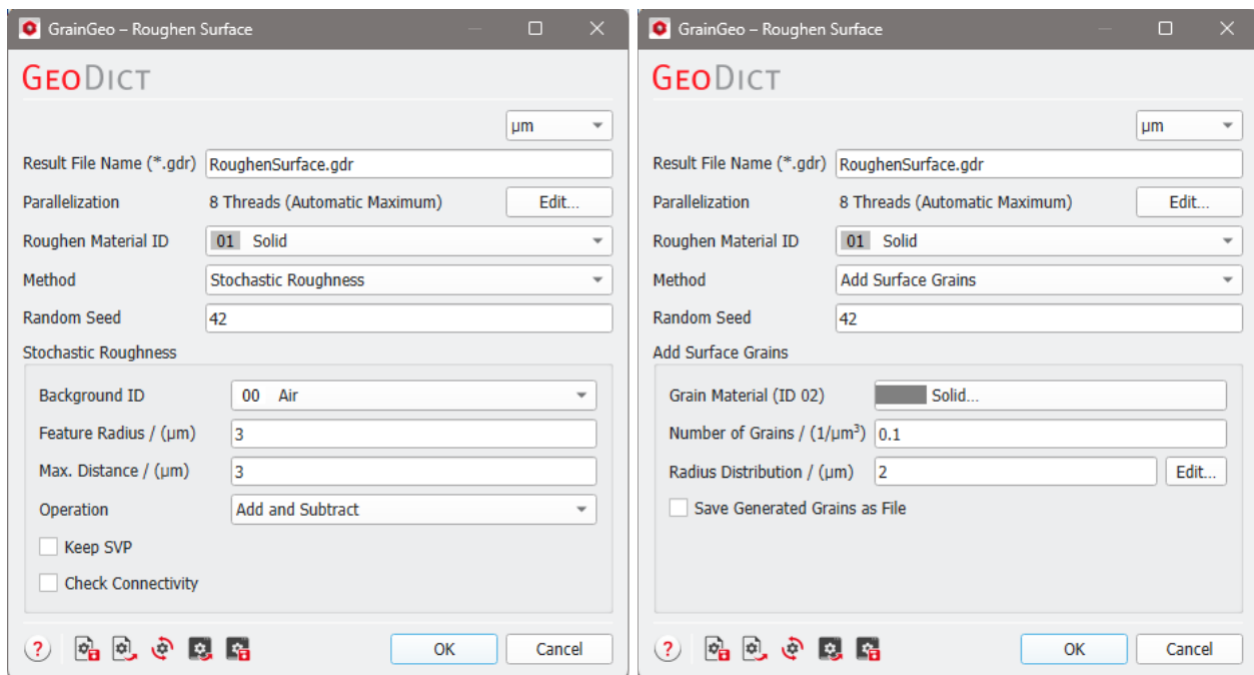
The Roughen Surface command:

- [Options](#)¹⁸⁷
Define the parameters for the surface roughening.
- [Results](#)¹⁹⁸
View the results in the Result Viewer.

1.9.1 Options

Clicking the Options' **Edit...** button opens the **Roughen Surface** options dialog. Clicking **OK** closes the dialog and returns to the GrainGeo section. Clicking **Generate** starts the process of surface roughening.

Two different methods can be chosen to roughen the surface. Using **Stochastic Roughness**, a Gaussian random field is produced to determine which voxels to add or subtract from the structure. With **Add Surface Grains**, small grains are added to the surfaces of the structure.



The parameters are described in groups:

- [General Options](#)¹⁸⁸
Define general parameters as result file name, parallelization, and the method for the surface roughening.
- [Stochastic Roughness](#)¹⁹²
Define the parameters specifying the stochastic roughness.
- [Add Surface Grains](#)¹⁹⁵
Define the parameters specifying the adding of grains to the surface.



- Opens the corresponding User Guide section.
- Saves the settings to a GeoDict settings file (*.gps).
- Loads the settings from a GeoDict settings file (*.gps) or a GeoDict result file (*.gdr).
- Resets all parameter settings to the built-in default settings.
- Resets all parameter settings to the saved start-up settings.
- Saves the current parameter settings as start-up settings.

Each option is explained by a tooltip which appears when resting the mouse over the icon.

General Options

At the top left of the dialog, the name for the file containing the generation results can be

entered in the **Result File Name (*.gdr)** box. The default name can be kept, or a new name can be chosen, fitting the current project.

The result files are saved in the chosen project folder (**File** → **Choose Project Folder**, in the **Menu bar**). If a GeoDict result file (*.gdr) with the given name already exists in the project folder, a warning message is shown at the start of the creation process. You can either decide to rename the chosen file name to a new one, to cancel the generation process, to overwrite or to back up the old file. When nothing is selected, GeoDict uses the **Back-Up** option after a waiting time.

The available units (m, cm, mm, μm , nm and Inch) are selectable from the pull-down menu at the top right of the dialog. When the units are changed, the entered values are adjusted automatically.

The screenshot shows a dialog box with the following fields and controls:

- Units: μm (pull-down menu)
- Result File Name (*.gdr): RoughenSurface.gdr
- Parallelization: 8 Threads (Automatic Maximum) with an Edit... button
- Roughen Material ID: 01 Solid (pull-down menu)
- Method: Add Surface Grains (pull-down menu)
- Random Seed: 42

✓ **Parallelization**

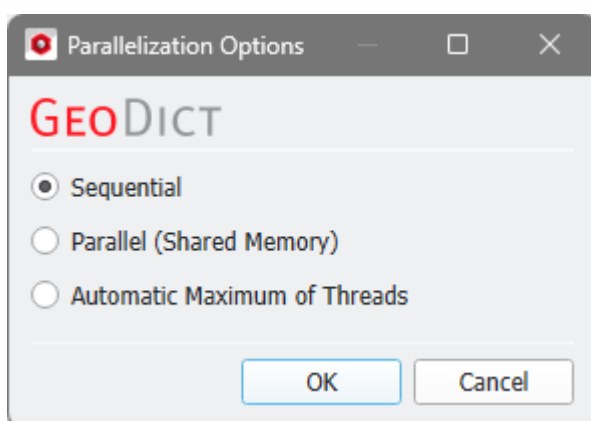
Control how many threads are used for the computation. Parallelization is possible if your license and hardware allow it.

The **Parallelization Options** dialog opens when clicking the **Edit** button and you can choose between **Sequential**, **Parallel (Shared Memory)**, or **Automatic Maximum of Threads**.

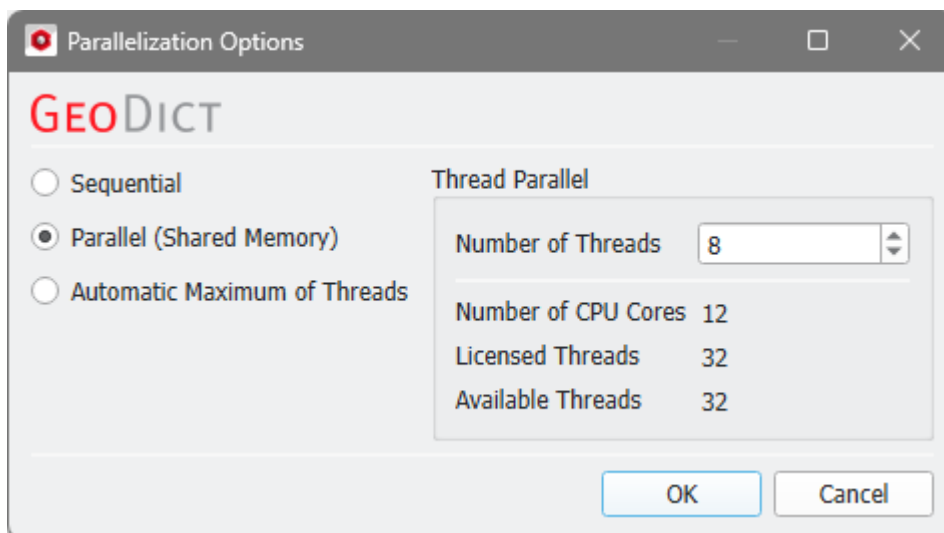
The screenshot shows a dialog box with the following fields and controls:

- Parallelization: 12 Threads (Automatic Maximum)
- Edit... button

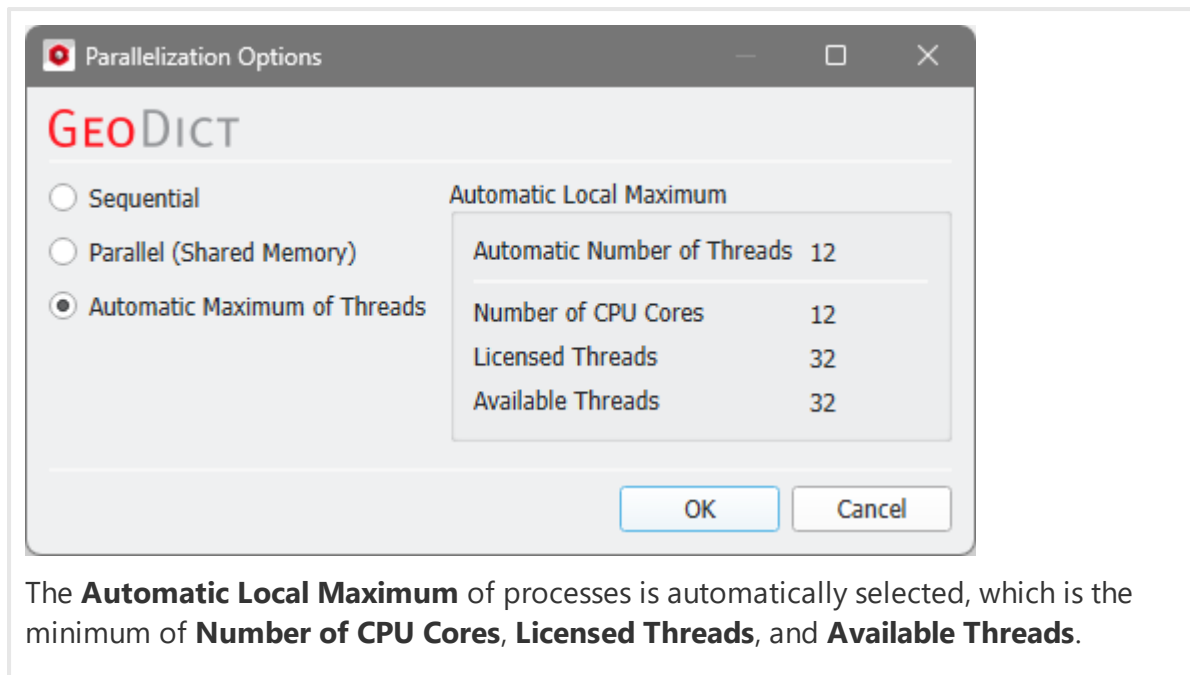
Selecting **Sequential** will not apply parallelization and only one thread is used for the computation.



When **Parallel (Shared Memory)** is selected, the **Number of Threads** can be entered. Below, the **Number of CPU Cores** that the current machine has, the maximum number of **Licensed Threads** and the number of those licensed threads that are available (**Available Threads**) are shown in the dialog. Of course, the maximal number of parallel processes you can use, is the smallest of those three numbers.



If **Automatic Maximum of Threads** is selected, the number of parallel processes is automatically selected for optimal speed, based on the CPU cores and licensed parallel processes.



✓ Roughen Material ID

From the **Roughen Material ID** pull-down menu, choose one material to be roughened from the materials present in the structure. If the structure consists of several materials, each material is treated separately.

✓ Method

Select [Stochastic Roughness](#)^[192] or [Add Surface Grains](#)^[195] as the **Method** to be used for the roughening process from the pull-down menu. Using **Stochastic Roughness**, a Gaussian random field is produced to determine which voxels to add or subtract from the structure. With **Add Surface Grains**, small grains are added to the surfaces of the structure.

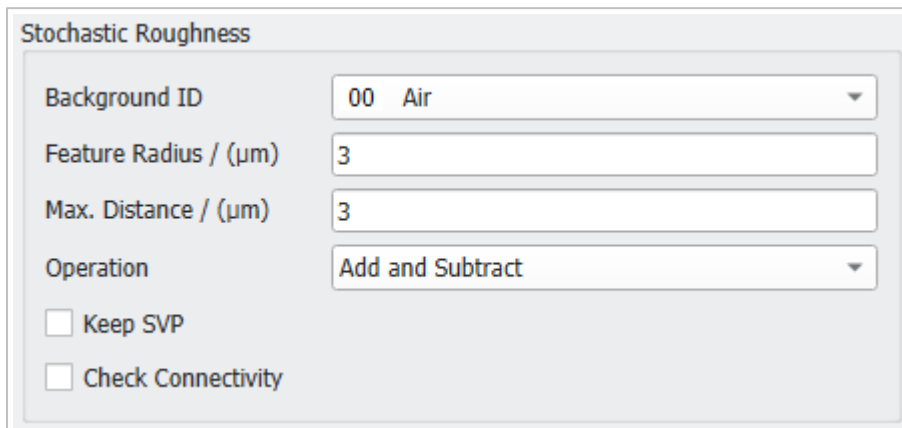
✓ Random Seed

Random Seed initializes the random number generator behind the surface roughening. Changing its value produces different sequences of random numbers and hence, different realizations of the surface roughening. If all settings are equal, generating with the same Random Seed value produces the identical roughening.

Stochastic Roughness

Stochastic Roughness roughens the surface of the Material ID selected with the [Roughen Material ID](#)^[191]. This is done by adding and/or subtracting voxels in the surface following a stochastic distribution.

The parameters in the **Stochastic Roughness** panel specify the roughening process. A stochastic field is created and segmented depending on the given parameters. It works similar to the [Stochastic Field Thresholding](#)^[143].

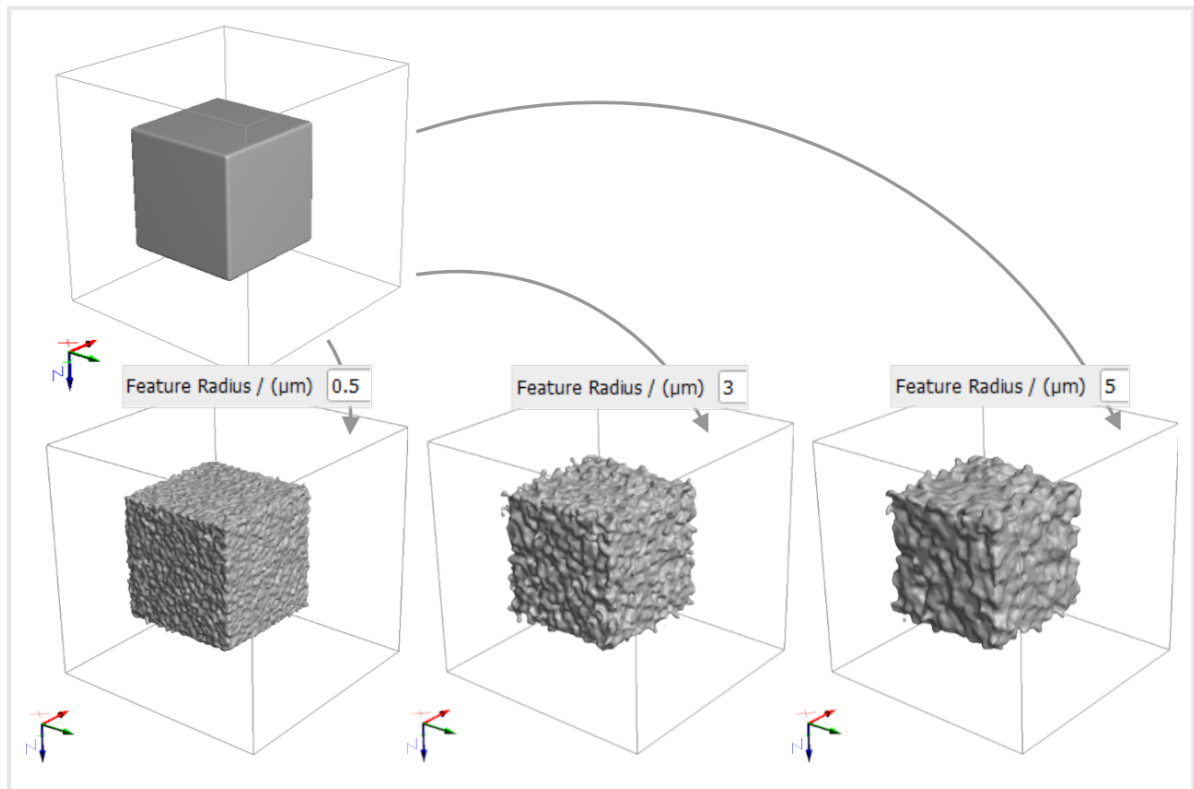


✓ Background ID

Only the area where the selected Material ID ([Roughen Material ID](#)^[191]) and the **Background ID** touch is defined as surface and thus, roughened.

✓ Feature Radius

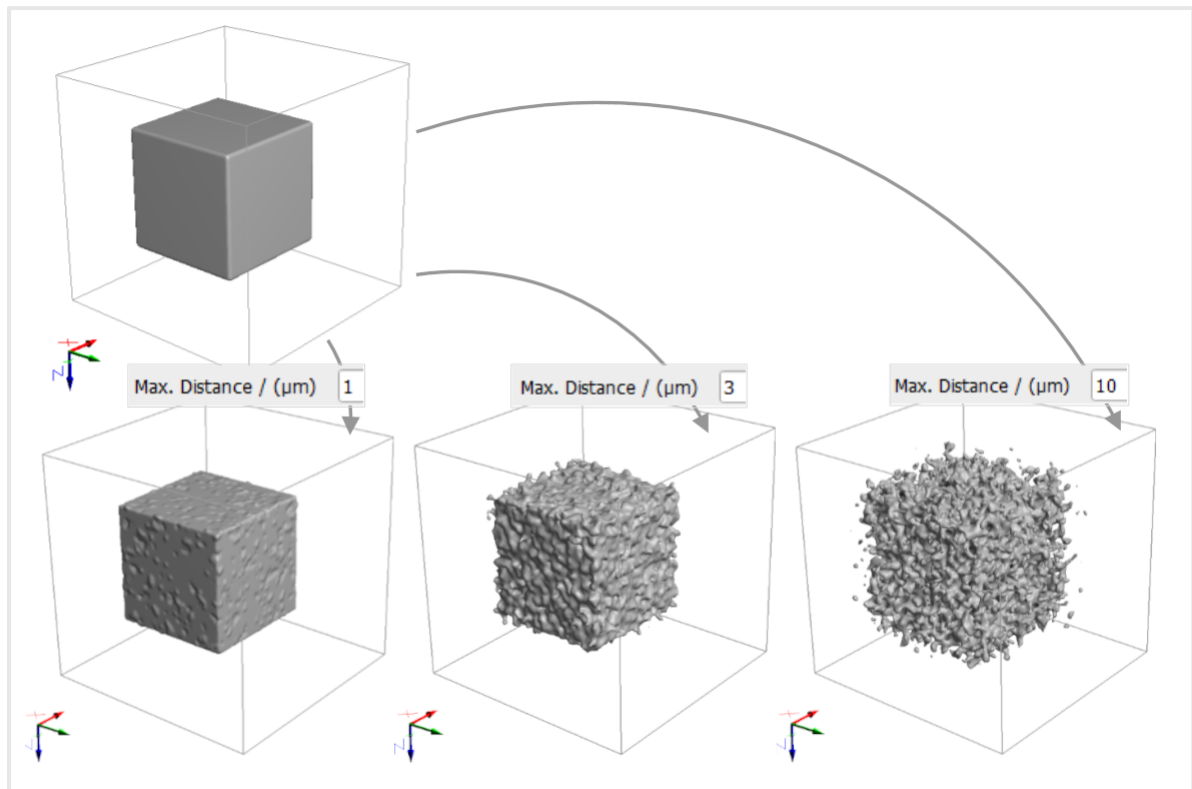
Change the **Feature Radius** to change the size of the added and subtracted features. The **Feature Radius** is the 99.7 percentile radius of the features, similar to a maximum grain radius.



✓ Max. Distance

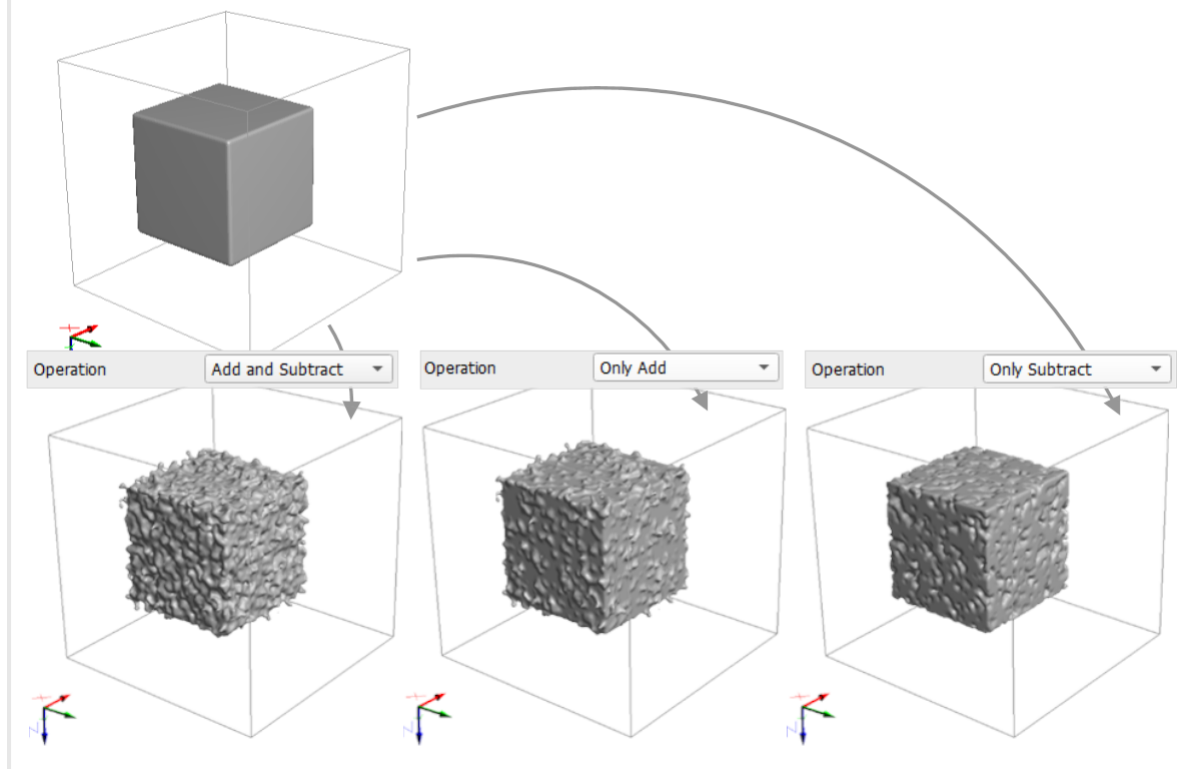
The **Max. Distance** specifies the displacement of the features from the surface, influencing the layer height. If the **Maximum Distance** is chosen higher than the selected **Feature Radius**, not all features are connected to the surface, unless [Check Connectivity](#)¹⁹⁵ is selected.

This can be observed in the following figure on the last structure with a max. distance of 10 μm and a feature radius of 3 μm .



✓ Operation

Select which **Operations** should be allowed for roughening. By default, Adding and Subtracting features is allowed. But it is also possible to choose **Only Add** or **Only Subtract** from the pull-down menu.



✓ Keep SVP

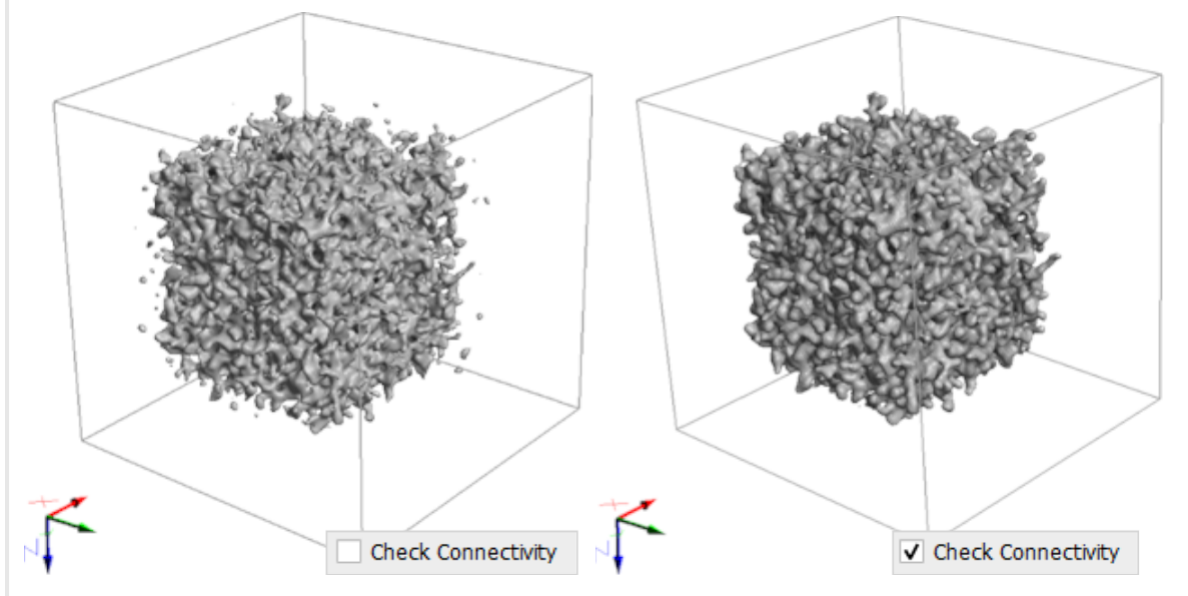
If **Add and Subtract** is selected, the checkbox **Keep SVP** is available. Check to keep the original solid volume percentage of the structure by using the same number of voxels for adding and subtracting.

Operation Add and Subtract ▼

☐ Keep SVP

✓ Check Connectivity

If **Check Connectivity** is selected, all features will be connected to the original structure even if the chosen [maximum distance](#)^[193] is very high.



Add Surface Grains

Add Surface Grains roughens the surface by adding grains on the surface of the Material ID selected with [Roughen Material ID](#)^[191].

Add Surface Grains

Grain Material (ID 02) Solid...

Number of Grains / ($1/\mu\text{m}^3$) 0.1

Radius Distribution / (μm) 2 Edit...

☐ Save Generated Grains as File

The added grains get the next free Material ID and the overlap between the added grains and the [Roughen Material ID](#)^[191] is defined following the rules described for Intersecting Material IDs in the Graphical User Interface User Guide.

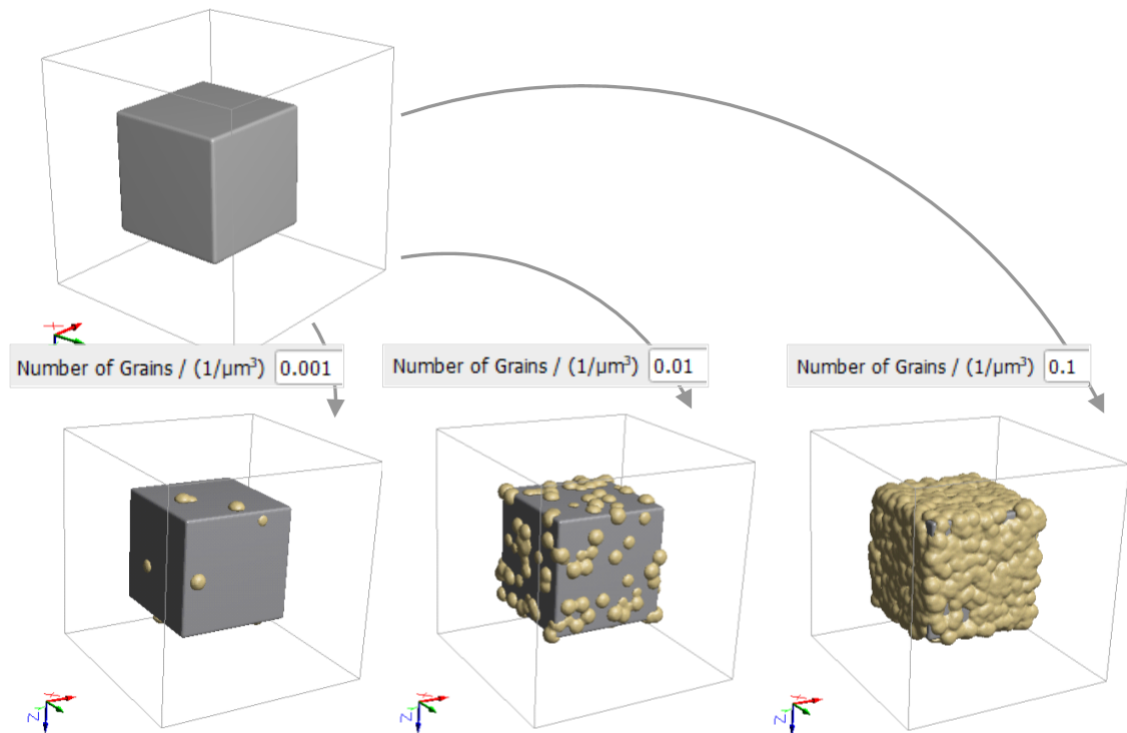
✓ Grain Material

Choose a **Grain Material** for the added surface grains from the material database. The next available Material ID is assigned to the grains and the material of the grains can be selected from the database after clicking the button. For example, if the structure contains one material with Material ID 01, the grains are assigned to Material ID 02.

✓ Number of Grains

The parameters **Number of Grains** per volume (given in $1/\mu\text{m}^3$) defines the number of grains added to a certain material in the domain.

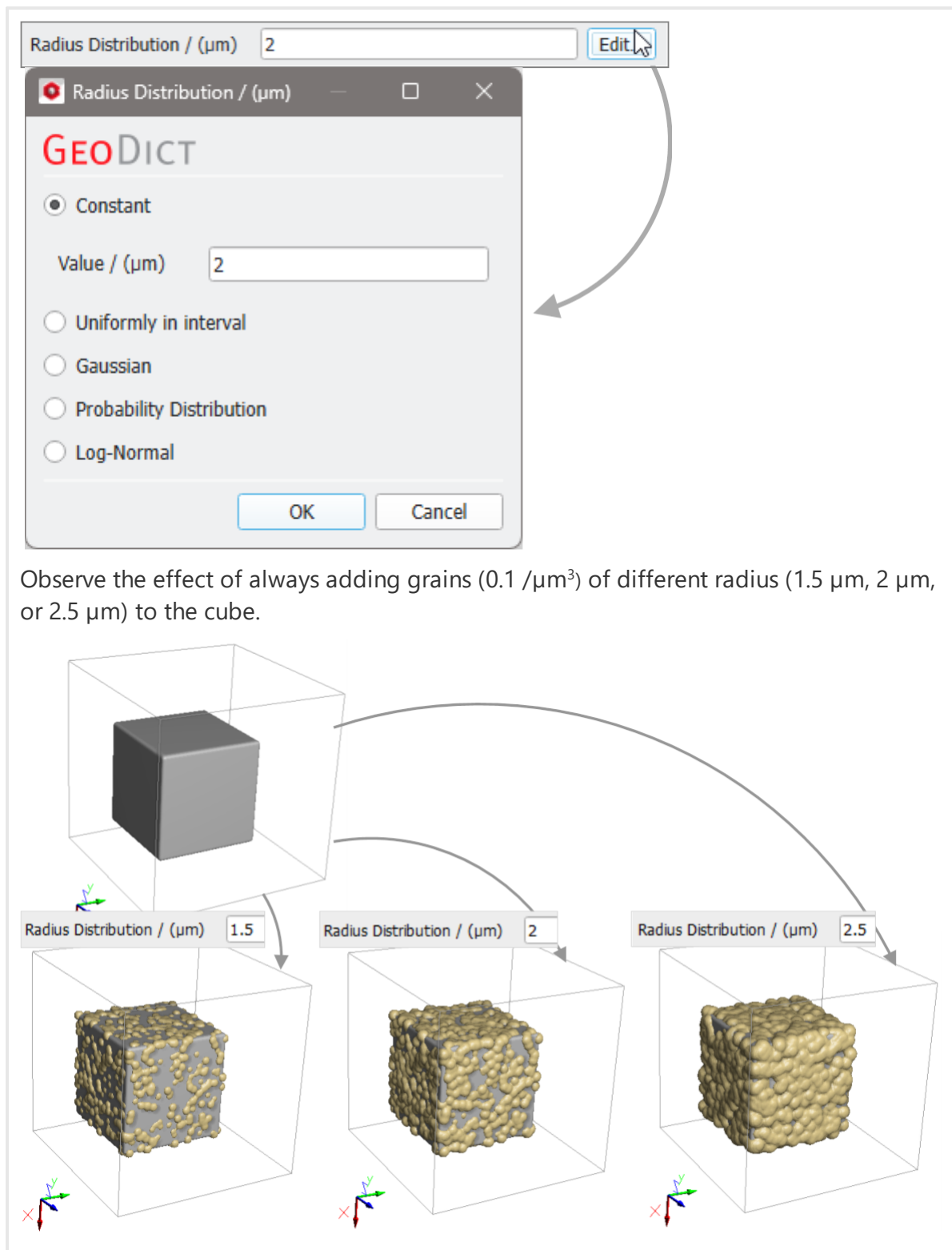
Observe now the effect of adding different amounts of grains with a radius of $3\ \mu\text{m}$ to a cube.



✓ Radius Distribution

The parameter **Radius Distribution** defines the size of the grains added to a certain material in the domain.

By clicking the **Edit...** button, the **Radius Distribution** of the grains can be set to be a **Constant** value, or to follow a [distribution](#)⁸¹ (Uniformly in interval, Gaussian, Probability Distribution, or Log-Normal).



Observe the effect of always adding grains ($0.1 / \mu\text{m}^3$) of different radius ($1.5 \mu\text{m}$, $2 \mu\text{m}$, or $2.5 \mu\text{m}$) to the cube.

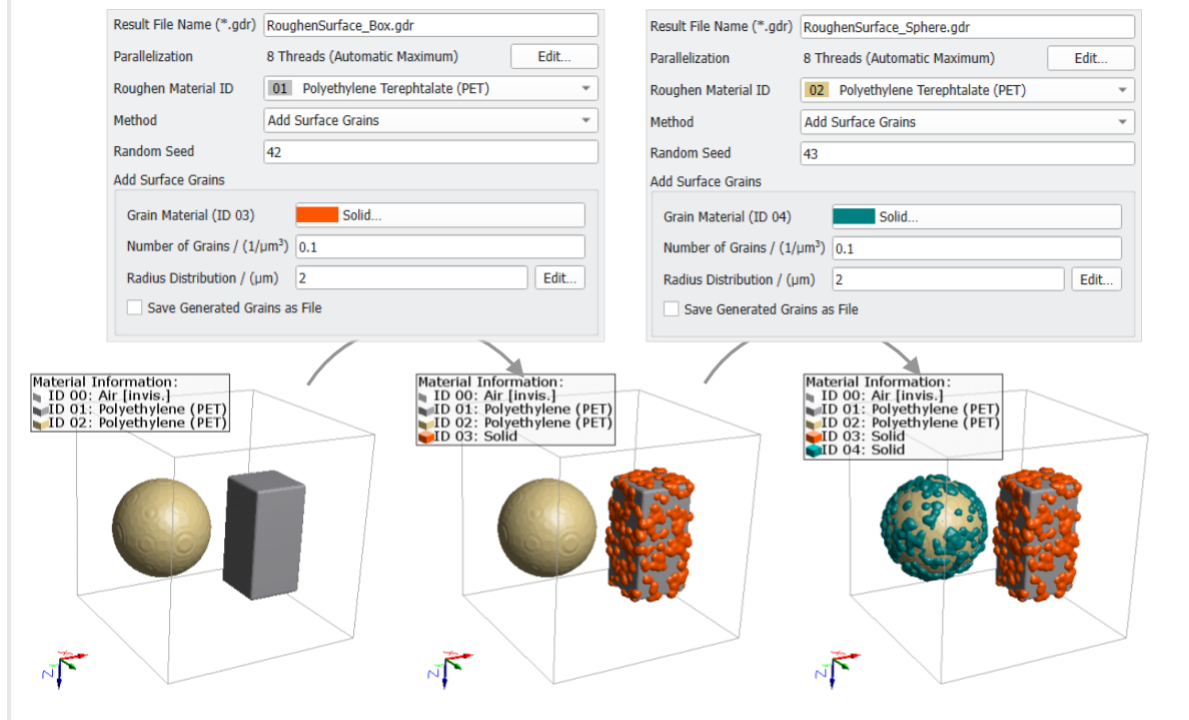
✓ Save Generated Grains as File

When **Save Generated Grains as File** is selected, the added surface grains are saved as **SurfaceGrains.gad** structure file in the result folder. This file contains the grains' analytic data.

✓ Example

As a simplified example, observe the addition of grains with radius 2 μm to objects (box and sphere) with different Material IDs. The grains are added in two steps, first to Material ID 01 (box), and then to Material ID 02 (sphere).

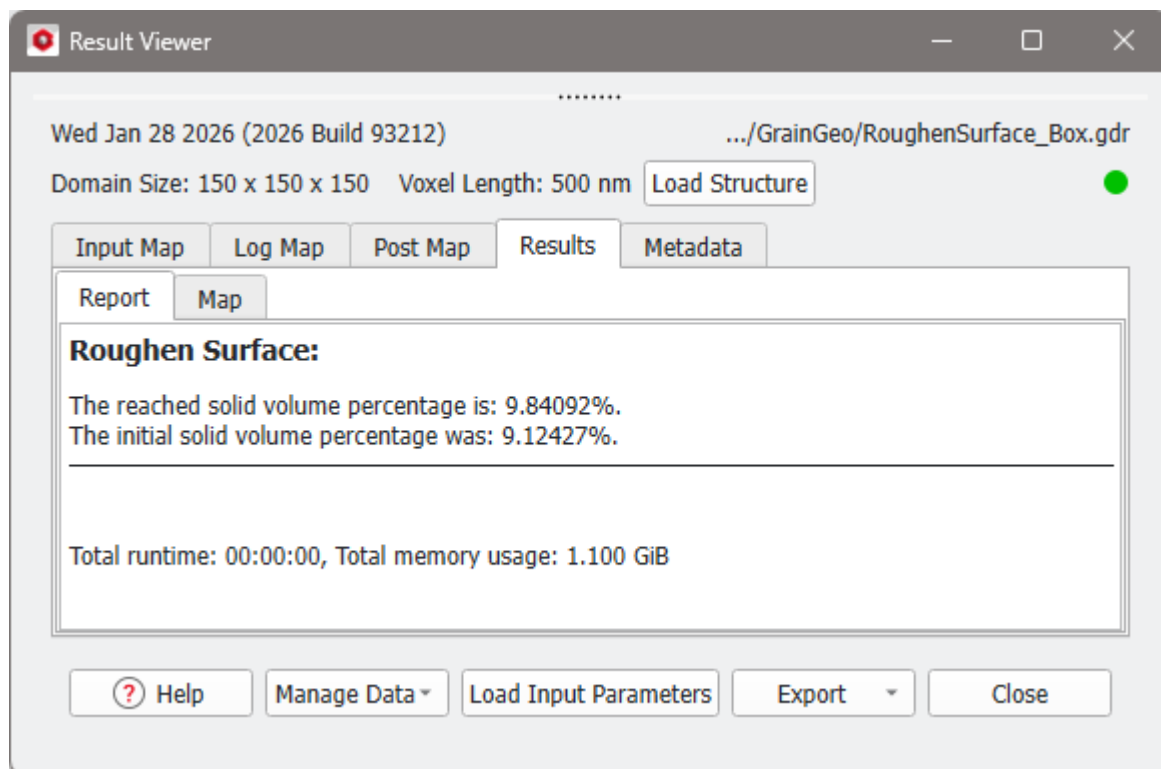
The **Number of Grains** added is 0.1 grains/ μm^3 (1 grain for every 10 μm^3 of the domain).



1.9.2 Results

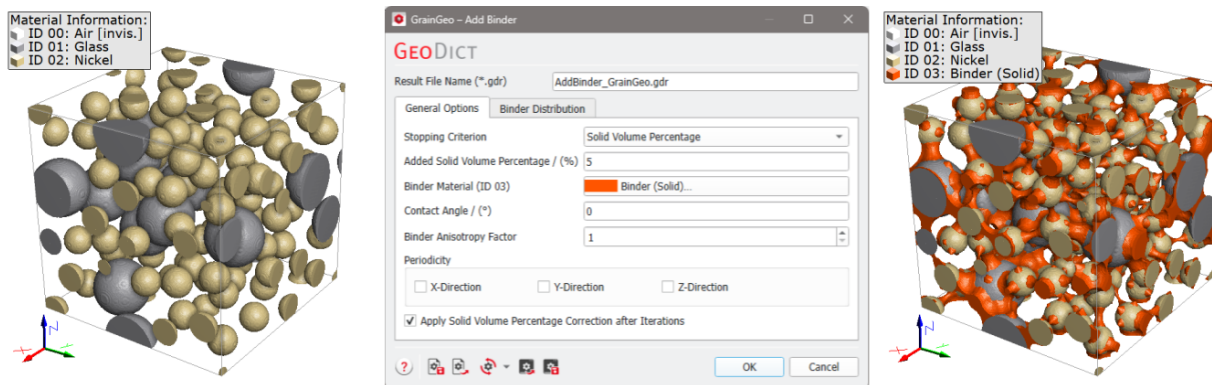
The structure with roughen surfaced is shown in the visualization area. Learn more about visualization in GeoDict in the **Visualization** User Guide.

The result file is automatically opened in the Result Viewer and shows the original and resulting solid volume percentage in the **Results - Report** tab. Find more information on GeoDict result files in the **Result Viewer** User Guide.



1.10 Add Binder

Binder provides structural integrity to structures with grains of all shapes and is, therefore, an important processing additive for battery electrodes, grain packs, ceramics, and hard-metal sintering processes.



Adding binder to a structure means adding material in the shape of a concave meniscus in the pore space where surfaces in that structure's material get close together. If there is no pore material in the structure, a warning is given.

For hollow objects, such as cellulose fibers, curved cellulose fibers, hollow fibers, curved hollow fibers, and hollow spheres, the algorithm under **Add Binder** needs analytic data (**GAD objects**) to discern that the empty voxels inside the fibers are not part of the pore space. Without analytic data, i.e., when using voxelized models, binder is also added inside the hollow fibers, which is physically inaccurate.

The **Add Binder** command:

- [Options](#)²⁰⁰
Define the Add Binder parameters.
- [Results](#)²¹³
View the Add Binder results.

1.10.1 Options

Clicking the **Options' Edit...** button opens the **Add Binder** dialog.

At the top of the **Add Binder** dialog, the name for the file containing the results of adding binding can be entered in the **Result File Name (*.gdr)** box. The default name can be kept, or a new name can be chosen, fitting the current project.

Clicking **OK** in it closes the dialog and returns to the module section. Clicking **Generate** starts the process.

The options are organized into tabs:

- [General Options](#)^[201]
Define shape and material of the binder.
- [Binder Distribution](#)^[210]
Define how the binder should be distributed throughout the domain.

General Options

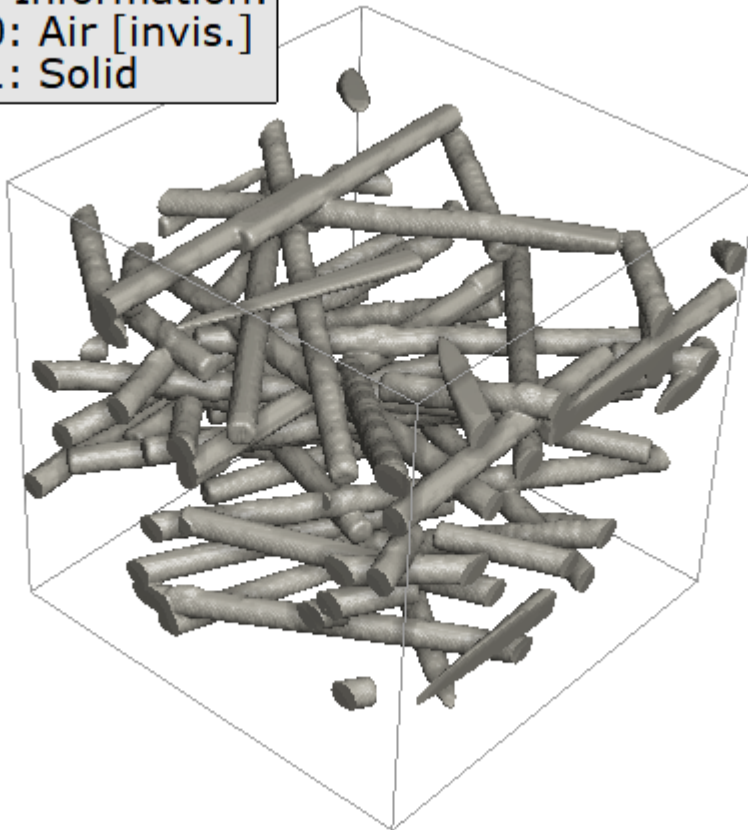
Define the general options, as the amount of binder to be added, the material and stopping criteria.

General Options	Binder Distribution
Stopping Criterion	Solid Volume Percentage
Added Solid Volume Percentage / (%)	10
Binder Material (ID 02)	 Binder (Solid)...
Contact Angle / (°)	0
Binder Anisotropy Factor	1
Periodicity	
☐ X-Direction ☐ Y-Direction ☐ Z-Direction	
☒ Apply Solid Volume Percentage Correction after Iterations	

Stopping Criterion

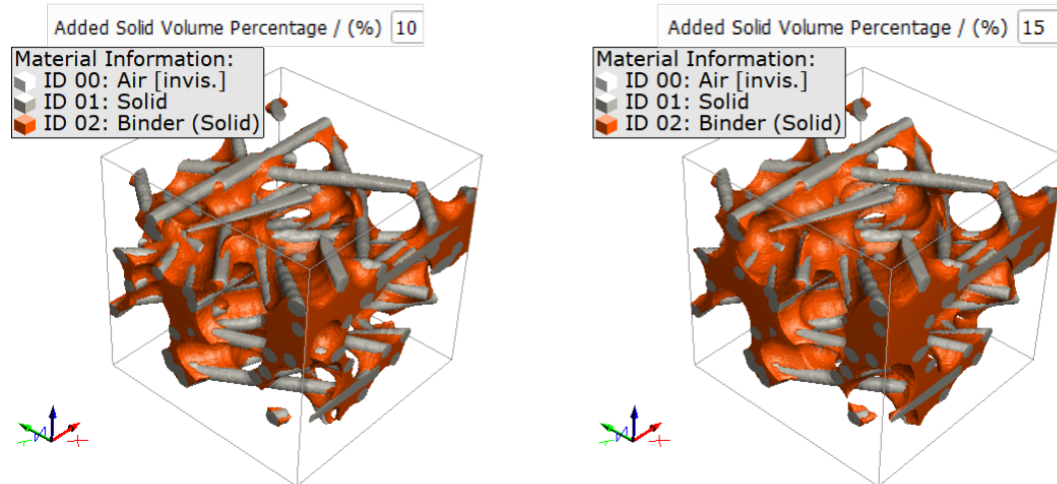
You may choose the most practical stopping criterion when adding binder. The chosen **Stopping Criterion** interrupts the addition of binder when it is reached. The possible stopping criteria are **Solid Volume Percentage**, **Weight Percentage**, and **Grammage**.

Material Information:
 ID 00: Air [invis.]
 ID 01: Solid



☒ Solid Volume Percentage

The process is stopped if the binder volume reaches the desired **Added Solid Volume Percentage**.



✓ Weight Percentage

The process is stopped if the weight of binder reaches a certain percentage of the weight of material. See [below](#) ²⁰⁴ how to select a material for the binder.

It is necessary to set the density for the structure's material (**Material Density**) and for the binder material (**Binder Density**) both in g/cm^3 , as well as the desired (weight) percentage of binder material to structure material (**Binder Weight Percentage**, in %). That is, a binder weight percentage of 20 means that there are 20 g of binder added per 100 g of objects in the structure.

Stopping Criterion	Weight Percentage
Binder Weight Percentage / (%)	20
Material Density / (g/cm^3)	1
Binder Material (ID 02)	 Binder (Solid)...
Binder Density / (g/cm^3)	2.70009

In the following example, two types of binder (high density: 5 g/cm^3 and low density: 0.5 g/cm^3) are added to a structure material with a density of 1.1399 g/cm^3 . Setting a binder weight percentage of 20% (20 g binder/100 g objects), the amount of binder material deposited is much larger when the binder is less dense.

Material Information:
ID 00: Air [invis.]
ID 01: Solid
ID 02: Binder (Solid)

Material Information:
ID 00: Air [invis.]
ID 01: Solid
ID 02: Binder (Solid)

Stopping Criterion: Weight Percentage

Binder Weight Percentage / (%) 20

Material Density / (g/cm³) 1.1399

Binder Material (ID 02) Binder (Solid)...

Binder Density / (g/cm³) 5

Stopping Criterion: Weight Percentage

Binder Weight Percentage / (%) 20

Material Density / (g/cm³) 1.1399

Binder Material (ID 02) Binder (Solid)...

Binder Density / (g/cm³) 0.5

For **Weight Percentage**, when **Manual** or **Undefined** are selected, you must enter the density of the binder (**Binder Density (g/cm³)**). If a material is selected from the database, the **Binder Density** of the binder material is automatically entered. If a manual material is used frequently, it is useful to save it to the material database.

✓ Grammage

The addition of binder stops when the **Added Grammage** (material and binder, g/m²) is reached.

See [below](#) ²⁰⁴, how to select a material for the binder.

Stopping Criterion Grammage

Added Grammage / (g/m²) 10

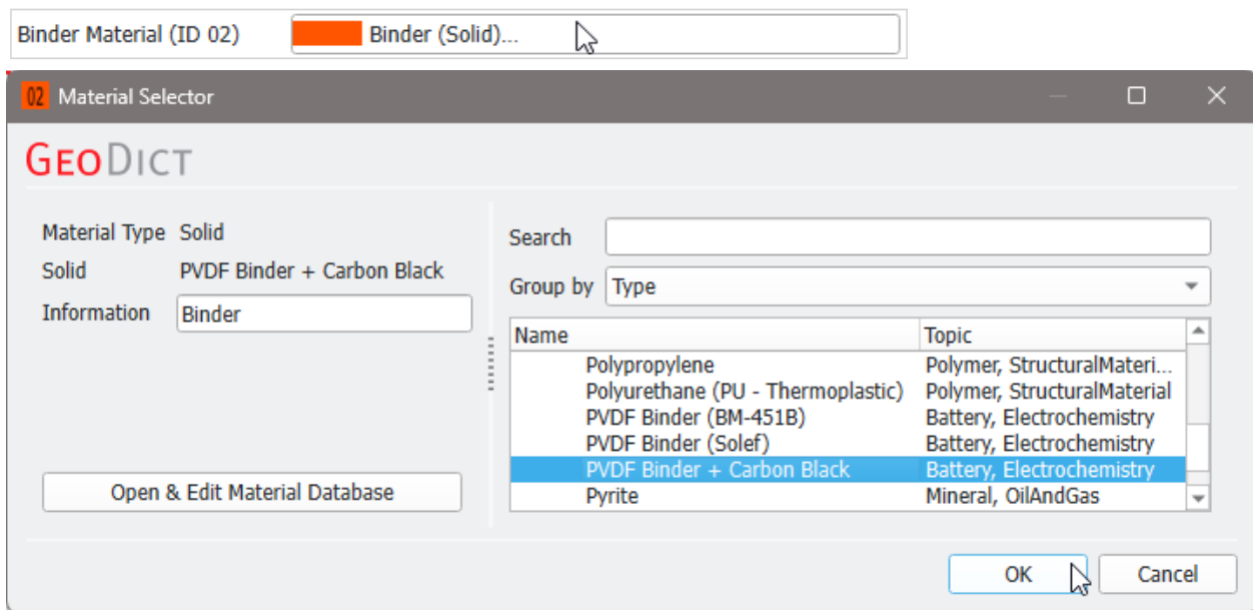
Binder Material (ID 02) Binder (Solid)...

Binder Density / (g/cm³) 2.7

For grammage, when manual or undefined are selected, the density of the binder is not automatically taken from the database and you must enter it manually (**Binder Density (g/cm³)**). If a manual material is used frequently, it is useful to save it to the material database.

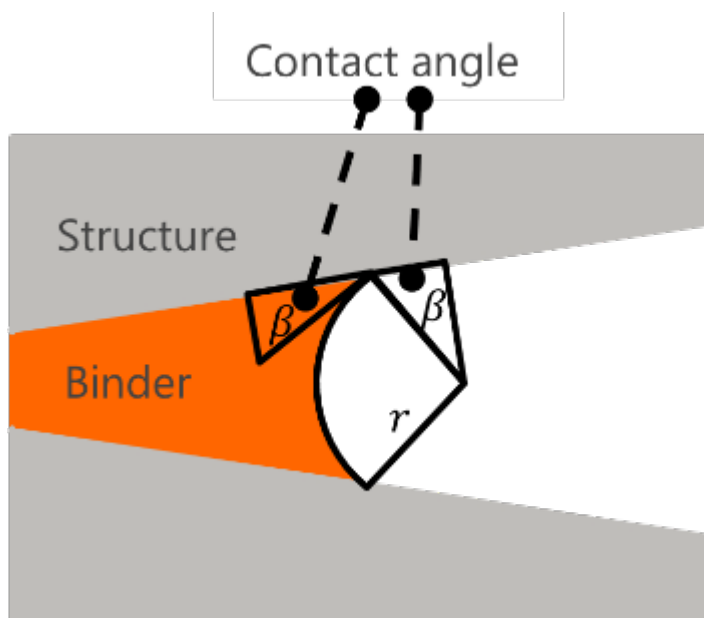
Binder Material

The **Binder Material** is assigned to the next available Material ID, and the appropriate material to be used as binder should be selected from the material database by clicking the button.



Contact Angle

The **Contact Angle** defines the angle in which the binder is deposited in relation to the materials in the structure. Values between 0° and 60° are accepted. When entering values larger than 60°, the value will be changed to 60° automatically. The contact angle helps to optimize and realistically model the addition of binder.



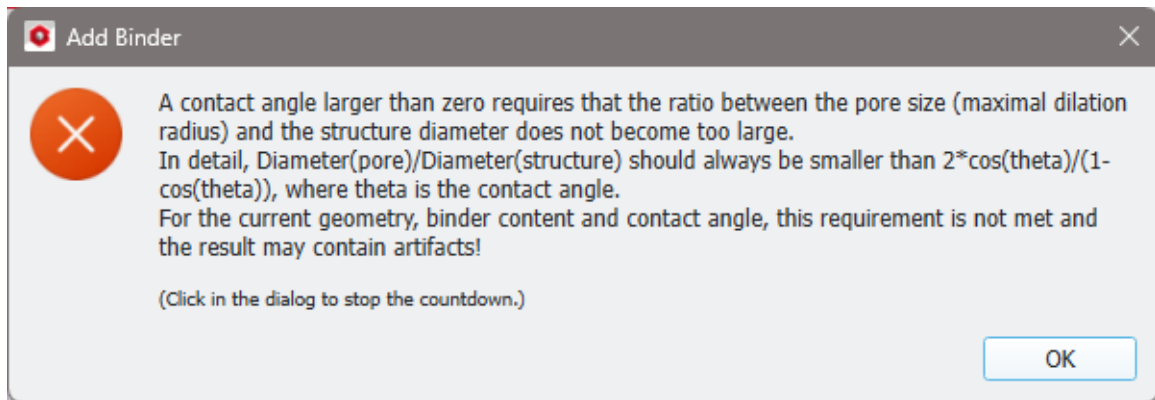
✓ Requirements for large contact angles

The contact angle must fulfill the following requirement:

$$\frac{\text{Diameter(Pore)}}{\text{Diameter(Structure)}} < \frac{2 \cos(\theta)}{1 - \cos(\theta)}$$

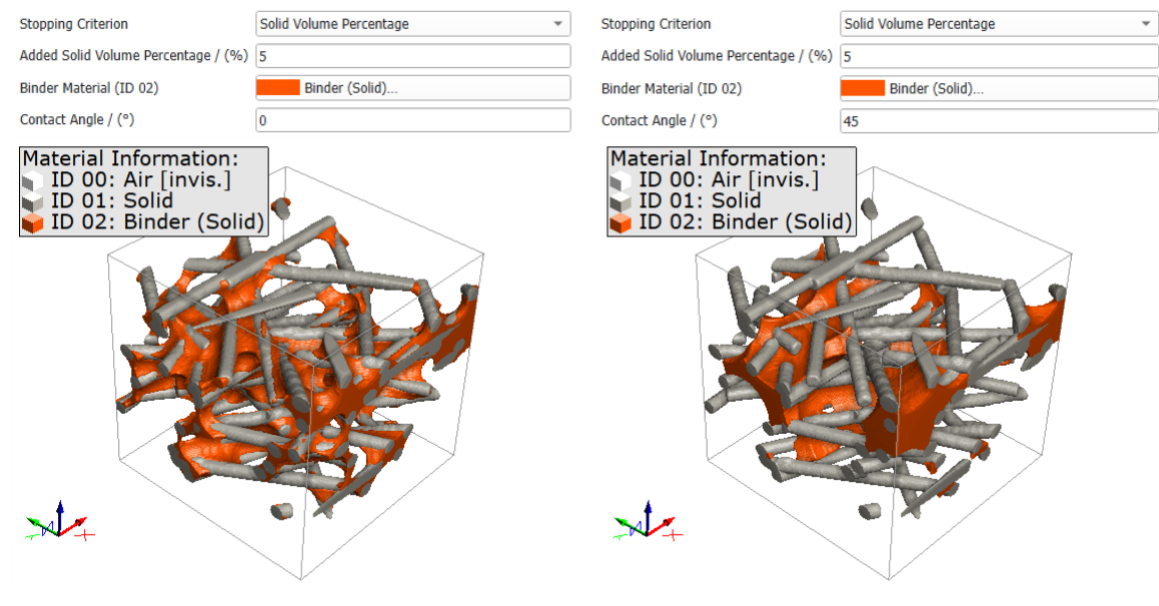
(10) Contact
Angle
Requirement

where θ is the contact angle and Diameter(Pore) means the maximal dilation radius. If this requirement is not met, a warning message appears. It is recommended to inspect the resulting structure to detect artifacts.



✓ Contact Angle Example

Observe the effect of adding binder with a **Contact Angle** of 0° or 45°.



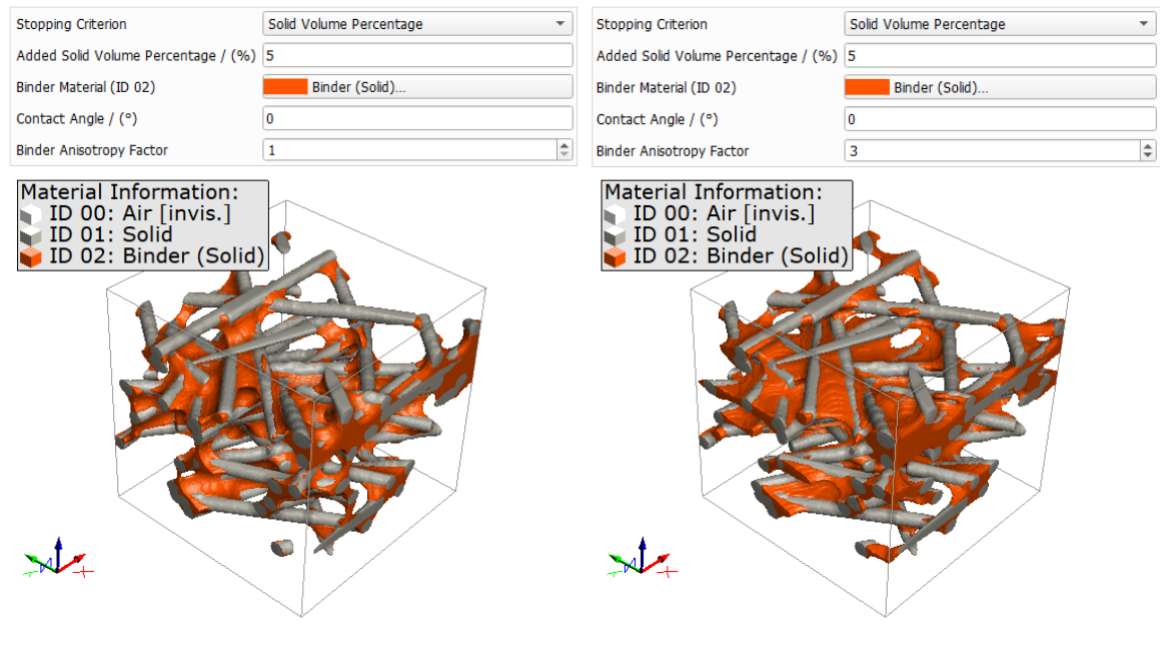
Binder Anisotropy Factor

The **Binder Anisotropy Factor** allows to control the grade of binder anisotropy in the X-Y-plane. If the factor is the default value of 1, the binder is distributed isotropically. By choosing larger values, the binder is distributed in the XY-plane but then, the contact angle value is not

accurate anymore.

✓ Binder Anisotropy Factor Example

Observe the effect of changing the **Binder Anisotropy Factor** from (the default) 1 to 3 when adding binder. With a binder anisotropy factor of 3, the binder is added in the direction of the XY-plane.



Periodicity

When the 3D-structure model is periodic in one or more directions, the binder can be added periodically: in all directions, only in the selected direction (**Periodic X**, **Periodic Y** and/or **Periodic Z**), or non-periodically. Adding binder periodically in certain direction(s) only makes sense if the 3D-structure model is periodic in that/those direction(s).

Periodicity
☐ X-Direction ☐ Y-Direction ☐ Z-Direction

Apply Solid Volume Percentage / Weight Percentage / Grammage Correction after Iterations

The algorithm adds binder until the iteration stops according to the given stopping criterion. Thus, the given value for **Solid Volume Percentage** / **Weight Percentage** / **Grammage** is usually not reached precisely and there are few cases, where the algorithm even does not converge.

If the amount of binder should be reached perfectly, it can be corrected by checking **Apply**

Solid Volume Percentage Correction after Iterations, Apply Weight Percentage Correction after Iterations or **Apply Grammage Correction after Iterations** depending on the chosen stopping criterion.

Selecting this option adds or removes binder surface voxels after the iterations are stopped until the given binder value is reached precisely.



Important! Using the correction feature reduces the **Contact Angle** precision.

General Options

Binder Distribution

Stopping Criterion

Solid Volume Percentage

Added Solid Volume Percentage / (%)

5

Binder Material (ID 02)

 Binder (Solid)...

Contact Angle / (°)

0

Binder Anisotropy Factor

1

Periodicity

☐ X-Direction
 ☐ Y-Direction
 ☐ Z-Direction

☒ Apply Solid Volume Percentage Correction after Iterations

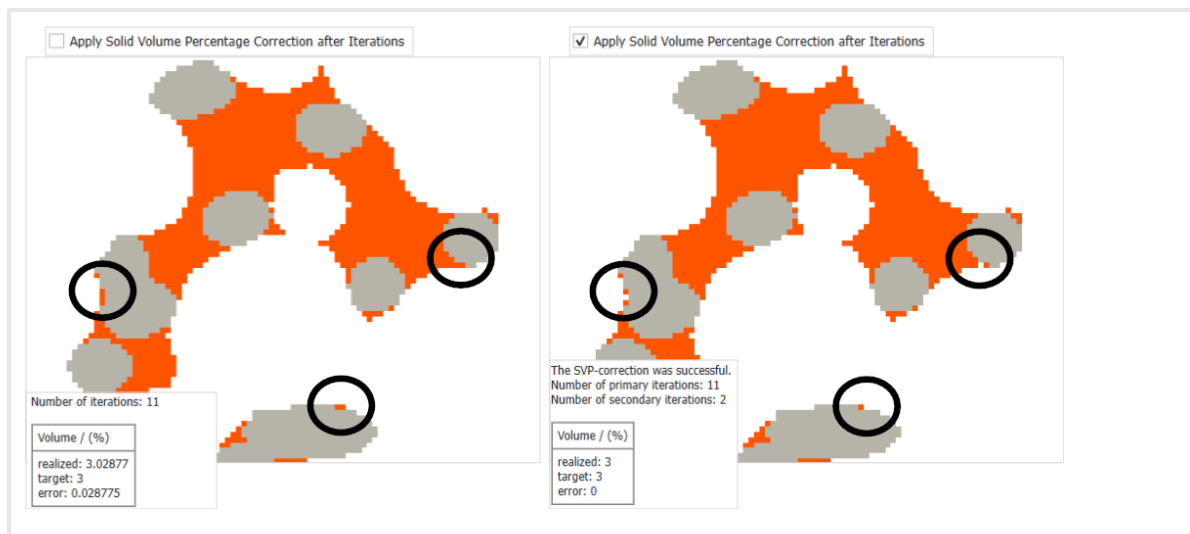
↓

☒ Apply Weight Percentage Correction after Iterations

☒ Apply Grammage Correction after Iterations

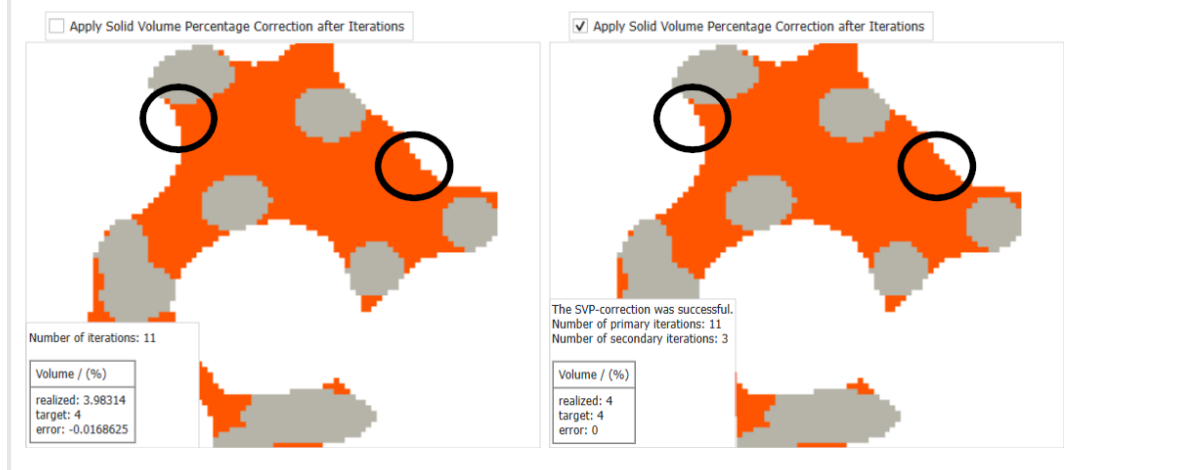
✓ Binder amount larger than target

If the realized amount of binder after the iterations is larger than the target value, voxels are removed from exposed positions, i.e., voxels with only one contact to another binder voxel.



✓ Binder amount smaller than target

In the other case, if the amount of binder is smaller than the target value, the algorithm adds voxels on positions with the most binder voxel neighbors.



✓ Algorithm

In detail, the algorithm applies small dilations and erosions to keep a smooth surface. In detail four steps are performed:

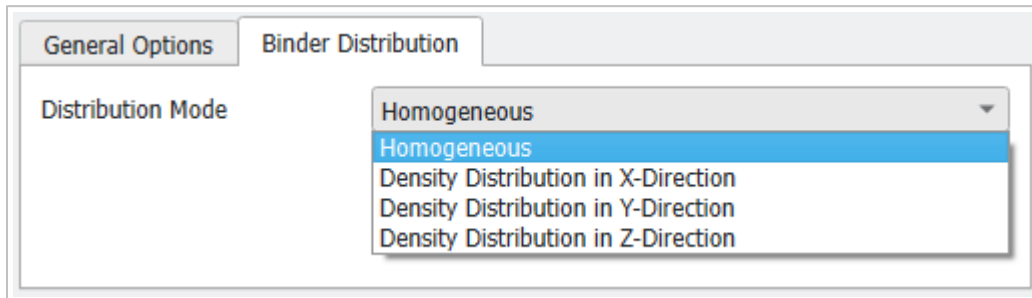
1. First, a voxel-zone at the surface is defined by the smallest possible dilation / erosion.
2. Within this voxel zone the algorithm again applies dilations / erosions. This reduces the voxel zone further.
3. Afterwards only a small surface layer remains that is maximal one voxel thick.
4. These remaining voxels are randomly reassigned.

The random reassignment is done to prevent biased change of the curvature.

Binder Distribution

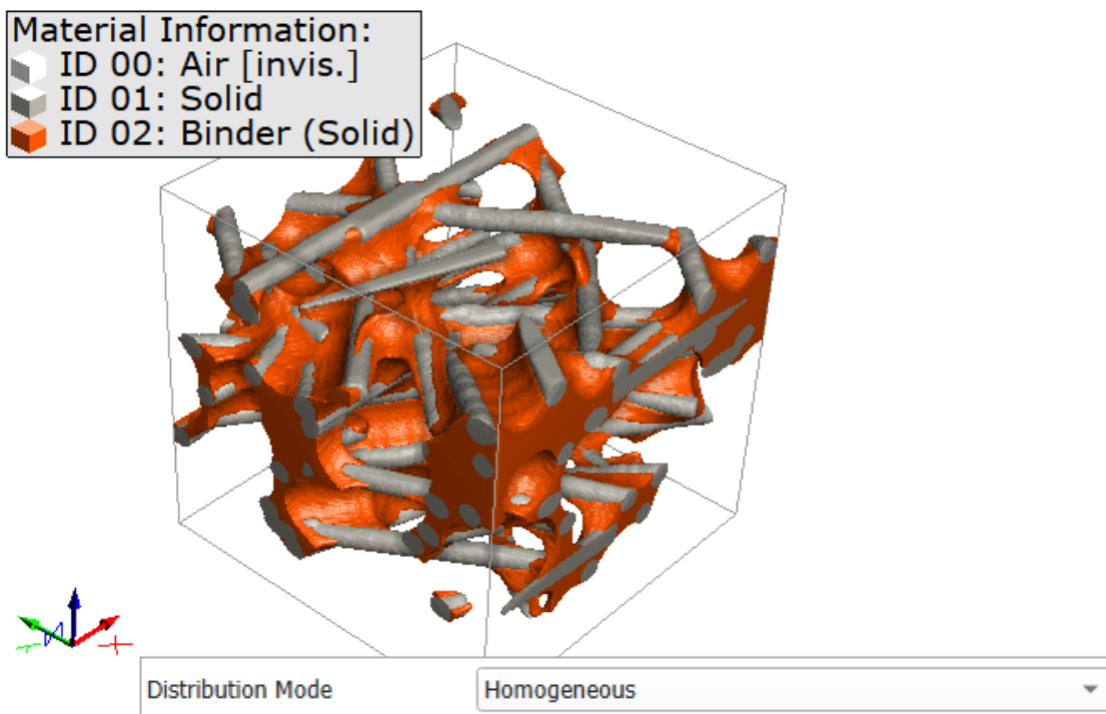
In real life, the process of adding binder to the material is affected by gravity and the viscosity of the binder, leading to inhomogeneous distributions. This effect can be modeled by defining a distribution of the binder under the **Binder Distribution** tab.

The binder either can be distributed homogeneously throughout the domain or follow a distribution in X-, Y- or Z- direction.



Homogeneous

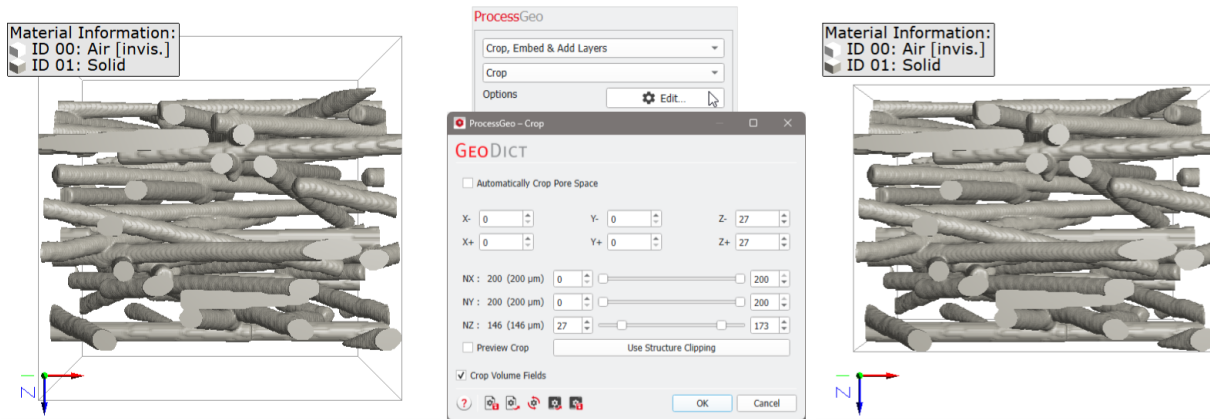
The default distribution is **Homogeneous**, but it can be changed to a **Density Distribution** to allow the modeling of inhomogeneity. For the default case, the binder is distributed homogeneously throughout the domain.



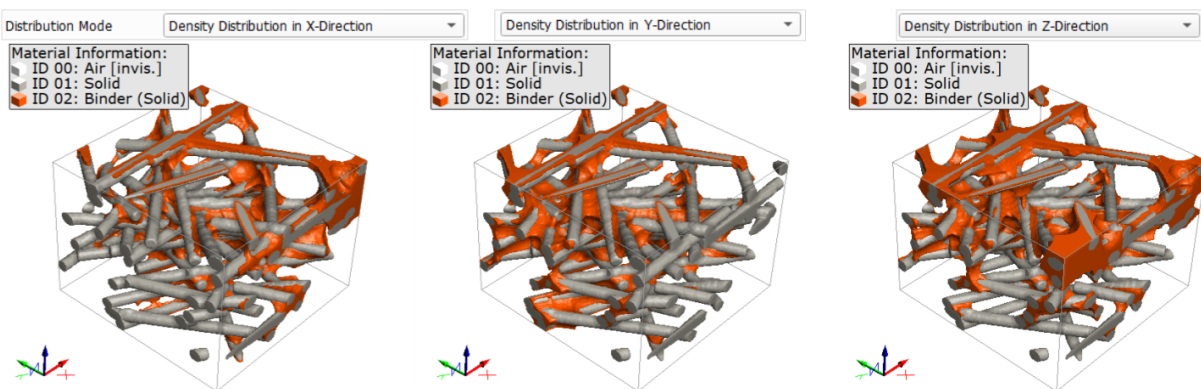
Density Distribution

To model a **Density Distribution**, no inlet or outlet should be left in the structure. If the

structure has an inlet or outlet in the chosen direction, remove it by cropping with **Model - ProcessGeo - Crop, Embed & Add Layers - Crop**. This is necessary because the algorithm strives to reach the desired binder amount for each sub-segment and will try to add binder in the empty domain. Alternatively, the amount of binder might be set to zero for these segments.



Select the direction for the desired density distribution.



In the examples we consider a density distribution in Z-direction. Then, the **Number of Rows** defines the number of Z-segments. To change the number of segments, change the **Number of Rows** to the number of segments desired.

Distribution Mode: Density Distribution in Z-Direction

Z-layer (min , max)	Relative Density
Z-layer 1 (0 , 16)	0
Z-layer 2 (16 , 32)	0.25
Z-layer 3 (32 , 48)	0.5
Z-layer 4 (48 , 64)	0.75
Z-layer 5 (64 , 81)	1
Z-layer 6 (81 , 97)	1.25
Z-layer 7 (97 , 113)	1.5
Z-layer 8 (113 , 129)	1.75
Z-layer 9 (129 , 146)	2

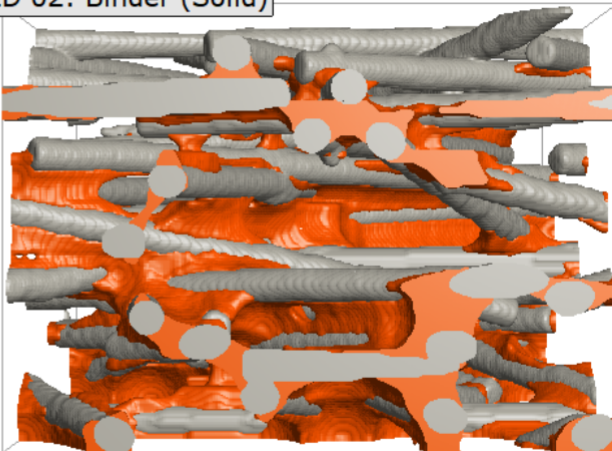
Probability Sum: Normalize

Number of Rows: 9

Load... Save...

Material Information:

- ID 00: Air [invis.]
- ID 01: Solid
- ID 02: Binder (Solid)

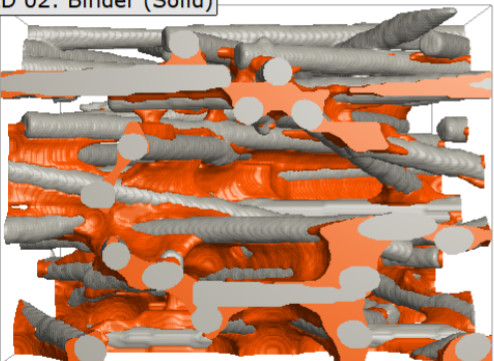


In each section the binder is generated separately according to the rules defined in the **General Options** tab. The **Added Solid Volume Percentage / (%)** is scaled with the normalized **Relative Density** given in the table of **Binder Distribution**.

Added Solid Volume Percentage / (%) 5

Material Information:

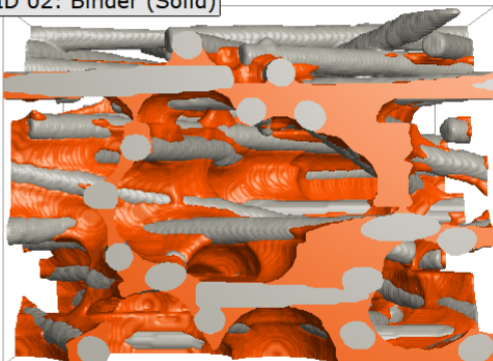
- ID 00: Air [invis.]
- ID 01: Solid
- ID 02: Binder (Solid)



Added Solid Volume Percentage / (%) 10

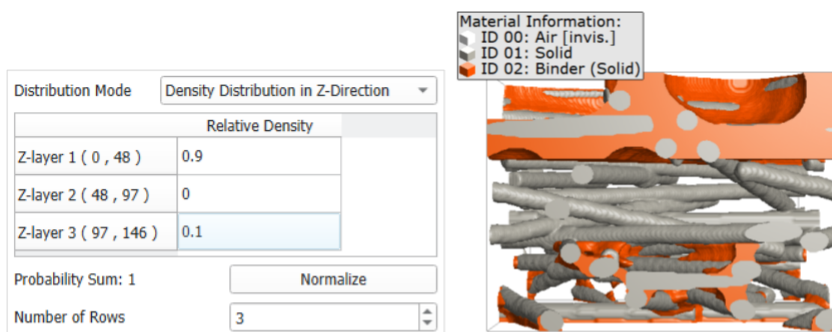
Material Information:

- ID 00: Air [invis.]
- ID 01: Solid
- ID 02: Binder (Solid)



The **Binder Distribution** can be entered in form of a ratio in the **Relative Density** table.

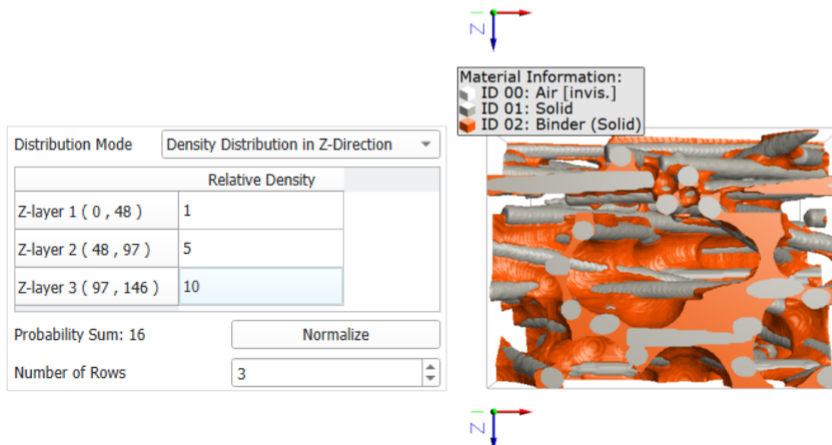
In the images below, three different segments are clearly discernible with a binder distribution according to the relative values given in the table.



90% of the binder is distributed in the Z-layers 0-48.

0% of the binder is distributed in the Z-

10 % of the binder is distributed in the Z-

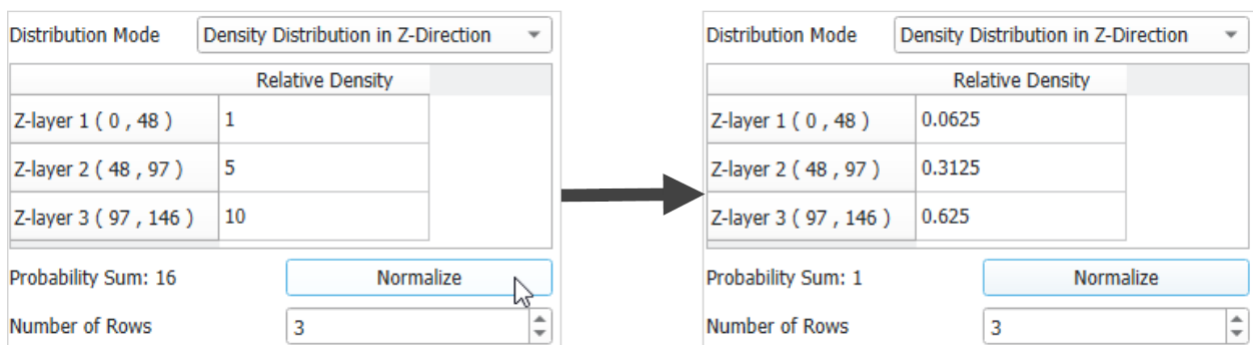


6% of the binder is distributed in the Z-layers 0-48.

31% of the binder is distributed in the Z-

63% of the binder is distributed in the Z-

Clicking the **Normalize** button ensures the Relative Density values sum up to one.

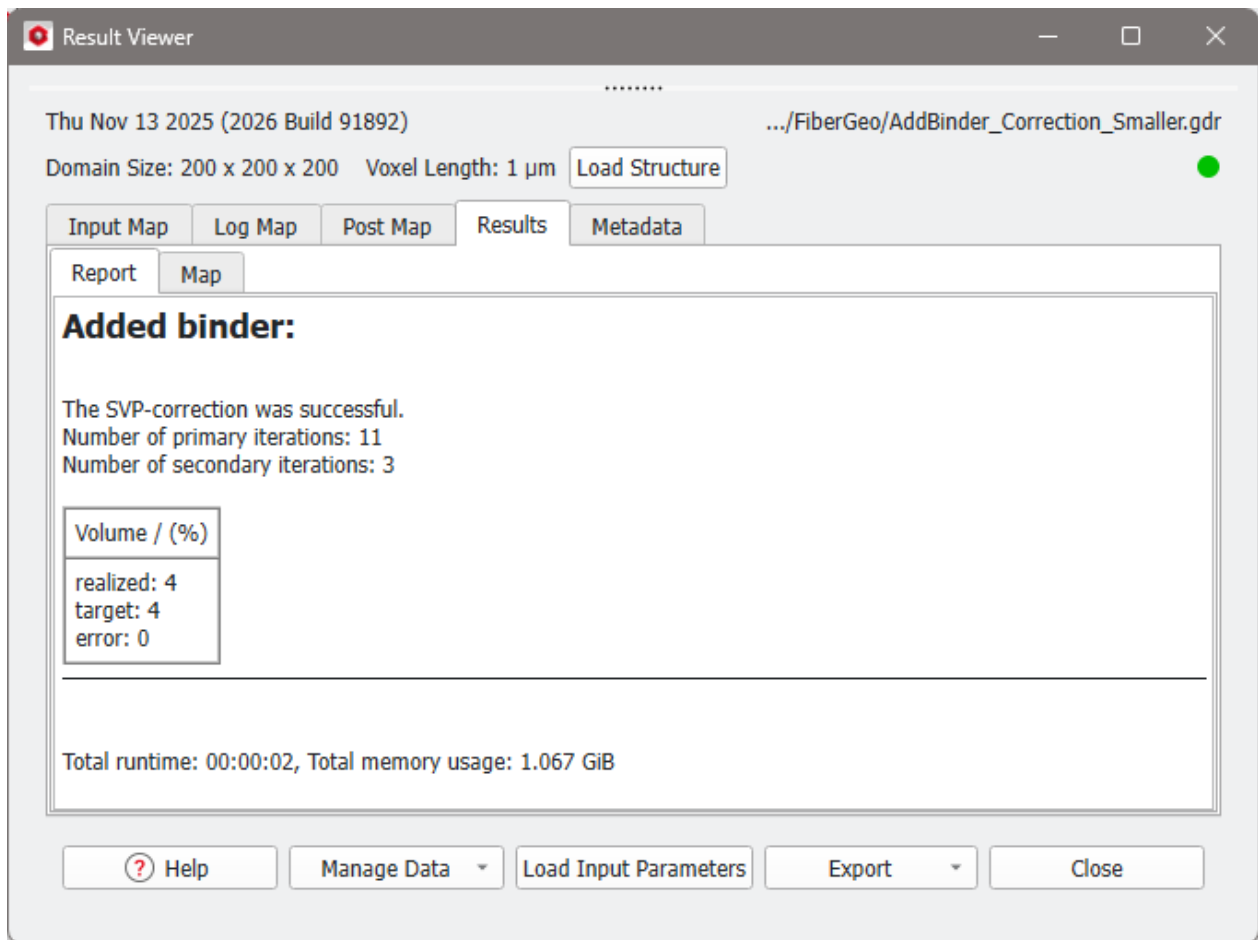


With the buttons **Load...** and **Save...** the distribution can be loaded/saved as text file which can be opened with other software as, e.g., Microsoft Excel.

1.10.2 Results

After the binder generation, the new structure with added binder is shown in the visualization area and the result file (*.gdr) is opened in the Result Viewer.

The **Results - Report** tab shows information about the binder generation, as number of iterations, target binder volume and realized binder volume.



If **Weight Percentage** or **Grammage** were selected as **Stopping Criterion**, additionally the realized and target binder weight percentage and grammage are given.

Volume / (%)	Grammage / (g/m ²)	Weight / (%)
realized: 3.46524	realized: 20	realized: 20
target: ---	target: ---	target: 20
error: ---	error: ---	error: 2.59463e-05

If a non-homogeneous binder distribution was defined, the binder volumes additionally are given for each defined layer.

Added binder:

Volume / (%)	Grammage / (g/m ²)	Weight / (%)
realized: 1.27263 target: --- error: ---	realized: 19.9999 target: --- error: ---	realized: 19.9999 target: 20 error: -5.52607e-05

Layer 1

The SVP-correction was successful.

Volume / (%)	Grammage / (g/m ²)	Weight / (%)
realized: 3.62099 target: --- error: ---	realized: 53.9998 target: --- error: ---	realized: 53.9998 target: 54 error: -0.00017705

Layer 2

No binder to add.
The SVP-correction was skipped.

Volume / (%)	Grammage / (g/m ²)	Weight / (%)
realized: 0 target: --- error: ---	realized: 0 target: --- error: ---	realized: 0 target: 0 error: 0

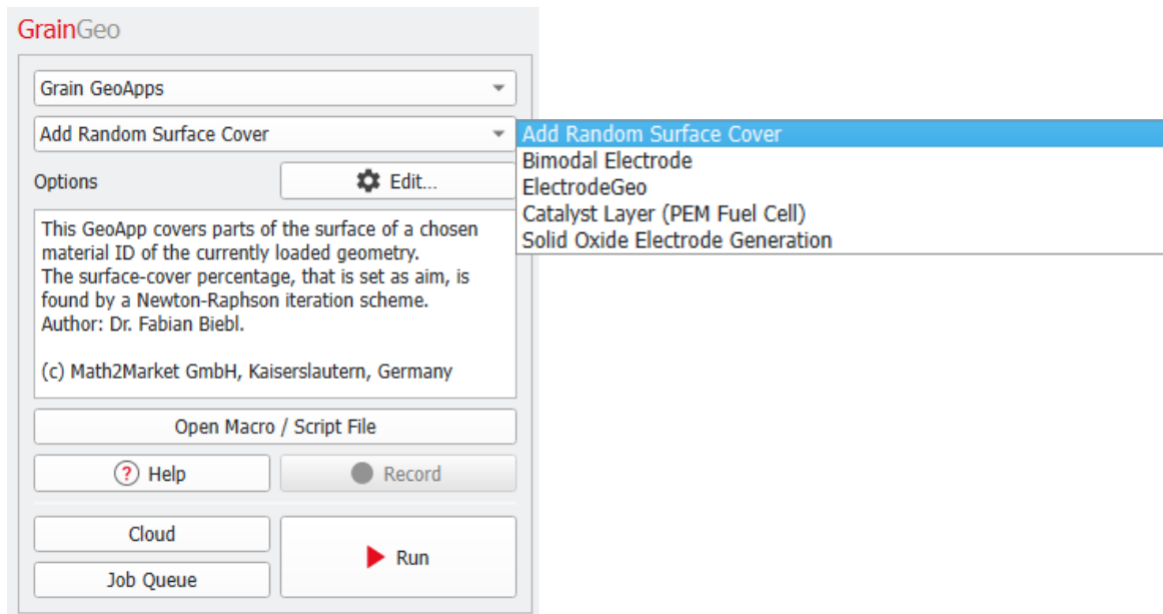
Layer 3

The SVP-correction was successful.

Volume / (%)	Grammage / (g/m ²)	Weight / (%)
realized: 0.196888 target: --- error: ---	realized: 6.00001 target: --- error: ---	realized: 6.00001 target: 6 error: 1.12676e-05

1.11 Grain GeoApps

Find a selection of **Grain GeoApps**. They are also available in different sections of the GeoApp menu. There, you can also add your own GeoApps.



The following apps are available from the GrainGeo section:

- [Add Random Surface Cover](#)^[216]
Cover the surface of the current structure randomly. Define covered surface area and layer thickness.
- [Bimodal Electrode](#)^[218]
Generates anode and cathode structures, which consist of one or two types of solid spherical, elliptical, or polyhedral particles. Define grain size distributions, solid carbon black and binder domain (CBD), and fluid electrolyte.
- [ElectrodeGeo](#)^[226]
Generates an electrode from different materials.
- [Catalyst Layer \(PEM Fuel Cell\)](#)^[228]
Create a model of the catalyst layer of a PEM fuel cell.
- [Solid Oxide Electrode Generation](#)^[230]
Generate three-phase microstructures typically observed for SOFC / SOEC electrodes, but also for all-solid-state battery electrodes.

1.11.1 Add Random Surface Cover

The **Add Random Surface Cover** GeoApp covers part of the surface of a selected material ID from the currently loaded geometry. The surface-cover percentage, that is set as aim, is found by a Newton-Raphson iteration scheme.



Modules needed to run this GeoApp:

MatDict, GrainGeo

Click **Edit** to open the **Add Random Surface Cover** parameter dialog.

Select a **Result File Name** fitting to the current project.

The random surface is created using GeoDict's [Gaussian Random Field Generator](#)^[238]. Control the **Typical Size of Surface Patches**, which changes the standard deviation of the Gaussian field. Additionally, define the **Thickness of the Cover**.

Set the **Approximate Percentage of the Cover**, which controls the surface coverage percentage. The algorithm tries to iterate until the correct surface coverage percentage is reached. The **Maximum Error for Cover Percentage** is a stopping criterion for this iteration. If the surface coverage percentage is within this error bound, the computation will be considered finished. Another stopping criterion is the **Max. Number of Iterations for Calculation**. If the number of iterations exceeds this parameter, the computation will be considered finished.

Then define all materials involved in the computation. The **Material ID to Cover** defines the material ID that should be covered. The added surface cover will have the set **Material ID of Surface Cover**. The **Material ID to Reassign** is the material that the algorithm uses as space for the surface coverage. This is typically the pore space ID 00.

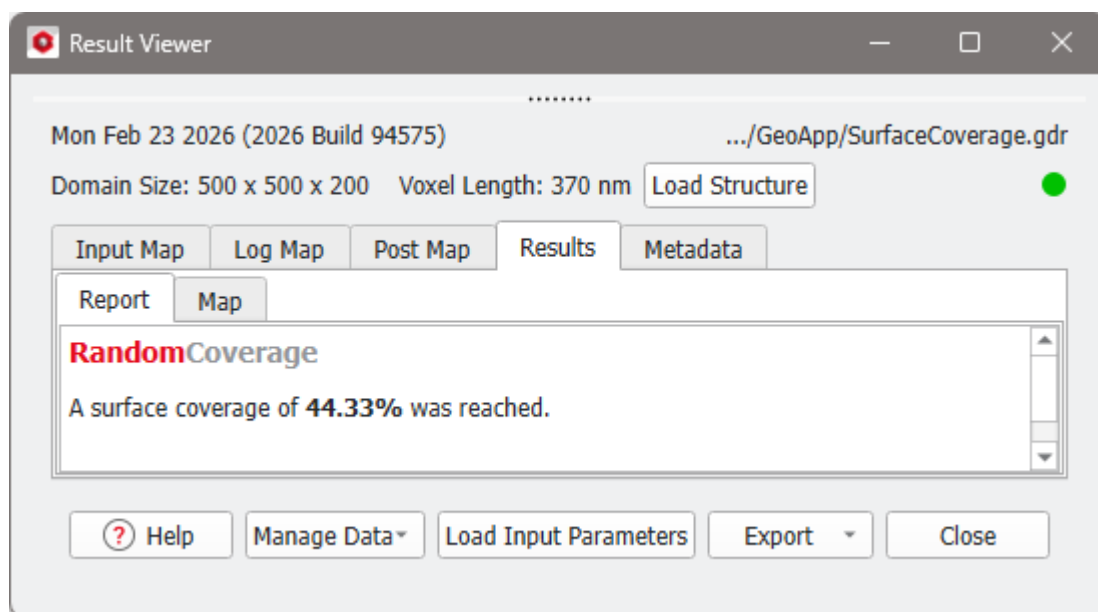
The **Random Seed** for the Gaussian Random Field Generator can affect how the surface cover looks like and how it is positioned.

Parameter	Value
Result File Name (*.gdr)	SurfaceCoverage
Typical Size of Surface Patches / (m)	2e-06
Thickness of the Cover / (m)	1e-06
Approximate Percentage of the Cover / (%)	45
Maximum Error for Cover Percentage / (%)	1
Maximum Number of Iterations for Calculation	1000
Material ID to Cover	1
Material ID of Surface Cover	4
Material ID to Reassign	0
Random Seed (Affects Cover Position)	42

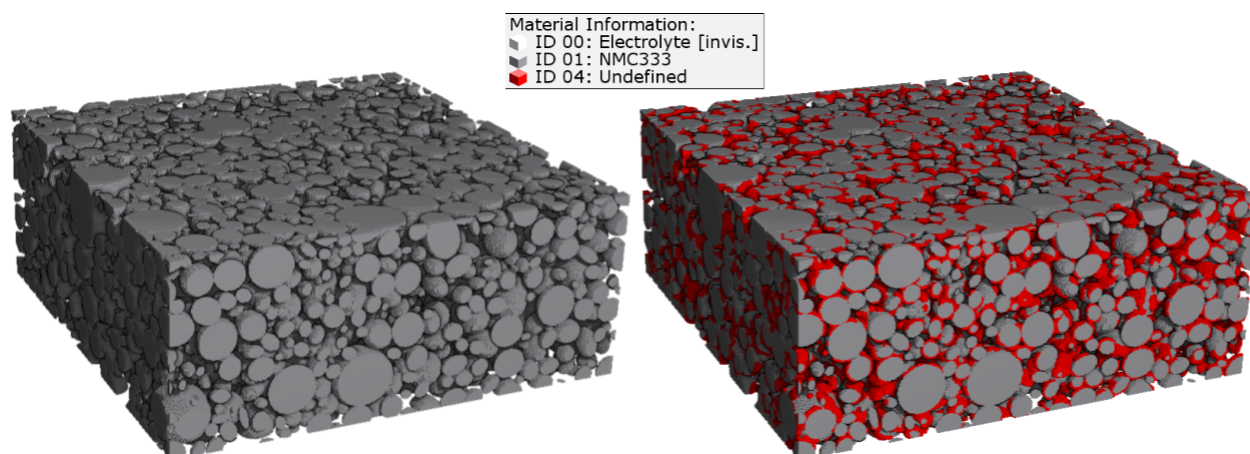
After defining all parameters click **OK** to close the dialog, go back to the GeoApp section, and click **Run**.

Results

After the **Add Random Surface Cover** app finishes the result file is loaded in the **Result Viewer**. In the result file the reached surface coverage is stated. Below you see the exemplary result for creating a surface cover on a cathode structure using the settings shown above. Here, the target for the surface coverage percentage was 45%.



The resulting covered structure is loaded in the visualization area. This structure as well as the result of the Gaussian Random Field is saved to the result folder.



1.11.2 Bimodal Electrode

The **Bimodal Anode** app generates a battery electrode structure, which consists of up to two types of solid spherical, elliptical, or polyhedron particles, solid carbon black and binder domain (CBD) and fluid electrolyte – the constituent materials can be selected from the

material database. The recipe of the electrode considers the grain size distribution of the particles, the ratio between particle types, binder mass percentage and target porosity or target areal loading (mAh/cm²) of the electrode.



Modules needed to run this GeoApp:

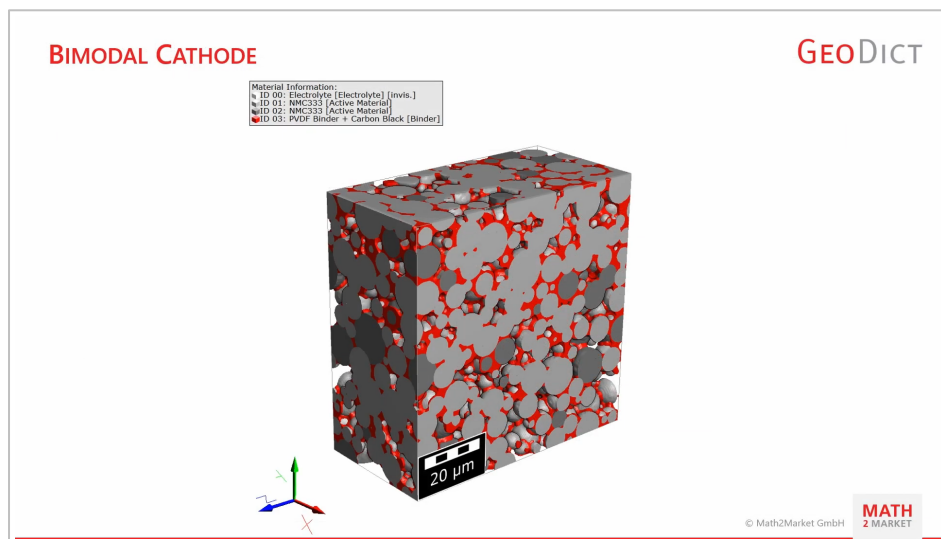
GrainGeo

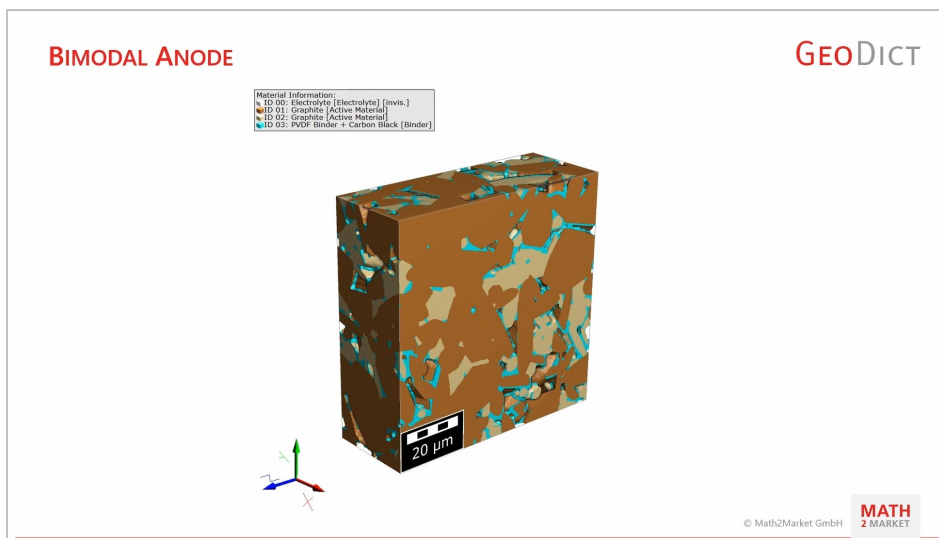


Note! Also have a look at our [website](#) for more information.

Video Tutorial: Creating a Digital Bimodal Cathode and Anode for GeoDict 2023

Since GeoDict 2026, the two GeoApps Bimodal Anode and Bimodal Cathode were merged into one app: Bimodal Electrode. Other than that, the parameters are the same in GeoDict 2023.

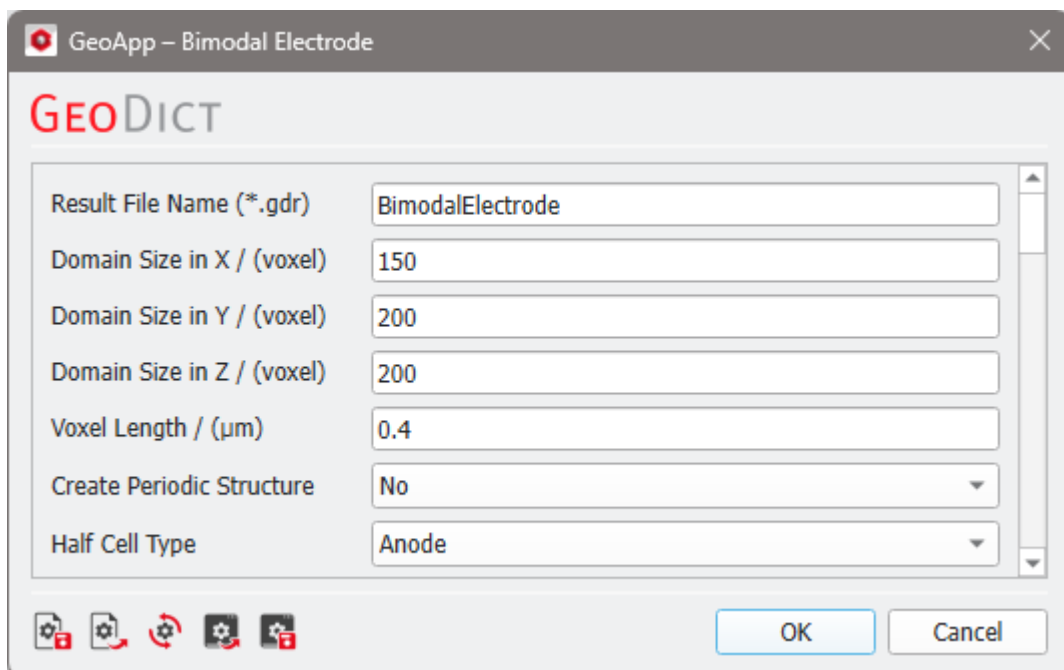




Parameters

Clicking **Edit** opens the **Bimodal Electrode Parameters** dialog. Clicking **Run** creates the electrode.

Enter a **Result File Name** for the bimodal electrode.



The electrode parameters are organized into groups described in the following. The **Particle Type** parameters depend on the selected **Half Cell Type**. For anodes ellipsoidal or polyhedral particle shapes are used, while the cathode always consists of spherical particles.

✓ Domain

Set the **Domain Size** in voxels for the **X**-, **Y**-, and **Z**-direction and enter a **Voxel Length**.

Result File Name (*.gdr)	BimodalElectrode
Domain Size in X / (voxel)	150
Domain Size in Y / (voxel)	200
Domain Size in Z / (voxel)	200
Voxel Length / (μm)	0.4
Create Periodic Structure	No
Half Cell Type	Cathode

The structures periodicity can be adjusted in each of the three directions by choosing **Yes** for **Create Periodic Structure**.

Create Periodic Structure	Yes
☐ X-Direction ☒ Y-Direction ☒ Z-Direction	

For **Half Cell Type**, select to create a **Cathode** or an **Anode**. The two types differ in the particle shape and the default materials.

✓ Particle Type 1

Select the **Material** for the active material for particle type 1.

Define the diameter distribution with D-values.

For anodes D-values are specified separately for shortest, intermediate, and longest axis of particles: **D10**, **D50**, **D90**, and fitted to Log-Normal distribution.

For cathodes the D-values **D10**, **D50**, **D90**, **Lower Bound**, and **Upper Bound** describe the spheres' diameters, and are fitted to Log-Normal distribution.

The **Lower** and **Upper Bounds** are also fitted to Log-Normal distribution but assigned once for all diameters within one particle type. They can be set as D1- and D99-values of corresponding measurements.

Half Cell Type: **Anode**

Particle Type 1 (Anode)

Material: **Graphite (Solid)...**

D10 of the Shortest Diameter / (μm): **6**

D10 of the Intermediate Diameter / (μm): **10**

D10 of the Longest Diameter / (μm): **15**

D50 of the Shortest Diameter / (μm): **11**

D50 of the Intermediate Diameter / (μm): **16**

D50 of the Longest Diameter / (μm): **23**

D90 of the Shortest Diameter / (μm): **18**

D90 of the Intermediate Diameter / (μm): **27**

D90 of the Longest Diameter / (μm): **42**

Lower Bound / (μm): **2**

Upper Bound / (μm): **56**

Half Cell Type: **Cathode**

Particle Type 1 (Cathode)

Material: **NMC333 (Solid)...**

D10 / (μm): **3**

D50 / (μm): **6**

D90 / (μm): **10**

Lower Bound / (μm): **2**

Upper Bound / (μm): **12**

✓ Add Particle Type 2

With **Add Particle Type 2**, a second active material can be added to the structure.

If **No** is used (default), an electrode structure with one active material type is created.

If **Yes** is selected, the macro enables creating a bimodal structure, where **Ratio of Particle Type 2** is defined in m% (mass percentage), and grain size distribution can be predefined using their own D-values.

Add Particle Type 2 (Anode): **Yes**

Ratio of Particle Type 2 / (m%): **20**

Material: **Graphite (Solid)...**

D10 of the Shortest Diameter / (μm): **4**

D10 of the Intermediate Diameter / (μm): **5**

D10 of the Longest Diameter / (μm): **8**

D50 of the Shortest Diameter / (μm): **5**

D50 of the Intermediate Diameter / (μm): **8**

D50 of the Longest Diameter / (μm): **12**

D90 of the Shortest Diameter / (μm): **9**

D90 of the Intermediate Diameter / (μm): **14**

D90 of the Longest Diameter / (μm): **20**

Lower Bound / (μm): **1**

Upper Bound / (μm): **41**

Add Particle Type 2: **Yes**

Ratio of Particle Type 2 / (m%): **20**

Material: **NMC333 (Solid)...**

D10 / (μm): **5**

D50 / (μm): **9**

D90 / (μm): **12**

Lower Bound / (μm): **3**

Upper Bound / (μm): **15**

✓ Structure

For anodes, all particles in the structure can be generated either with **Ellipsoids** or with **Polyhedrons** based on ellipsoids.

The **Orientation** of particles is specified by the main diagonal tensor orientation in the global coordinate system XYZ. Corresponding values of **Orientation Tensor XX, YY** or **ZZ** are set as the probabilities for the orientations in the three axial directions. The sum of all three tensor components should always be 1. For more information on

orientation tensors, refer to [GrainGeo - Orientation](#)⁶⁵.

For cathodes, the particles always have spherical shape and thus, no particle shape or orientation can be selected.

Structure (Anode)	Structure (Cathode)
Select Particle Shape: Polyhedron	Select Material for Electrolyte: Electrolyte...
Orientation Tensor XX: 0.2	Select Material for CBD: PVDF Binder + Carbon Black (Solid)...
Orientation Tensor YY: 0.4	CBD Mass Percentage / (m%): 10
Orientation Tensor ZZ: 0.4	
Select Material for Electrolyte: Electrolyte...	
Select Material for CBD: PVDF Binder + Carbon Black (Solid)...	
CBD Mass Percentage / (m%): 10	

Additionally for both electrode types, **Select Materials for Electrolyte** and **CBD** and define the **CBD Mass Percentage** in m%.

✓ Criteria to Match

Choose the Criterion to Match. The default criterion **Porosity** allows to define the desired porosity of the electrode.

As an alternative, **Loading** allows to define the desired areal loading of the electrode in mAh/cm².

In both cases, structure generation is repeated within **Maximum Number of Tries** until the desired porosity or areal loading is reached within a given **Tolerance** in %. If the target porosity or loading was not reached, GeoDict saves and displays the result of the last generation try.

Choose the Criterion to Match: Porosity	Choose the Criterion to Match: Loading
Porosity of the Electrode / (%): 30	Loading of the Electrode / (mAh/cm ²): 2.8
Tolerance / (%): 3	Tolerance / (%): 3
Maximum Number of Tries: 2	Maximum Number of Tries: 2

Enter **Value of Random Seed**: By default, the seed for generating the structure will be randomly chosen. If you choose **Yes**, you can enter a random seed manually. Entering the same **Random Seed** will result in an identical structure.

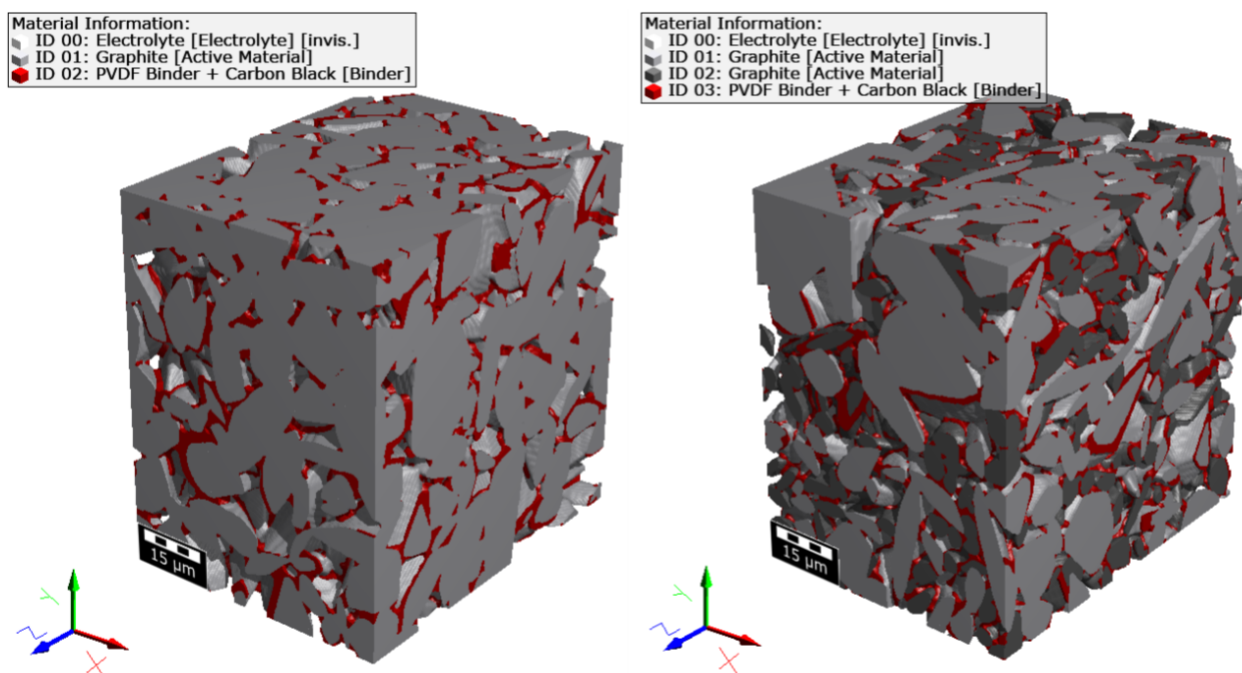
Enter the Value of Random Seed	Yes
Random Seed	247163

The parameters which **Specify Generation Stopping Criteria** for the particles creation are **Target Particle Overlap**, **Iterations**, and **Maximum Generation Time**. They are active by default and can be changed if needed.

Specify Generation Stopping Criteria		Yes
Target Particle Overlap / (%)	1	
Iterations	100	
Maximum Generation Time / (hours)	6	

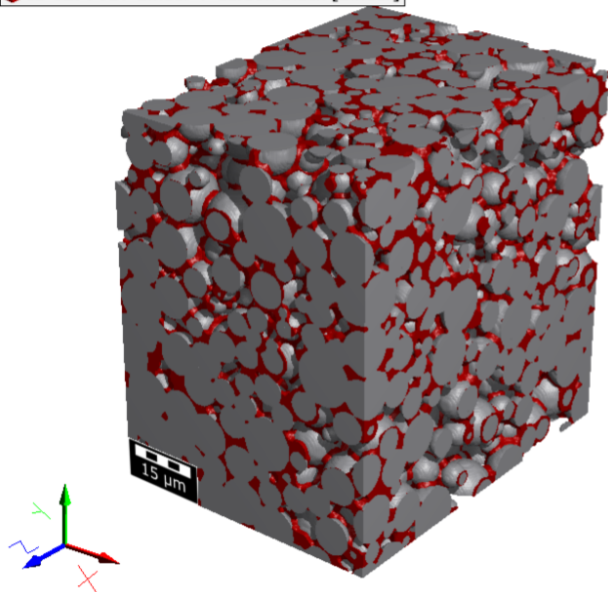
Results

In the figure below, on the left, a monomodal battery anode is shown and on the right, a bimodal battery anode is shown. Both are generated with the respective default settings. Of course, the half cell type must be set to anode and for the bimodal anode, the second particle type was enabled. For comparability, the random seed was enabled and set to 21.

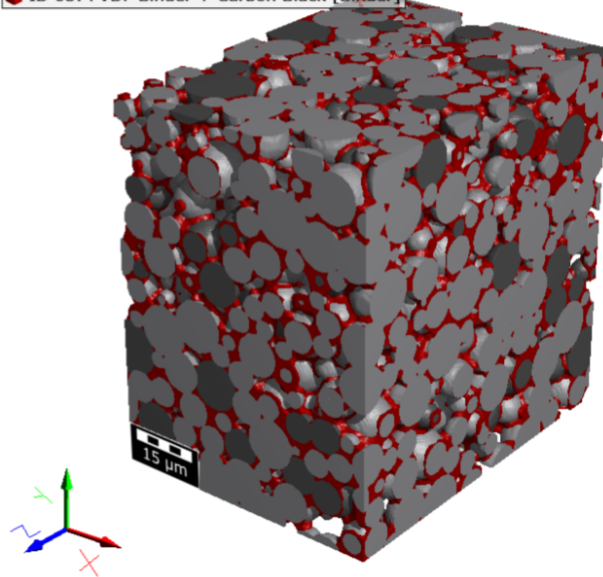


In the figure below, on the left, a monomodal battery cathode is shown and on the right, a bimodal battery cathode is shown. Both are generated with the respective default settings. Of course, the half cell type must be set to cathode and for the bimodal cathode, the second particle type was enabled. For comparability, the random seed was enabled and set to 20.

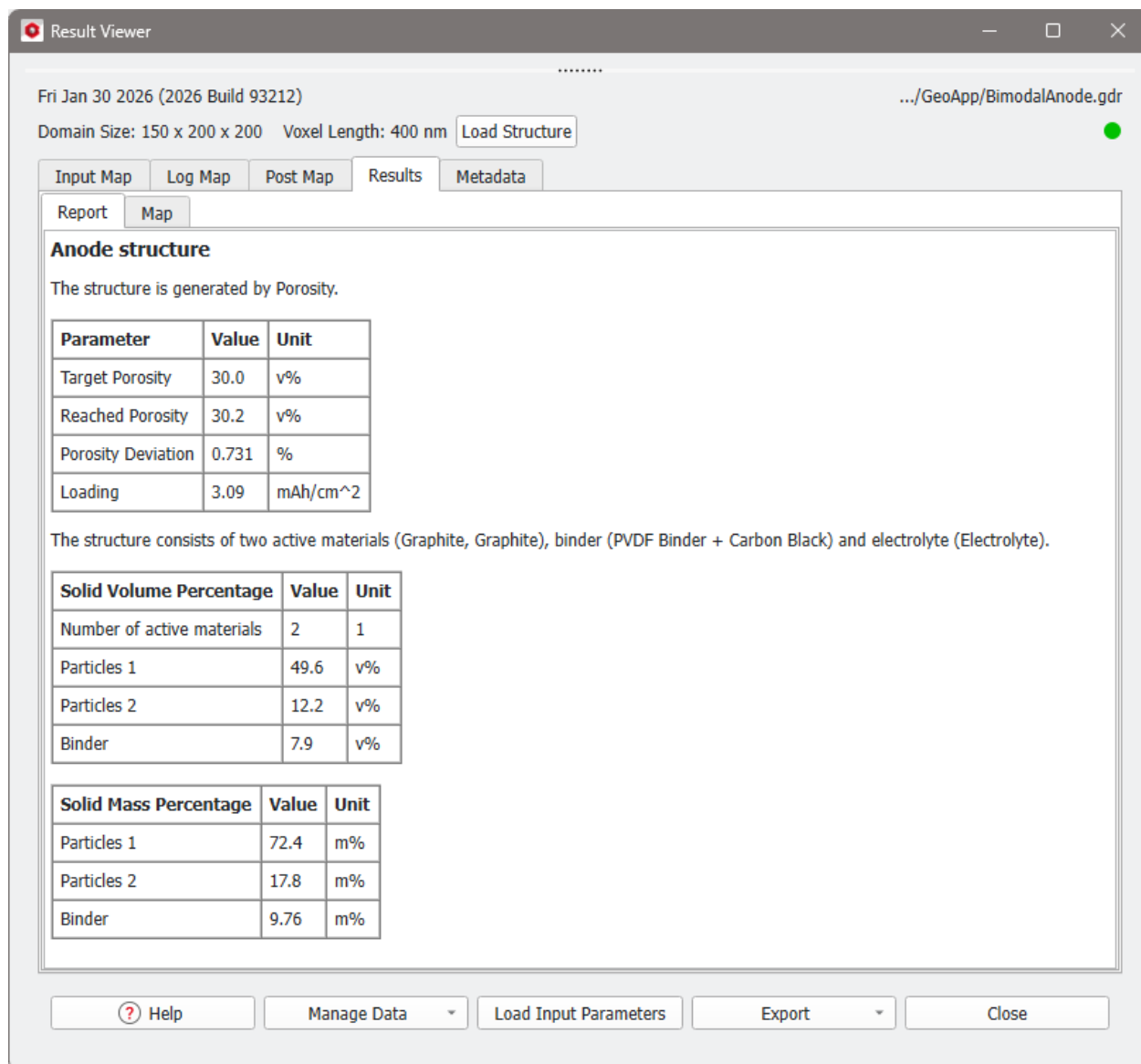
Material Information:
ID 00: Electrolyte [Electrolyte] [Invis.]
ID 01: NMC333 [Active Material]
ID 02: PVDF Binder + Carbon Black [Binder]



Material Information:
ID 00: Electrolyte [Electrolyte] [Invis.]
ID 01: NMC333 [Active Material]
ID 02: NMC333 [Active Material]
ID 03: PVDF Binder + Carbon Black [Binder]



The result file is opened in the **Result Viewer** when the generation is finished, and the Report tab provides information about the structure generation.



1.11.3 ElectrodeGeo

The **ElectrodeGeo** app generates an anode according to the given materials and solid volume percentages.

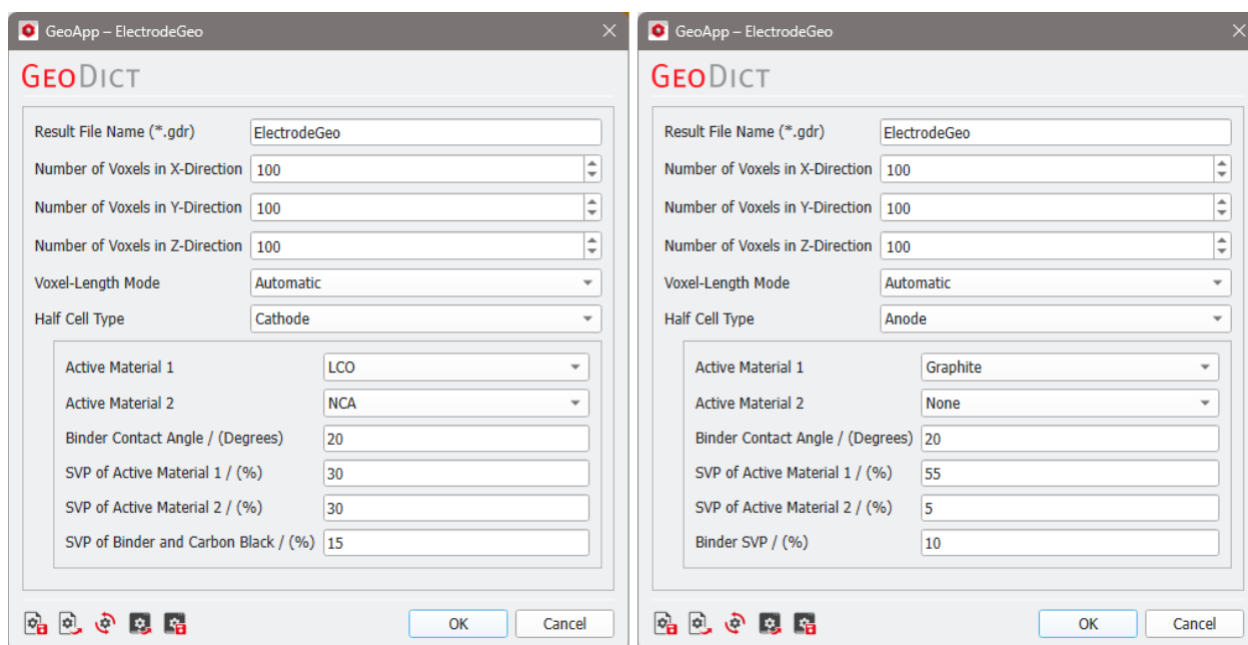


Modules needed to run this GeoApp:

GrainGeo

Parameters

Clicking **Edit** opens the **ElectrodeGeo** Parameters dialog.



Enter a **Result File Name** for the resulting GeoDict result file (*.gdr) and the result folder containing the generated electrode structure.

Two active materials can be set. If only one active material is needed, set the **Active Material 2** to **None**.

For the anode active materials select between **Graphite**, **Si**, and **LTO**. For the cathode active materials choose from the materials **LCO**, **LMO**, **NCA**, and **NMC**.

Define the volume dimensions as **Number of Voxels** in the three directions.

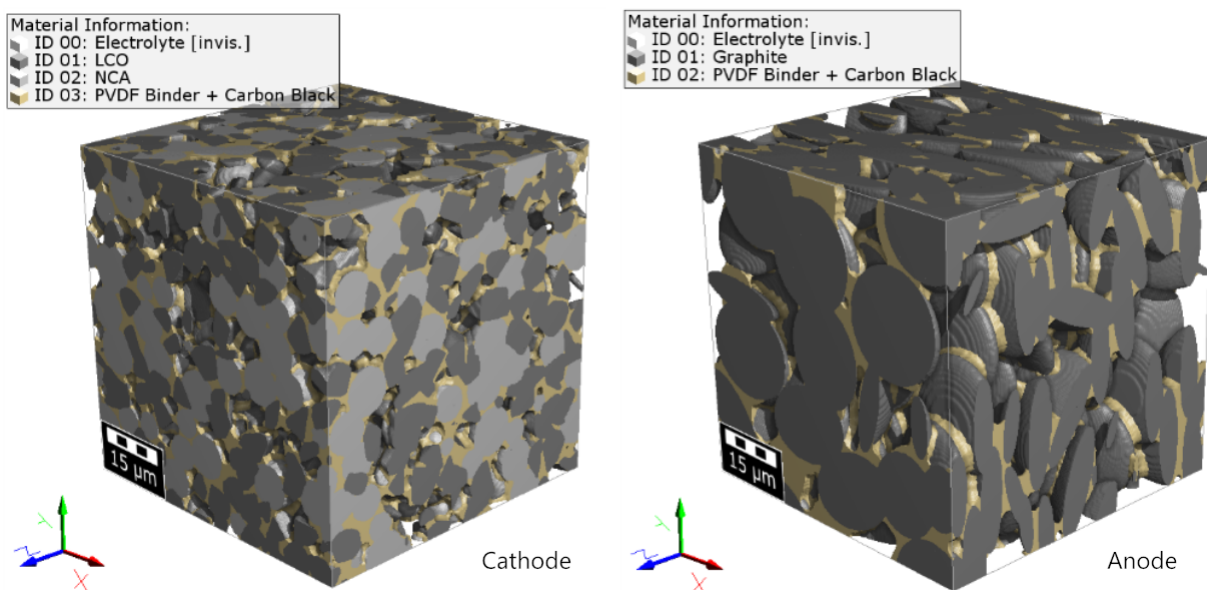
Determine the solid volume percentages (**SVP**) for the active materials and the binder.

The voxel length can either be given manually or it can be set to automatically fitting the other parameters. For this, choose the corresponding **Voxel-Length Mode**. Two active materials can be set. If only one active material is needed, set the **Active Material 2** to **None**.

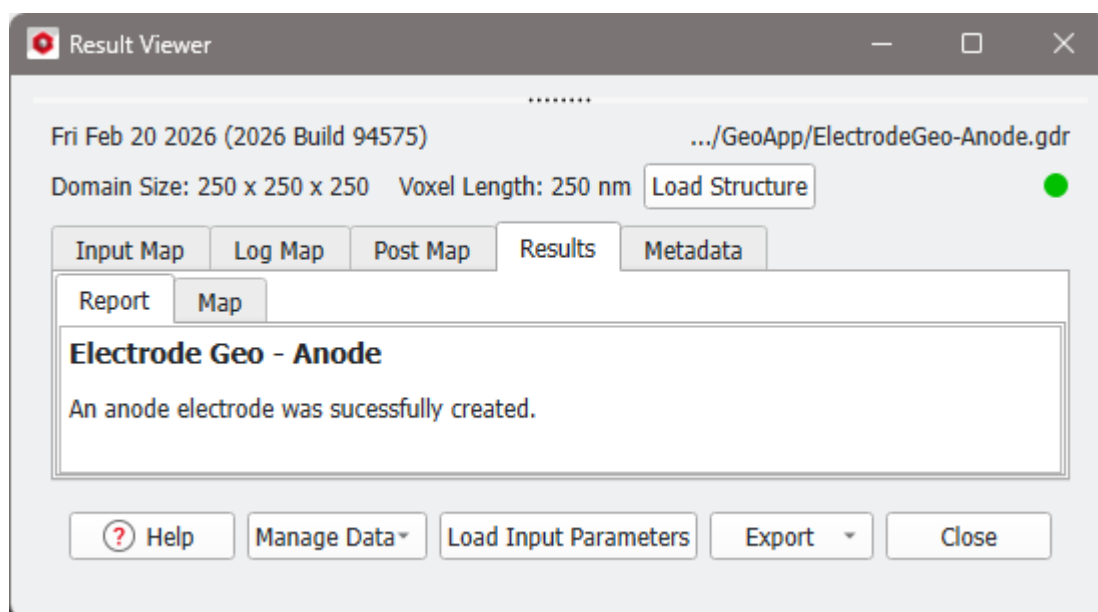
Results

Clicking **Run** creates the electrode.

Below find the default electrodes generated with the default settings, except for a larger domain size (250x250x250 voxel).



When the structure generation is finished, the result file is shown in the **Result Viewer** and the structure is saved to the result folder.



1.11.4 Catalyst Layer (PEM Fuel Cell)

The **Catalyst Layer (PEM Fuel Cell)** app creates a model of the catalyst layer of a PEM fuel cell.



Modules needed to run this GeoApp:

GrainGeo

Parameters

Clicking **Edit** opens the **Catalyst Layer (PEM Fuel Cell) Parameters** dialog.

GeoApp – Catalyst Layer (PEM Fuel Cell)

GEO DICT

Result File Name (*.gdr)

Dimensions

Voxel Length / (nm)

NX / (voxel)

NY / (voxel)

NZ / (voxel)

Material - Particles

Particle Name

Solid Volume Percentage / (%)

Material - Ionomer

Ionomer Name

Solid Volume Percentage / (%)

Random Seed

Enter a **Result File Name** for the generated result file (*.gdr) and the corresponding result folder.

Then, set the **Voxel Length** in nm and the domain size in Voxel in the three directions using the parameters **NX**, **NY**, and **NZ**.

Finally, set the parameters for the **Particles** and **Ionomer Materials** by defining the **Name** and their **Solid Volume Percentage**.

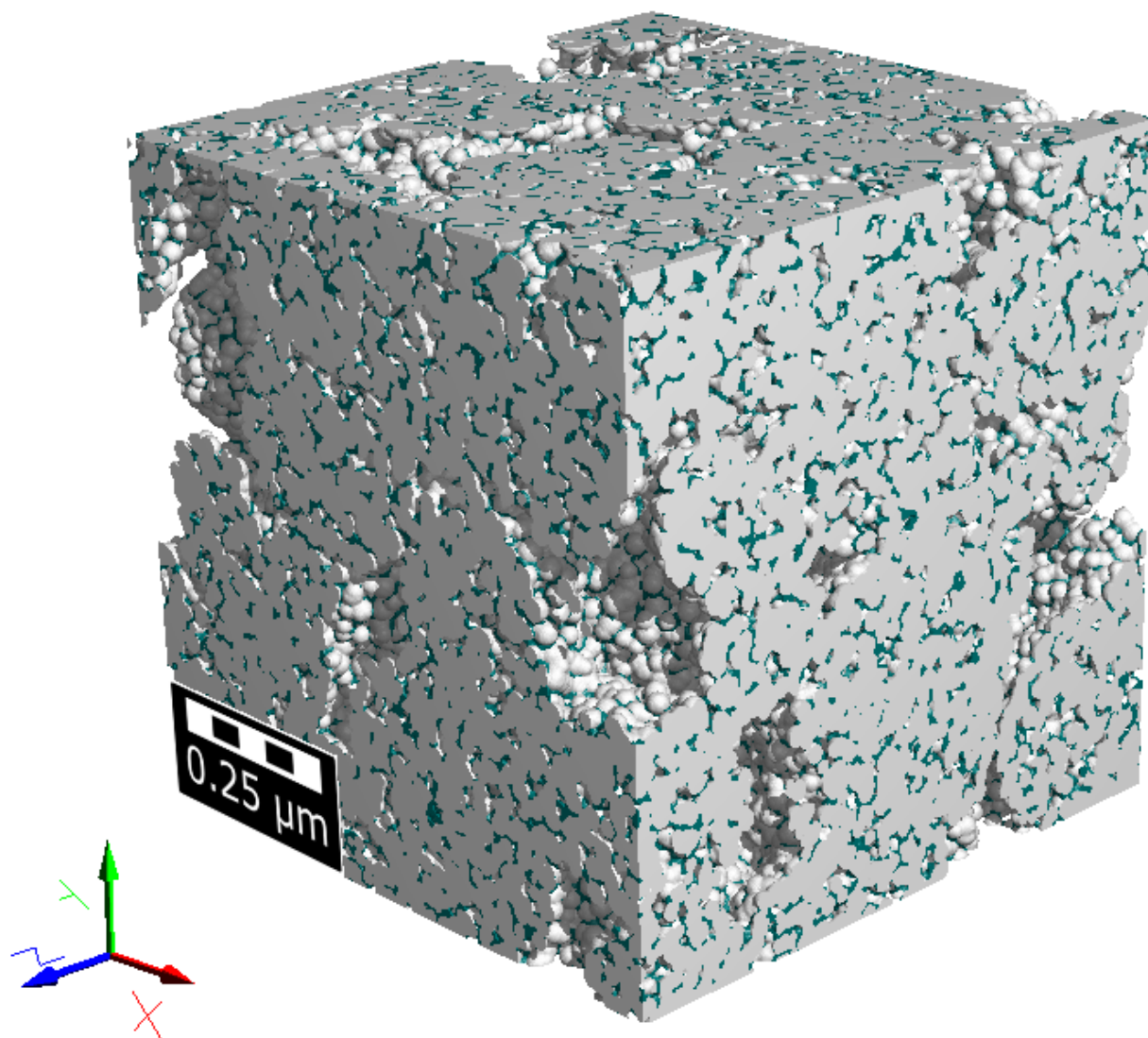
For both materials you can change the material information by editing the **Particle Name** and **Ionomer Name**. The materials will both be set to manual but through the material information they still get individual names.

Choose a different **Random Seed**, to generate a different structure but with the same statistical properties.

Results

Clicking **Run** creates the catalyst layer and saves the structure file in the result folder..

Material Information:	
	ID 00: Air [invis.]
	ID 01: Carbon Particles (Solid)
	ID 02: Ionomer (Solid)



1.11.5 Solid Oxide Electrode Generation

The **Solid Oxide Electrode Generation** app uses stochastic geometric modeling to generate three-phase microstructures (2 solids and 1 pore phase) typically observed for SOFC / SOEC electrodes. Of course you can use this GeoApp also for other structures with similar geometric properties, for example for a solid state electrode.

The app generates two independent Gaussian random fields (GRF) to facilitate a bi-gaussian or exponential random field. Find more information about Gaussian Random fields in [GrainGeo - Generate Gaussian Random Fields](#)^[238]. This two-dimensional field is thresholded into three phases according to the specified volume fractions (under [Random Field 1 and 2](#)^[233]) and contact angles (under [Change Expert Settings](#)^[233]), where the latter determine the wetting

behavior of the phases. The approach is based on work of Marmet et al., 2023.



Modules needed to run this GeoApp:

FiberGeo or GrainGeo

Parameters

Click **Edit** to open the **Solid Oxide Electrode Generation Parameters** dialog.

Enter a **Result File Name** for the generated result file (*.gdr) and the corresponding result folder.

The parameters are organized in groups.

GeoApp – Solid Oxide Electrode Generation

GEODICT

Result File Name (*.gdr)

Dimensions

Voxel Length / (m)

NX

NY

NZ

Random Field 1

Material

Correlation Function

Solid Volume Fraction / (%)

Standard Deviation / (voxel)

Random Seed

Random Field 2

Material

Correlation Function

Solid Volume Fraction / (%)

Standard Deviation / (voxel)

Random Seed

Solid Volume Fraction Tolerance / (%)

☐ Change Expert Settings

OK Cancel

✓ Dimensions

Define the domain sizes for the structure to generate. These are also applied to the two GRFs. The domain size is given by the number of voxels in X-, Y-, and Z-direction (**NX**, **NY**, and **NZ**) and the **Voxel Length** in **m**.

Dimensions

Voxel Length / (m)

2e-08

NX

200

NY

200

NZ

200

✓ Random Field 1 and 2

The structure contains two materials. For both define the following parameters.

Click on the **Material** boxes to select a material from the GeoDict material database.

Choose if the **Correlation Function** that defines the random field should be **Gauss** or **Exponential**. Find examples for Gauss and Exponential fields in the [GrainGeo](#)^[244] User Guide.

The two random fields represent two solid phases. Each phase has its own **Solid Volume Fraction** (SVF) for the resulting structure. Note that the sum of the two solid phases must be less than 100%. The remaining percentage (100 - SVF1 - SVF2) specifies the porosity of the electrode structure.

The **Standard Deviation** for the correlation functions can be defined. Higher values lead to larger pores.

Changing the **Random Seed** creates a different random field but with the same statistical properties.

The mean value for the random fields is always set to 0.

Random Field 1

Material

8YSZ (Solid)...

Correlation Function

Gauss

Solid Volume Fraction / (%)

37.5

Standard Deviation / (voxel)

10

Random Seed

1

Random Field 2

Material

Nickel (Solid)...

Correlation Function

Gauss

Solid Volume Fraction / (%)

37.5

Standard Deviation / (voxel)

10

Random Seed

10

✓ Solid Volume Fraction Tolerance

The **Solid Volume Fraction Tolerance** specifies how close the generation process approximates the target values given for [Solid Volume Fraction](#)^[233].

✓ Change Expert Settings

Check **Change Expert Settings** to edit additional settings.

Adopt Phase Interface smoothing: applies a Gaussian filter to the previously generated or loaded GRFs. This way, the phase boundaries created by thresholding are smoothed. If this option is not checked, the **Filter Factors** are set to 0%.

☒ **Adopt Phase Interface smoothing**

Filter Factor for GRF1 / (%)

Filter Factor for GRF2 / (%)

Change Threshold Angle Parameters: The thresholding angles between the three resulting phases can be set. Their setting differentiates the two solid phases between wetting and non-wetting behavior. The values are optional and have commonly used defaults (neutral wetting behavior). See Marmet et al., 2023 for further details. If not checked, the default values are used.

☒ **Change Threshold Angle Parameters**

Threshold Angle Alpha / (°)

Threshold Angle Beta / (°)

Threshold Angle Gamma / (°)

Smoothing of the final Result: To dilute the boundary between two phases, a smoothing based on voxels is applied. Dilation is used to coat neighboring voxels from another material. Doing this vice-versa between two phases, the boundary is smoothed. For this purpose, the dilation between two of the three phases can be stated. Note that at least one pair of phases needs to have a dilation radius >0 for any smoothing to commence.

☒ **Smoothing the final Result**

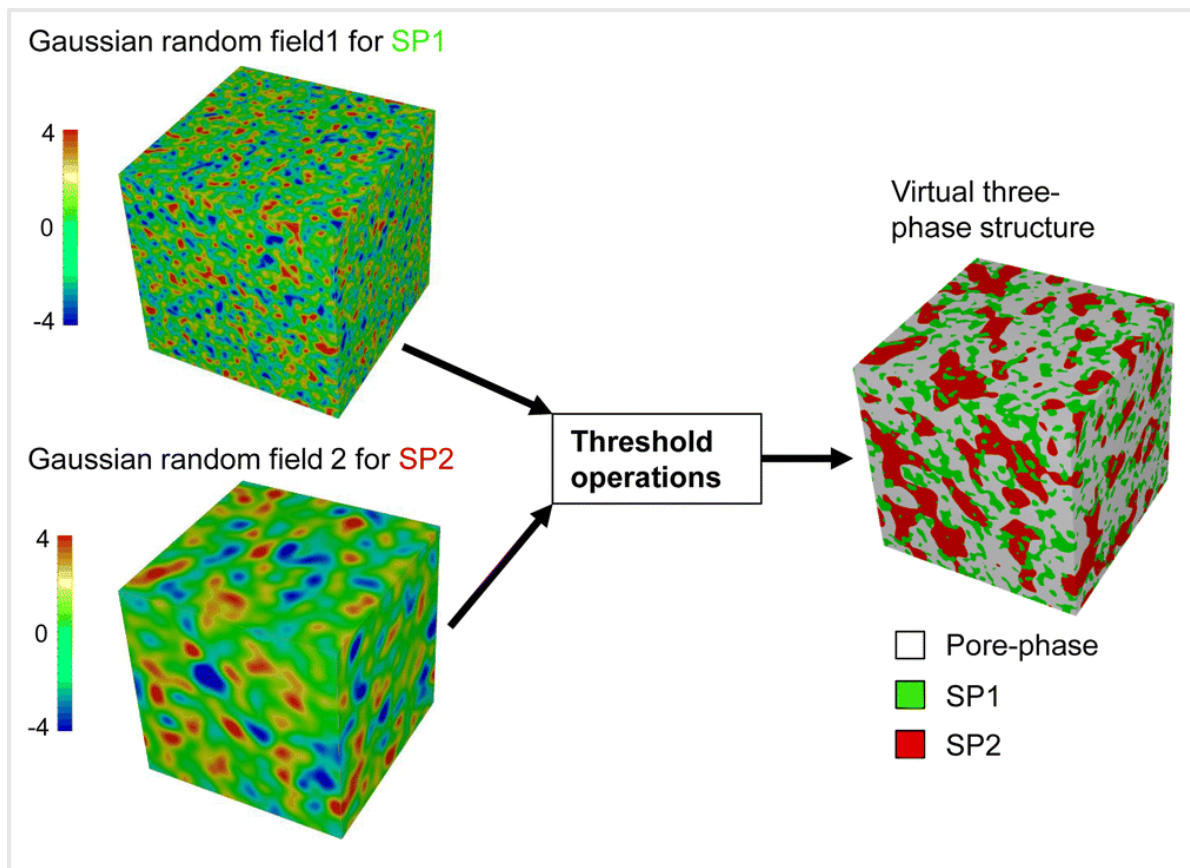
Dilation Radius between Pore and GRF 1 / (voxel)

Dilation Radius between Pore and GRF 2 / (voxel)

Dilation Radius between GRF 1 and GRF 2 / (voxel)

✓ Algorithm

The figure below (see also Marmet et al., 2023, Figure 3) illustrates the virtual structure generation with pluri-Gaussian random fields. Two GRFs are combined with threshold operations to achieve three phases with defined phase volume fractions and wetting behavior.



Results

Clicking **Run** starts the solid oxide electrode generation.

When the structure generation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically.

The **Results - Report** tab displays a report about the resulting structure.

Result Viewer

Fri Feb 20 2026 (2026 Build 94575) .../GeoApp/SolidOxideElectrode.gdr

Domain Size: 200 x 200 x 200 Voxel Length: 20 nm

Input Map Log Map Results

Report Map

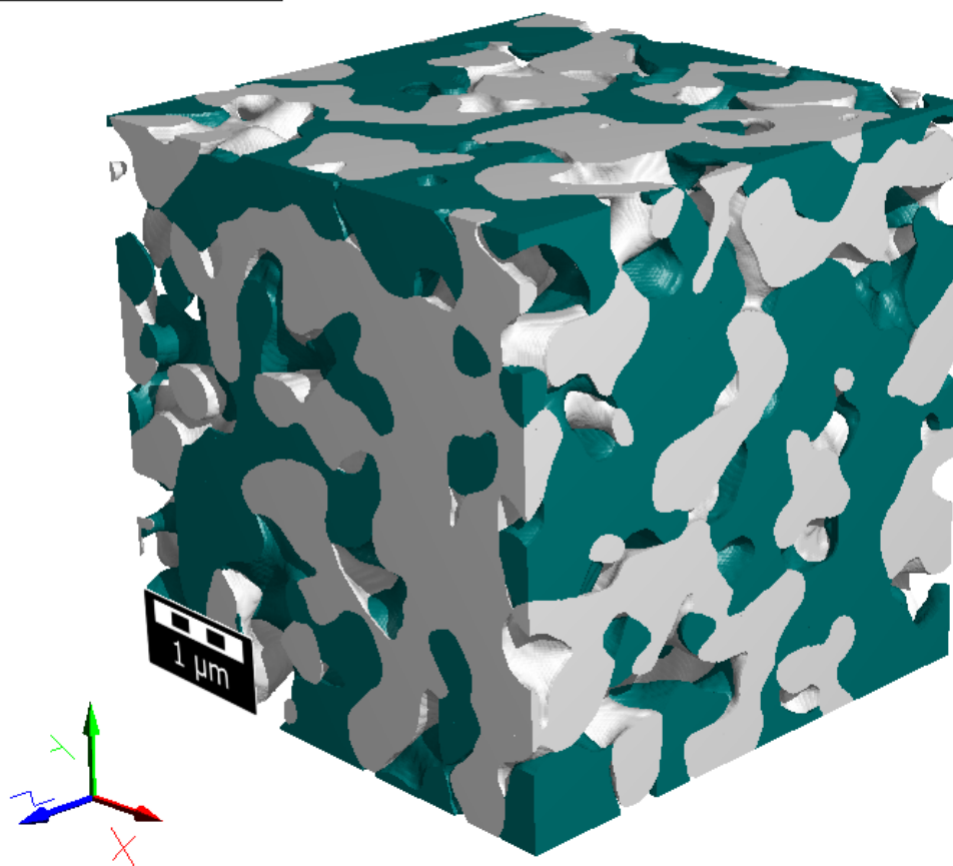
Solid Oxide Electrode

Successfully created a solid oxide electrode structure with the parameters given in the table below:

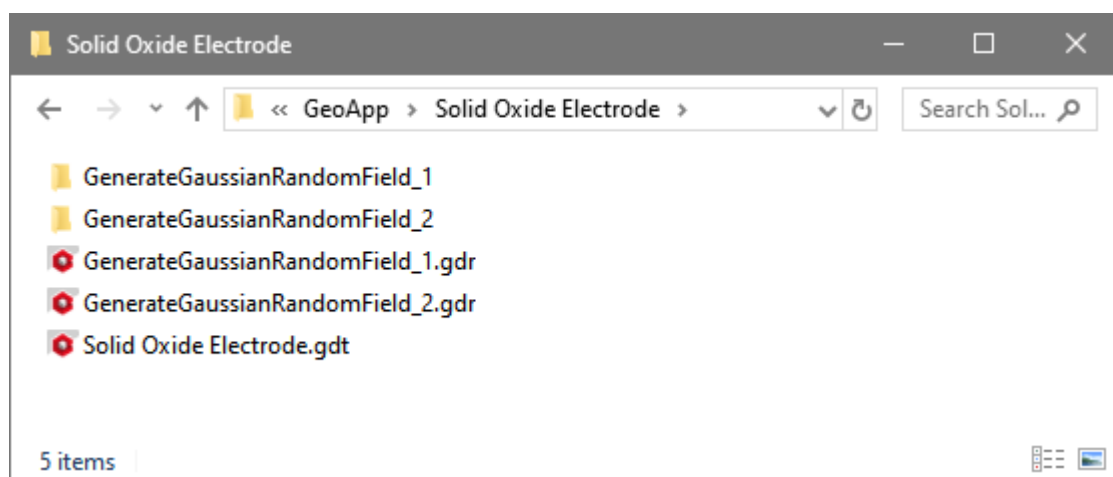
Description	Variable	Unit	Value
Number of voxels in X-Direction	NX	voxel	200
Number of voxels in Y-Direction	NY	voxel	200
Number of voxels in Z-Direction	NZ	voxel	200
Voxel Length	Voxel Length	nm	20.0
Standard deviation of the GRF of solid phase 1	Standard Deviation SP1	voxel	10.0
Standard deviation of the GRF of solid phase 2	Standard Deviation SP2	voxel	10.0
Random seed for the GRF of solid phase 1	Random Seed GRF1	-	1
Random seed for the GRF of solid phase 2	Random Seed GRF1	-	10
Predefined solid volume fraction of solid phase 1	SVF SP1 def	%	37.5
Predefined solid volume fraction of solid phase 2	SVF SP2 def	%	37.5
Tolerance for the solid volume fractions	SVF Tolerance	%	0.01
Angle between the threshold areas of solid phases 1 and 2	Alpha	°	45
Angle between the threshold areas of solid phase 2 and pore phase	Beta	°	0
Angle between the threshold areas of solid phase 1 and pore phase	Gamma	°	0
Dilation radius between pore phase and solid phase 1	Dilation Radius 0 1	voxel	0
Dilation radius between pore phase and solid phase 2	Dilation Radius 0 2	voxel	0
Dilation radius between solid phase 1 and solid phase 2	Dilation Radius 1 2	voxel	0
Standard deviation for the Gaussian filter for SP1	Sigma Gauss Filter SP1	voxel	0.25
Standard deviation for the Gaussian filter for SP2	Sigma Gauss Filter SP2	voxel	0.25
Realized solid volume fraction of solid phase 1	SVF SP1	%	37.5
Realized solid volume fraction of solid phase 2	SVF SP2	%	37.5
Realized threshold 1 to achieve the defined volume fractions	Threshold 1		0.03973199999999991
Realized threshold 2 to achieve the defined volume fractions	Threshold 1		0.002467124999999939
Realized total porosity	Epsilon tot	%	25.0

The generated solid state electrode structure is shown in the visualization area of GeoDict:

Material Information:
ID 00: Pore [invis.]
ID 01: 8YSZ
ID 02: Nickel

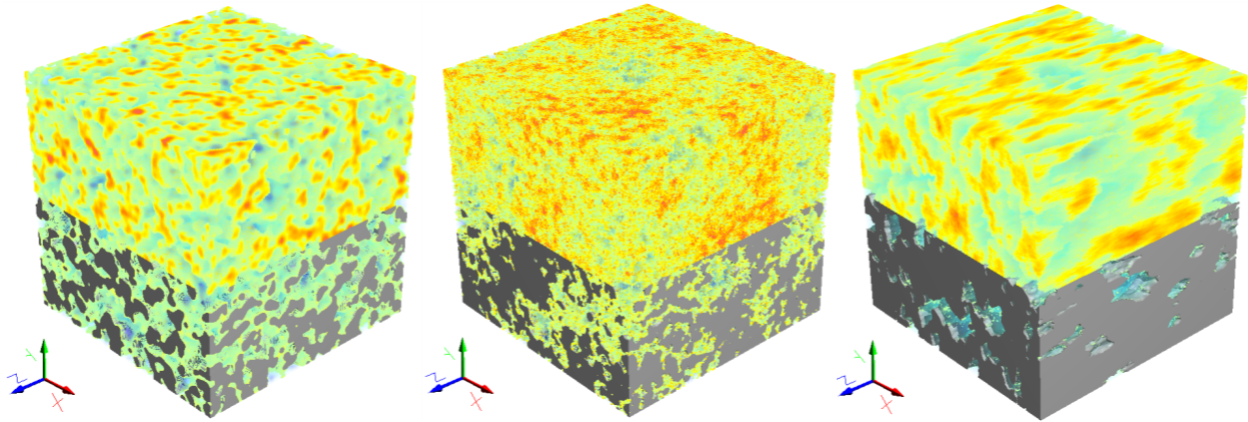


The result folder contains the GRFs and the electrode structure file.

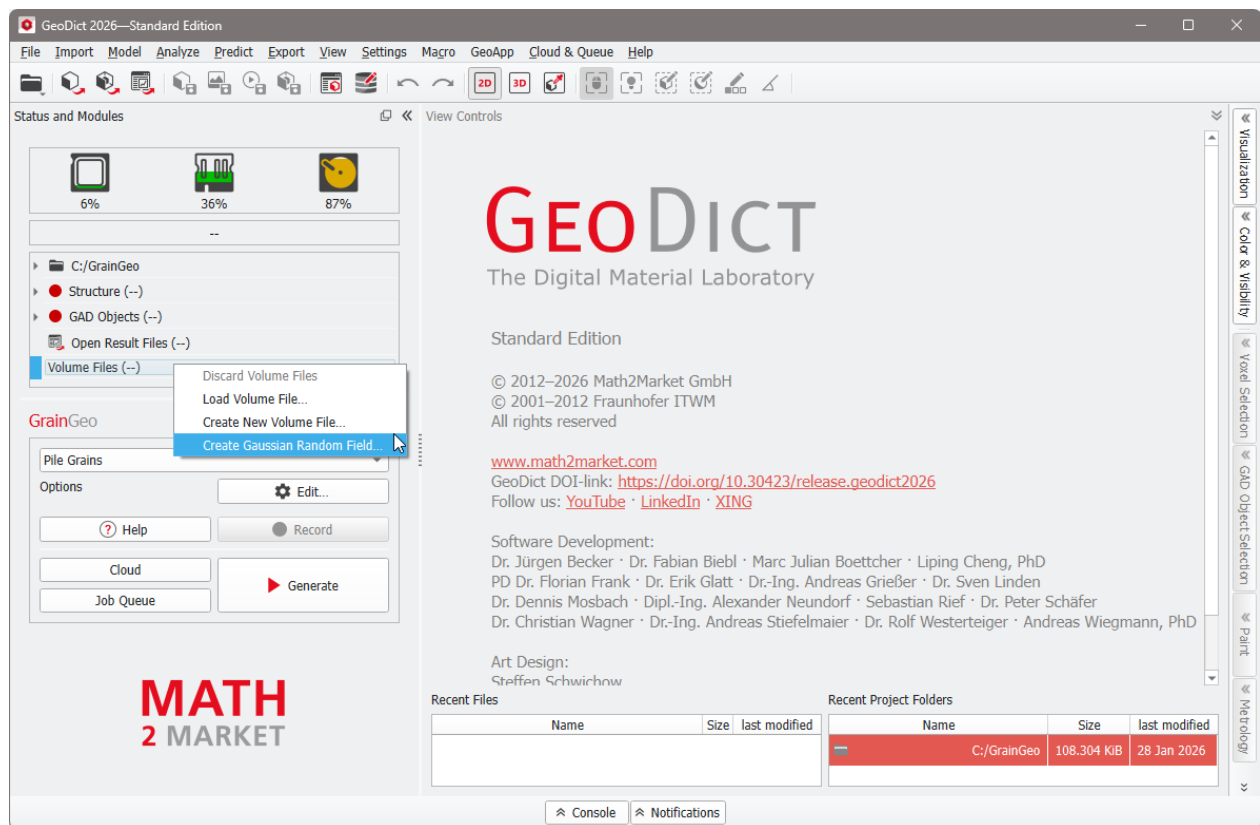


1.12 Gaussian Random Field Generator

Generate **Gaussian random fields** and threshold them afterwards to obtain structures.



To open the **Gaussian Random Field Generator**, right-click on **Volume Field** in the **Project Status** section in the left-hand side of GeoDict and select **Create Gaussian Random Field....**



The Gaussian Random Field command:

- [Theoretical Background](#)²³⁹
What are Gaussian Random Fields and what to do with them.
- [Options](#)²⁴¹
Define the parameters for the random field generation.
- [Results](#)²⁵¹

The Gaussian Random Field command:

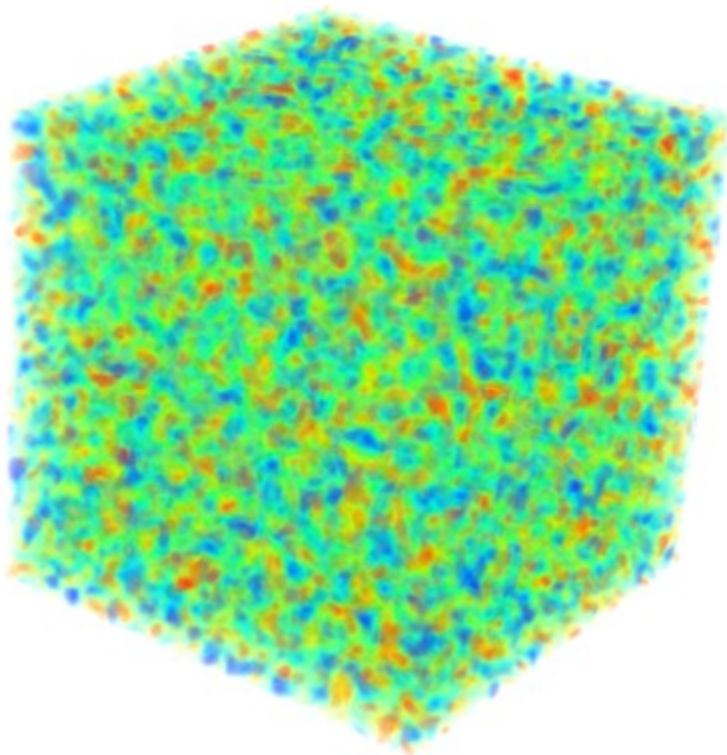
How to load a Gaussian Random Field and segment it to a structure.

1.12.1 Theoretical Background

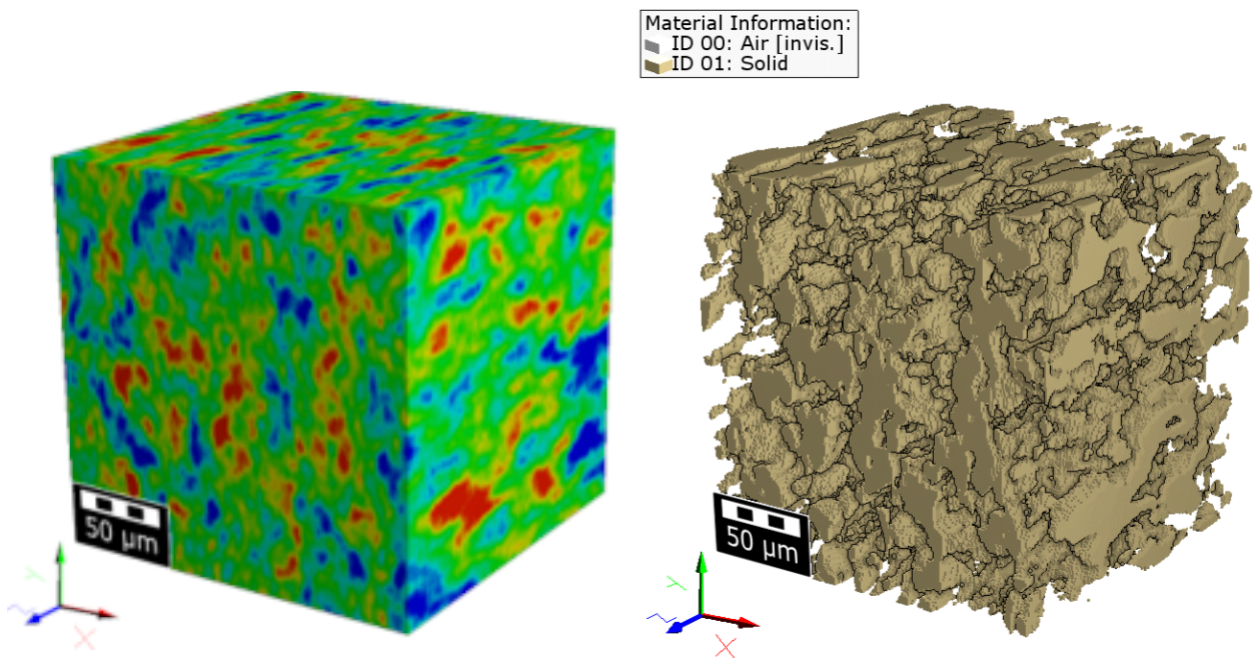
Generate **Gaussian random fields** and threshold them to obtain structures.

A **Gaussian random field** describes a volume field with correlated noise. This means the probability of similarity between two values decreases exponentially with their distance. In the **Gaussian Random Field Generator** in GeoDict, several Gauss functions can be combined to define a random field.

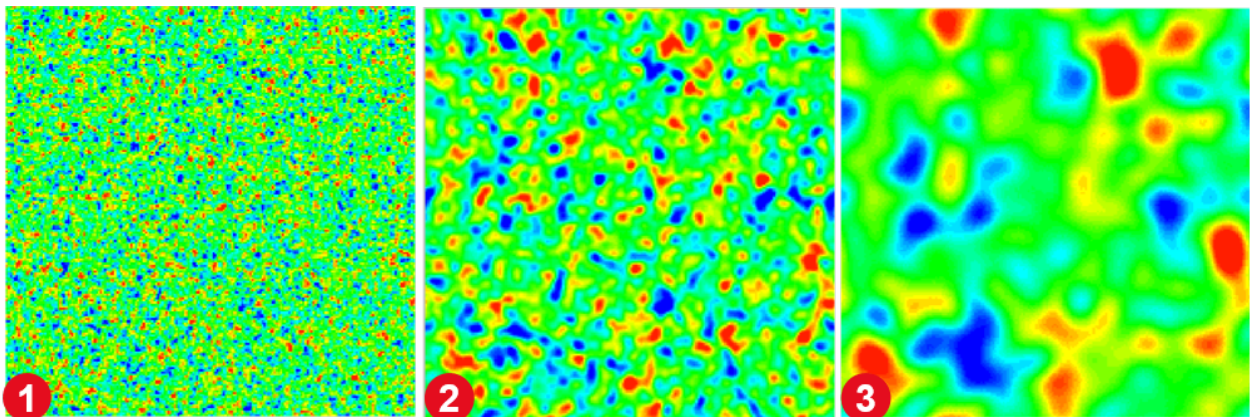
In the image below, a scalar Gaussian random field in a jet color gradient is shown. The corresponding Gaussian function has a standard deviation of 3.



The Gaussian random field can then be segmented to a structure as shown [here](#) 



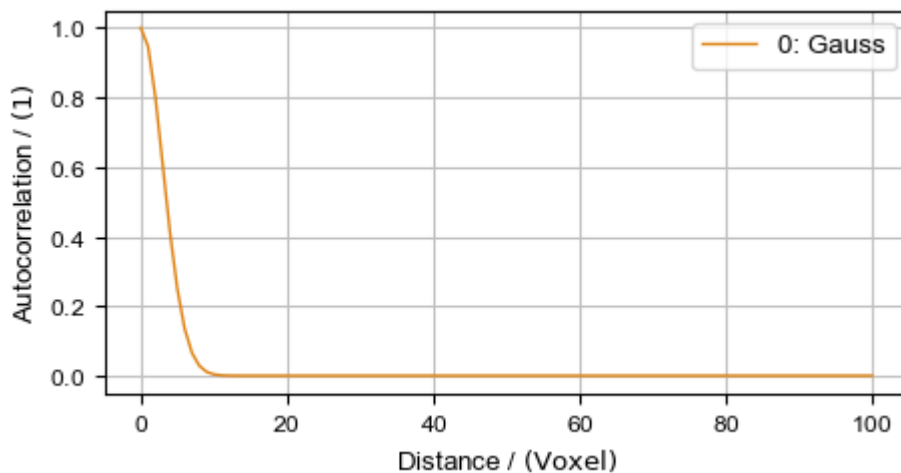
In the following example observe different forms of noise.



1. Uncorrelated noise, all values are independent.
2. Noise following a spatial correlation. The values are correlated with their spatial neighborhood.
3. Noise following a spatial correlation with a large correlation length.

The spatial correlation can be specified with an autocorrelation graph. For each distance between two voxels the probability of similarity, also called covariance, is described.

In the **Gaussian Random Field Generator**, you may define several autocorrelation functions to generate a custom random field.

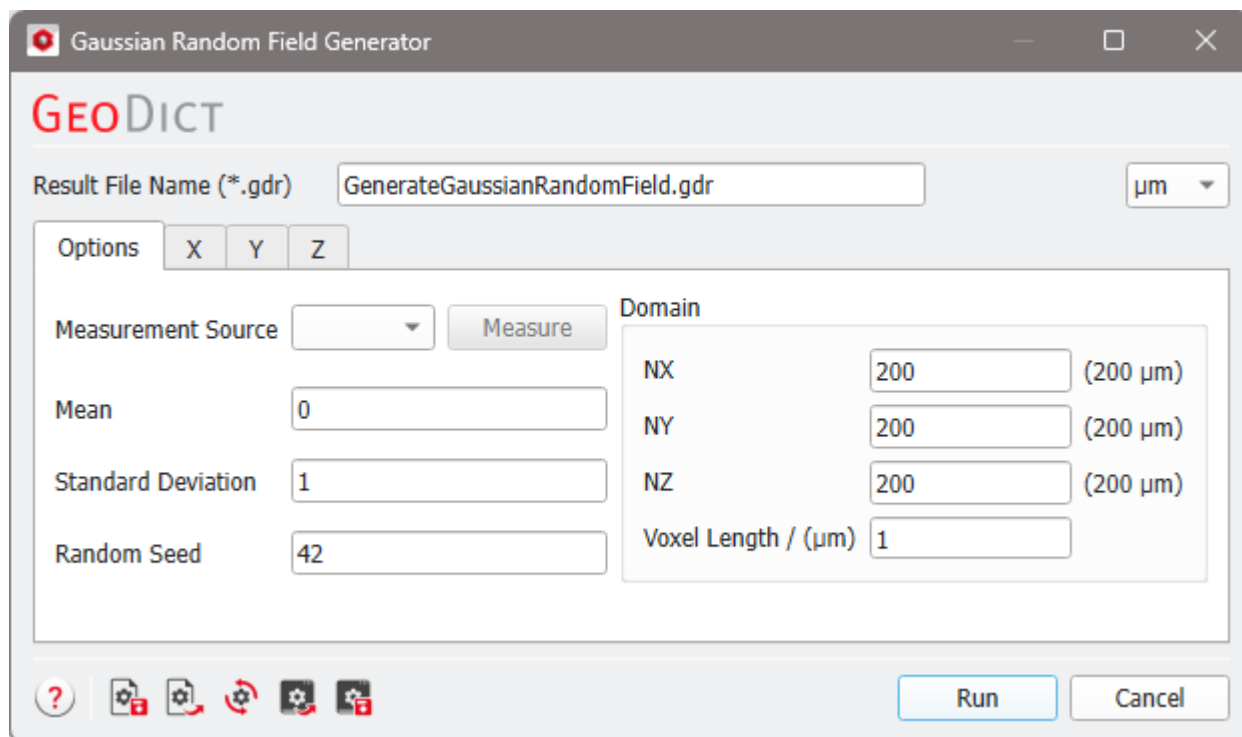


1.12.2 Options

At the top left of the dialog, the name for the file containing the generation results can be entered in the **Result File Name (*.gdr)** box. The default name can be kept, or a new name can be chosen, fitting the current project.

The result files are saved in the chosen project folder (**File** → **Choose Project Folder**, in the **Menu bar**). If a GeoDict result file (*.gdr) with the given name already exists in the project folder, a warning message is shown at the start of the creation process. You can either decide to rename the chosen file name to a new one, to cancel the generation process, to overwrite or to back up the old file. When nothing is selected, GeoDict uses the **Back-Up** option after a waiting time.

The available units (m, cm, mm, μm , nm and Inch) are selectable from the pull-down menu at the top right of the dialog. When the units are changed, the entered values are adjusted automatically.

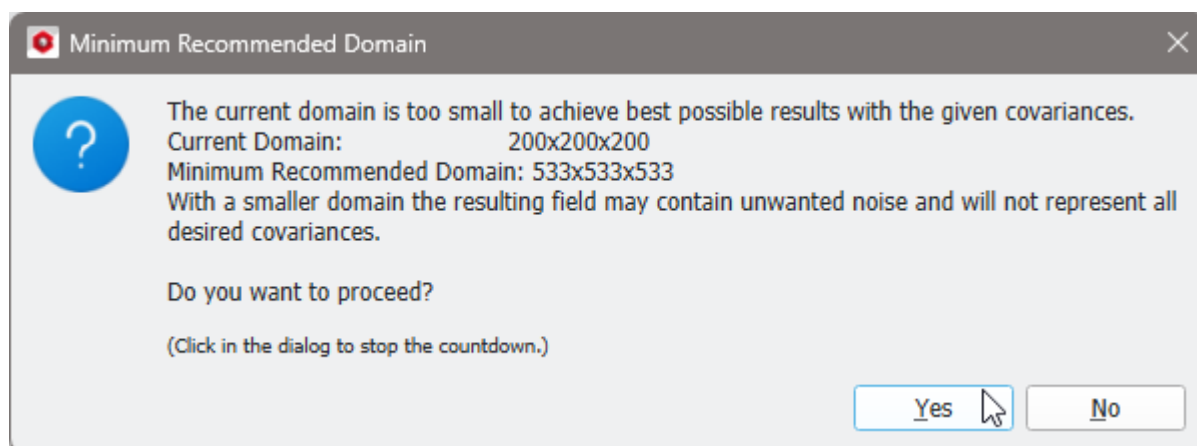


The parameters are organized into tabs:

- [Options](#)^[243]
Determine general properties of the resulting structure, such as size and resolution.
- [Autocorrelation Settings](#)^[244]
Define the autocorrelation parameters for the three axial directions X, Y, and Z.

After setting all autocorrelation functions as desired for all three directions, clicking **Run** generates the **Gaussian random field**.

If the [domain parameters](#)^[244] are not large enough to represent the given covariances, a warning dialog appears. Decide if the generation should proceed or if it should be aborted. Changing the domain size accordingly improves the accuracy.



Options

The geometric properties of the desired random field are accessible under the **Options** tab. The parameters are grouped in the parameters defining the general randomness and the **Domain** parameters.

Options X Y Z

Measurement Source Measure

Mean

Standard Deviation

Random Seed

Domain

NX (200 μm)

NY (200 μm)

NZ (200 μm)

Voxel Length / (μm)

Randomness Parameters

✓ Measurement Source

If a volume field is loaded, a **Measurement Source** can be selected. This is useful, for example, if a scan with a random field-like structure should be reproduced with a different realization of the same statistical properties. Clicking **Measure** then computes the autocorrelation for the volume field values and adds the corresponding graph in the X, Y, and Z tabs as **Measured Covariance**. In the **Options** tab the **Mean value** and the **Standard Deviation** of the selected field are also entered automatically.

Measurement Source Measure

If the volume field is not given in the right data type and thus does not show up in the pull-down menu, it can be transformed. Therefore, right-click on the field in the **Project Status** and select **Math Operation**.

In the **Math Operation** dialog select **Convert to Data Type** from the first and **Float Single-Precision** from the second pull-down menu.

Project Status

- C:/GrainGeo
- Structure (--)
- GAD Objects (0)
- Statistics
- Constituent Materials (1)
- Open Result Files (1)
- Volume Files (1)
 - hard001.png (257x257x256, 1 μm)
 - Image

Math Operation

Input Field: Gray Values

Math Operation:

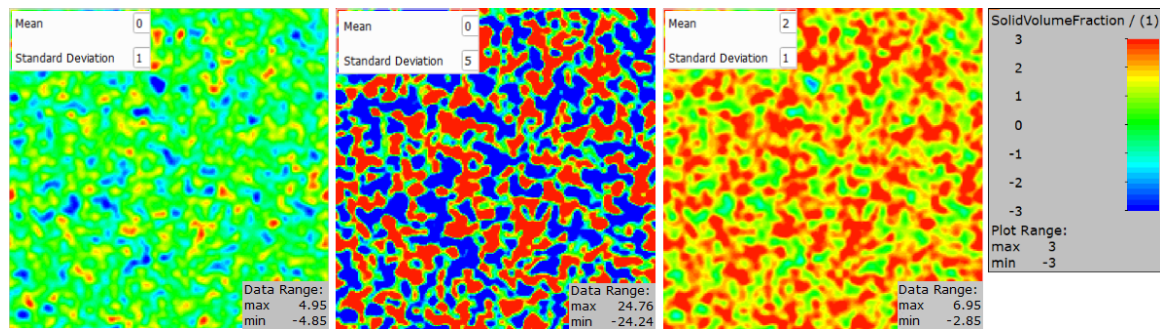
New Data Type:

Run Cancel

✓ Mean value and Standard Deviation

To generate a new custom random field, enter the desired **Mean** value and **Standard Deviation** manually. These values correspond to the generated random field and define the value range in it.

In the following observe how the data range changes for different mean values and standard deviations while all other parameters are kept the same.



✓ Random Seed

Random Seed initializes the random number generator behind the field generator. Changing its value produces different sequences of random numbers and hence, different realizations of the specified random field. If all settings are equal, generating with the same **Random Seed** value produces the identical random field. **Random Seed** must be a non-negative integer number.

Domain Parameters

The **Domain** panel contains the parameters defining the structure size (**NX**, **NY**, and **NZ**) in combination with the resolution (**Voxel Length**).

NX, **NY**, and **NZ** are the number (N) of voxels in X, Y, and Z directions.

The **Voxel Length** is the size of one voxel in the chosen units. Varying the values for **NX**, **NY**, and **NZ** has the effect of changing the size of the structure in the given direction.

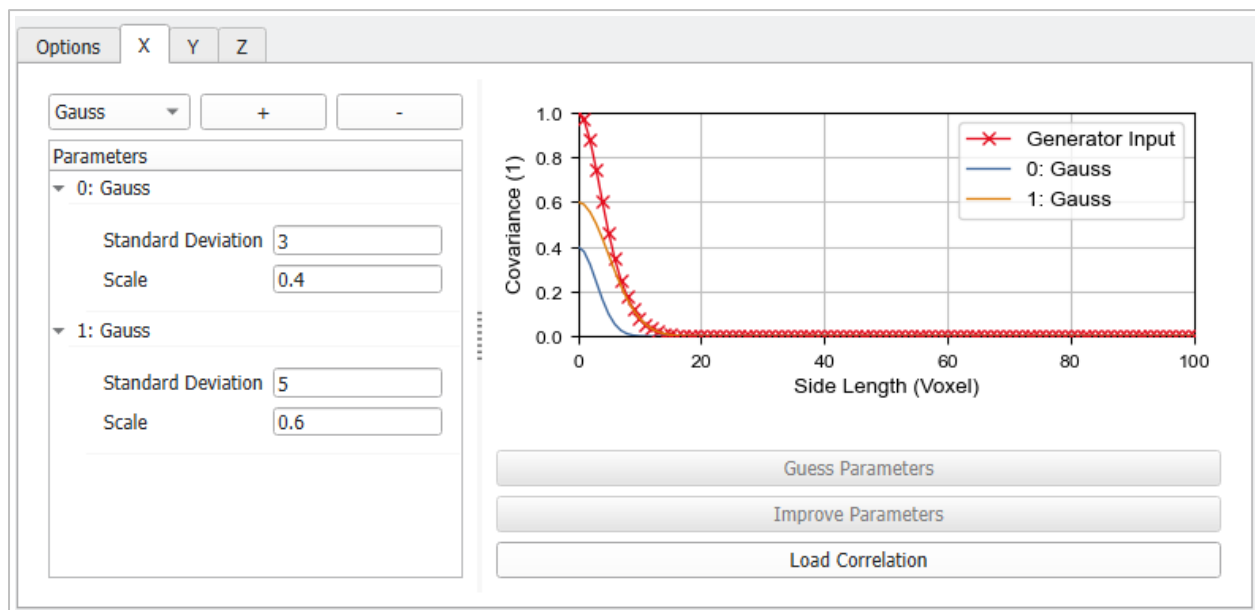
Low values for **Voxel Length** in combination with high values for **NX**, **NY**, and **NZ** increase the resolution, but also increase computational time. After setting the values of **NX**, **NY**, **NZ**, and **Voxel Length**, the physical structure size is automatically displayed in the chosen units.

If a scan should be statistically reproduced, use the same voxel length here.

Autocorrelation Settings

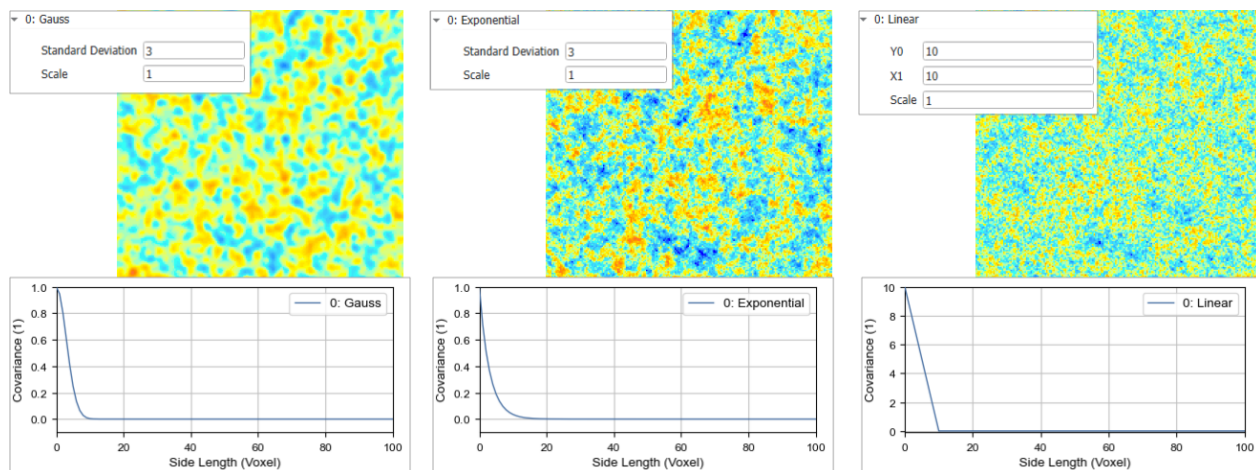
In these tabs the covariances for the corresponding directions are defined.

Define several autocorrelation functions in the left panel and view a preview of the current **Generator Input** function on the right. The generator input is the sum of the defined elements in the **Parameters** panel and defines the resulting covariance for the random field.



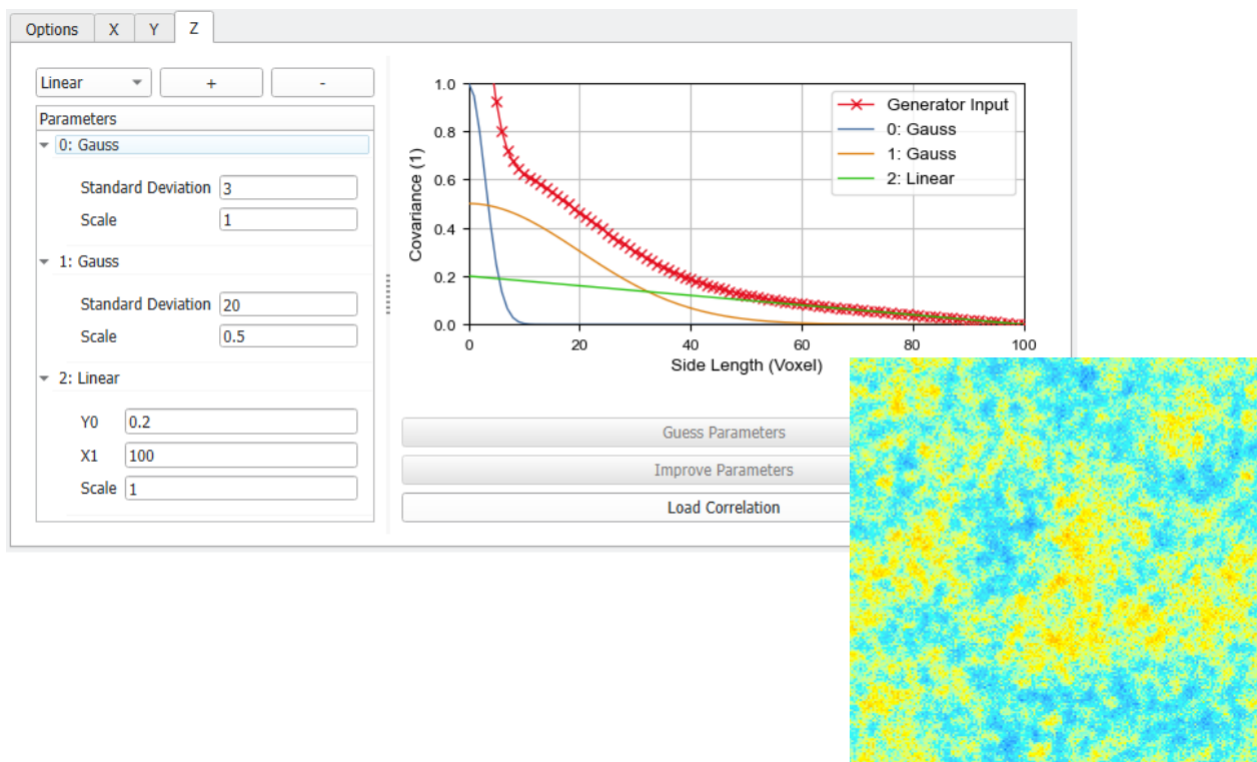
The **Side Length** defines the length of correlated areas in voxel. The **Covariance** value displays the relative amount of areas with the given side length.

Either **Linear**, **Gauss**, or **Exponential** functions can be added. Select them from the pull-down menu in the upper left corner and click . To remove a function, select it in the **Parameters** panel and click .



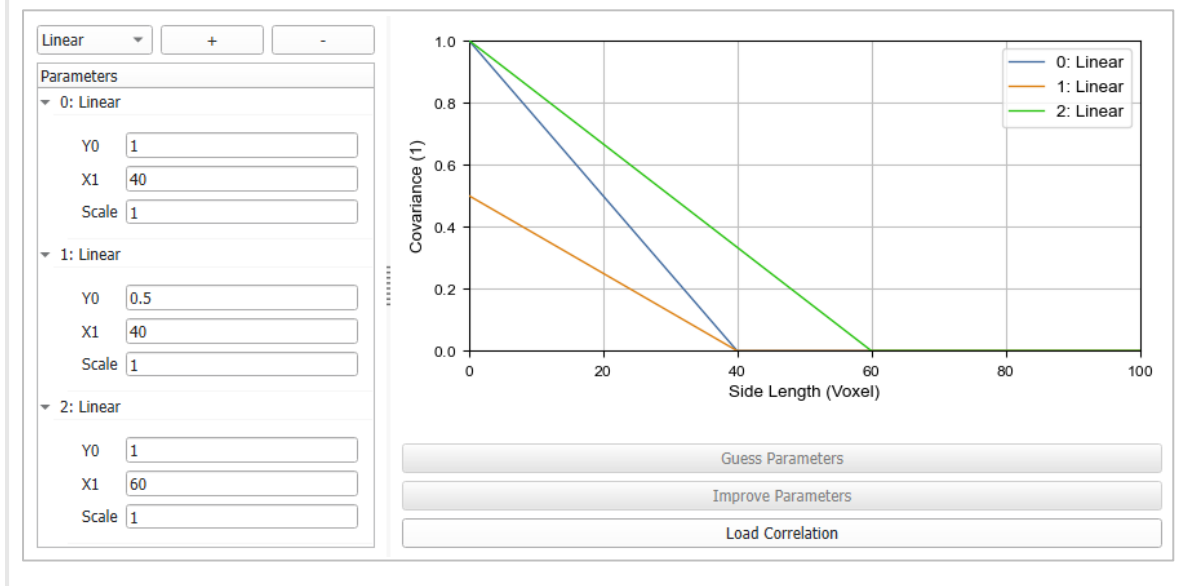
The corresponding graphs are shown on the right with the same name and update automatically whenever a parameter is changed.

The **Generator Input** then is the normalized sum of all the functions and defines the autocorrelation of the generated Gaussian random field. It is also possible to combine the different function types. Below two Gauss functions were combined with a Linear function.



✓ Linear function parameters

For **Linear** functions define the intercept of the linear function with the Y-axis (**Y0**) and the X-axis (**X0**) and multiply this function with the factor given for **Scale**.



✓ Gauss function parameters

In the **Parameters** panel for **Gauss** functions, define **Standard Deviation** and **Scale**.

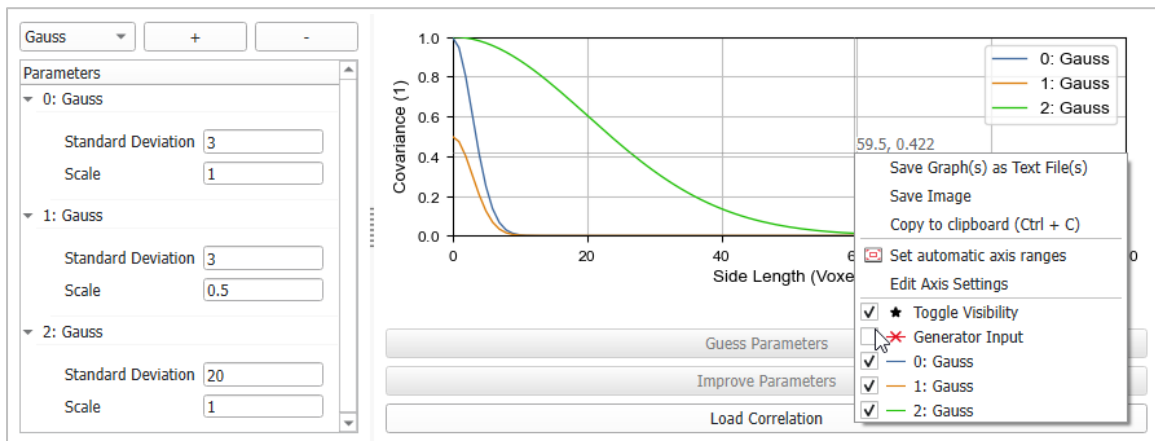
Standard Deviation controls the range for **Side Length**. Note, that the standard deviation here directly refers to the corresponding **Gauss** function, while the standard

deviation in the **Options** tab defines the value range in the generated **Gaussian Random Field**.

Scale controls the range for the **Covariance**, being a factor multiplied to the **Gauss** function.

In the following example, observe the impact of scale and standard deviation on the graphs. The generator input visualization was turned off by right-clicking in the plot and deselecting **Generator Input**.

To learn more about how to edit plots in GeoDict refer to the Result Viewer User Guide.



✓ Exponential function parameters

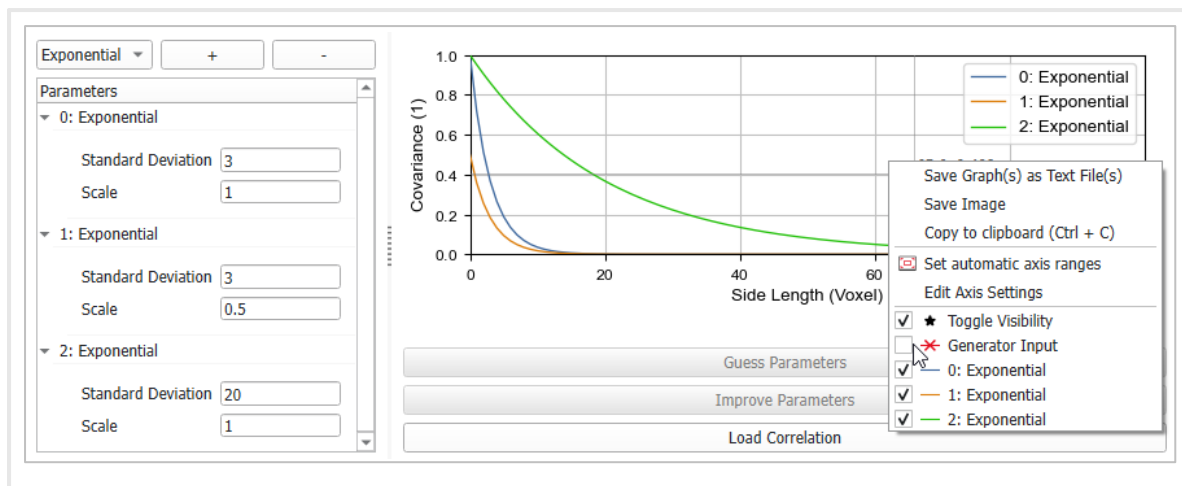
In the **Parameters** panel for **Exponential** functions, define **Standard Deviation** and **Scale**.

Standard Deviation controls the range for **Side Length**. Note, that the standard deviation here directly refers to the corresponding **Exponential** function, while the standard deviation in the **Options** tab defines the value range in the generated **Exponential Gaussian Random Field**.

Scale controls the range for the **Covariance**, being a factor multiplied to the **Exponential** function.

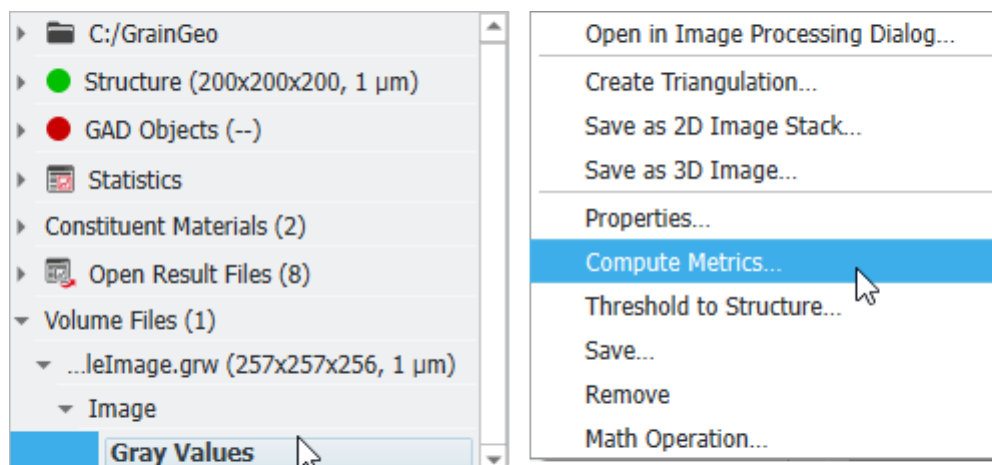
In the following example, observe the impact of scale and standard deviation on the graphs. The generator input visualization was turned off by right-clicking in the plot and deselecting **Generator Input**.

To learn more about how to edit plots in GeoDict refer to the Result Viewer User Guide.



✓ Load Correlation, Guess Parameters, and Improve Parameters

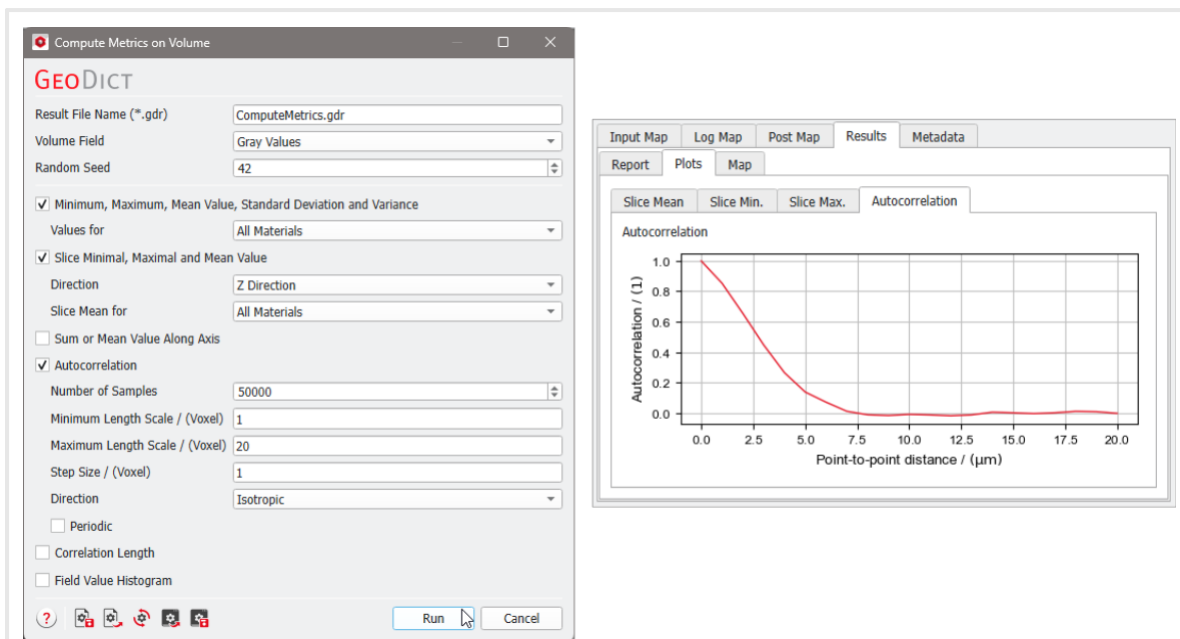
While loading the autocorrelation values in the [Options](#) ²⁴³ tab is usually the easiest possibility, autocorrelations can also be loaded from GeoDict result files generated with **Compute Metrics**, available from the **Project Status** by right-clicking on the volume field to analyze.



In the **Compute Metrics** dialog select **Minimum**, **Maximum**, **Mean Value**, **Standard Deviation** and **Variance**, and **Autocorrelation** and define the parameters as needed.

For example, if the autocorrelation in the current field is different for the three directions, compute the metrics for each direction separately. Therefore, for **Direction** select **X-**, **Y-**, or **Z-Direction** instead of **Isotropic**.

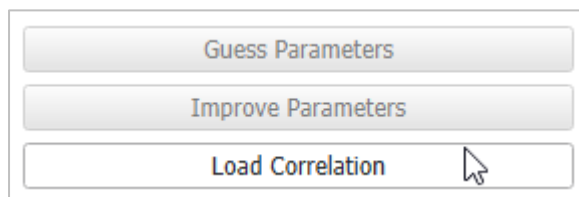
Clicking **Run** computes the standard deviation, mean value, and autocorrelation function for the chosen volume field.



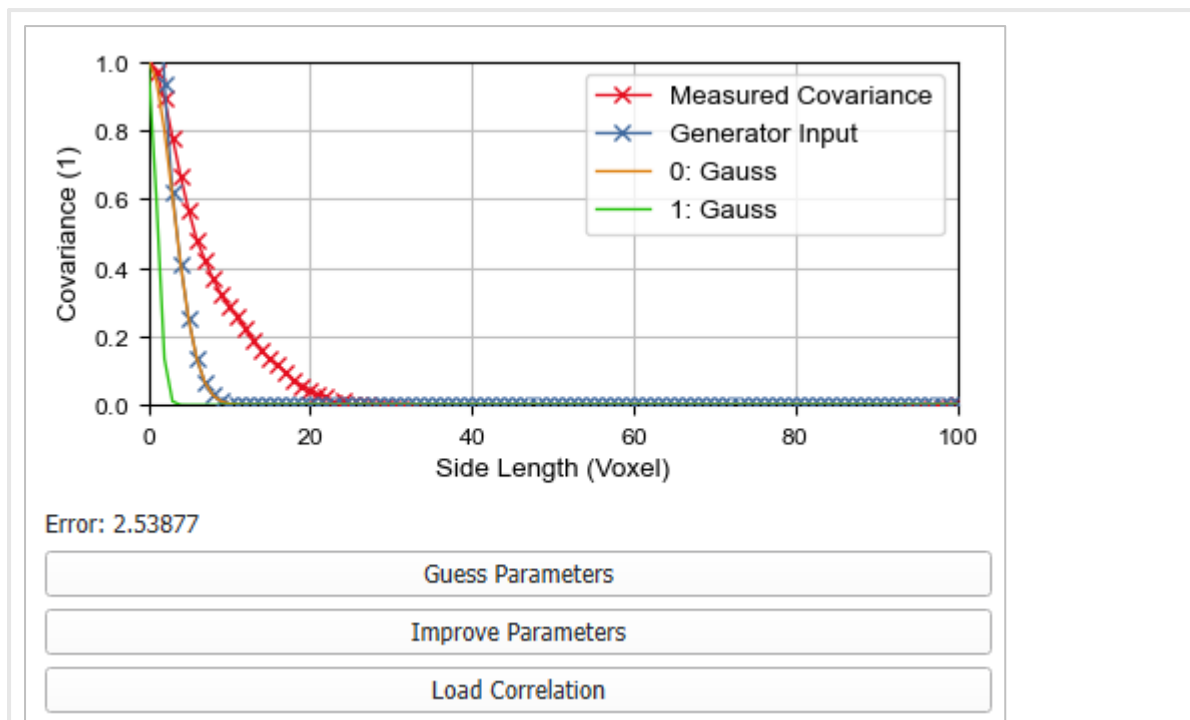
In the **Gaussian Random Field Generator** enter the **Standard Deviation** and **Mean** manually in the **Options** tab as given in the **Compute Metrics** result file.



Then, move to each of the **X**, **Y**, and **Z** tabs and load the computed autocorrelations. Therefore, click **Load Correlation** and browse for the **Compute Metrics** result.

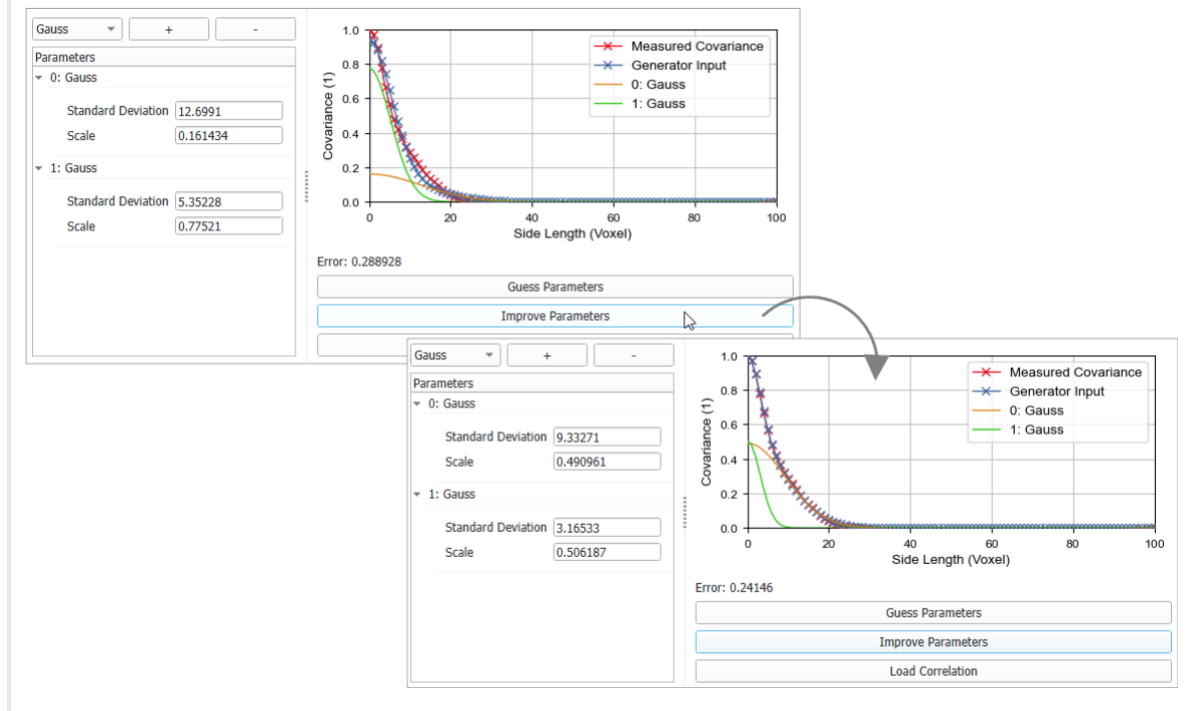


If an autocorrelation was loaded either from the current volume field or from a metrics result, in the plot a graph for the **Measured Covariance** is added and the buttons **Guess Parameters** and **Improve Parameters** become available. Additionally, below the plot the **Error** between the measured covariance and the current generator input is displayed. It is computed as the sum of squared deviations for all data points in the curve.



The number and type of functions needed to fit the measured covariance must be defined. After adding the needed number of **Gauss**, **Exponential**, or **Linear** functions, clicking **Guess Parameters** tries different parameters to fit the measured covariance. Automatically, the first best guess of the algorithm is entered for the parameters.

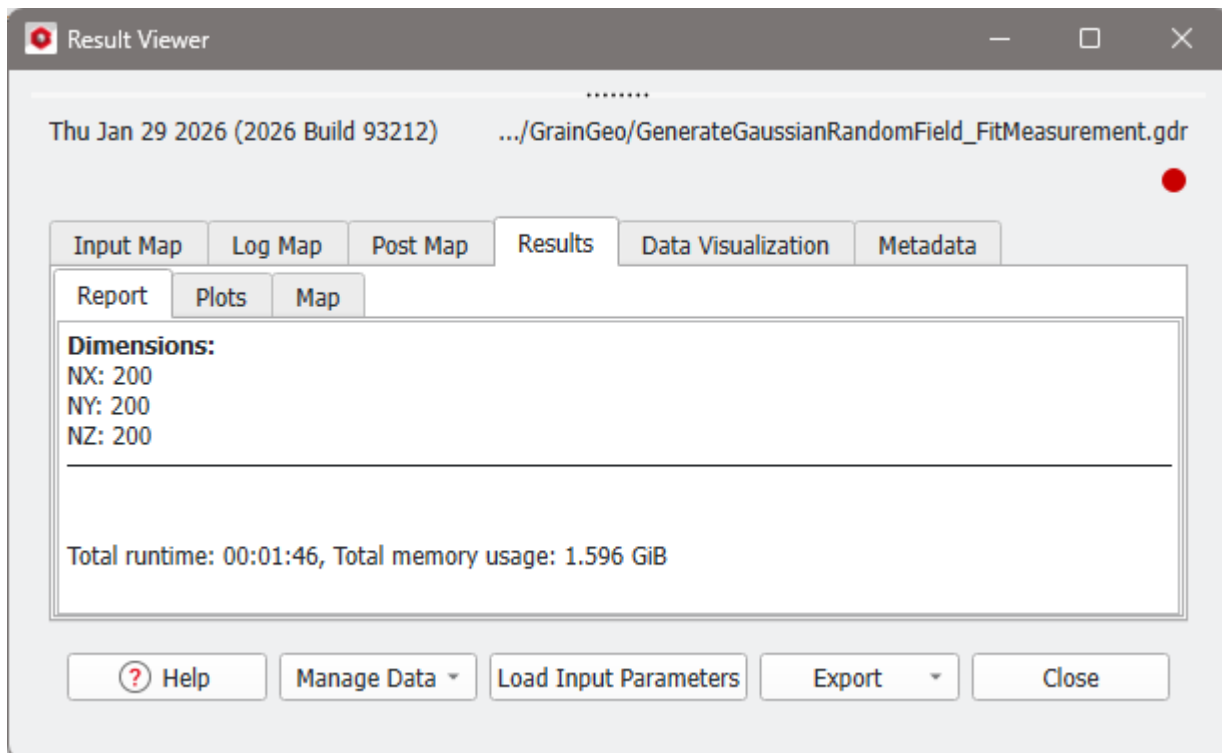
It can be necessary to click **Improve Parameters** several times, if the **Generator Input** does not fit the **Measured Covariance** with the desired accuracy.



1.12.3 Results

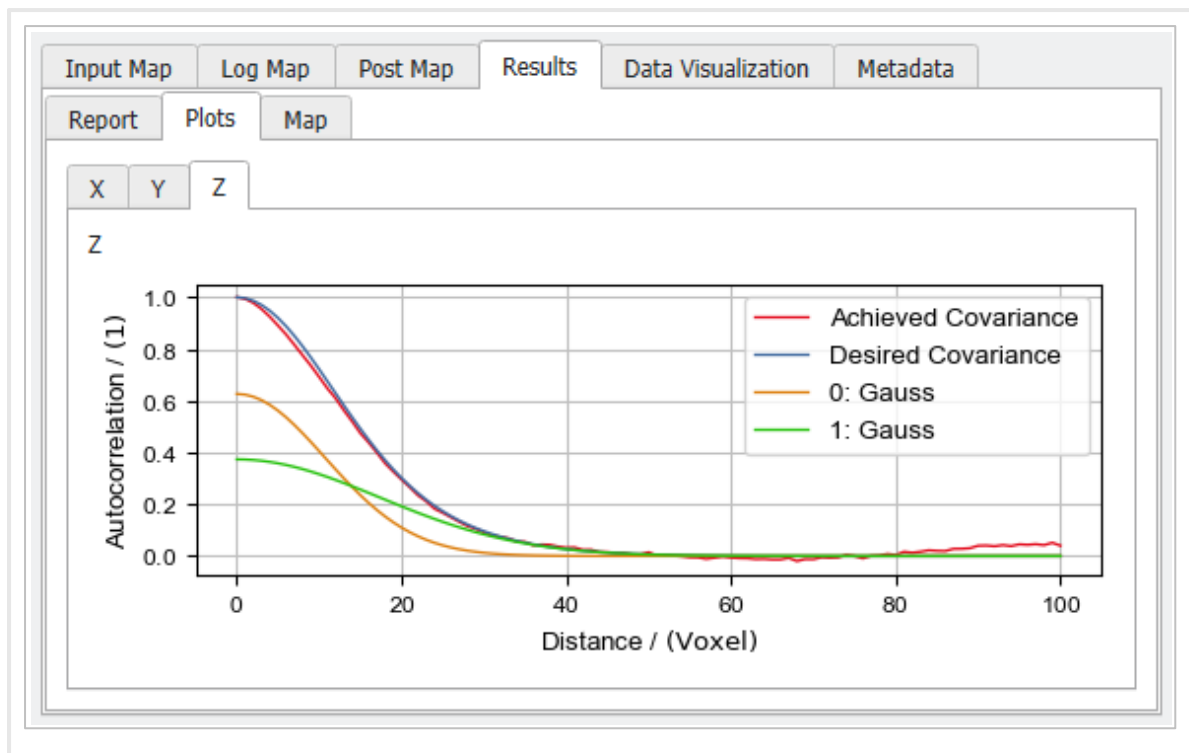
Generating a Gaussian random field produces a GeoDict result file (*.gdr) and a result folder with the same name. Both are saved in the chosen project folder (**File** → **Choose Project Folder...** in the menu bar).

The GeoDict **Result Viewer** opens for the result file and in the **Results – Report** subtab find the dimensions of the generated field.



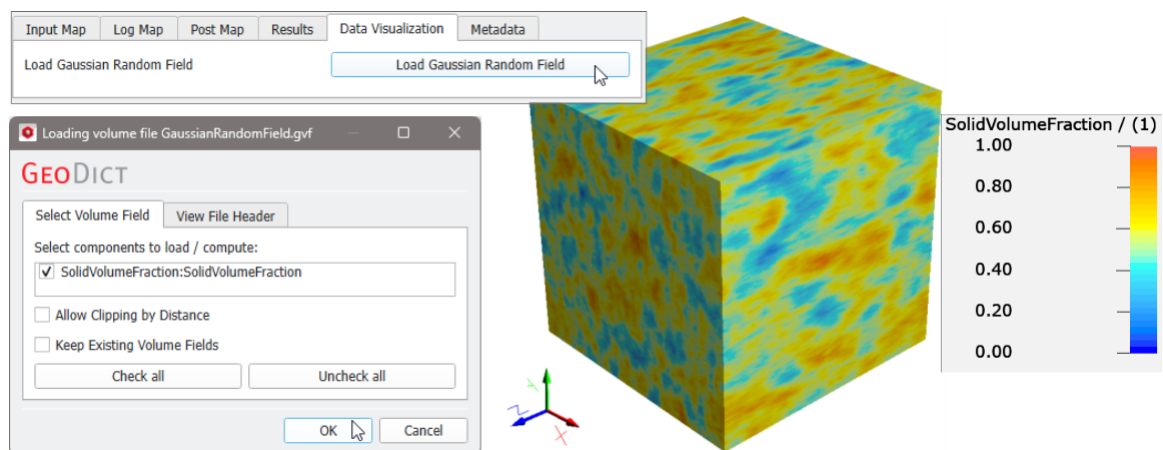
✓ Plots

View the achieved covariances for the three dimensions in the **Plots** subtab of the Results tab. The red graph shows the **Achieved Covariance** in the resulting Gaussian random field. The blue plot shows the **Desired Covariance** which is the **Generator Input** prepared in the **Gaussian Random Field Generator**. How many numbered plots appear depends on the settings in the generator dialog. Here, the desired covariance is the sum of two **Gauss** functions.



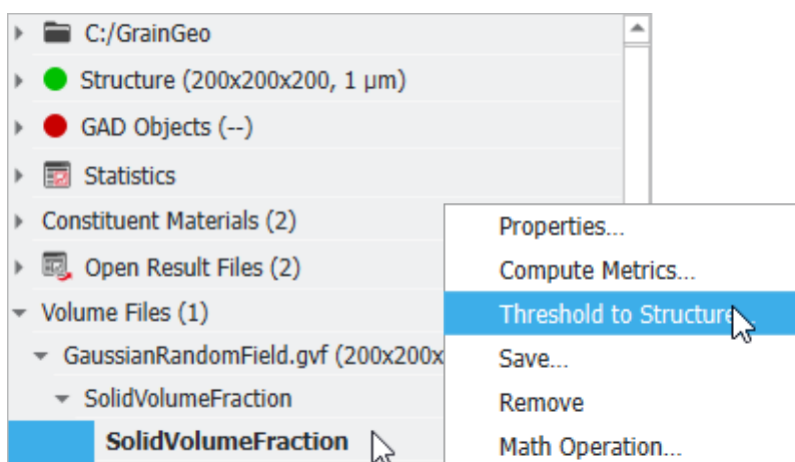
✓ Data Visualization and Thresholding

The Gaussian Random Field is visualized in GeoDict after the generation but can also be loaded at any time from the **Result Viewer**. In the **Data Visualization** tab click **Load Gaussian Random Field** and in the **Loading Volume File** dialog click **OK**.

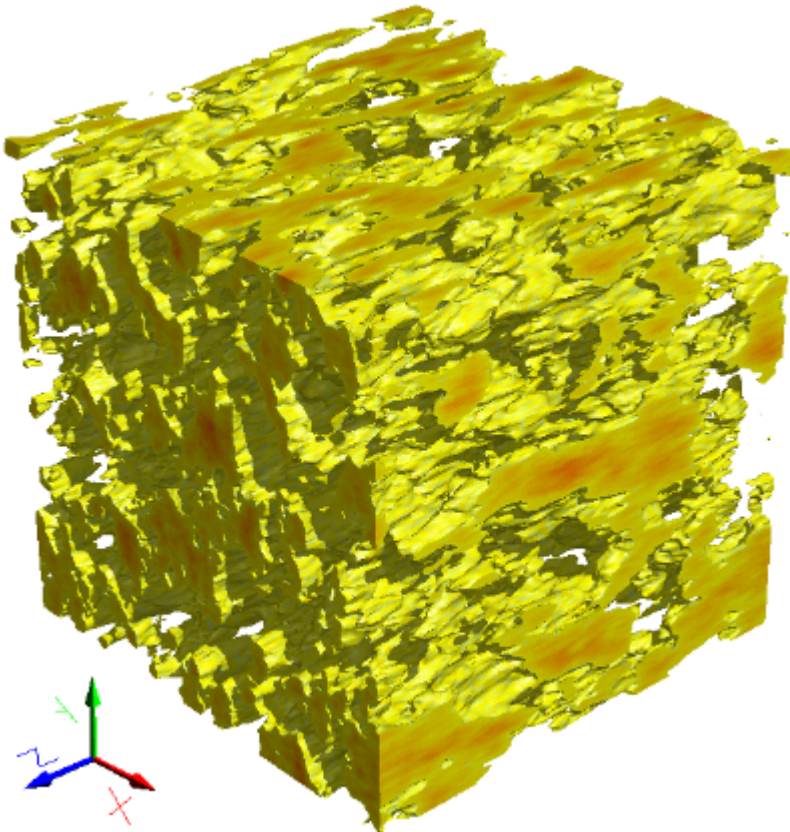


To learn more about visualization in GeoDict, refer to the Visualization User Guide.

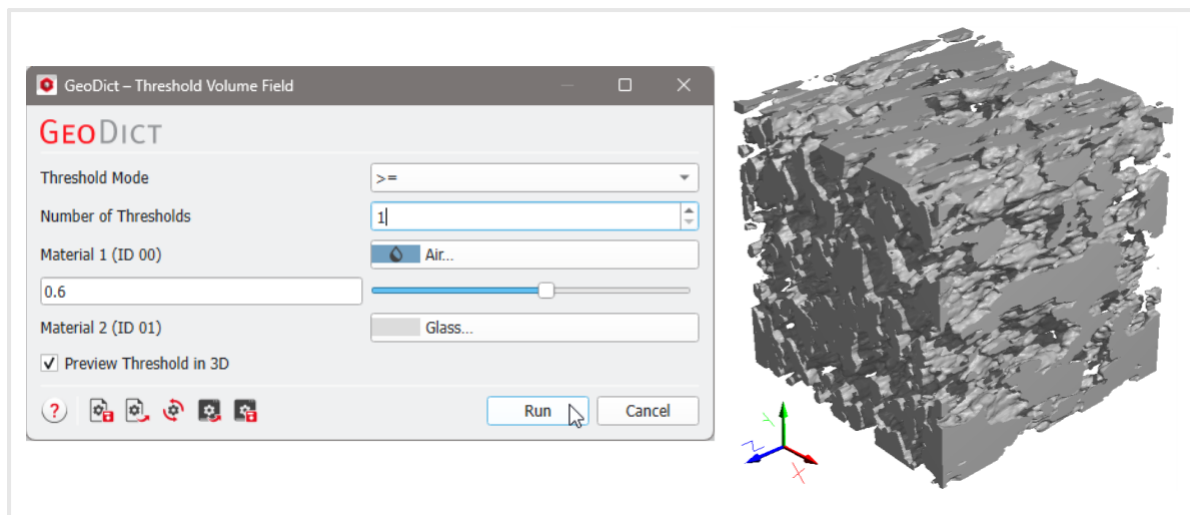
This volume field can be transformed into a structure by right-clicking on the field in the **Project Status** and selecting **Threshold to Structure**.



For one threshold, the resulting structure can be previewed in 3D. Voxels with values below a selected threshold will be converted to a solid/Material ID01, while voxels with values above the threshold will be assigned to pore/Material ID00.



Edit the parameters as desired, and click **Run**.



1.13 References

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