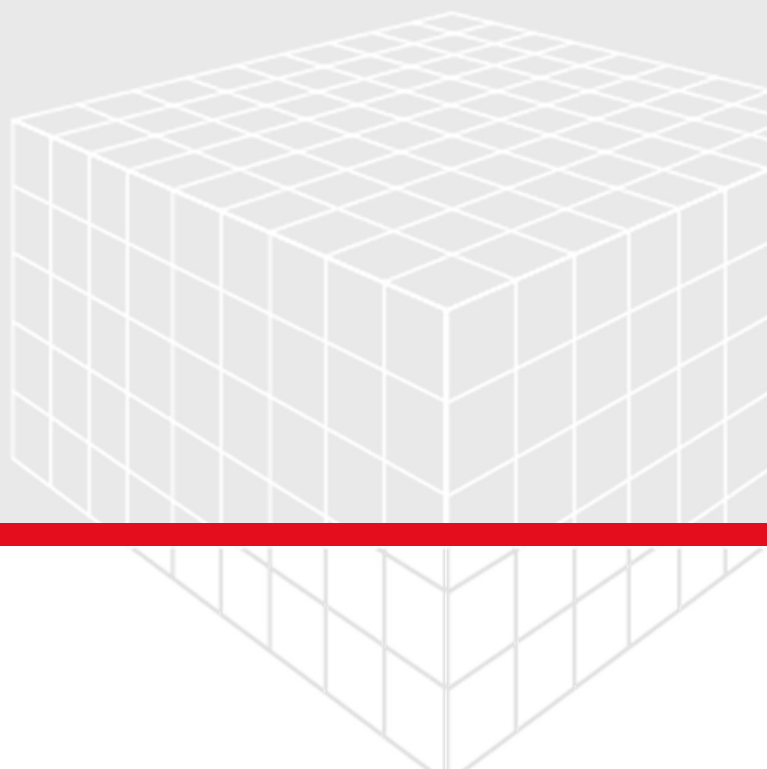


GeoApps

User Guide

GEODICT Release 2026

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GEO DICT

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1 GeoApps

GeoDict offers great automation possibilities to enhance productivity in the form of GeoApps. All steps done in GeoDict are recorded in macros. The GeoApp menu in GeoDict gives access to several pre-defined macros for workflows that are often requested. Additionally, you can add own recorded and edited parameter macros to create custom GeoApps for frequent workflows.

The **GeoApp** menu in the menu bar gives access to many GeoApps, grouped into **Shared GeoApps** and **My GeoApps**.

The GeoApps delivered with GeoDict are described shortly in the following. Please ask support@math2market.de if you want to know more details about the specific parameters used in these apps and the functionality they provide.

Run **Modules** specific GeoApps for several modules, which can also be found in the corresponding module sections.

The **Shared GeoApps** are groups of apps delivered with GeoDict and, later, apps that you create or modify to be shared with your colleagues.

Under **My GeoApps** is an example GeoApp provided by Math2Market and, later, the local GeoApps you created for your private use. The **My GeoApps** are placed in the GeoDict settings folder.



New in GeoDict 2026

- GeoApps are rearranged:
 - Several GeoApps were moved to the Scripting Examples
 - Module specific GeoApps are also copied to GeoApp groups
 - The sub entries in the GeoApp menu now follow the same naming scheme for each group
- Several new apps - find more information in the specific topics
- Some apps were renamed - find more information in the specific topics

Discover the following GeoDict topics:

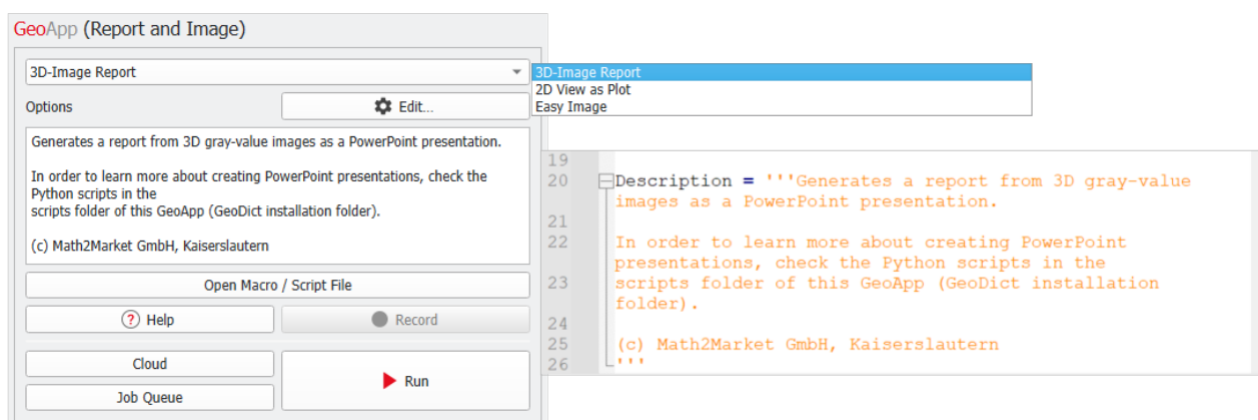
- [General GeoApps](#)⁶
Compute physical properties, create images, reports, and gray value images, and modify structures.
- [Digital Twin GeoApps](#)⁶⁸
GeoDict offers several GeoApps to automatically generate statistical digital twins matching various geometrical and physical properties.
- [Battery GeoApps](#)⁹⁹
Create realistic anode and cathode structures for a battery.

Discover the following GeoDict topics:

- [Composites GeoApps](#)¹²²
Create structures as glass-fiber enforced plastic and laminates.
- [Digital Rock Physics \(DRP\) GeoApps](#)¹²⁷
Run simulations on rocks, as for example quality control and nuclear magnetic resonance.
- [Filtration GeoApps](#)¹⁷⁵
Create filters and compute special filtration simulations.
- [Fuel Cell and Electrolyser GeoApps](#)¹⁸⁹
Generate components of fuel cells and electrolyzers.
- [Additive Manufacturing GeoApps](#)²⁰¹
Generate structures from additive manufacturing.
- [Woven Mesh Materials GeoApps](#)²³⁰
Generate and analyze woven mesh materials.
- [3rd Party GeoApps](#)²³⁴
GeoApps created by 3rd parties.
- [Adding Custom GeoApps](#)²³⁵
Learn how to add your own custom GeoApps.
- [References](#)²⁴⁰
List of references used in the GeoApp User Guide.

Selecting one of the GeoApps groups opens the corresponding **GeoApp** module section, located left of the visualization area. It contains a pull-down menu listing the available GeoApps for this particular GeoApp group.

GeoDict macros corresponding to the simulations are called and executed when the GeoApps are run. These macros are available in the **GeoApp** folder in the GeoDict installation folder. GeoApps may be opened with a text editor, to observe their syntax and the steps involved in the simulation.



When selecting one of the available GeoApps, the description area displays a report about the app. In the corresponding GeoPy script, this report content can be found inside the apostrophes after **Description = '''**. For the **3D-Image Report.py** app from the GeoApp

module **General** → **Report and Image**, the text in the macro and the description area is shown above.

Click the **Options' Edit ...** button to edit the parameters of the macro.

By clicking **Open Macro / Script File**, the macro file containing all steps for the app simulations can be accessed in a text editor. For detailed information about GeoPy and editing GeoDict macros refer to the GeoPy scripting user guide.

After setting the input parameters for the selected GeoApp, clicking **Run** starts the execution.



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 General GeoApps

Use the **General GeoApps** to compute physical properties, create images and reports, generate gray value images, and modify structures.



New in GeoDict 2026

- The [Material Dissolution](#)^[44] GeoApp is new in GeoDict 2026 and allows you to simulate the dissolution of solids in your structure.
- The **Property Prediction** group has been divided into [Geometric Properties](#)^[6] and [Physical Properties](#)^[18].
- The following GeoApps are not new to GeoDict but are now sorted under the **General** GeoApps menu:
 - [Identify Fractures](#)^[14]
 - [Air Permeability Test](#)^[19]
 - [Concentration Dependent Diffusivity](#)^[21]
 - [Stiffness Estimation](#)^[23]
 - [Upscaling Mercury Injection Capillary Pressure](#)^[25]
 - [Upscaling Relative Permeability](#)^[29]
 - [Hysteresis](#)^[32]
 - [Contact Detachment](#)^[36]
 - [Distribute Material IDs](#)^[60]

Find the following General GeoApp groups:

- [Geometric Properties](#)^[6]
Compute geometric properties.
- [Physical Properties](#)^[18]
Compute physical properties.
- [Report and Image](#)^[47]
Save images and create PowerPoint reports.
- [Structure Generation](#)^[54]
Generate gray value images, add a random surface cover to a structure, and correct contacts.

1.1.1 Geometric Properties

Use the **Geometric Properties** GeoApps to calculate non-physical properties of your structure.

The following Geometric Properties GeoApps are shipped with GeoDict:

- [Compute Tortuosity](#)^[7]

The following Geometric Properties GeoApps are shipped with GeoDict:

Compute pore space tortuosity using different approaches.

- [Compute Fractal Dimension](#)^[13]

Compute the fractal dimension of the solid materials of a loaded geometry.

- [Identify Fractures](#)^[14]

Analyze the pore morphology and segment the chosen material into fractures, small and large pores.

Compute Tortuosity

The **Compute Tortuosity** GeoApp uses different approaches, as described in [Holzer et al., 2023](#)^[240], to calculate the tortuosity of the pore space in a chosen computation direction. Additionally, a geometric analysis can be performed and effective transport properties on the macroscale can be predicted based on [Holzer et al., 2013](#)^[240].



Modules needed to run this GeoApp (depending on the selected options):

PoroDict + MatDict, DiffuDict, ConductoDict, FlowDict, AddiDict

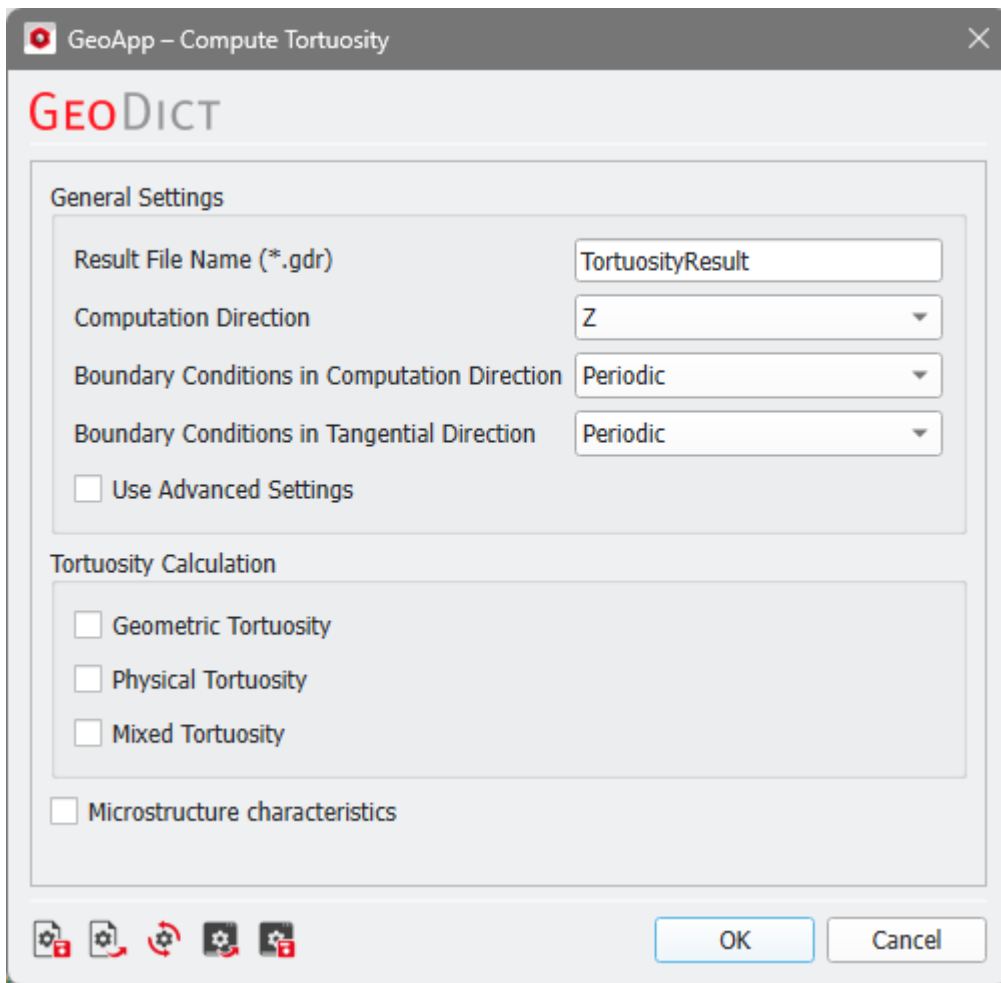


Note! Also have a look at our [website](#) for more information.

Generally, three different kinds of tortuosity can be computed:

- **Geometric Tortuosity**, which is directly derived from the microstructure,
- **Physical Tortuosity** or physics-based tortuosity, which is indirectly derived by transport mechanisms,
- **Mixed Tortuosity**, which uses a mixture of determinations based on geometric analysis and physical transportation phenomena.

Click **Edit** to open the **Compute Tortuosity** parameter dialog.



Select a **Result File Name** and the **Computation Direction** in the **General Settings** panel. Also, the **Boundary Conditions in Computation Direction** and **in Tangential Direction** must be defined.

After activating **Use Advanced Settings** you can define the **Parallelization**, the **Bin Sizes** for **Streamlines** and **Porosimetry & Granulometry**, the **In- / Outlet Length for Stokes Flow**, and **Dense Sampling of Streamlines**.

☒ Use Advanced Settings

☐ Use Maximum Parallelization

DiffuDict Parallelization	8
ConductoDict Parallelization	8
FlowDict Parallelization	8
PoroDict Parallelization	8

Streamline Bin Size

Porosimetry and Granulometry Bin Size

In- / Outlet length for Stokes Flow

☐ Use a Dense Sampling of Streamlines

In the **Tortuosity Calculation** panel, select the properties to be computed.

☒ Geometric Tortuosity

There are two options available for the **Geometric Tortuosity**. These tortuosity values are derived directly from the morphological characteristics of the analyzed structure and are defined solely by the structure.

The general definition of the **Geometric Tortuosity** is the comparison of the effective geometric path length L_{eff} to the shortest geometric path length L_0 :

$$\tau = \frac{L_{eff}}{L_0} \quad (1) \text{ Geometric Tortuosity}$$

The geometric tortuosity options are:

- **Geodesic Tortuosity** in PoroDict: Computing the mean geodesic tortuosity from the percolation pathway starting from every voxel in the inlet, i.e., the shortest path in pore space is compared to the direct path.
- **Percolation Path Tortuosity** in PoroDict: Computing the mean value of the percolation pathways with the 50 largest diameters, i.e., the length of the path of large particles (largest possible diameters) through the structure (median axis) is compared to the direct path.

☒ Physical Tortuosity

There are four options available for the **Physical Tortuosity**. These tortuosities are indirectly derived and do not use the geometric path lengths:

$$\tau \neq \frac{L_{eff}}{L_0} \quad (2)$$

Physical tortuosities are determined using effective properties to deduce a tortuosity value indirectly. Therefore, the effects of microstructure such as bottleneck effects are included. A physical tortuosity is only meaningful if it is based on a transport phenomenon that is relevant to the simulated material. Thus, different tortuosities can be determined depending on the dominating transport mechanism: diffusion of molecules or ions, conductivity of electrons, etc.

Consider, for example, the effective diffusion of gas through a porous membrane compared to the gas's self-diffusion. In this case, the diffusion tortuosity is of interest, as described in the DiffuDict user guide. GeoDict can output both, the value for the tortuosity τ and the value of the tortuosity factor κ by comparing the effective diffusion to self-diffusion:

$$\tau_{indir,diff} = \sqrt{\kappa_{indir,diff}} = \sqrt{\frac{\varepsilon}{D_{rel}}} \quad (3)$$

where ε is the porosity and D_{rel} the relative diffusivity due to the porous-media dependent part of the effective diffusion. The numbers τ and κ can be converted in each other by the general relation between them:

$$\tau = \sqrt{\kappa} \quad (4)$$

The available physical tortuosities are:

- **Diffusional Tortuosity** in DiffuDict: Diffusion as indirect, physical approach (see also [Epstein, 1989](#)^[240]). The tortuosity will be extracted from the DiffuDict **Laplace** or **Knudsen** Diffusion result files, respectively.
- **Conduction Tortuosity** in ConductoDict: **Electrical** or **Thermal** conductivity as indirect, physical approach (see also [Ullman et al., 1982](#)^[241]). The tortuosity will be extracted from the respective ConductoDict result file.

✓ Mixed Tortuosity

There are five options available for the **Mixed Tortuosity**. The mixed tortuosities are derived from a mixed determination including the geometrical analysis of streamlines and pathways from simulations of diffusion, flow, advection, etc. The available mixed tortuosities are:

- **Tortuosity from Laplace Diffusion Flux** in DiffuDict (see also [Tye, 1983](#)^[241]): The mean value of the DiffuDict Laplace diffusion flux streamlines and/or the tortuosity is calculated based on the volume average of the DiffuDict Laplace diffusion flux.
- **Tortuosity from Electrical Current Density and Thermal Heat Flux** in ConductoDict: The mean value of the streamline length of the ConductoDict streamlines and/or the tortuosity is calculated based on the volume average of the electrical current density and thermal heat flux.
- **Tortuosity from Stokes Flow Velocity** in FlowDict (see also [Duda et al., 2011](#)^[240]): The mean value of the streamline length of FlowDict Stokes flow velocity streamlines and/or the tortuosity is calculated based on the volume average of FlowDict Stokes flow velocity.
- **Tortuosity from Advection Particle Path Length** in AddiDict: Computes the mean value of the particle path length for advection.
- **Tortuosity from Particle Diffusion Path Length** in AddiDict: The mean value is calculated based on effective isotropic diffusivity.

✓ Microstructure Characteristics

In addition to the different tortuosities, the **Compute Tortuosity** GeoApp can calculate **Microstructure characteristics**. Three options are available:

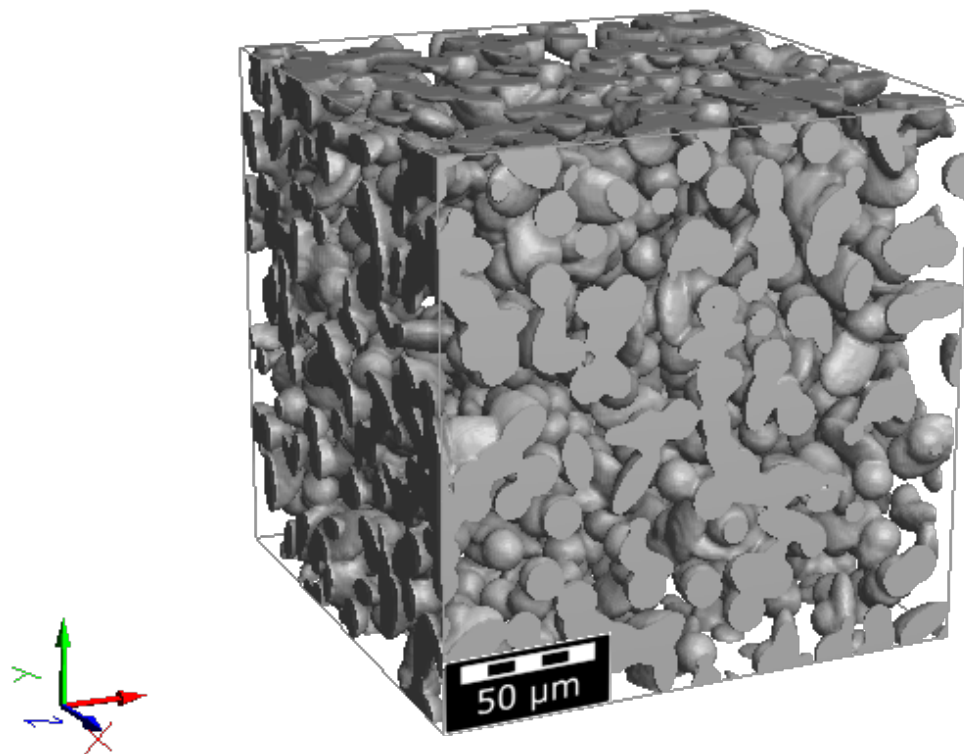
- **Characteristic Diameters from Granulometry** in PoroDict: Computing D10, D50, and D90.
- **Characteristic Diameters from Porosimetry** in PoroDict: Computing D10, D50, and D90.
- **Surface Area** in MatDict: Specific surface area between pore space and solid materials.

Results

Below the exemplary results for the following structure are shown.

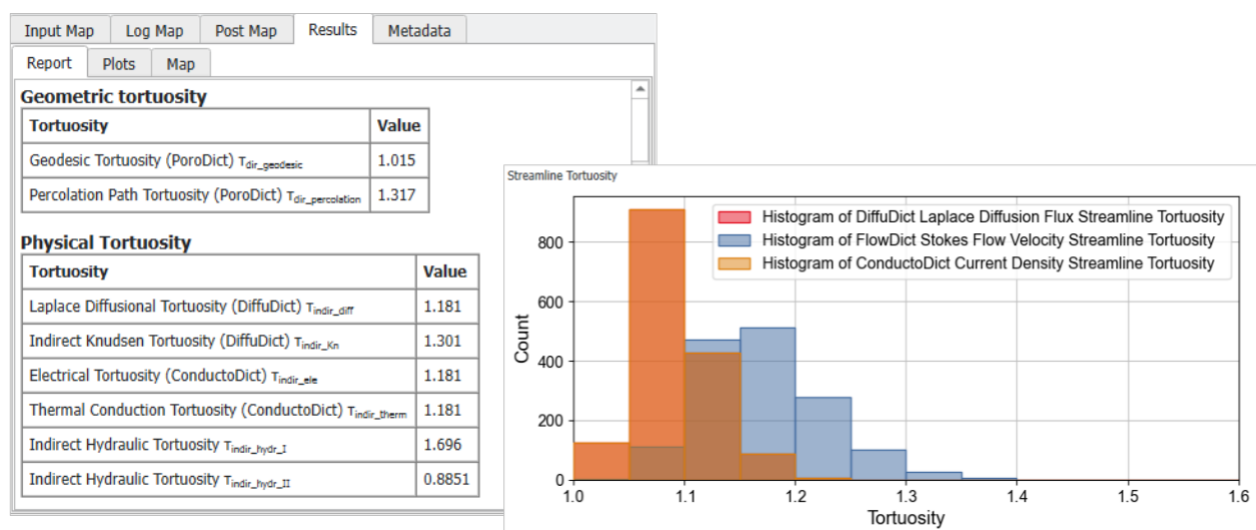
Material Information:

-  ID 00: Air [invis.]
-  ID 01: Solid

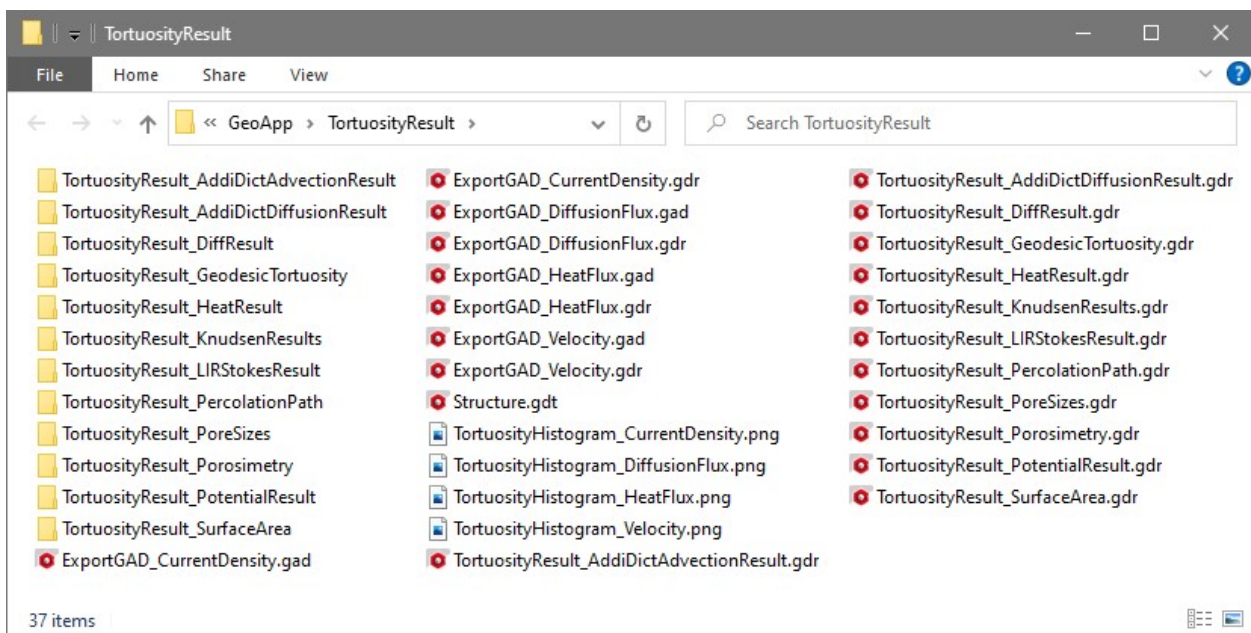


The result file's **Result Viewer** opens automatically when the **Compute Tortuosity** app finishes. The result file provides detailed information about the formulas used to calculate the different tortuosities, the microstructure characteristics, the pore phase and transport properties, as well as those used to predict effective transport properties.

Depending on the selection in the **Compute Tortuosity** parameter dialog, the respective results are given in tables. If the calculation of the tortuosity based on streamlines was selected, the evaluation of streamline length is shown as a **Streamline Tortuosity** plot.



Additionally, the corresponding result folder contains the detailed GeoDict results for all selected tortuosity computations.



Compute Fractal Dimension

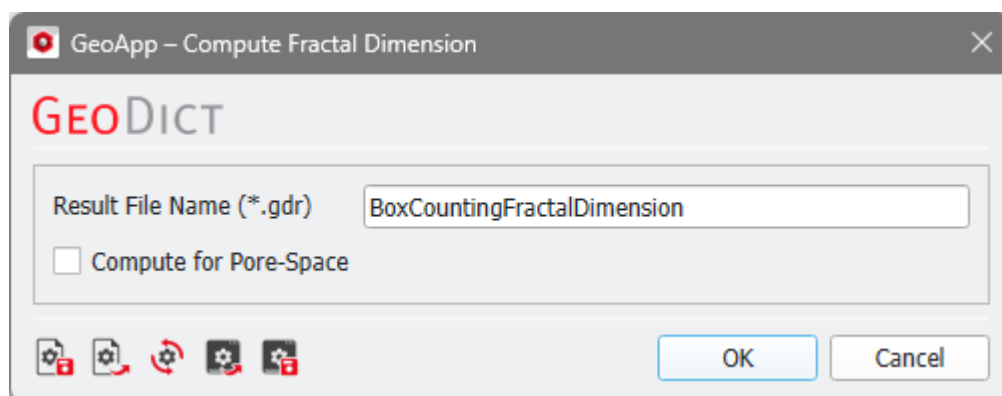
The **Compute Fractal Dimension** GeoApp calculates the fractal dimension of the solid materials or the pore space of a loaded geometry. It mathematically describes the complexity of the current structure by analyzing how it changes in detail with respect to a change in scale. The used method is the box-counting algorithm. The fractal dimension is another measure for microstructures and is used, e.g., to characterize carbon particle agglomerates. The GeoApp executes the MatDict command 3D Inhomogeneity several times with increasing side length of the boxes.



Modules needed to run this GeoApp:

Porodict

Click **Edit** to open the **Compute Fractal Dimension** parameter dialog.



Select a **Result File Name**, then decide whether to compute the fractal dimension for the pore

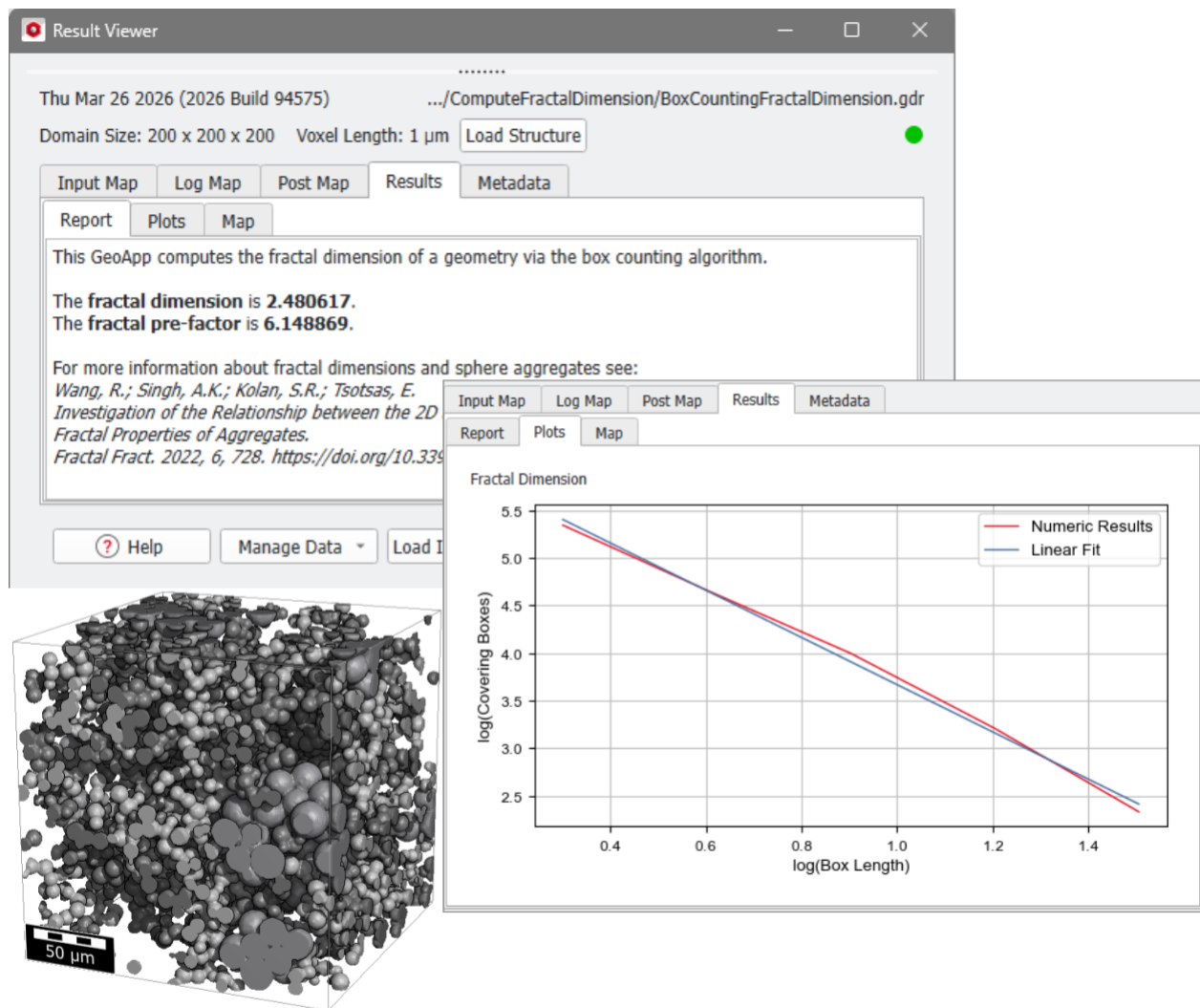
space or solid materials by checking or unchecking **Compute for Pore-Space**, respectively.

Results

The result file opens in the **Result Viewer** when the **Compute Fractal Dimension** app is finished.

The result file shows the **fractal dimension** and the **fractal pre-factor** described by [Wang et al. \(2022\)](#).

In the plots tab find the fractal dimension visualized in a 2D plot.



Identify Fractures

The **Identify Fractures** GeoApp analyzes the pore morphology and segments the selected material ID into fractures, small, and large pores. The GeoApp applies multiple runs of Identify Pores and its corresponding post-processing to distinguish between pores and fractures.



Modules needed to run this GeoApp:

Porodict

Click **Edit** to open the **Identify Fractures Parameters** dialog.

The **Identify Fractures** GeoApp has two main features. The first feature, **Separate fractures from pores by the following features**, segments the selected **Pore/Fracture Material ID** into fracture and pore phases. The second feature, **Segment pore sizes**, allows differentiation between small and large pores. When both features are activated, differentiation of pore sizes is performed only on the pore phase, not the fracture phase.

GeoApp – Identify Fractures

GEODICT

Result File Name (*.gdr)

Pore/Fracture Material ID

☒ Separate fractures from pores by the following features

☒ Start from previous run with identical Result File Name

☒ Use Surface to Volume Ratios

Apply threshold of (fracture <):

☒ Use Krumbein Sphericities

Apply threshold of (fracture <):

☒ Use Sheppard Sphericities

Apply threshold of (fracture <):

☒ Use Aspect Ratio

Apply threshold of (fracture <):

Post Processing

Number of features that must apply (>=)

☒ Obtain Properties of the identified Fracture

Parameters for Pore Separation

☒ Segment Pore Sizes

Separate small from large Pores By

For fracture identification, void spaces in a structure are considered fractures if the values are below the chosen **Threshold** for each parameter. These parameters can be modified if necessary. The default threshold values may already correctly segment fractures. To improve the results, adjust the threshold values according to the current structure. In the **Post Processing** section, choose the **Number of features** required to identify a fracture phase. This number must always be smaller than or equal to the number of activated features. When

Obtain properties of the identified fracture is activated, an additional instance of **Identify Pores** is executed on the previously identified fractures.

If the **Identify Fractures** GeoApp is executed on a structure but the segmentation needs improvement, it should be re-executed iteratively to obtain the best result. This can be done by re-running the app with different values until a sufficient result is achieved. To save time, activate **Start from previous run with identical Result File Name**. This skips the first **Identify Pores** instance and uses the previously created *.gdr file to execute post-processing.

Click **OK** to close the dialog, go back to the GeoApp section, and click **Run**.

Results

When the computation is finished, and the checkbox of **Obtain properties of the identified fracture** is checked, the **Result Viewer** of the result file (*.gdr) opens automatically. Find the results in the **Results - Report**, **Results - Plots**, and **Pore Visualization** tabs. The result file is created using PoroDict - Identify Pores.

The screenshot shows the PoreFind Result Viewer interface. At the top, there are tabs: Input Map, Log Map, Post Map, Results (selected), Pore Visualization, Create Videos, and Metadata. Below these, there are sub-tabs: Report (selected), Plots, and Map. The main content area displays the following information:

PoreFind

Main results

- Number of pores: **40100**.
- Number of pore contacts: **516** (total pore contact area: 2.59666 mm²).
- The index image "**Pores.g32**" contains the identified pores with their pore tags. These tags are integers ranging from 1 to 40100.
- All mean values, all standard deviations, all D10 values, all D50 values, all D90 values, and all histogram values are calculated by **weighting** with the **pore volume**. The weighting can be changed in the post-processing widget.

Pore volume percentage statistics

Step	Pore volume percentage
Initial Pore Structure	13.2683 %
Watershed with minimal diameter	13.2683 %
Pore reconnection	13.2683 %

Pore volume statistics

	Minimum	Maximum	Mean value	Standard deviation
Volume	28652.6 μm ³	12.1901 mm ³	4.02416 mm ³	4.57397 mm ³

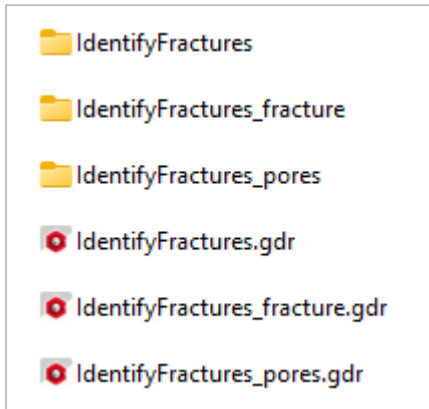
Three result files and result folders are generated and can be found in the main result folder.

The prefix is based on the chosen **Result File Name** (default is IdentifyFractures). The **IdentifyFractures** folder contains the results of the Identify Pores instance which was executed

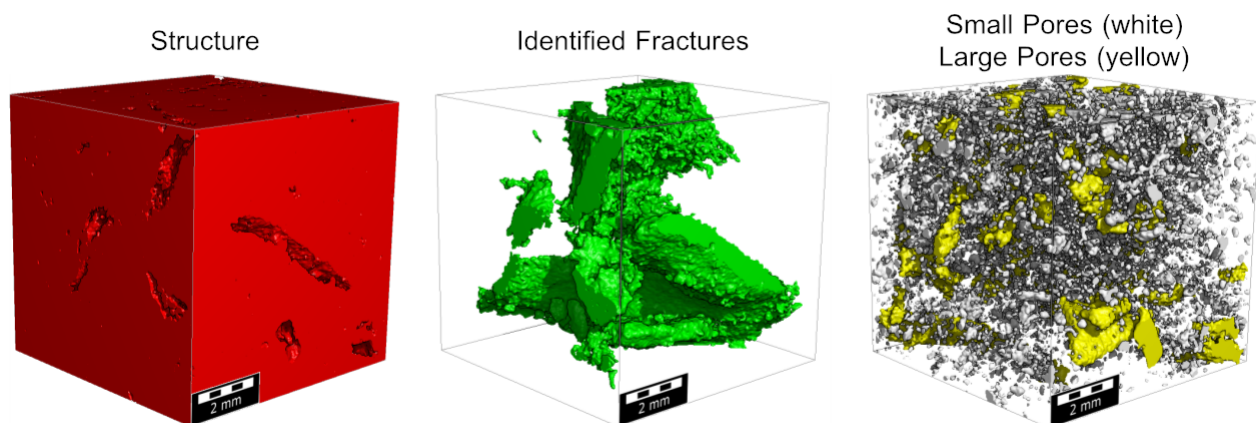
on the structure. The thresholding of the fractures by features, is executed on the contained IdentifyFractures.gdr.

When **Obtain properties of the identified fracture** is activated, the IdentifyFractures_fracture folder contains results of the respective **Identify Pores** run.

When **Segment pore sizes** is activated, the pores in the structure are segmented by their **Volume** or **Equivalent diameters** (IdentifyFractures_pores). In this case, the folder IdentifyFractures_pores is created which contains the Identify Pores run performed on the pores.



The following example shows how fractures and pores can be separated. The pore space belonging to an identified fracture is assigned to the corresponding material phase. The remaining pore space, which does not belong to a fracture, is divided into large and small pores based on their **Volume** or **Equivalent diameters**.



1.1.2 Physical Properties

Use the **Physical Properties** GeoApps to calculate various physical properties of your structure.

Topics of this section

- [Air Permeability Test](#)^[19]
Compute the air volume that passes through your structure per time and surface area.
- [Concentration Dependent Diffusivity](#)^[21]
Approximate a diffusion process where the local diffusivity depends on the concentration of

Topics of this section

the diffusing species.

- [Stiffness Estimation](#)²³
Estimate the stiffness for one constituent material, if the stiffness of the complete structure is known.
- [Upscaling Mercury Injection Capillary Pressure](#)²⁵
Conduct a MICP experiment for structures containing both resolved and unresolved porous materials.
- [Upscaling Relative Permeability](#)²⁹
Predict relative permeability and capillary pressure curves for structures containing both resolved and unresolved porous materials.
- [Hysteresis](#)³²
This GeoApp executes the drainage and imbibition algorithms alternately.
- [Contact Detachment](#)³⁶
Simulate the detachment of contacts between objects.
- [Material Dissolution](#)⁴⁴
Simulate the dissolution of your structure.

Air Permeability Test

Air Permeability is an important factor in the performance of textile materials, e.g., gas filters or fabrics for air bags.



Modules needed to run this GeoApp:

FlowDict



Know how! The *air permeability* is the air volume that passes through the media per time and surface area. It therefore has the unit $\text{cm}^3/\text{min}/\text{cm}^2$ or $\text{ft}^3/\text{min}/\text{ft}^2$ and thus describes an average flow velocity through the media at a standardized pressure drop. It is not to be confused with the material property *permeability* that is used in Darcy's law which has the unit m^2 or Darcy.

Select **Air Permeability Test** from the pull-down menu and click the **Option's Edit...** button to open a dialog to enter or edit the simulation options. Choose a **Result File Name** for the result file (*.gdr) fitting to your current project.

Input Mode

Two different **Input Mode** are available to prescribe the pressure drop for the simulation. Either enter a pressure drop manually or select one of the norms that define a pressure drop

for the measurement. The pressure drop is applied in Z-direction on the current 3D structure.

Input Mode: Manual
Pressure Drop / (Pa): 125

Input Mode: Permeability_Norm
Permeability Norm: ASTM D737-18 125 Pa

ASTM D737-18 125 Pa
DIN EN ISO 9073-15:2008-08 100 Pa
DIN EN ISO 9073-15:2008-08 125 Pa
DIN EN ISO 9073-15:2008-08 200 Pa
ISO 9237:1995 50 Pa
ISO 9237:1995 100 Pa
ISO 9237:1995 200 Pa
ISO 9237:1995 500 Pa

Computation Method: Direct Simulation

If you select **Direct Simulation** as **Computation Method**, the Navier-Stokes command is used to simulate the air flow at the prescribed pressure drop. The boundary conditions and all solver parameters are automatically selected by the app.

Result File Name (*.gdr): AirPermeabilityTest-ISO-500Pa-Direct.gdr
Input Mode: Permeability_Norm
Permeability Norm: ISO 9237:1995 500 Pa
Computation Method: Direct_Simulation

You can find the computed air permeability in the first line of the report.

Report Plots Map

Z-direction

Air permeability at 500 Pa: 547.338 cm³/s/cm², or 1077.43 ft³/min/ft².
Average (superficial) flow velocity at 500 Pa: 5.47338 m/s.
Volume flow rate: 5473.38 l/(s m²)
Reynolds number 12.0681 for characteristic length 3.35857e-05 m.
Asymptotic estimate of average flow velocity: 5.47814 m/s.

Computation Method: Forchheimer Approximation

If the media has a low flow resistivity, the air velocities may become very high at the prescribed pressure drop. In some cases, the flow might become turbulent, and the **Direct Simulation** might not converge. In these situations, select **Forchheimer Approximation** as

Computation Method.

Select two lower pressure drops (**Pressure Drop 1** and **Pressure Drop 2**), which will be used for the extrapolation. The first value can be very small, but the second can be selected as high as possible (but low enough that convergence of the solver is still achieved).

The screenshot shows a web form with the following fields and values:

- Result File Name (*.gdr): AirPermeabilityTest-ISO-500Pa-Forchheimer.gdr
- Input Mode: Permeability_Norm
- Permeability Norm: ISO 9237:1995 500 Pa
- Computation Method: Forchheimer_Approximation
- Pressure Drop 1 / (Pa): 10
- Pressure Drop 2 / (Pa): 100

The app uses the Navier-Stokes command to simulate the air flow at the prescribed pressure drops. The boundary conditions and all solver parameters are automatically selected by the app. Afterwards, the app uses the Forchheimer Approximation command to estimate the air permeability. You can find the result at the bottom of the report. Note, that the air permeability is reported as velocity in m/s here.

The screenshot shows the 'Report' tab of the GeoApp interface. The report content is as follows:

Forchheimer equation for predicted Experiment:
 $\Delta P = 67.6922 u + 3.98417 u^2$

For $-dp/dx = \mu u/\kappa + \rho u^2/\kappa_1$
where κ is Darcy permeability, κ_1 is inertial permeability, μ is dynamic viscosity, ρ is fluid density, and L is medium thickness.

Darcy permeability $\kappa = \mu * L / f1 = 1.834e-05 * 0.001 / 67.6922 \text{ m}^2 = 2.70932e-10 \text{ m}^2$.
Inertial permeability $\kappa_1 = \rho * L / f2 = 1.204 * 0.001 / 3.98417 \text{ m} = 0.000302196 \text{ m}$.

The estimation is 5.56417 m/s for 500 Pa.

Concentration Dependent Diffusivity

The **Concentration Dependent Diffusivity** script approximates a diffusion process where the local diffusivity depends on the concentration of the diffusing species. This is achieved by using the existing constant diffusivity solver in an iterative process, where the local diffusivity in one iteration depends on the local concentration computed in the previous iteration.



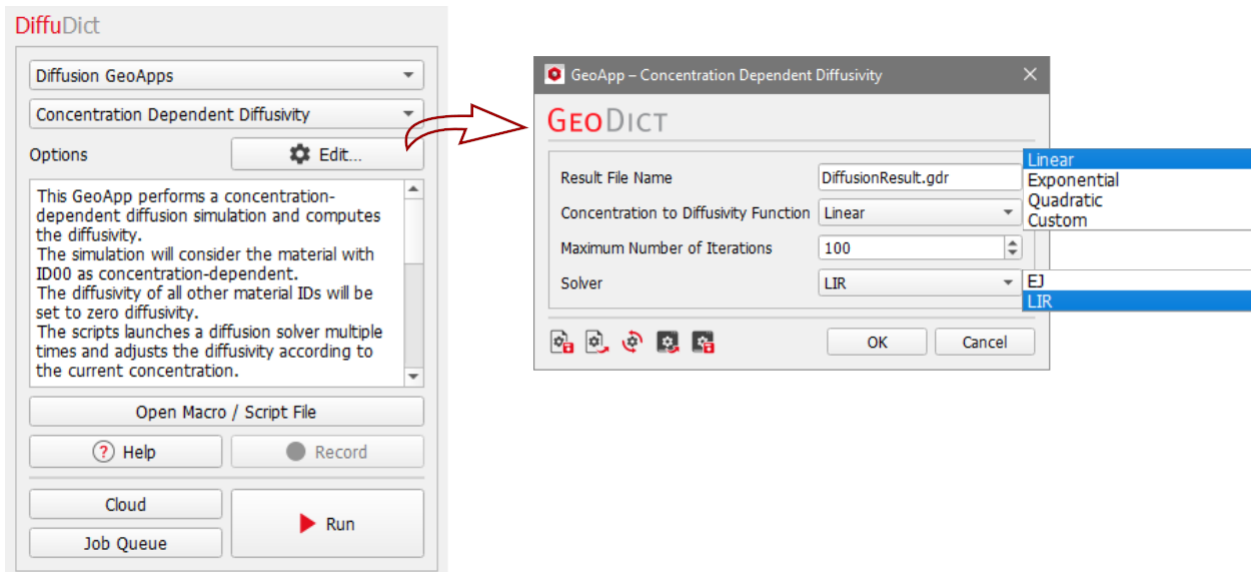
Modules needed to run this GeoApp:

DiffuDict

The window below the selection box shows the description of the script and its input parameters. Click **Open Macro / Script File** to open the underlying Python script in a text editor. Be aware that administrator privileges would be required to change the macro if GeoDict has been installed in the default location for all users.

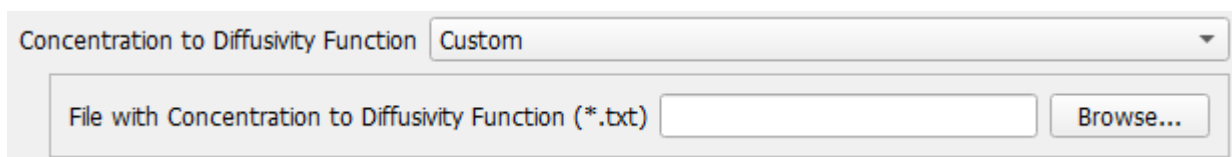
Click **Run** to start the computation. When the simulation is finished, a DiffuDict result file is opened in the **Result Viewer**.

Click **Edit...** to open the dialog to adjust the available parameters.



Under **Concentration to Diffusivity Function**, define how the diffusivity depends on concentration. **Linear**, **Exponential**, and **Quadratic** are predefined concentration to diffusivity functions. These predefined functions are stored as text file in the GeoDict installation folder in the subfolder `c:\Program Files\Math2Market GmbH\GeoDict 2026\GeoApps\General\Physical Properties\DiffusivityFuncs`.

If you want to define your own concentration to diffusivity function select **Custom**.



Create a text file (*.txt) describing the relationship between diffusivity value (D_i) and concentration value (u_i) as follows:

```
QuadraticDiffusivity.txt
1 u_i 0.1, 17817.94801, 23757.26402, 31676.35202, 42235.13603, 56313.51471, 75084.68628,
2 D_i -1, 0.000317479, 0.000564408, 0.001003391, 0.001783807, 0.003171212, 0.00563771,
```

For example, copy one of the predefined files to a project specific file location and edit it in a text editor. Since the diffusivity is given in bins of a specific range, the number of elements differs by 1 with respect to the number of concentration values. Therefore, the diffusivity value-pairs must start with a sentinel, e.g., (0.1, -1), followed by the desired values. Due to the iterative process described below, after the sentinel 15 different value pairs must be given.

The **Maximum Number of Iterations** can be specified in order to increase the degree of

convergence. For the solver choose between the **EJ** and the **LIR** solvers.

The effective diffusivity of the material for the chosen concentration difference is always computed in z-direction according to

$$\text{div}(D(u)\nabla u) = 0 \quad (5)$$

Here, u is the concentration and D the concentration-dependent diffusivity. For the surfaces, no-slip boundary conditions are applied. In Z-direction, constant Dirichlet-boundary conditions are applied where the constants are taken from the given diffusivity file as minimum and maximum values. In the tangential directions, symmetric boundary conditions are used. The solution to the non-linear equation (5) is found in an iterative manner by dividing the pore space into 15 different materials according to the values of u and assigning diffusivity, then solve a linear approximation to (5) for u and repeat until convergence is reached, i.e., when the distribution of the materials does not need to be adjusted anymore for the newly computed u .

Please contact support@math2market.de for more help and information regarding concentration dependent diffusivity simulations, if you are interested in this topic.

Stiffness Estimation

The **Stiffness Estimation** GeoApp estimates the stiffness for one constituent material, if the stiffness of the complete structure is known.



Modules needed to run this GeoApp:

ElastoDict-FeelMath

Click **Edit...** to open the **Stiffness Estimation Parameters** dialog .

The result file name can be entered in **Result File Name (*.gdr)**.

The **Compute Direction** (X, Y, or Z) for the stiffness and the **Orientation Mode** are defined in their drop-down menus. Refer to the ElastoDict Deformations solver settings for more details. In this example, the stiffness in Z-Direction of material with ID 01 is estimated.

The material stiffness of the structure in the given direction is set in **Target Stiffness in given Direction / (GPa)**.

Enter the ID number of the material for which the stiffness should be estimated in **Estimate Stiffness for Material ID**.

The stopping criteria is defined in **Tolerance / (%)**. If the relative error for the estimated structure stiffness is smaller than the specified tolerance, the estimation stops.

After all parameters are set, click **OK** to close the **Stiffness Estimation** parameters dialog and click **Run** to start the estimation.

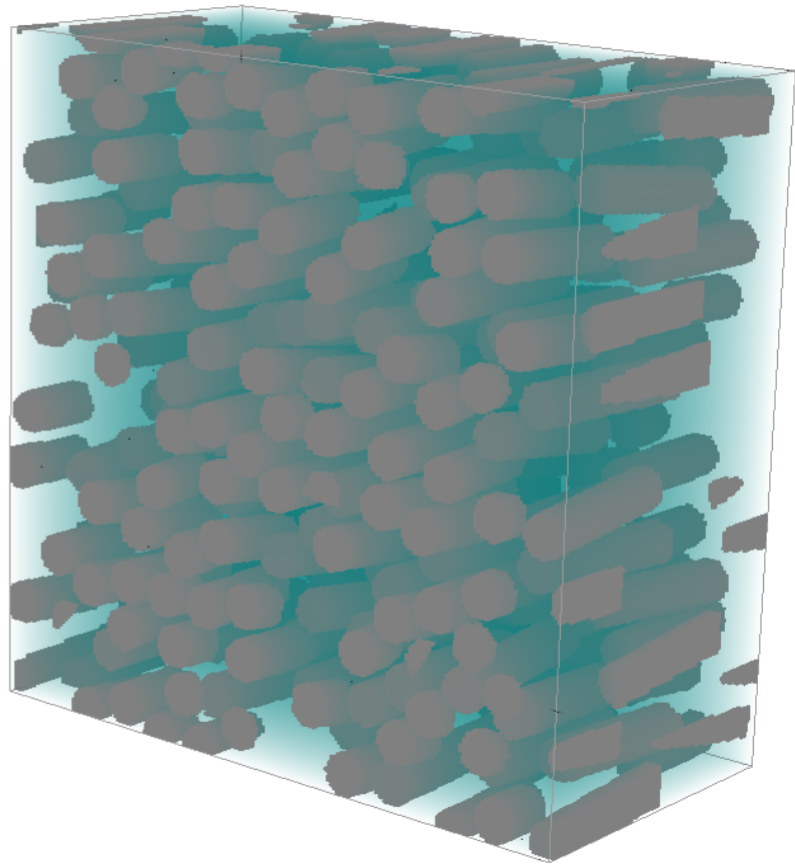
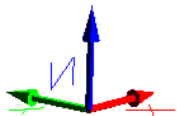
Results

The estimation result is documented among others in the **Results** tab of the **Result Viewer**. The table shown in the **Report** tab summarizes the GeoApp results. In addition to the user-defined target stiffness of the structure, the stiffness reached during the fitting process is shown.

Input Map	Log Map	Post Map	Results	Data Visualization	Metadata
Report Map					
Estimate stiffness for Material00					
Parameter	Value	Unit			
Target Stiffness	7.2	GPa			
Reached Stiffness	7.159	GPa			
Stiffness Deviation	0.5675	%			
Estimated Stiffness for Material00	4.429	GPa			
Number of iterations	2				

In this example, the stiffness of the epoxy matrix (material ID00) of a composite structure is estimated. The table displayed in the **Results - Report** subtab shows that the estimated overall structure stiffness (**Reached Stiffness**) is 7.159 GPa with a defined **Target Stiffness** of 7.2 GPa. The **Estimated Stiffness for Material00**, which is the stiffness for the epoxy matrix, is 4.429 GPa. The fitting process in this example took 3 iterations.

Material Information:
ID 00: Epoxy (3501-6)
ID 01: Glass



Upscaling Mercury Injection Capillary Pressure

The **Upscaling MICP** GeoApp is a comprehensive solution for analyzing complex porous media, effectively bridging the gap between small-scale, detailed experiments and large-scale, practical applications. This capability is essential for improving the precision of simulations, enhancing material performance predictions, and making informed decisions in various industrial and research contexts.

This GeoApp computes the MICP on structures with unresolved porous materials. For those materials, no exact fluid distribution can be calculated as the location of the pores is unknown. However, you can determine or measure the capillary pressure curve of the porous material at a higher scale and use this information for the computations in the GeoApp.



Important! The structure you want to analyze must contain at least one porous material phase.



Modules needed to run this GeoApp:

SatuDict, GeoApp-Upscaling MICP

The screenshot shows a dialog box titled "GeoApp – Upscaling Mercury Injection Capillary Pressure". Inside, the "GEO" part of the "GEO" logo is in red. The dialog contains the following fields and controls:

- Result File Name:** A text box containing "Upscaling Mercury Injection Capillary Pressure".
- Inflow Side:** A dropdown menu showing "All-sides".
- Load .gdrs to assign Capillary Pressure Curves to Porous Materials:** An unchecked checkbox.
- Breakthrough considered at Saturation / (%):** A text box containing "15".
- Parallelization:** A dropdown menu showing "Maximum".
- Buttons:** "OK" and "Cancel" buttons at the bottom right.
- Icons:** A row of five icons (gear, folder, refresh, undo, redo) at the bottom left.

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

Below, choose from which domain sides the mercury may intrude the structure. Either **All-sides** can be chosen, or one specific domain side (e.g., z+) is available.

Next, you have to define from which source the capillary pressure curve values are taken.

✓ **Load .gdrs to assign Capillary Pressure Curves to Porous Materials**

This screenshot shows a detailed view of the section where the checkbox "Load .gdrs to assign Capillary Pressure Curves to Porous Materials" is checked. It contains the following elements:

- MaterialID01 Capillary Pressure:** A text box for "Capillary Pressure (*.gdr)" and a "Browse..." button.
- MaterialID02 Capillary Pressure:** A text box for "Capillary Pressure (*.gdr)" and a "Browse..." button.
- MaterialID03 Capillary Pressure:** A text box for "Capillary Pressure (*.gdr)" and a "Browse..." button.
- Breakthrough Model:** A dropdown menu showing "Saturation".
- Breakthrough considered at Saturation / (%):** A text box containing "15".

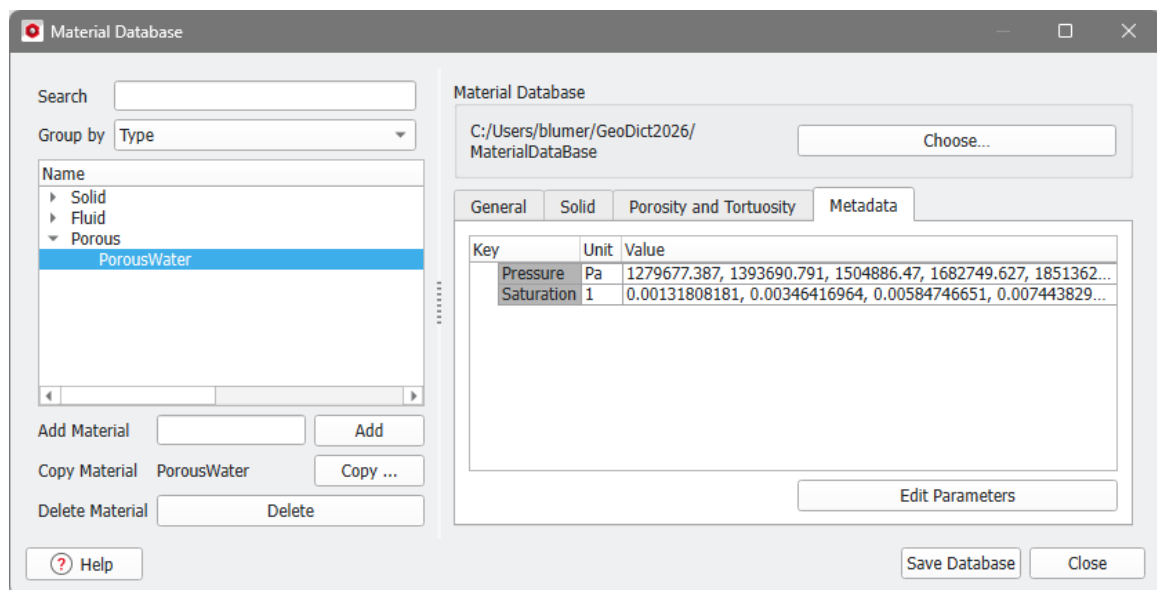
Load pre-computed result files of Capillary Pressure for all porous material phases according to the Material IDs. For the materials you have to specify at which saturation

the porous region is filled enough to establish a continuous pathway through the material securing capillary connectivity.

With the **Breakthrough Model** you decide to either use a fixed **Saturation** (enter the value under **Breakthrough considered at Saturation**), or the **Thomeer** fit based on the Capillary Pressure Curve result files is used.

✓ Define capillary pressure values in the material properties

With this option you have to add and edit the porous material in the Material Database. Enter the pressure and saturation values in the Metadata tab and use the keys **Pressure** and **Saturation**, respectively.

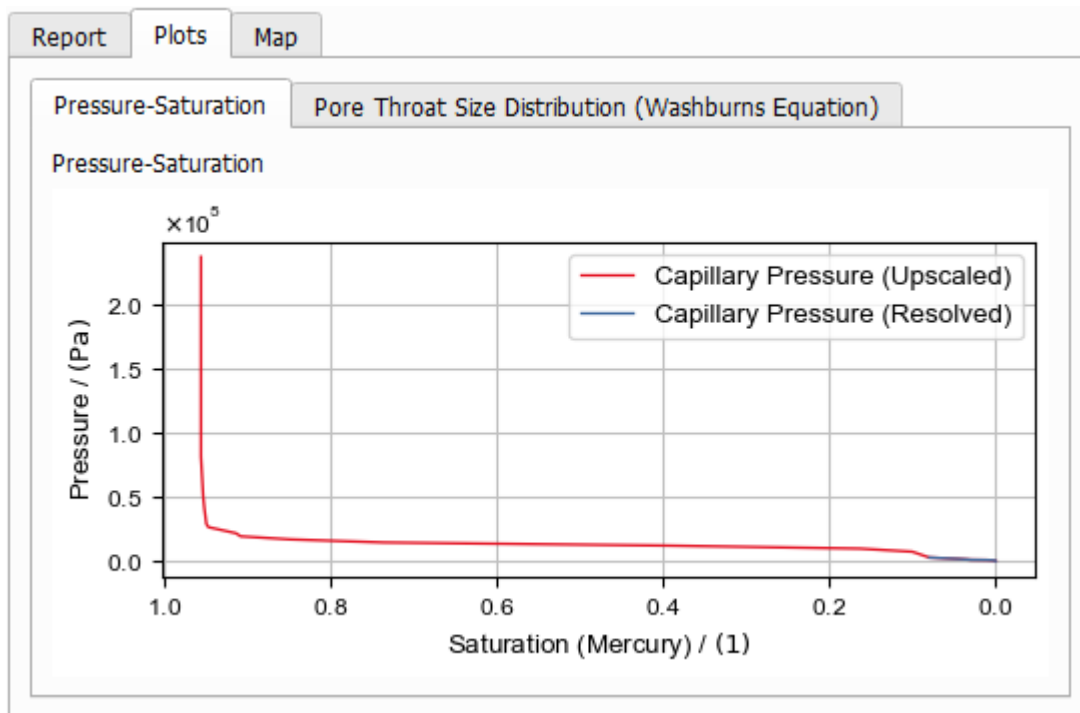


In this case, no choice of **Breakthrough Model** is available, you can only enter a value for **Breakthrough considered at Saturation**.

For the **Parallelization** of the execution either use the **Maximum** number of cores or enter a **Manual** value.

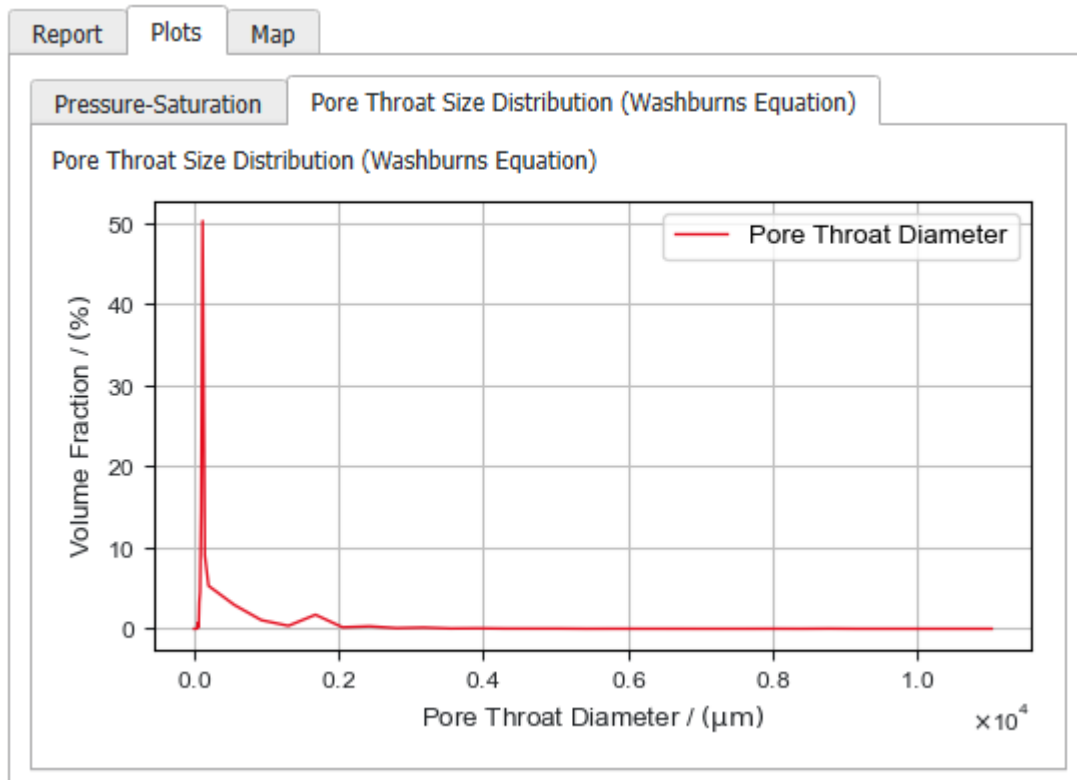
Results

The result file shows the capillary pressure curve, where the resolved part, which could be calculated with the Mercury Porosimetry & Capillary Pressure command, and the upscaled (unresolved) part are marked.



Note! No residual is left in the structure, except the closed pores, which cannot be filled with mercury as they are not connected to any inflow side. Thus, the mercury saturation is not exactly 100%.

Additionally, the pore throat size distribution calculated with the Washburn equation is given as in the result file of the MICP command.



Upscaling Relative Permeability

The **Upscaling Relative Permeability** GeoApp allows you to compute relative permeability and capillary pressure curves for structures containing both resolved and unresolved porous materials. For the unresolved materials you need to pre-compute the capillary pressure curve and relative permeability on a higher resolution scale.



Modules needed to run this GeoApp:

SatuDict, GeoApp-Upscaling Relative Permeability

GeoApp – Upscaling Relative Permeability

GEODICT

Result File Name: UpscalingRelativePermeability

Inflow Side: z-

Invading Fluid: Water (Distilled)...

Displaced Fluid: Air...

Surface Tension: 0.0728

Compute Relative Permeability for Saturations: 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9

Porous Material Properties

MaterialID01

Capillary Pressure (*.gdr): Browse...

Relative Permeability (*.gdr): Browse...

MaterialID02

Capillary Pressure (*.gdr): Browse...

Relative Permeability (*.gdr): Browse...

MaterialID03

Capillary Pressure (*.gdr): Browse...

Relative Permeability (*.gdr): Browse...

Breakthrough considered at Saturation / (%) 15

Fluid Phase

☒ Invading Phase

☒ Displaced Phase

Parallelization: Maximum

OK Cancel

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

Below, choose the **Inflow Side**, which defines from which domain side the invading fluid may enter the structure.

The **Invading Fluid** and the **Displaced Fluid** must be chosen from the Material Selector. Note, that the displaced fluid must be present in the loaded structure.

The **Surface Tension** between the fluids works as described for Capillary Pressure Curve.

To **Compute Relative Permeability for Saturations** you enter the saturations as comma separated list. They work in the same way as for the Relative Permeability command.

For the **Porous Material Properties** you have to load a Capillary Pressure Curve and a Relative Permeability result file (*.gdr) for each of the porous material phases. Up to three porous materials can be present in the structure and they have to be assigned the Material IDs 01, 02, or 03.



Important! We strongly recommend, that the capillary pressure curve result files are computed with the same fluids and surface tension as entered in this dialog. Otherwise the phase distribution and thus the permeability may not be correct. The contact angles of the fluids are taken from the capillary pressure curve result files.



Important! For the relative permeability result files select the computational direction according to the Inflow Side you want to choose in this dialog. This means if you choose **z-** as inflow plane, you have to compute the relative permeability in **Z** direction.

The two parameters, **Breakthrough considered at Saturation** and **Parallelization** are explained in Upscaling Mercury Injection Capillary Pressure.

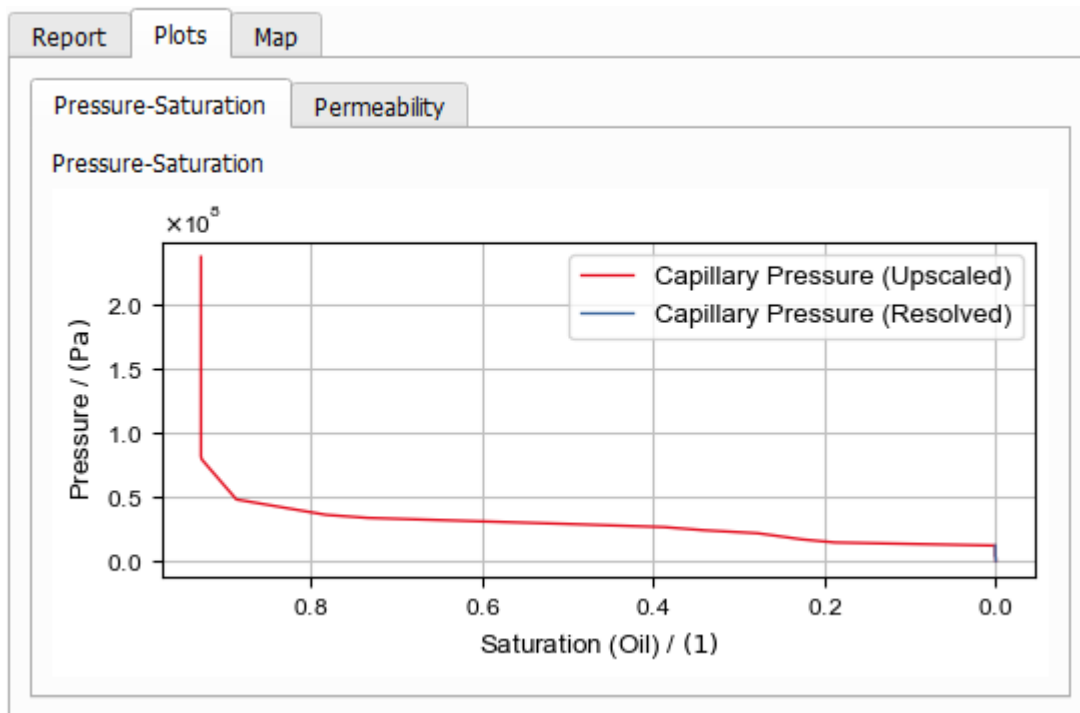
Additionally, you can check whether the Relative Permeability should be computed for the **Invading Phase** and/or the **Displaced Phase**.

During the calculation, first a capillary pressure curve is computed, where the displaced fluid can leave a residual. For the resolved pores, the saturation points from this run are taken for the relative permeability calculation, where the entered saturation points are approximated as in the Relative Permeability command.

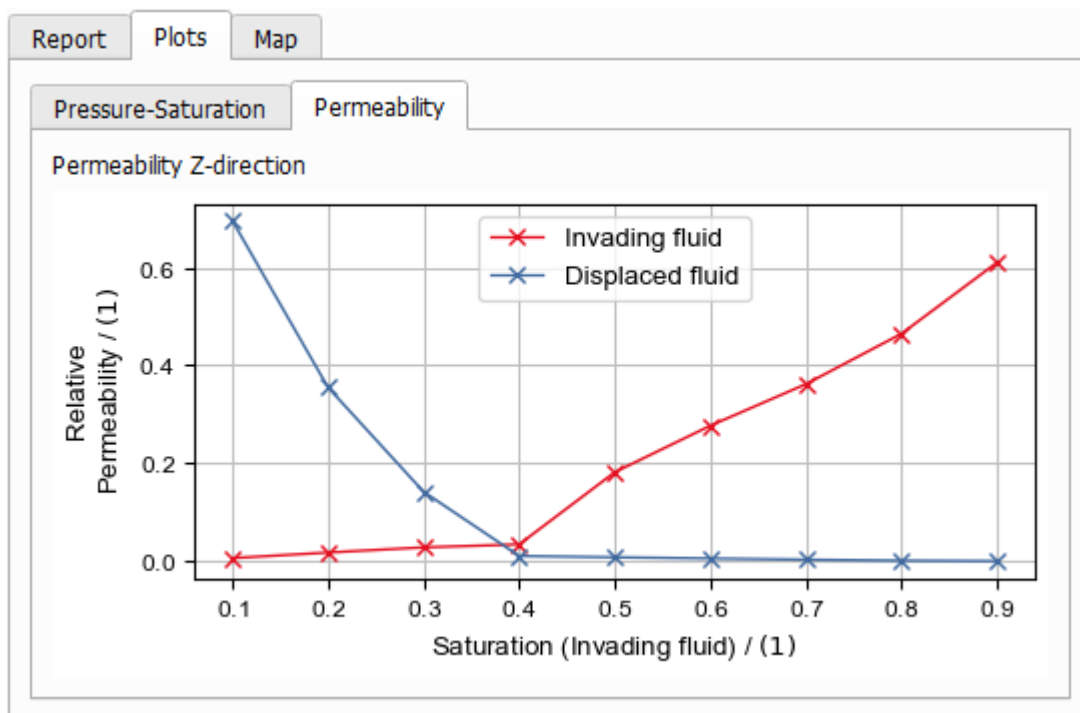
For the unresolved porous materials, the input result files are used for the capillary pressure curve and the relative permeability values.

Results

In the result file, the **Pressure-Saturation** plot shows the capillary pressure curve with the parts for the resolved and unresolved parts similar as in the Upscaling MICP GeoApp.



The **Permeability** plot is the same as for the Relative Permeability Plot.



Hysteresis

The **Hysteresis** GeoApp performs a hysteresis simulation of the SatuDict functionalities Drainage and Imbibition (both with invading fluid connected to a reservoir and the displaced fluid can leave a residual) in succession. This GeoApp repetitively runs the Capillary Pressure command in the same way as it was explained in Capillary Pressure with Hysteresis Effect until the chosen **Number of Cycles** is reached.



Modules needed to run this GeoApp:

SatuDict

After clicking **Edit...**, enter the **Hysteresis Result File Name** and the necessary parameters.

GeoApp – Hysteresis

GEO DICT

Hysteresis Result File Name (*.gdr)

Hysteresis Cycle

Number of Cycles

☒ Start with Drainage

☐ Use Dynamic Pore Morphology

Fluid phases

Wetting Phase

Non-Wetting Phase

Capillary Pressure Curve computation - Parameters

Interfacial Tension / (N/m)

Contact Angle Mode

Contact Angle for Material ID 1 / (°)

Contact Angle for Material ID 2 / (°)

Contact Angle for Material ID 3 / (°)

Contact Angle for Material ID 4 / (°)

Boundary conditions

Drainage - invading phase boundary

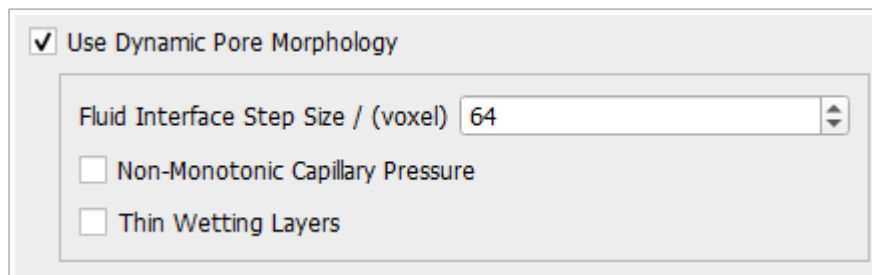
Imbibition - invading phase boundary

Parallelization

✓ Hysteresis cycle

Enter the desired **Number of Cycles**, which means the number of SatuDict computations. The minimum value is 2, so that at least one drainage and one imbibition simulation will be performed. Check the box **Start with Drainage?** to first compute a drainage simulation, otherwise an imbibition will be simulated at the beginning. In the example shown above, 3 SatuDict simulations are done: first a drainage, followed by an imbibition, and finally a secondary drainage.

You can decide to **Use Dynamic Pore Morphology**, which has the same options as in the Capillary Pressure Curve command. Additionally, you can set the **Fluid Interface Step Size** as in the Solver Parameters tab of Capillary Pressure Curve.



✓ Fluid phases

With **Wetting Phase** and **Non-Wetting Phase** select the fluids involved.



Important! If you start the computations with a **Drainage** simulation, the **Wetting Phase** must be present in the loaded structure. Similarly, if you decide to start with an **Imbibition** simulation, the **Non-Wetting Phase** has to be present at the beginning. The reason is, that in the simulations the corresponding fluid will be displaced.

✓ Capillary Pressure Curve computation - Parameters

Set the **Interfacial Tension**, the **Contact Angle Mode**, and the **Contact Angle** with respect to the **Wetting Phase** for up to four solid material phases. The parameters are similar to those from Capillary Pressure Curve, except that the contact angle mode Constant Contact Angle is not available here.

✓ Boundary conditions

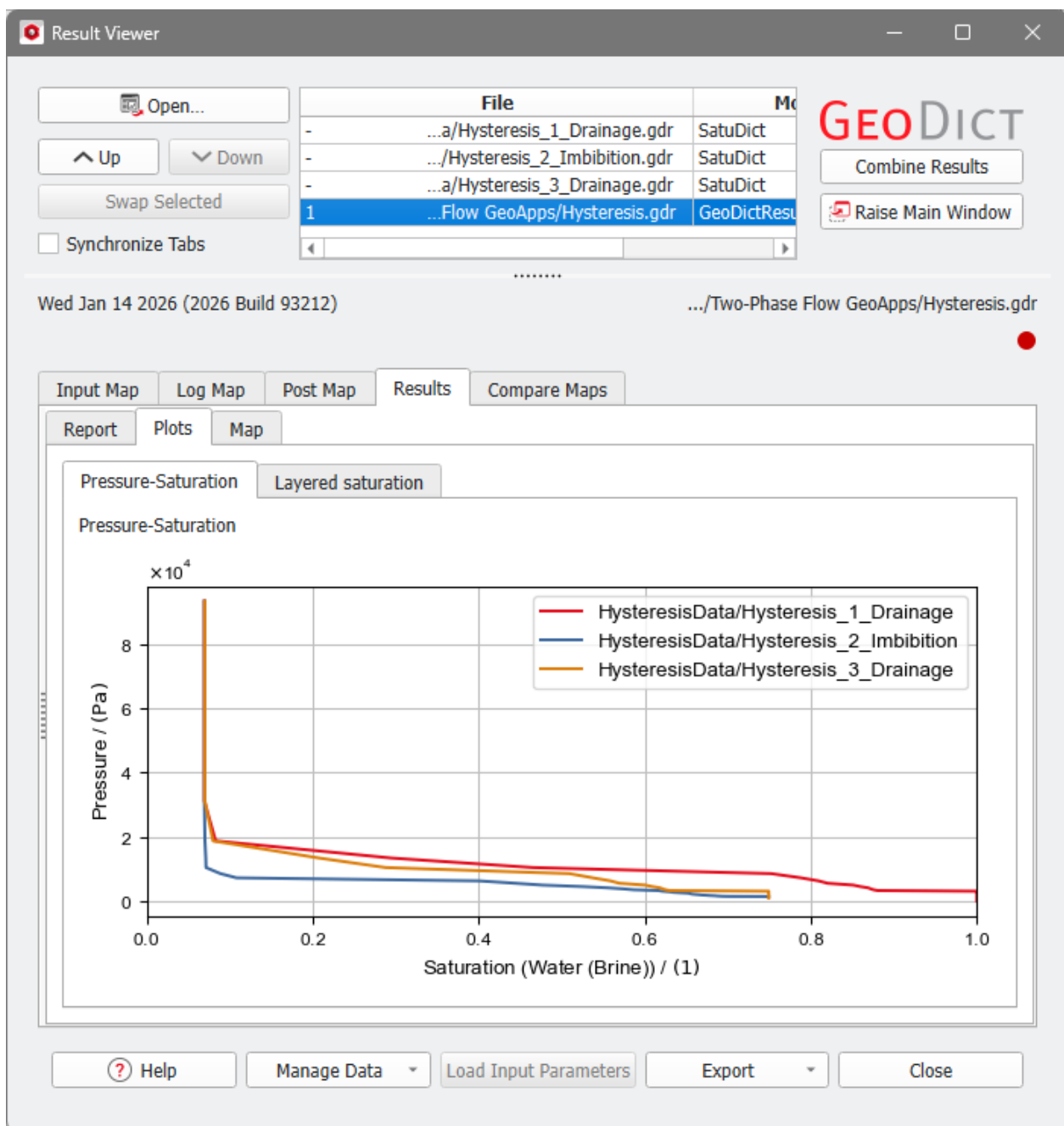
Select the **invading phase boundary** for both Drainage and Imbibition. The other five domain boundary sides are set to **Displaced Fluid Outlet** (see also Boundary Conditions).

✓ Parallelization

Choose to compute with **Maximum** parallelization or set a **Manual** number of threads.

Results

After the **Hysteresis** computation has finished, the Result Viewer opens. The Header section box lists all the Imbibition and Drainage result files of each cycle. The hysteresis result file is an automatically combined result file showing the Pressure-Saturation curves in a single plot.



Contact Detachment

The **Contact Detachment** GeoApp allows using the work in progress version of the contact detachment feature. With this feature, it is possible to simulate detaching of contacts between objects in ElastoDict - Deformations simulations.



Modules needed to run this GeoApp:

ElastoDict-FeelMath

Click **Edit...** to open the **Contact Detachment** parameters dialog.

GeoApp – Contact Detachment

GEO DICT

Experiment Type:

Result File Name (*.gdr):

Uniaxial Experiment:

Tensile Strain / (%):

Tensile Steps:

Load Direction:

☒ Keep Gray Value Image

Resampling:

☒ Allow Contact Detachment

☒ Detach Initial Contacts

☒ Calculate Surface Normals

Contact Penalty Factor:

Shear Contact Penalty Factor:

Object Mode:

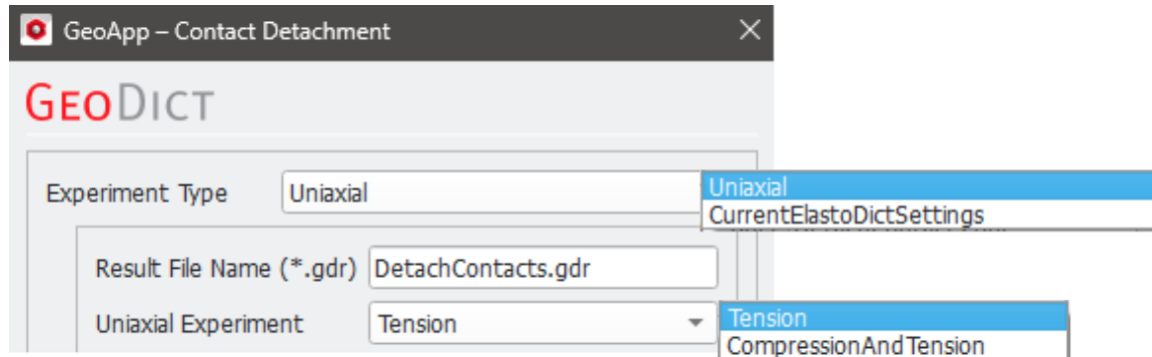
☐ Adaptive Time Steps

☒ Analyze Geometry

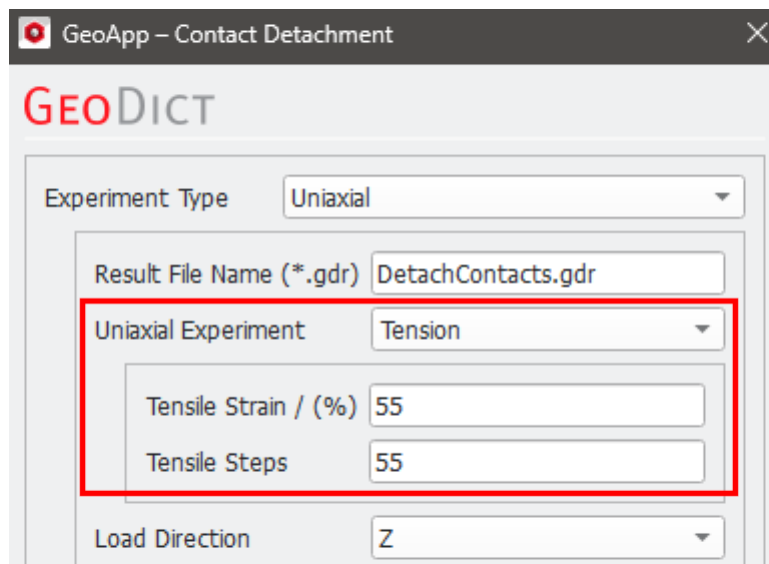
OK Cancel

✓ Experiment Type

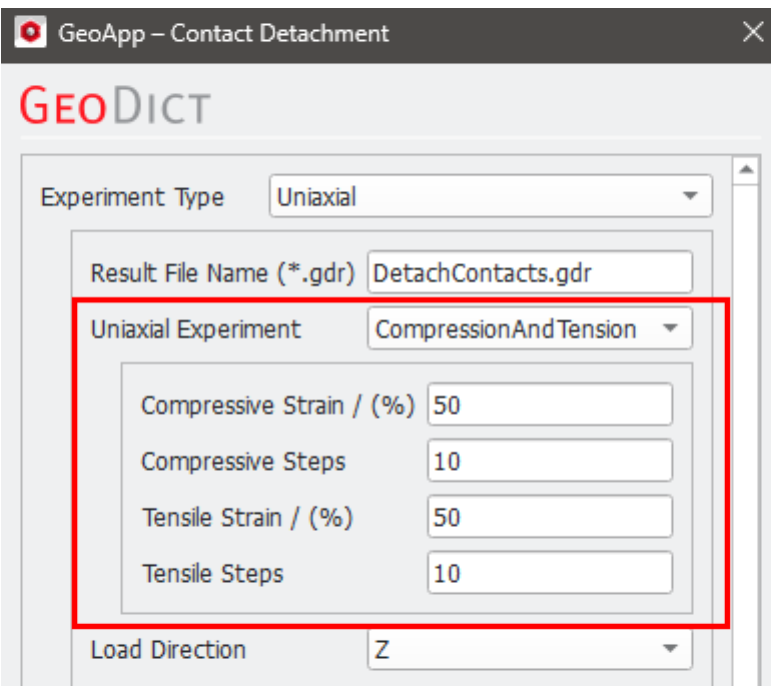
In the GeoApp it is either possible to directly set a uniaxial tensile experiment, a combined compressive/tensile experiment, or to use the current settings of ElastoDict Deformations.



The tensile experiment is chosen by selecting **Tension** in the dropdown menu. The experiment is defined by the maximal tensile strain (in percentage with respect to the original geometry) and the number of steps to apply this strain.



For the **Compression and Tension** experiment, a compression is applied to the geometry, followed by a tension. Again, both deformations are defined by the maximal strain (in percentage with respect to the original geometry) and the number of steps for each deformation.



GeoApp – Contact Detachment

GEODICT

Experiment Type: Uniaxial

Result File Name (*.gdr): DetachContacts.gdr

Uniaxial Experiment: CompressionAndTension

Compressive Strain / (%): 50

Compressive Steps: 10

Tensile Strain / (%): 50

Tensile Steps: 10

Load Direction: Z

☒ Keep Gray Value Image

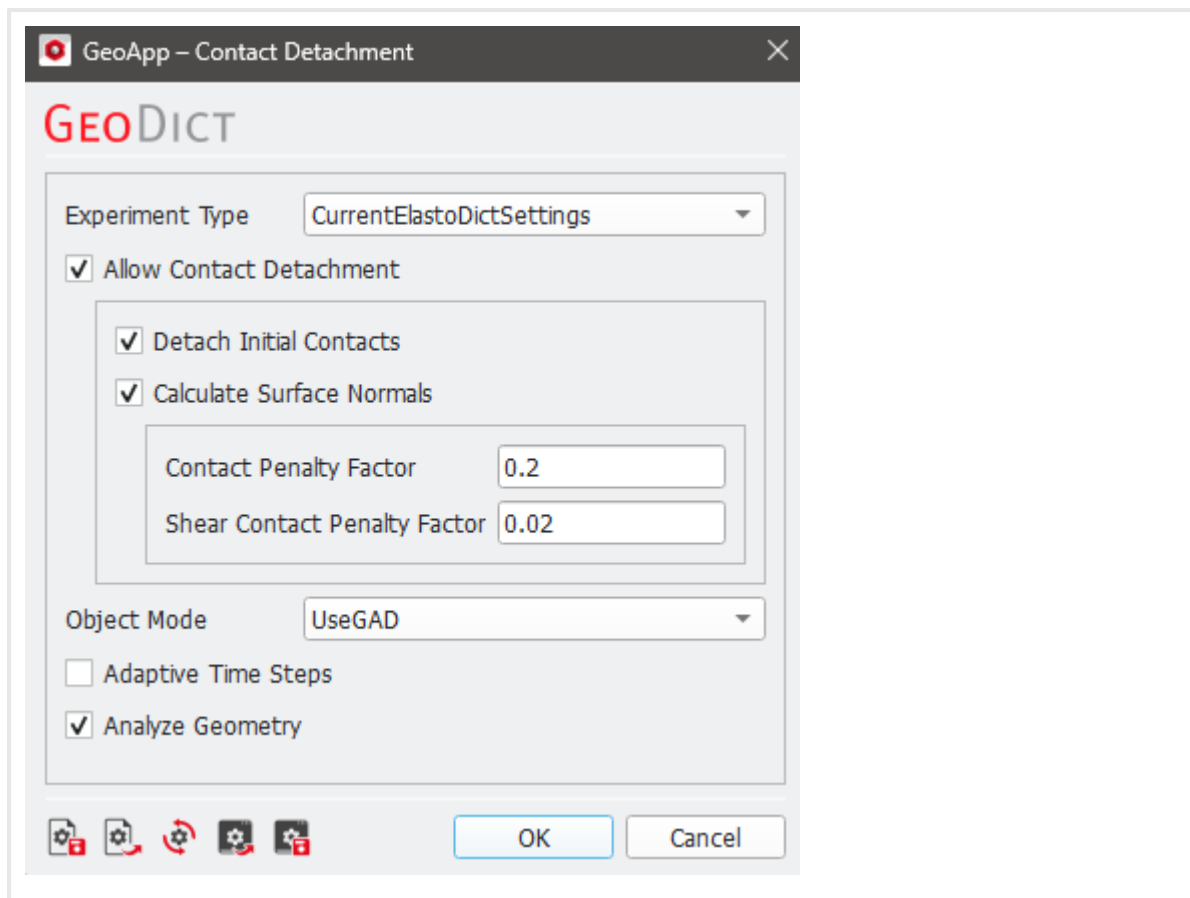
Resampling: Automatic

For both experiments the **Load Direction** can be chosen (X, Y, or Z).

To keep the accurate volume fraction information for each material ID and update these in the memory, the **Keep gray value image** box can be checked. Although this option requires more memory, it results in more accurate deformation of the geometry if many small steps are computed. If this option is not chosen the volume fractions are segmented into a structure in each deformation step and the volume fraction information is lost.

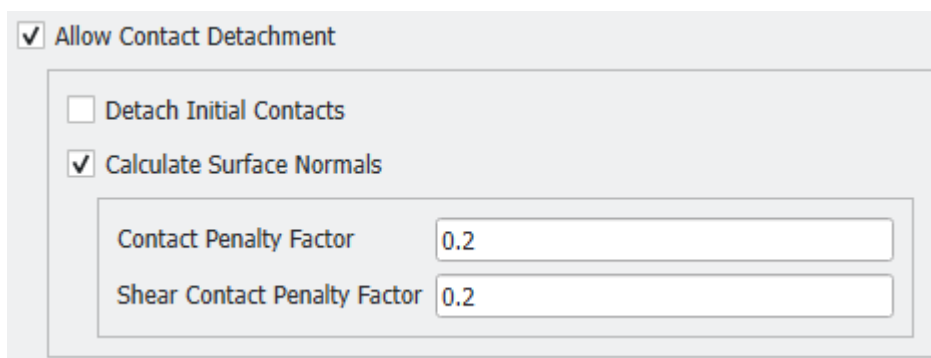
The **Resampling** options are explained under ElastoDict Deformation - Geometry Handling in more detail.

If you choose **CurrentElastoDictSettings**, the settings defined in the ElastoDict Deformations dialog will be used within the GeoApp. No additional adjustments can be made in this GeoApp dialog.



✓ Allow Contact Detachment

If the option **Allow Contact Detachment** is checked, a detachment between different objects during the simulation run is possible.



Detachment is detected as soon as the stress changes from compression to tension in the contact area.

By choosing **Detach Initial Contacts**, a detachment is allowed for all objects, especially also for those, which are attached to each other initially. Otherwise, only objects can be detached, which were detached initially but get attached to each other during the simulation.

To **Calculate Surface Normals** between objects check the corresponding option. Only

the tensile part of the surface normal is used for the detachment algorithm.

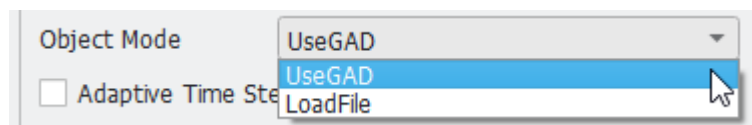
With the **Contact Penalty Factor** the detachment for contacts under normal load can be controlled. Choose a value between 0.0 (no resistance against detaching) and 1.0 (perfect contact). The higher the penalty factor, the later the detachment. Very small values can lead to convergence problems. For most cases the default value of 0.2 works well.

When **Calculate Surface Normals** is checked you can also define the **Shear Contact Penalty Factor**. With this parameter the detachment under shear load can be controlled. Choose a value between 0.0 (no resistance against detaching) and 1.0 (perfect contact). The higher the penalty factor, the later the detachment. Very small values can lead to convergence problems. For most cases the default value of 0.2 works well.

✓ Object Mode

This simulation requires information about the objects in the structure. This information can be provided in two ways:

1. As GAD objects (select **Object Mode - UseGAD**)
2. Via a G32 file (select **Object Mode - LoadFile**)



✓ Adaptive Time Steps

Since GeoDict 2026 it is possible to run the simulation with **Adaptive Time Steps**.

 A screenshot of a settings panel for 'Adaptive Time Steps'. At the top, there is a checkbox labeled 'Adaptive Time Steps' which is checked. Below this checkbox, there are three input fields: 'Initial Time Step' with the value '0.05', 'Minimal Time Step' with the value '0.01', and 'Maximal Time Step' with the value '0.5'.

Define the **Initial Time Step**, with which the solver starts the simulation. The number of iterations from the first step is kept as reference value. For all subsequent simulation steps the number of iterations is compared to this reference number of iterations: if it is much smaller, the time step size is increased. If it is much larger, the time step is discarded and restarted with a smaller time step size. As soon as the minimal time step size is reached, the solver finishes the step and proceeds with the next step.

The time step size is always kept within the predefined bounds: it will never exceed the predefined **Maximal Time Step** and never fall below the **Minimal Time Step**.

✓ Analyze Geometry

When the **Analyze Geometry** box is checked, GeoDict verifies the existence of a solid load path before beginning the simulation. This ensures that the geometry is properly connected as is typically intended.

☒ Analyze Geometry

In special cases, you can disable this check by unchecking **Analyze Geometry**. You may want to do this if you are using the same structure again or if you have already performed this check and know that a path exists.

Results

Click **OK** to close the **Contact Detachment Parameters** dialog. Then click **Run** to start the **Contact Detachment** simulation. The results are stored in the result file previously entered under the **Result File Name (*.gdr)** field of the **Contact Detachment Parameters** dialog.

After a successful run, the **Result Viewer** opens automatically showing the **Results - Report** subtab.

Mon Mar 2 2026 (2026 Build 94575) .../ElastoDict/DetachContacts.gdr

Domain Size: 64 x 64 x 64 Voxel Length: 250 nm Load Structure

Input Map Log Map Post Map Results Strain/Stress Visualization Create Videos Metadata

Report Plots Map

Coordinate system
The coordinate system of the experiment is aligned with the coordinate axis in GeoDict.

Average strain

Time / (s)	Temp. Change / (°C)	XX / (%)	YY / (%)	ZZ / (%)	YZ / (%)	XZ / (%)	XY / (%)	VonMises / (%)	Hydrostatic / (%)
0	0	0	0	0	0	0	0	0	0
1	0	-0.080948	-0.080948	1	-0.0044244	-0.0044244	0.0012284	1.081	0.279368
2	0	-0.15771	-0.15771	2	-0.010582	-0.010582	0.0024286	2.15787	0.561525
3	0	-0.2301	-0.2301	3	-0.021218	-0.021218	0.0033938	3.23053	0.846597
4	0	-0.29912	-0.29912	4	-0.029019	-0.029019	0.004353	4.29971	1.13392
5	0	-0.36364	-0.36364	5	-0.037652	-0.037652	0.0056163	5.36445	1.42424
6	0	-0.42196	-0.42196	6	-0.052677	-0.052677	0.0067691	6.42326	1.7187
7	0	-0.47675	-0.47675	7	-0.062675	-0.062675	0.0074965	7.47833	2.0155
8	0	-0.52649	-0.52649	8	-0.0762	-0.0762	0.0078526	8.52855	2.31567

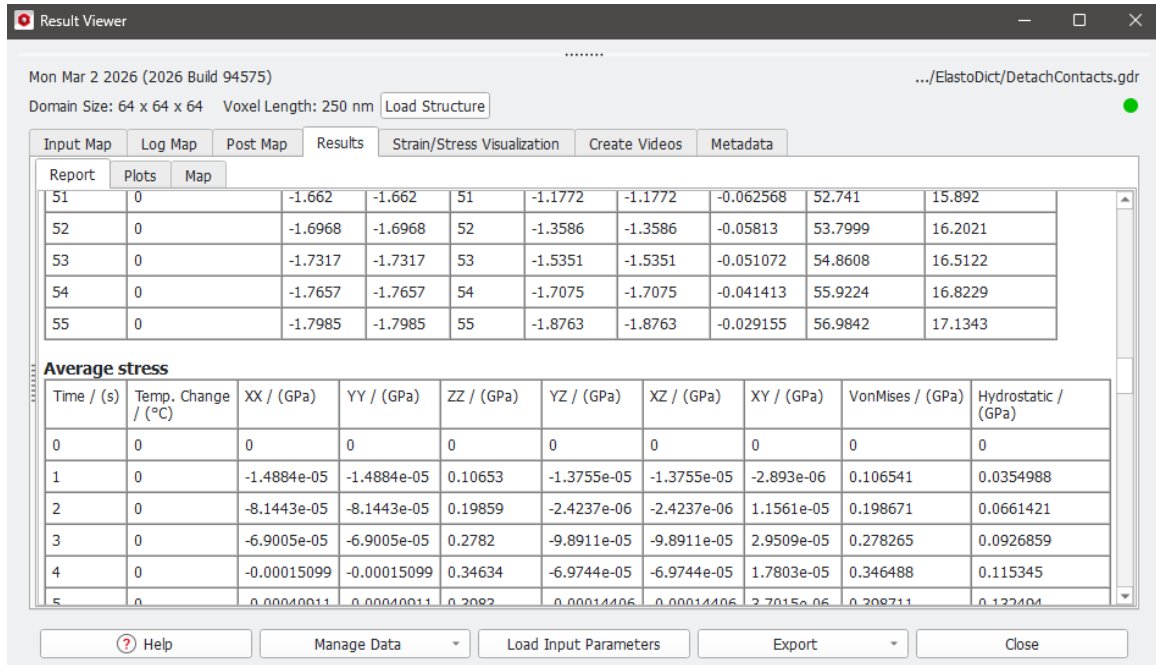
? Help Manage Data Load Input Parameters Export Close

In this example, a **Tension** experiment is simulated in which two objects are pulled in the Z-direction, resulting in object detachment.

✓ Report

The strain that the objects undergo is documented in the first table of the Report tab in

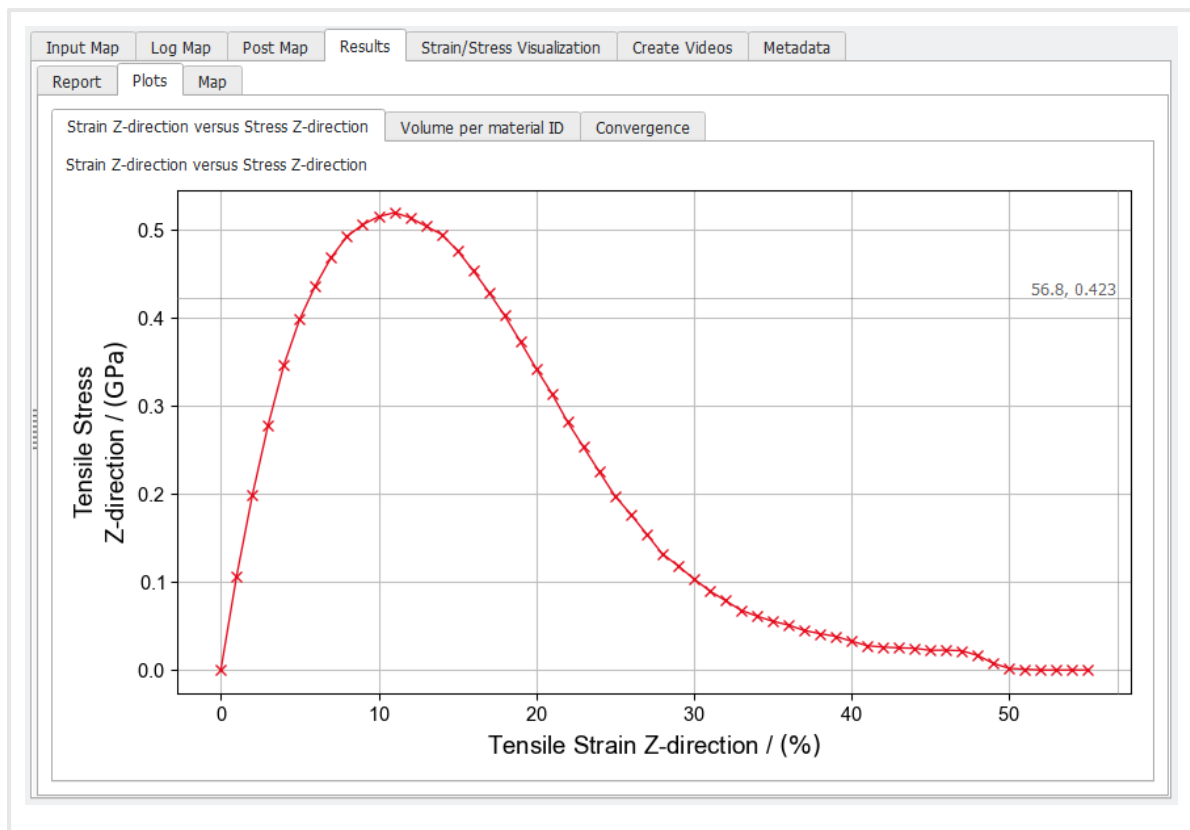
the Result Viewer. Since the **Uniaxial Experiment - Tensile** with a maximum strain of 55% was defined in the **Macroscopic Load** tab, the average strain values for the ZZ column start at 0% and end at 55% after 55 steps.



In the table below, the **Average stress** is displayed.

✓ Plots

The figure in the **Plots** subtab of the **Results** tab plots the tensile stress over tensile strain, which is a graphical representation of the table content in the [Report](#) tab. Tensile stress reaches its maximum at 11% strain and becomes zero at approximately 51% strain. At this point, the two objects begin to separate.



✓ Strain / Stress Visualization

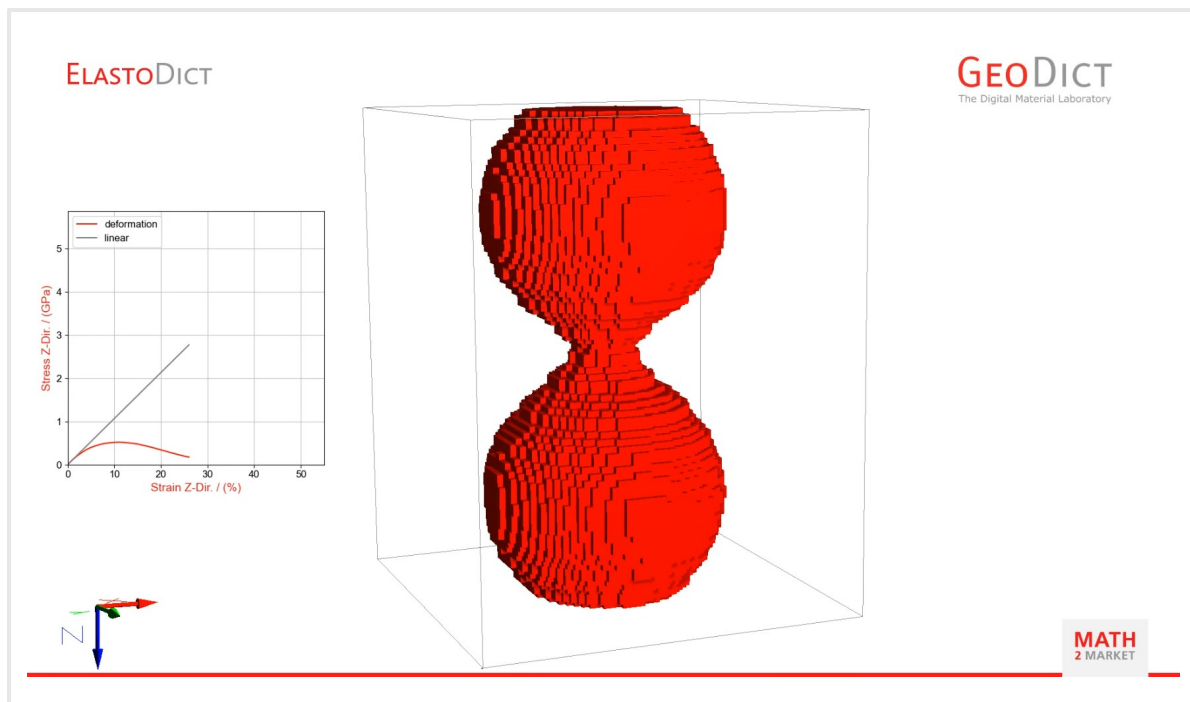
In the **Strain/Stress Visualization** tab, the different result files can be loaded according to the description for ElastoDict Deformations.



Know how! For this type of experiment, **Box Structure Rendering** might be a better choice since it allows for more precise observation of detachment, as seen in the pictures below.

✓ Create Videos

The detachment process can be visualized using the options found under the Create Videos tab.



Material Dissolution

The **Material Dissolution** GeoApp dissolves a structure. Material is removed step by step until everything has dissolved.



Modules needed to run this GeoApp:

GeoDict Base

GeoApp – Material Dissolution

GEODICT

Result File Name (*.gdr)

Dissolving Agent ID

Dissolution Rates

	Material ID	Dissolution rate (m/s)
1	1	7.5e-05
2	2	2.5e-05
3	3	0.0001
4	4	0.0001
5		

☐ Use Automatic Time Step

Time Step / (s)

☒ Use pre-defined View Settings

☒ Generate Video

OK Cancel

Select a **Result File Name** fitting to the current project.

The **Dissolving Agent ID** defines the material that will dissolve the other solid materials in the structure.

Define a **Dissolution Rate** for each solid material. This denotes the dissolution speed of each material in m/s.

Select the **Use Automatic Time Step** option to automatically select the smallest possible time step, based on the given dissolution rates. Disabling this option requires you to manually define a **Time Step** for each time batch.

Select the **Use pre-defined View Settings** option to set pre-defined camera and clipping settings for generating images. If this option is deactivated, the images will use the current view settings.

Select the **Generate Video** option to create a video detailing the dissolution progress from the saved image of each time step.

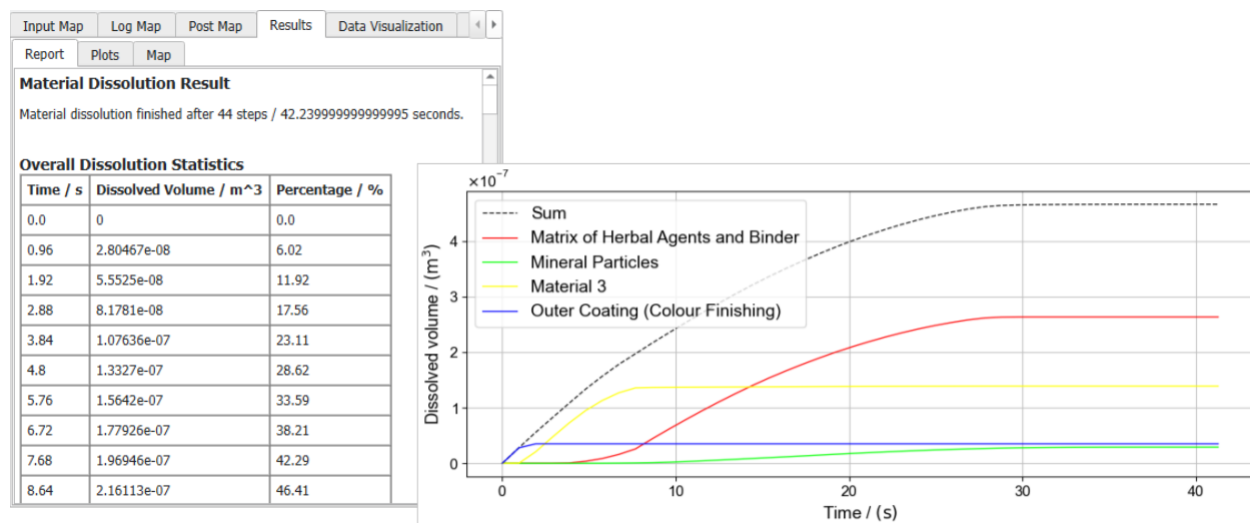
Results

Once the **Material Dissolution** simulation is complete, the corresponding result file will open automatically in the **Result Viewer**. The results folder contains intermediate/partially dissolved structures, generated images and video (if selected), and the input structure.

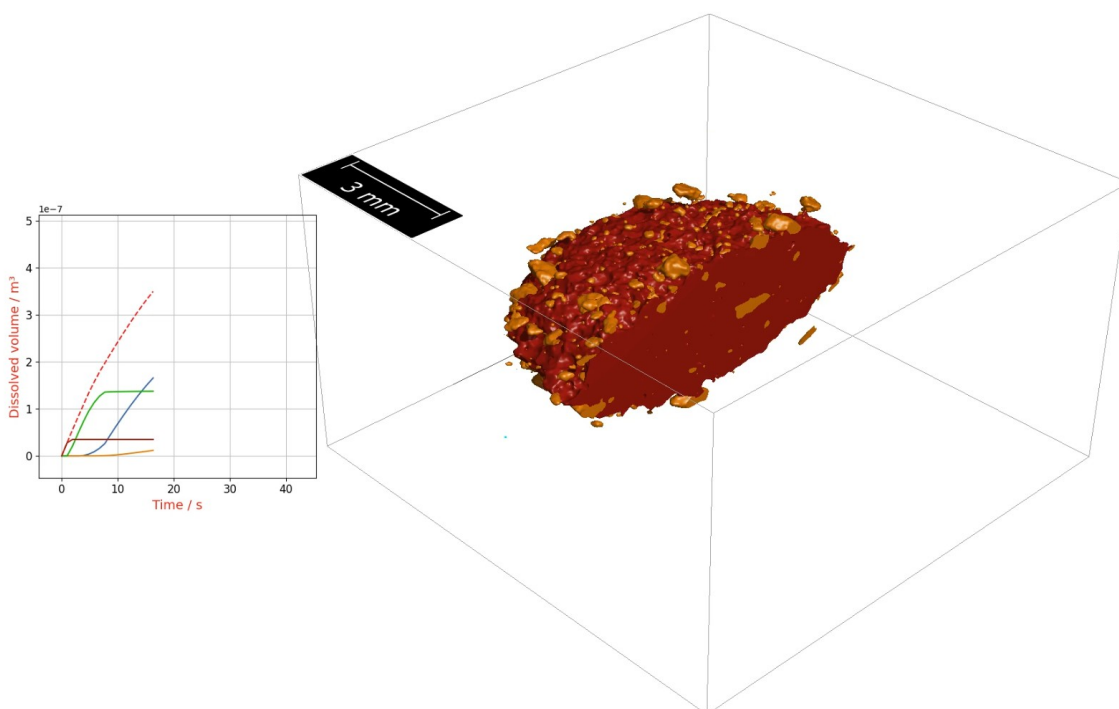
The **Report** tab displays the time at which dissolution finished at the top. Below, you will find tables showing the dissolved volume per time step for the overall structure and for each solid material ID.

Under the **Plots** tab, you will find a plot showing the dissolved volume of each solid material ID over time.

From the **Data Visualization** tab, you can load intermediate structures with partial dissolution.



If selected, the generated video can be found in the results folder. Below is a video showing the dissolution of a tablet containing herbal active ingredients that combat inflammation of the paranasal sinuses:



1.1.3 Report and Image

Use the **Report and Image** GeoApps to save images and create PowerPoint reports.

The following Report and Image GeoApps are shipped with GeoDict:

- [3D-Image Report](#)^[47]
Generate a report from 3D gray value images as a PowerPoint presentation.
- [2D View as Plot](#)^[49]
Save the 2D view of the current structure as a plot.
- [Easy Image](#)^[51]
Create a variety of media materials, e.g., for websites or presentations, based on proofed presets.

3D-Image Report

The **3D-Image Report** app generates a report from 3D gray value images as a PowerPoint presentation. To learn more about creating PowerPoint presentations, refer to GeoPy Scripting or check the Python scripts in the scripts folder of this GeoApp (`\GeoDict 2026\GeoApps\General\Report and Image`)



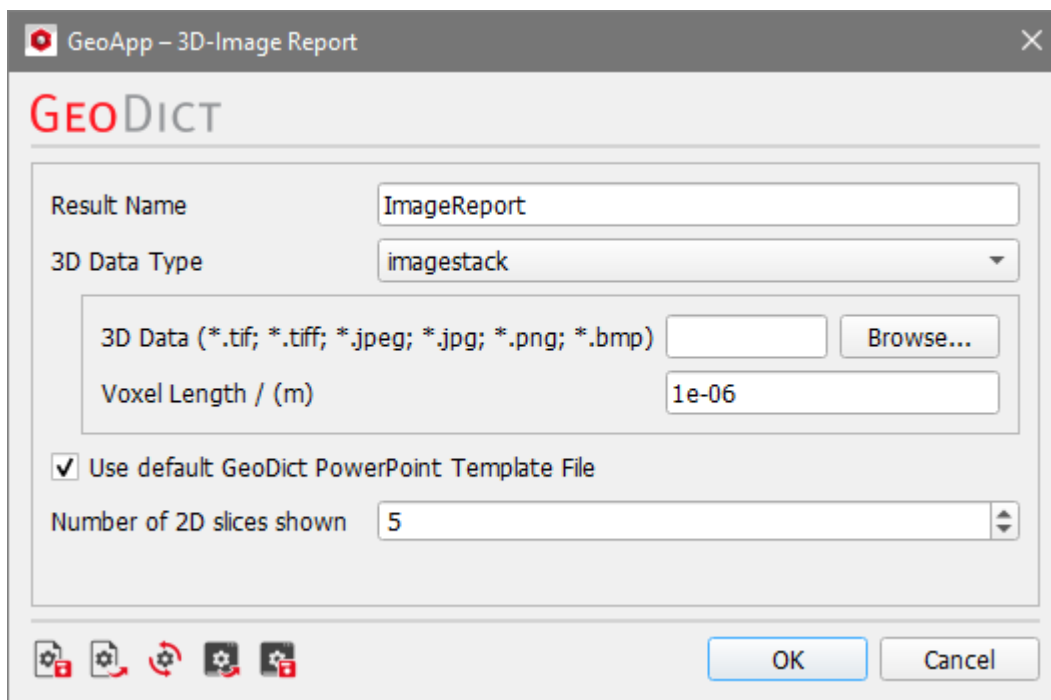
Modules needed to run this GeoApp:

ImportGeo-Vol

Click **Edit** to open the **3D-Image Report Parameters** dialog.

The input parameters include **Result Name**, **3D Data Type**, **Voxel Length**, **Use default GeoDict PowerPoint Template File**, and **Number of 2D slices shown**. Please find detailed explanations of the parameters and how to customize the PowerPoint Template File in our [GeoApp for 3D-Image PowerPoint reports](#) tutorial.

Browse for the dataset and select the file. For image stacks, select one of the images in the stack folder. Adjust the parameters as desired. Click **OK** to close the dialog, go back to the GeoApp section, and click **Run** to start the generation of the report.



Results

After the GeoApp run is finished, the generated PowerPoint report is saved to the result folder. The presentation contains a title slide, as well as the defined number of 2D image slices for each of the Z-, Y-, and X-directions. Three 2D videos can be accessed by clicking on the corresponding slide. The videos display the complete image data from each view axis. Carefully examining the PowerPoint slides in a loop may reveal previously unknown image artifacts.



2D View as Plot

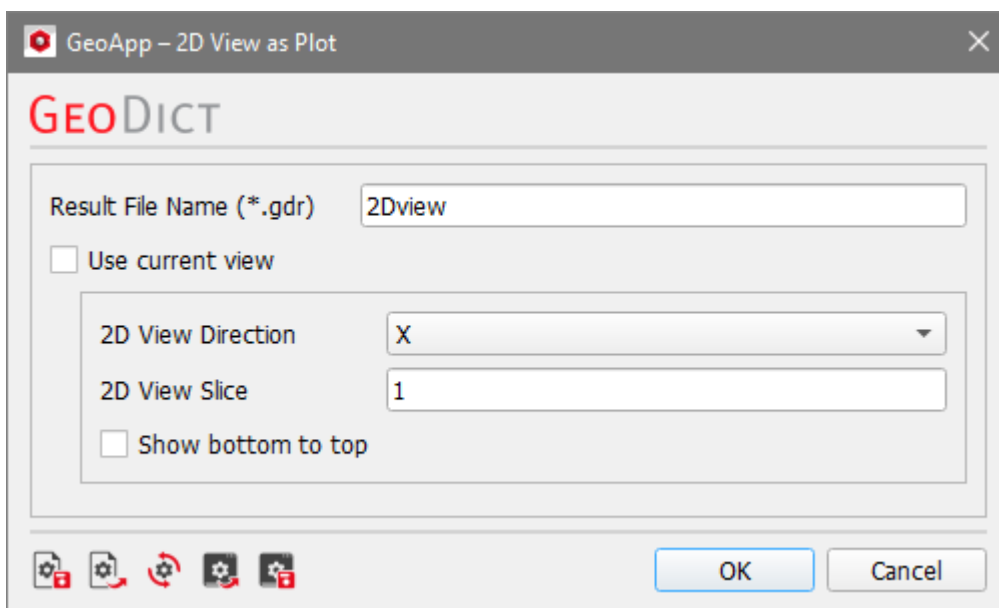
The **2D View as Plot** app saves the 2D visualization of the current structure as a plot. This plot is then contained in a GeoDict result file (*.gdr).



Modules needed to run this GeoApp:

GeoDict Base

Click **Edit** to open the **2D View as Plot** parameter dialog. Select a **Result File Name** fitting to the current project.

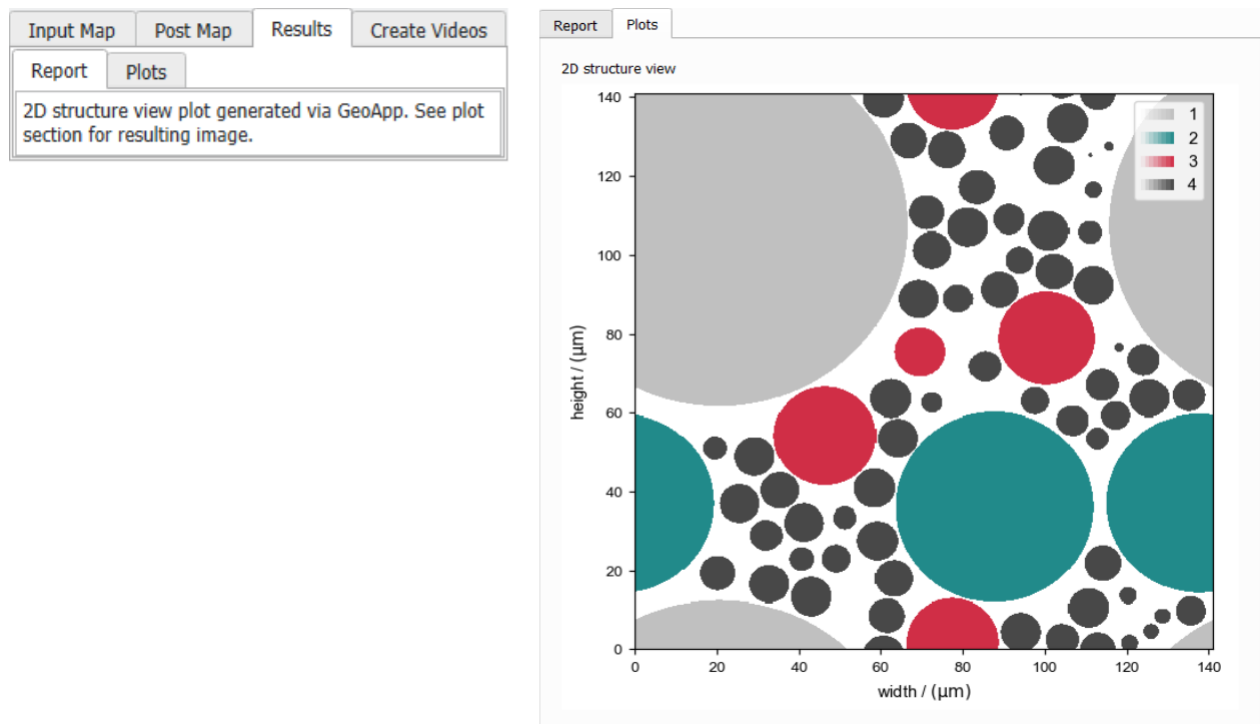


Check **Use Current View** to save a plot of the currently visualized 2D slice and view direction. If this option is unchecked, you will need to select the **2D View Direction**. Activate **Show**

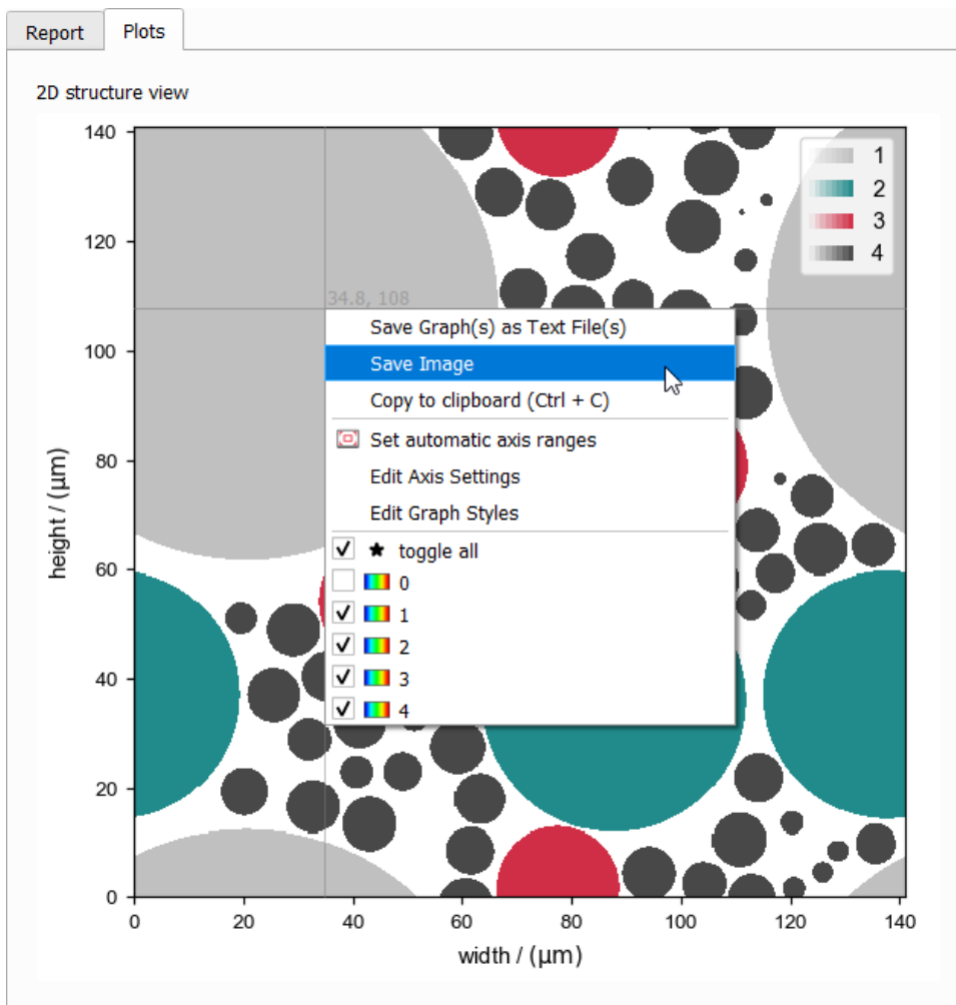
bottom to top to display the image accordingly. If this option is inactive, the image is shown top to bottom. Once you have defined these parameters, click **OK** to close the dialog box. Then, go back to the GeoApp section and click **Run**.

Results

When the image generation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically. The **Results - Report** tab only displays a short report. You find the resulting image from the 2D structure view in the **Result - Plots** tab.



Right-click in the plot to open a dialog providing several options for post-processing, as described in the Result Viewer user guide. The image is also saved as *.png in the corresponding result folder.



Easy Image

The **Easy Image** GeoApp is designed to guide you through the process of creating various types of media in an easy-to-understand way. It also saves the necessary data to recreate the media.



Modules needed to run this GeoApp:

GeoDict Base

Click **Run** to open the **Easy Image** dialog. Here, you can set the basic settings, such as **Image Name**, **Save Folder**, and **Image Preset** selection. Hover over each entry to see a tooltip with more information about that option.

Easy Image

GEODICT

Image Setup

Image Name: testEasyImage

Name Prefix:

Name Suffix:

Image Presets: Math2Market Module Images

Material ID Colors: Keep

Input Settings Mode: Quick-Mode

☐ Add Image Preset to image name

Save Files

Choose Save Folder: C:/GeoApp Browse...

☒ Create a folder to store the data in

☒ Save GeoDict Files

Overwrite Mode: Ask for Action

Description

Description:

☐ Reset the Viewport after finishing

OK Cancel

Under the **Image Presets**, you can also select special modes, such as the **Split Structure by Material** preset. With this preset, you can also save a video that visualizes the splitting process. If you would like to learn more, a video tutorial is available [here](#).

Additional dialogs appear during image creation to help you collect and save all the necessary GeoDict files. Other dialogs allow you to adjust the image setup. For example, the **Expert-Mode** dialog shown below allows you to change the camera and visualization effects.

Easy Image

GEO DICT

3D Options

Rotation HDG

38

Rotation ATT

22

Rotation BNK

-65

Local Rotation X

0

Local Rotation Y

0

Local Rotation Z

0

Position X

0

Position Y

0

Position Z

0

Structure Renderer

Keep

☒ Outlines

☒ Halos

☐ Global Lighting

☐ Reset Light

Field of View

20

Image Options

☐ Show Bounding-Box

☐ Show Scale-Bar

☐ Show Material Legend

☐ Show Volume Field Legend

Image Setup

☒ Create Image

Width

2048

Height

2048

☒ Transparency

☒ Crop Whitespace

Keep Whitespace around image in %

5

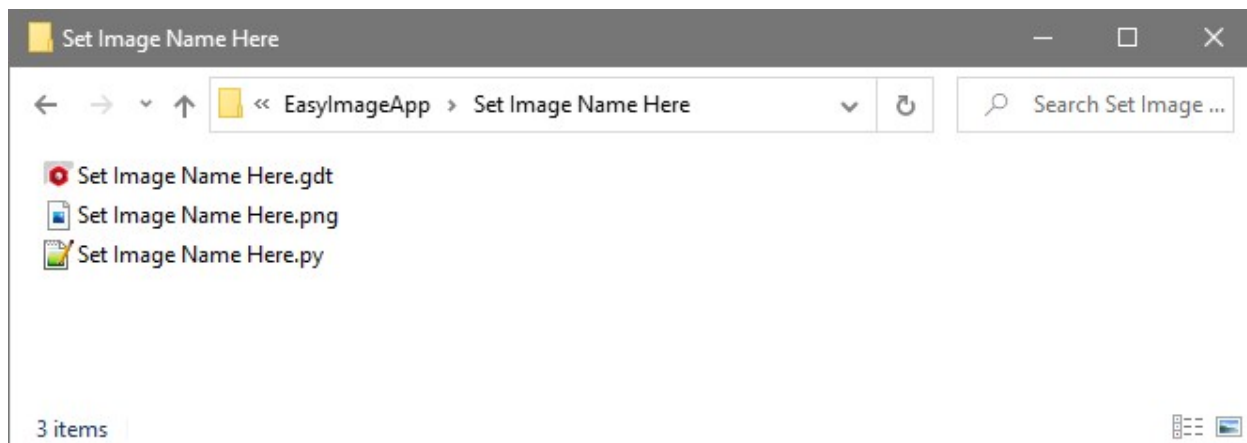


OK

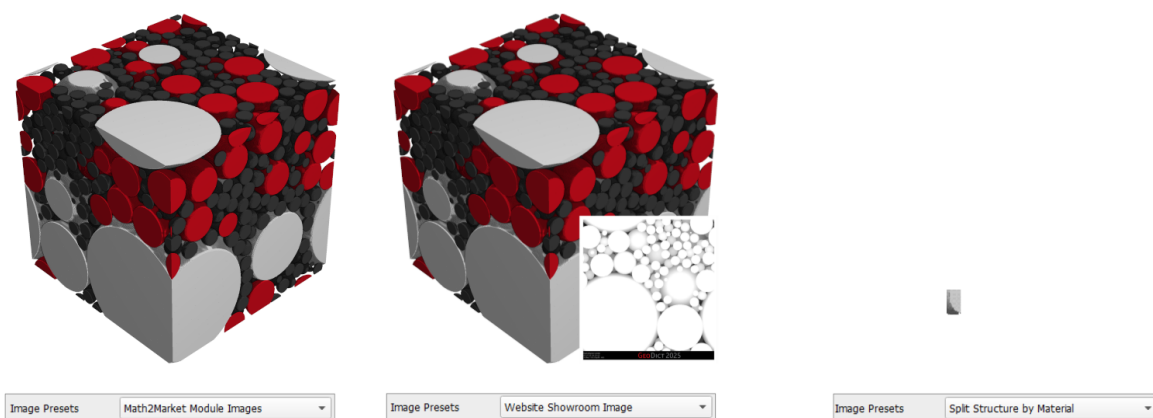
Cancel

Results

After creating an image with the **Easy Image** GeoApp, a folder with the previously selected **Image Name** will be created. The **Name Prefix** and **Name Suffix** are only applied to files stored in the folder. This allows you to quickly and easily create multiple versions in one place without duplicating necessary files. With all the files in one place and the image settings saved as a Python macro, you can reproduce images quickly and easily.



Here, three different **Image Presets** were used for the same structure, also available on our [website](#). The **Material ID Colors** were set to **GeoDict Highlight Colors**. All other parameters were kept at their default settings.



1.1.4 Structure Generation

Use the **Structure Generation** GeoApps to generate or modify structures.

The following Structure Generation GeoApps are shipped with GeoDict:

- [Generate Artificial CT](#) ⁵⁵
Generate gray value images from structure files and add artificial image artifacts, e.g., noise, ring artifacts, or curtaining.
- [Add Random Surface Cover](#) ⁵⁸

The following Structure Generation GeoApps are shipped with GeoDict:

Cover the surface of the current structure randomly.

- [Distribute Material IDs](#)⁶⁰
Assign multiple material IDs to the solid phase of the currently loaded geometry.
- [Contact Correction](#)⁶³
Adjust grain-to-grain contacts to reflect their true mechanical behavior.

Generate Artificial CT

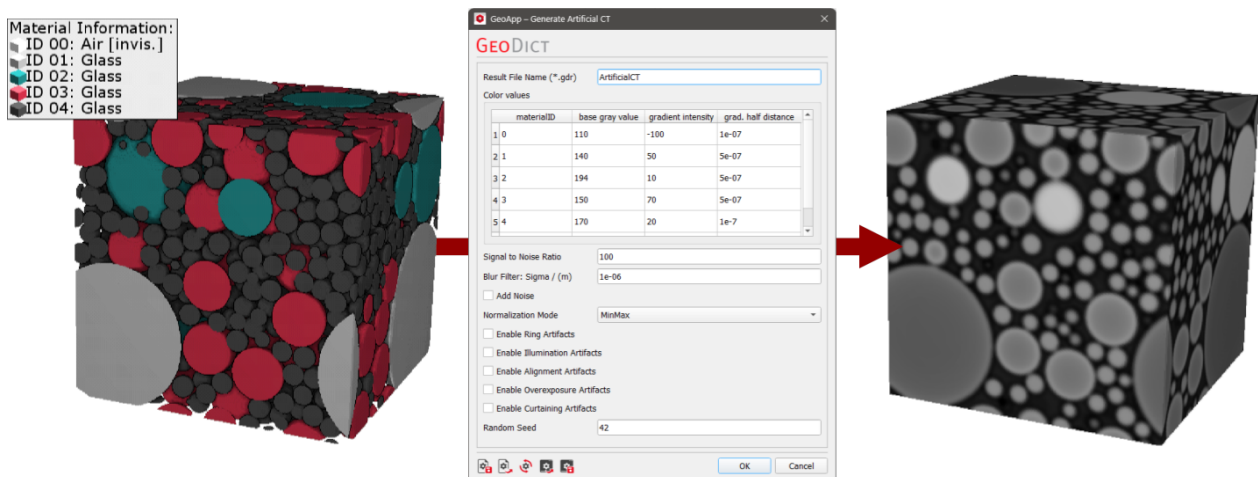
The **Generate Artificial CT** app creates a multi-material artificial CT based on the voxel geometry loaded in GeoDict.



Modules needed to run this GeoApp:

GrainGeo or FiberGeo, PoroDict

Click **Edit** to open the **Generate Artificial CT** parameter dialog.



General Parameters

Enter a **Result File Name** at the top of the dialog.

Use the **Color values** table to define the gray values for each material. The **base gray value** is the mean gray value for the each material in the generated gray value image. Define the **gradient intensity**, which determines whether the borders of the material will be lighter or darker. The **gradient half distance** defines the thickness of these border gradients.

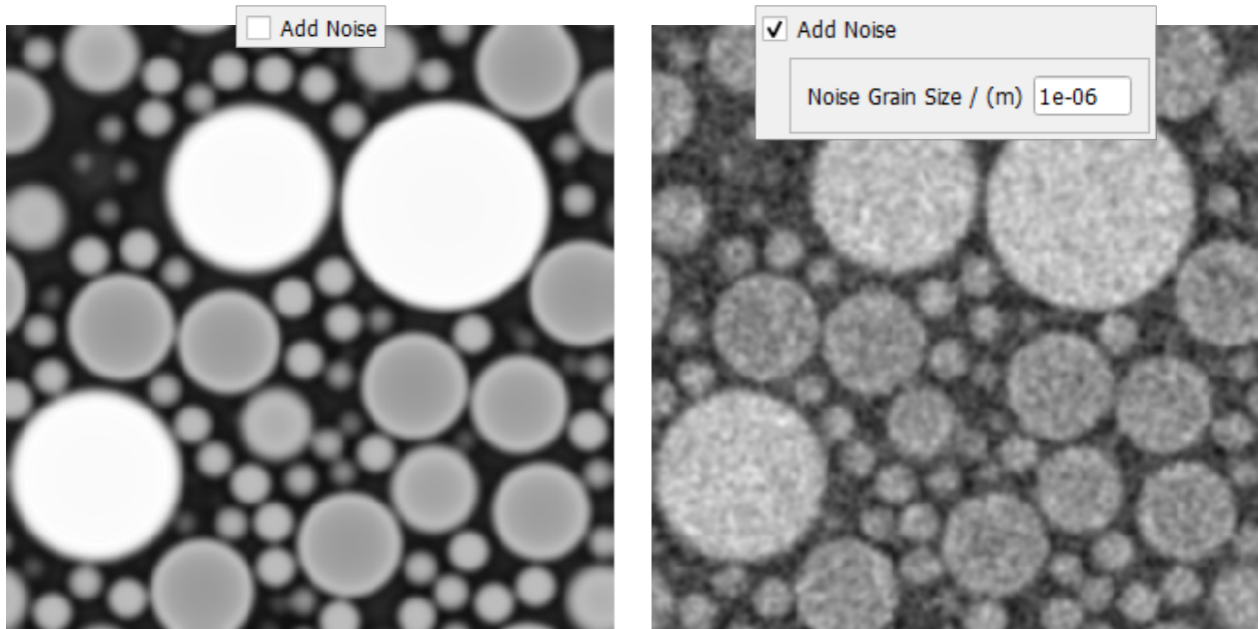


Note! The **Generate Artificial CT** app always creates an 8-bit image dataset (gray values between 0 and 255). If you want to create an 16-bit image dataset, create the 8-bit version first and then use the Sample to 8 / 16 bit functionality in ImportGeo-Vol.

Define the **Signal to Noise Ratio**, where higher values result in a clearer image, while lower values add more random noise.

The **Blur Filter: Sigma** defines the strength of the blurriness in the generated image.

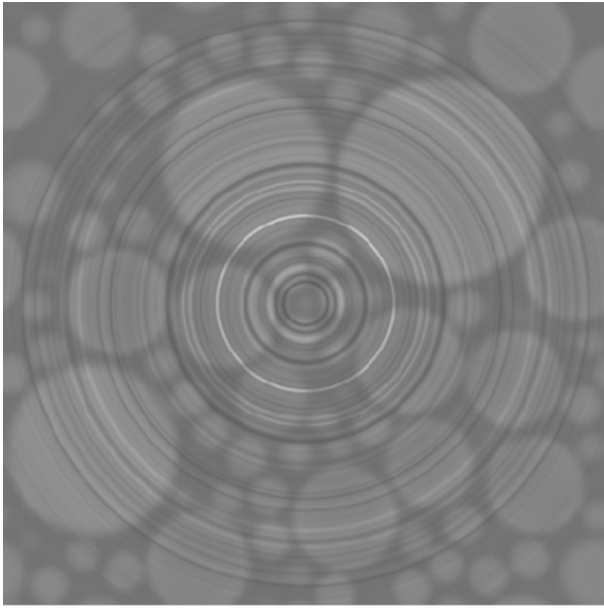
Decide whether to add **Noise**. Larger values of **Noise Grain Size** create larger patches of noise with similar gray values.



The **Normalization Mode** defines how the gray value image is normalized. It can be set according to **MinMax** gray values or to **0-255**.

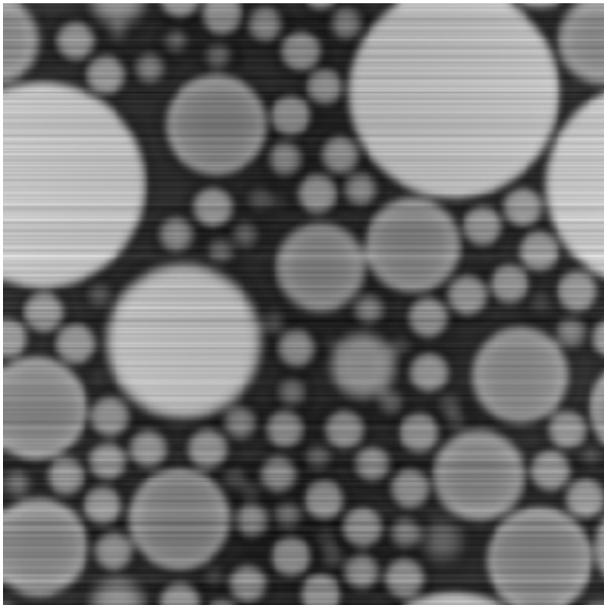
Add Artifacts

Five different types of artifacts can be added to the artificial CT images:



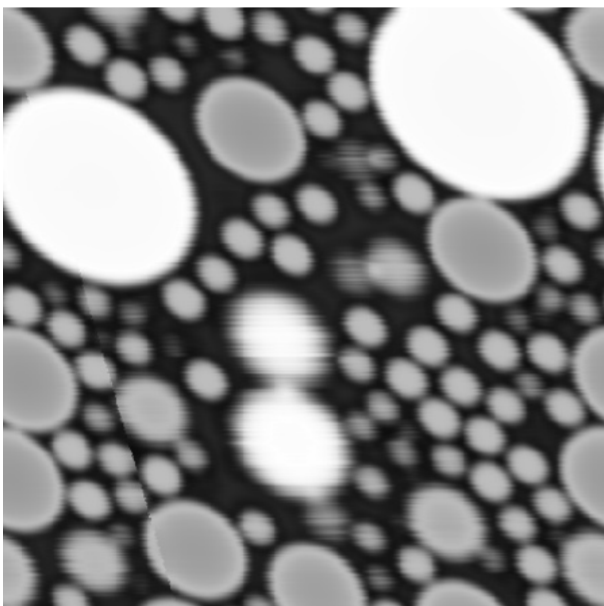
☒ Enable Ring Artifacts

Ring Strength / (%)	30
Maximal Ring Radius / (voxel)	300
Number of Ring Maxima	0
Angle Offset of Ring Maxima / (°)	20



☒ Enable Illumination Artifacts

Flickering Strength / (%)	15
Z-direction Vignette Strength / (%)	10
Gradient Strength / (%)	10



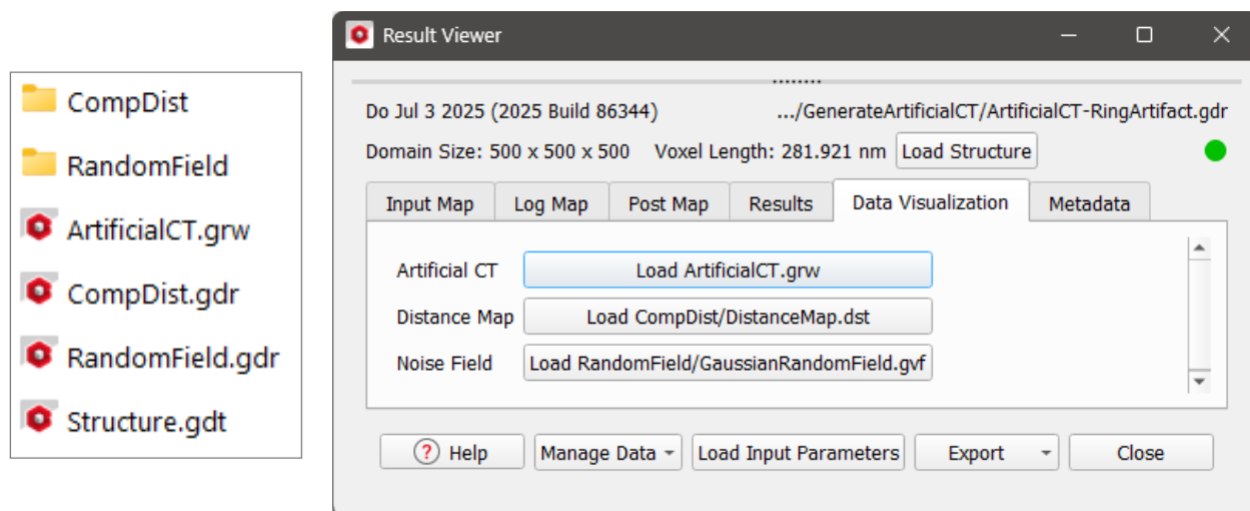
☒ Enable Alignment Artifacts

Maximal Random Misalignment / (voxel)	1
FIB-SEM Slice Shift / (voxel/slice)	0.3



Results

After the CT-generation is finished, the artificial CT-scan is loaded as volume field in the visualization area and the result file is opened in the Result Viewer. From the **Data Visualization** tab the **Artificial CT-scan**, the used **Distance Map**, and the **Noise Field** can be loaded.



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.

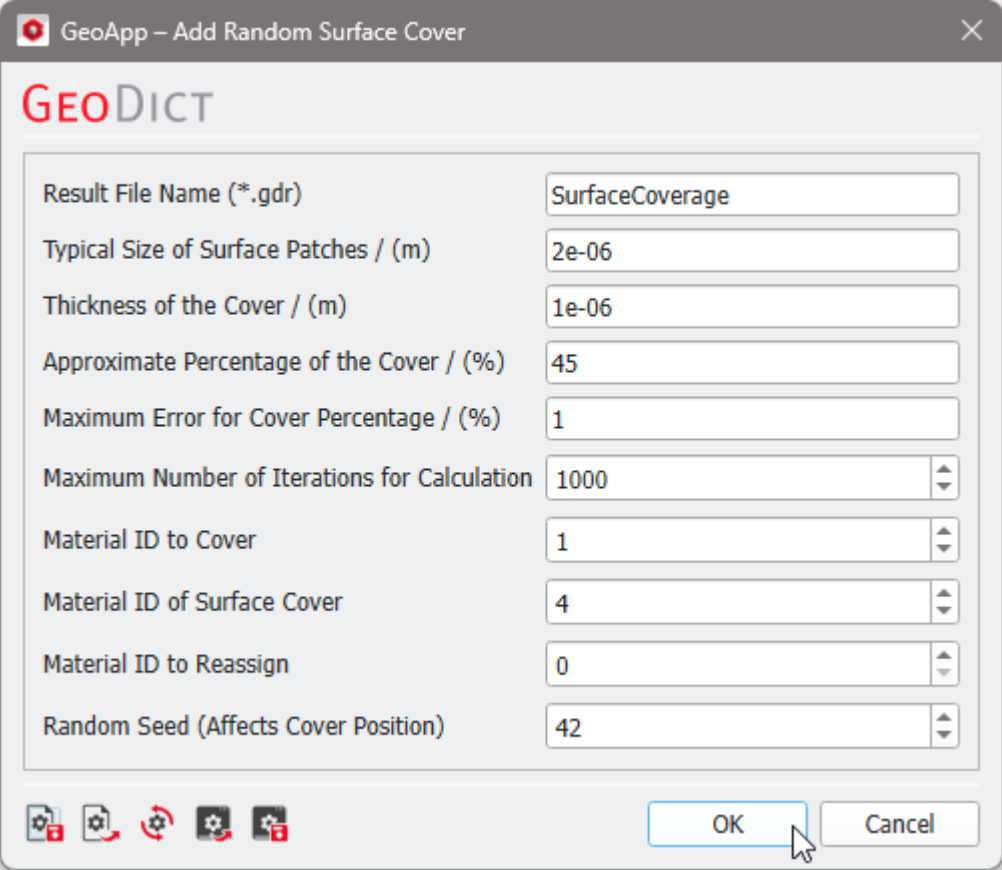
The random surface is created using GeoDict's Gaussian Random Field Generator. Control the **Typical Size of Surface Patches**, which changes the standard deviation of the Gaussian field. Additionally, define the **Thickness of the Cover**.

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.

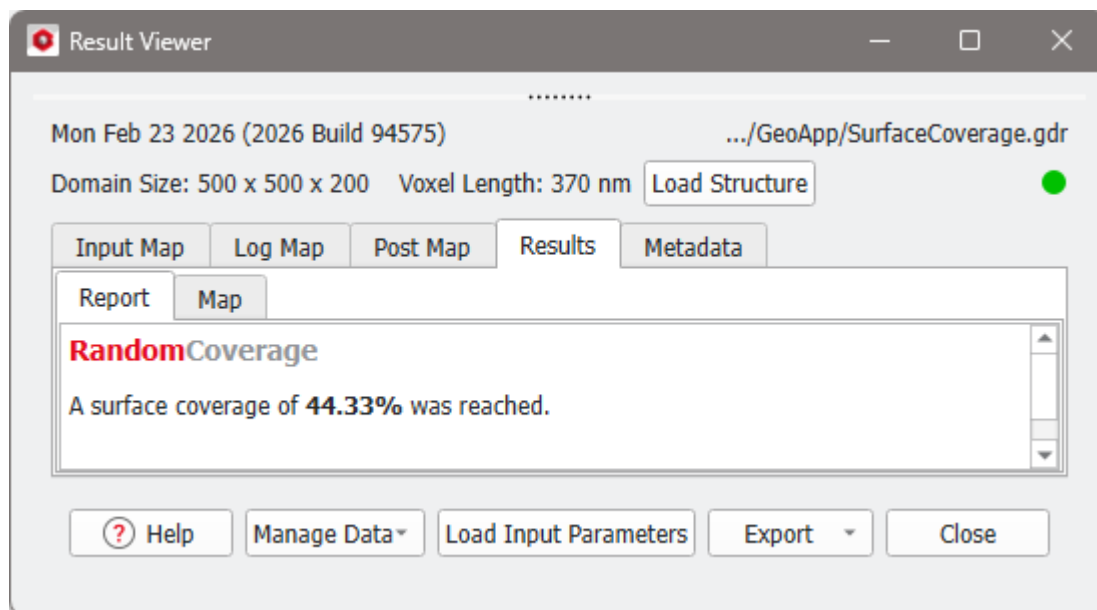


Parameter	Value
Result File Name (*.gdr)	SurfaceCoverage
Typical Size of Surface Patches / (m)	2e-06
Thickness of the Cover / (m)	1e-06
Approximate Percentage of the Cover / (%)	45
Maximum Error for Cover Percentage / (%)	1
Maximum Number of Iterations for Calculation	1000
Material ID to Cover	1
Material ID of Surface Cover	4
Material ID to Reassign	0
Random Seed (Affects Cover Position)	42

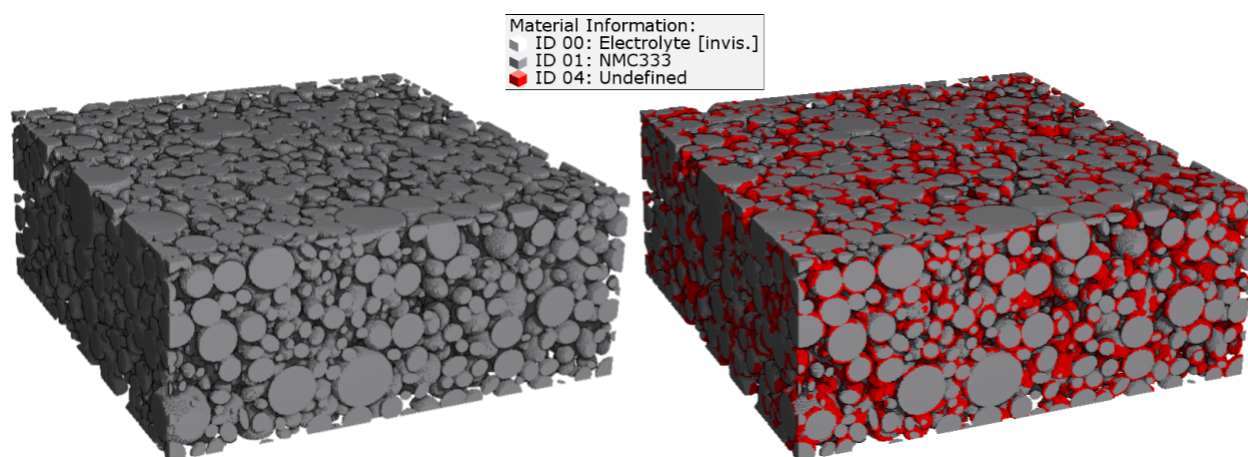
After defining all parameters click **OK** to close the dialog, go back to the GeoApp section, and click **Run**.

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.



Distribute Material IDs

The **Distribute Material IDs** GeoApp enables the assignment of multiple material IDs to the solid phase of the currently loaded geometry.

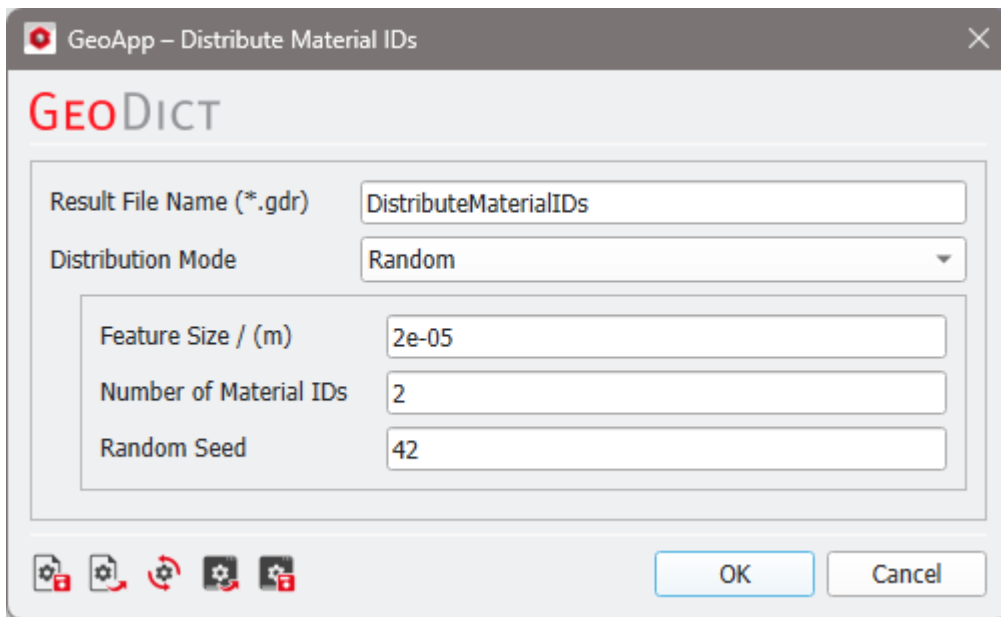
A common use of this tool is simulating electrospun fibers, where different surface charges are assigned to material IDs to model heterogeneous electrostatic behavior. When electrostatic effects are enabled, the Material Charge can be set as **Individual per material type**, which requires a heterogeneous material distribution.



Modules needed to run this GeoApp:

FiberGeo or GrainGeo

Select a **Result File Name** fitting to the current project.



Depending on the selected **Distribution Mode**, the GeoApp assigns material ID numbers to the 3D structure. It does not assign materials to those numbers. For example, if you select 20 as the **Number of Material IDs** in the app, you may have to assign a material and all the corresponding parameters to each of the 20 IDs.



Important! Be aware that the app changes the material IDs of all solid materials.

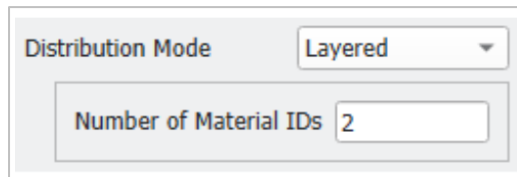
✓ Random

Material IDs are randomly assigned according to a Gaussian Random Field distribution. First, define the **Feature Size**, which is the correlation length that characterizes the Gaussian random field. Next, define the **Number of Material IDs** that will be present after the distribution is complete. Finally, define the **Random Seed** for the generator of the Gaussian random field.

✓ Layered

Material IDs are distributed in layers along the Z-axis. Specify the **Number of Material**

IDs that will be present once the distribution is complete.

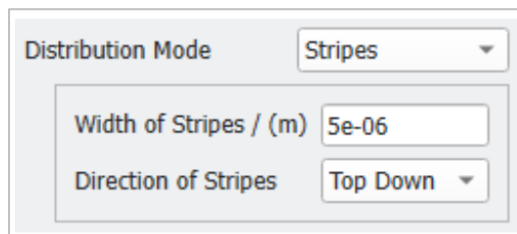


Distribution Mode: Layered

Number of Material IDs: 2

✓ Stripes

Material IDs are assigned in stripe patterns across the geometry. This mode requires GAD objects. Define the **Width of Stripes** that the GAD objects are split into. Then, define the **Direction of Stripes**.



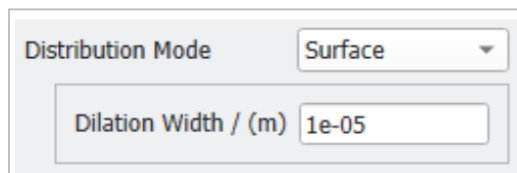
Distribution Mode: Stripes

Width of Stripes / (m): 5e-06

Direction of Stripes: Top Down

✓ Surface

Material IDs are assigned to the uppermost and lowermost voxels in the Z-direction, which can be followed by dilation. Specify the dilation of these uppermost and lowermost materials or "capped materials" via the **Dilation Width**.



Distribution Mode: Surface

Dilation Width / (m): 1e-05

Results

Once the computation is finished, a result file will be generated stating that the material IDs were assigned using the selected **Distribution Mode**. The generated structure is automatically loaded into GeoDict. You can load the **Input Structure** from the result viewer via the **Data Visualization** tab. The corresponding result folder contains the generated and input structures, as well as the Gaussian random field when using the **Random** distribution mode.

Input Map

Log Map

Post Map

Results

Data Visualization

Metadata

Report

Map

Material ID Distribution

Assignment of multiple material IDs to the solid phase with the "Random" mode.

Usable for example in electrostatic fiber cases.

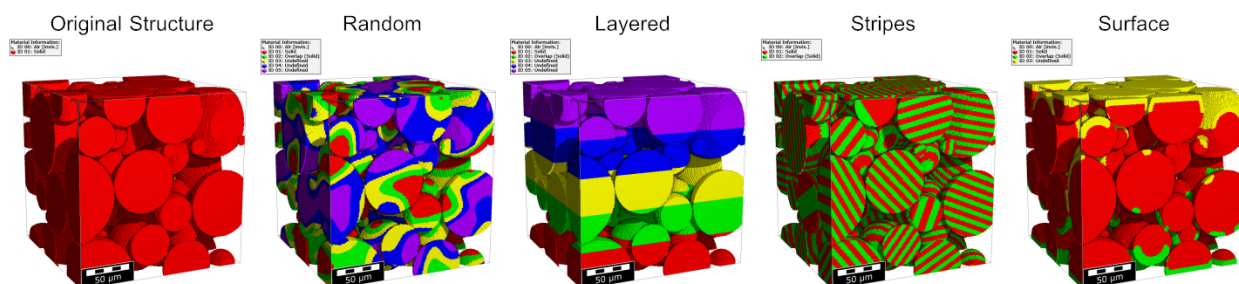
GenerateGaussianRandomField

GenerateGaussianRandomField.gdr

InputStructure.gdt

Structure.gdt

View results for the different distribution modes in the example below:



Contact Correction

The **Contact Correction** GeoApp adjusts grain-to-grain contacts to accurately reflect mechanical behavior by reducing stiffness through one of two methods. Both methods rely on the GrainFind's watershed-based grain segmentation, which accurately identifies grains and their contact zones.



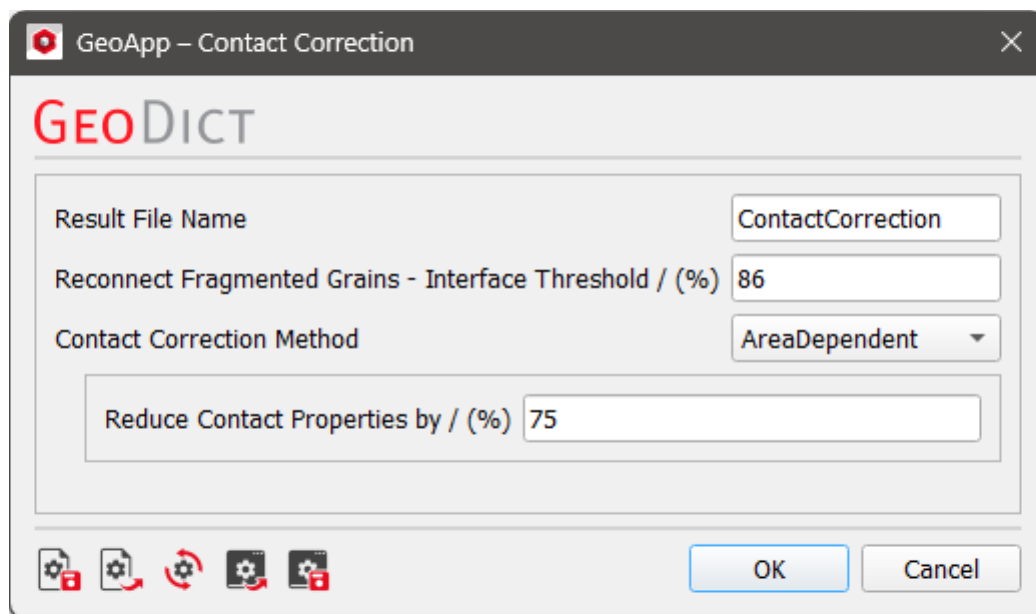
Modules needed to run this GeoApp:

GrainFind, MatDict

Click **Edit** to open the **Contact Correction** parameter dialog.

Select a **Result File Name** fitting to the current project.

Define the **Reconnect Fragmented Grains - Interface Threshold** value. This value determines which touching grain fragments that are merged. value of 0% merges all touching grains, while a value of 100% prevents any merging. Refer to the GrainFind user guide for more information on this parameter.

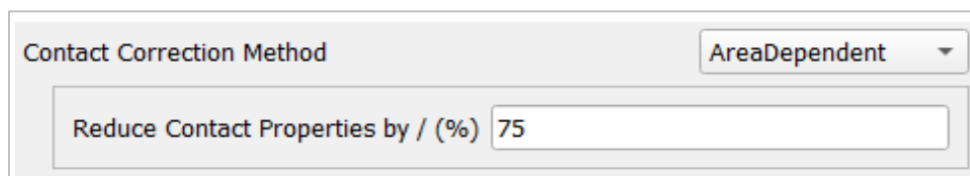


Then, select the **Contact Correction Method**. Two methods are available here:

✓ Area-Dependent

The **Area-Dependent Stiffness Reduction** is described in detail in [Halisch et al., 2025^{\[240\]}](#). This method maintains the original grain contact segmentation while modifying the mechanical properties to achieve realistic behavior by reducing the effective stiffness based on the relative size of the contact areas between grains.

When selecting this method, you must to define the **Reduce Contact Properties by** value. This percentage determines the reduction factor for the density, Young's modulus, and Poisson's ratio.



✓ Explicit

Using the **Explicit Contact Area Reduction** method ([Saxena et al., 2019^{\[241\]}](#)) involves physically eroding contact voxels to shrink contact zones. This method alters the porosity of the original structure, producing simulations that more closely resemble experimental conditions, even when working with resolution-limited imaging data.

When selecting this method, you must define the **Eroded Voxel Number**. This parameter controls the size of the voxel layer by which the contact zones between grains and pore space are eroded. Refer to the ProcessGeo user guide for more information on eroding voxels.

Contact Correction Method

Explicit

Eroded Voxel Number

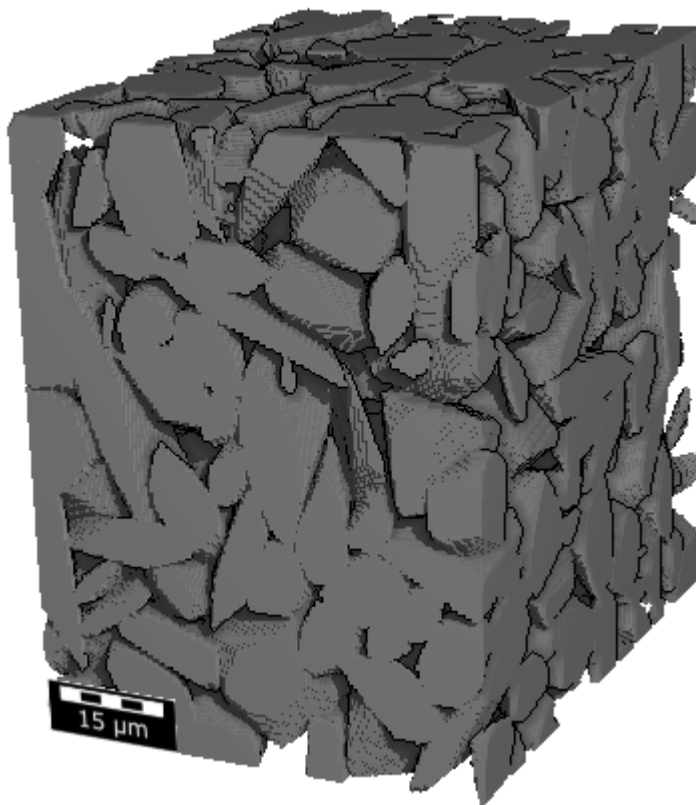
1

After defining all parameters click **OK** to close the dialog, go back to the GeoApp section, and click **Run**.

Results

Below the results from both methods are shown for an exemplary anode structure using the default settings.

Material Information:
 ID 00: Electrolyte [Electrolyte] [invis.]
 ID 01: Graphite [Active Material]

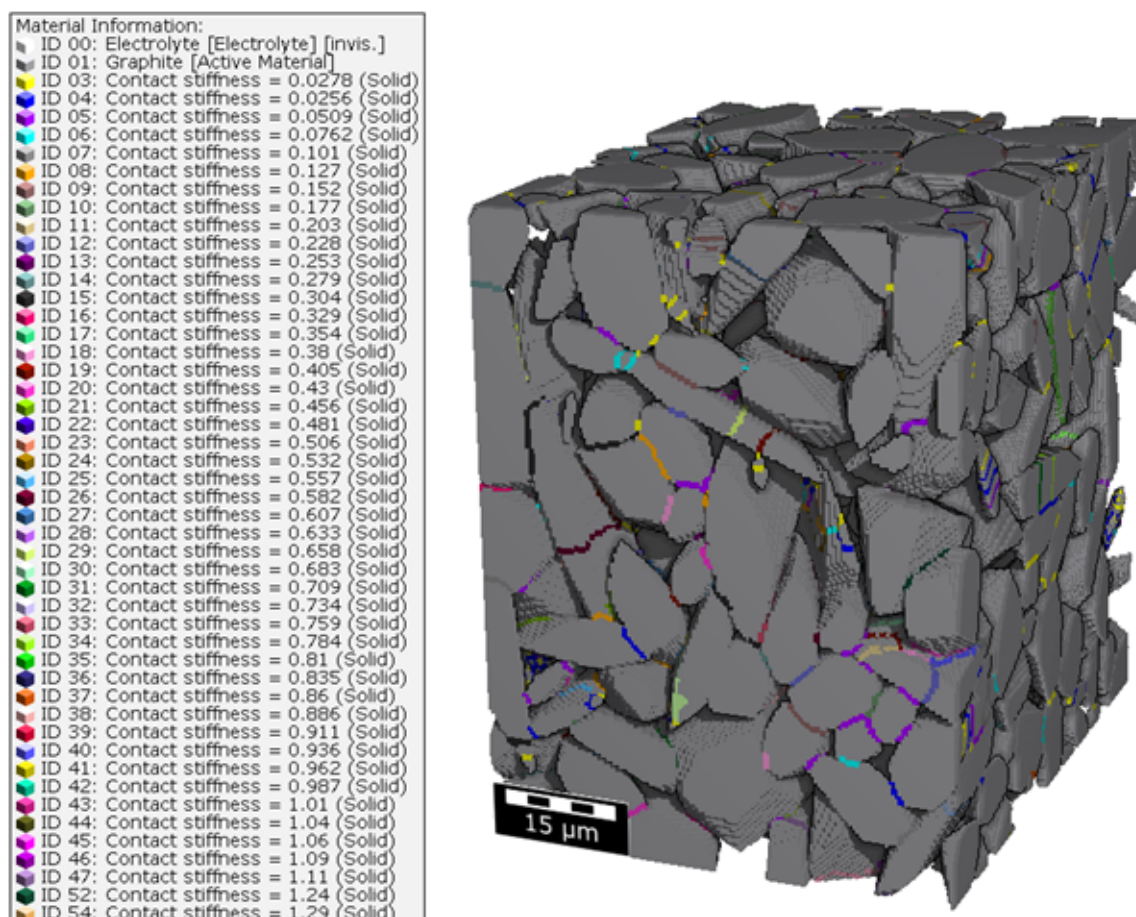


Area-Dependent

Once the **Contact Correction** app has finished, the result file loads in the **Result Viewer**. The result file lists the input parameters, and under the **Data Visualization** tab, you can load the contact-corrected structure. This structure is also automatically loaded into the visualization area at the end of the run.

In the contact-corrected structure, each contact area has its own material ID and individual mechanical properties that are based on its relative size. You can view the material properties in the material name or by viewing the Constituent Materials.

In the results folder, you will find additional results, such as Identify Grains, as well as the original and contact-corrected structures. Additionally, structures containing only contact areas or simple, weak contacts are available for loading.



✓ Explicit

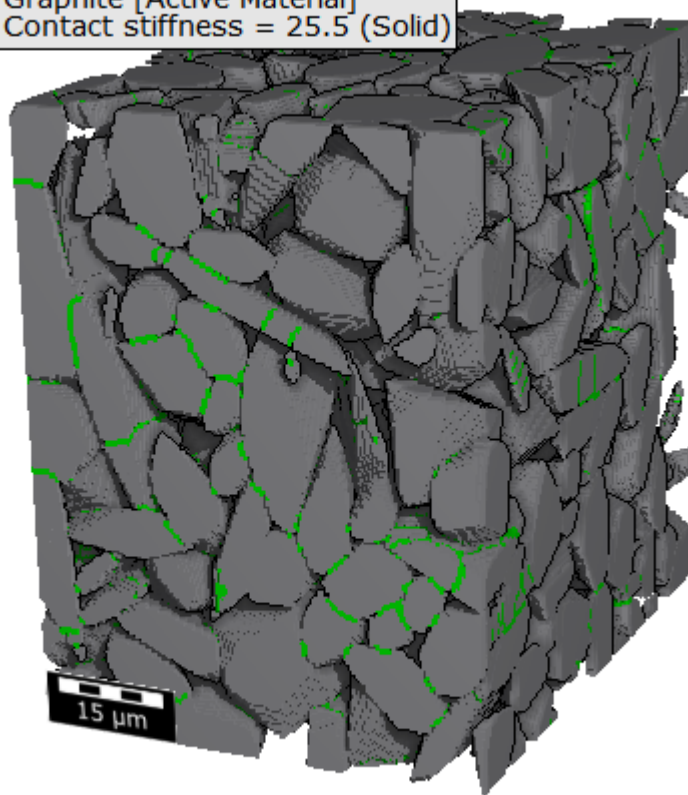
Once the **Contact Correction** app has finished, the result file loads in the **Result Viewer**. The result file lists the input parameters, and under the **Data Visualization** tab, you can load the contact-corrected structure. This structure is also automatically loaded into the visualization area at the end of the run. Additionally, the identified grain contacts are loaded as a volume field.

In the contact-corrected structure all identified and then eroded contact areas are assigned to a new material ID. This material has the same mechanical properties as the original material, but the area is reduced by the set number of voxels.

In the result folder, you find additional results (e.g., Identify Grains, or Percolation Path) as well as the original and contact-corrected structures.

Material Information:

-  ID 00: Electrolyte [Electrolyte] [invis.]
-  ID 01: Graphite [Active Material]
-  ID 02: Contact stiffness = 25.5 (Solid)



1.2 Digital Twin GeoApps

GeoDict offers several GeoApps to automatically generate statistical **Digital Twins** matching various geometrical and physical properties.

For this, the apps use structure generators from FiberGeo or GrainGeo to create 3D structures. These 3D structures are then compared with the available input structure. By varying the input parameters of the structure generators, the app searches for a best match with the input structure. Be aware that the optimization routine only searches for a best match in a given setup and parameter range. For example, the structure generator build into the app may assume that fiber cross sections are circular, and in that case, all resulting structures will have a circular fiber cross section.



New in GeoDict 2026

- The apps have been renamed and re-sorted in GeoDict 2026.
- The **Generate Granular Structure** app now has the possibility to use the [Add Binder](#)^[72] command during the structure generation and several more options for the selection of the [Random Field](#)^[71].
- The parameter optimization algorithm of the **Generate Granular Twin From 2D/3D** was improved and offers new options: In 2D [Out-Of-Plane 2D Permeability](#)^[78] can be used as matching criterion and the global optimization parameters are now selectable.

Find the following Digital Twin GeoApp groups:

- [Structure Generation](#)^[68]
Create digital twin structures.

1.2.1 Structure Generation

Use the **Structure Generation** GeoApps to create digital twin structures.

The following Structure Generation GeoApps are shipped with GeoDict:

- [Generate Granular Structure](#)^[69]
Create a 3D model with the structure generator used in the Generate Granular Twin apps.
- [Generate Granular Twin From 2D](#)^[74]
Creates a 3D statistical digital twin of a 2D slice from a granular microstructure.
- [Generate Granular Twin From 3D](#)^[86]
Creates a statistical digital twin of a 3D granular microstructure.
- [Generate Nonwoven Twin](#)^[96]
Create a statistical digital twin of a non-woven microstructure resembling defined stochastic geometrical properties of the original.

Generate Granular Structure

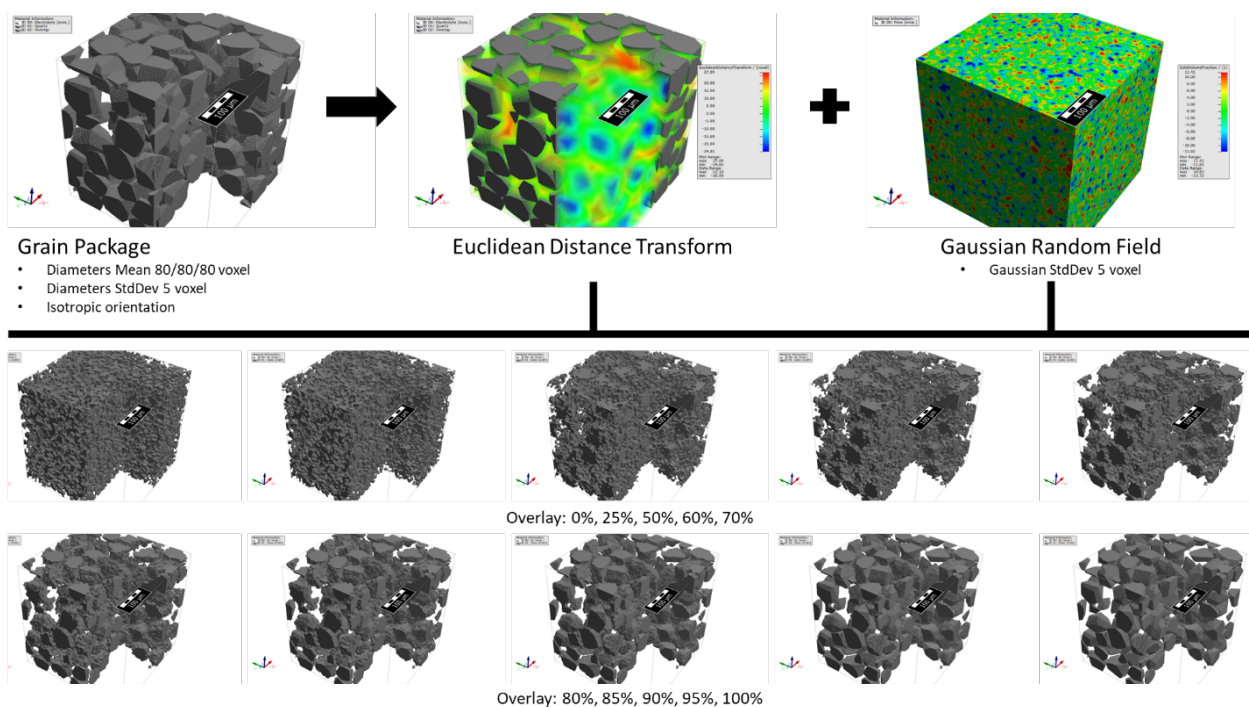
The **Generate Granular Structure** app uses stochastic geometric modeling on a grain-based distance field to generate a 3D structure model. The app uses the same structure generation algorithm as the [Generate Granular Twin From 2D](#)^[74] and the [Generate Granular Twin From 3D](#)^[86] apps. It can therefore be used to

- find an initial guess for the optimization run in one of the other apps, or
- generate digital twins with the parameters found in one of the other apps.

This generation is done in three steps:

1. A package of grains is generated by GrainGeo - Create Grains and removing overlap up to a certain degree. The grain generator uses spheres, ellipsoids or convex polyhedrons with enclosing ellipsoids, depending on the settings.
2. Based on this grain package, a Euclidean distance field is generated.
3. Using GrainGeo - Stochastic Field Thresholding, a random field is generated, overlaid with the Euclidean distance field and thresholded to reach the targeted porosity.

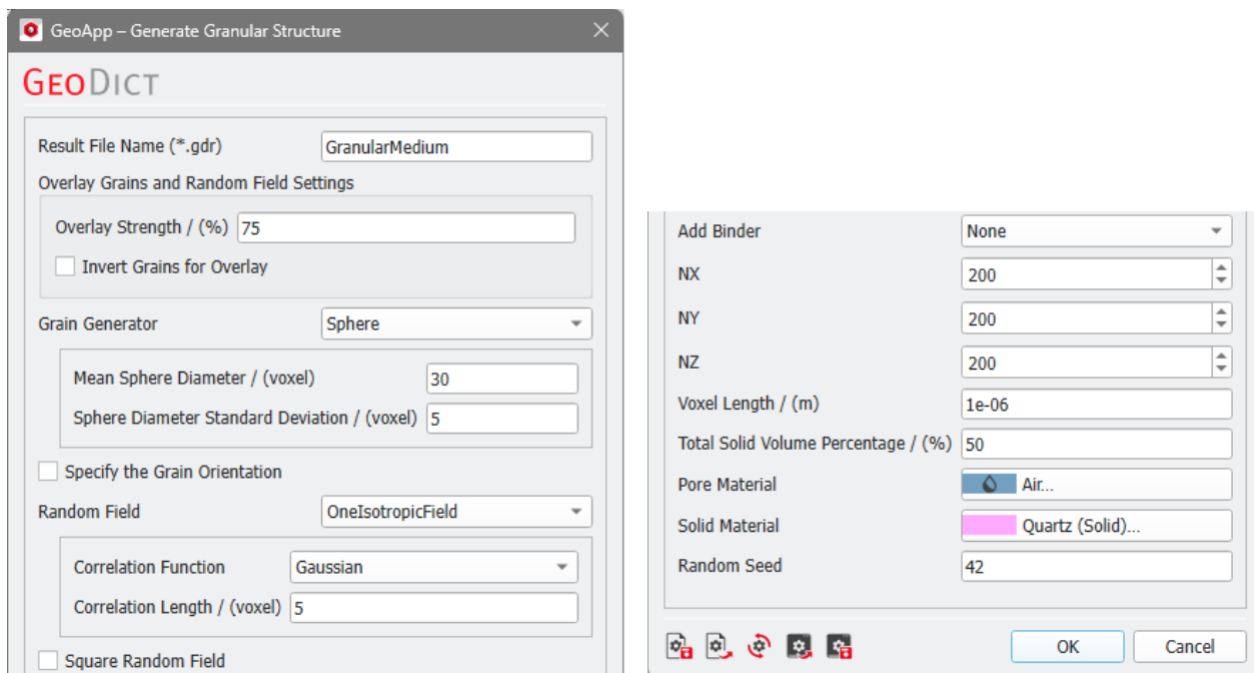
The figure below illustrates an example of different overlay strengths for a target with 30% solid volume percentage. After generation, the structure is cleansed to remove artifacts.



Modules needed to run this GeoApp:

GrainGeo

Clicking **Edit...** opens the **Generate Structure** dialog. At the top, define a **Result File Name** for the result file and the result folder containing the generated structure.



✓ Overlay Grains and Random Field Settings

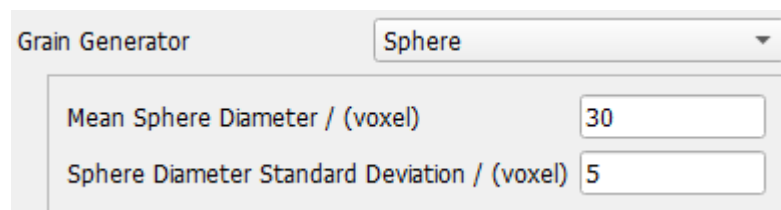
The **Overlay Strength** is the field overlay strength in percentage. At 100% overlay strength the result will only show the grain package, while at 0% overlay strength the result will show only the random field. If no **Random Field** is used, this value is automatically set to 100%. If no **Grain Generator** is used, this value is automatically set to 0%.

Check **Invert Grains for Overlay** to switch pore and solid material. In this case, the grain generator creates the pore space, and the background becomes the solid material.

✓ Grain Generator

Select the basic shape used to generate the 3D structure. Select **None** as **Grain Generator** to use only the **Random Field** for the structure generation. The app uses the GrainGeo - Create Grains command to create the grain structure. Be aware that all lengths are given in the unit voxel.

For the **Sphere** shape, the diameters are Gaussian distributed. Select the mean diameter and the standard deviation.



For the **Ellipsoid** shape, the first diameter is Gaussian distributed. Select the mean

diameter and the standard deviation. For the other two diameters, the same fixed aspect ratio is used. The selected aspect ratio must be between 0.25 and 1. Therefore, only prolate spheroid shapes are possible here.

The screenshot shows the 'Grain Generator' window with 'Ellipsoid' selected in the dropdown menu. Below the menu, there are three input fields: 'Mean Ellipsoid Diameter 1 / (voxel)' with a value of 40, 'Aspect Ratio' with a value of 0.6, and 'Ellipsoid Diameter Standard Deviation / (voxel)' with a value of 10.

For the **Convex Polyhedron** shape, an (prolate spheroid) ellipsoid is used as enclosing object with matching Enclosing Object Volume (see the GrainGeo user guide for details). Select the mean diameter and the standard deviation. For the other two diameters, the same fixed aspect ratio is used. Again, the selected aspect ratio must be between 0.25 and 1.

The screenshot shows the 'Grain Generator' window with 'ConvexPolyhedron' selected in the dropdown menu. Below the menu, there are three input fields: 'Mean Polyhedron Diameter 1 / (voxel)' with a value of 40, 'Aspect Ratio' with a value of 0.6, and 'Polyhedron Diameter Standard Deviation / (voxel)' with a value of 10.

✓ Specify the Grain Orientation

Each granular object is created with a random orientation. By default, the orientation is isotropic, and every direction has the same probability. Check the **Specify the Grain Orientation** box to define an anisotropic distribution of the object's orientation.

Define the orientation tensor as described for the Object Options of the GrainGeo - Create Grains command. The three **Orientation Tensor** parameters entered here correspond to the diagonal entries of the orientation tensor.

The tensor describes the distribution of the grain's main direction, which corresponds to the long axis of the prolate spheroid.

The screenshot shows a section titled 'Specify the Grain Orientation' with a checked checkbox. Below the title, there are three input fields: 'Orientation Tensor XX' with a value of 0.7, 'Orientation Tensor YY' with a value of 0.2, and 'Orientation Tensor ZZ' with a value of 0.1.

✓ Random Field

Select **None** as **Random Field** to use only the **Grain Generator** for the structure generation.

Select **OneIsotropicField** to use the GrainGeo - Stochastic Field Thresholding command to create a random field. With the **Correlation Function**, you can switch between the Isotropic Squared Exponential (Gaussian) generation mode and the Isotropic Exponential (Laplacian) generation mode.

Enter the **Correlation Length** for the selected random field

Random Field: OneIsotropicField

Correlation Function: Gaussian

Correlation Length / (voxel): 5

Select **TwoIsotropicFields** to use the GrainGeo - Stochastic Field Thresholding command to create a random field with the Custom Generation Option using two kernels. You can define the **Relative Influence** of the first kernel, select a **Correlation Function** for each kernel and give both **Correlation Lengths**.

Random Field: TwoIsotropicFields

Correlation Function 1: Gaussian

Correlation Length 1 / (voxel): 5

Relative Influence / (%): 50

Correlation Function 2: Gaussian

Correlation Length 2 / (voxel): 5

✓ Square Random Field

The created random field contains values distributed around mean value 0. Check **Square Random Field** to square these values, thus turning all values positive. Checking **Invert Squared Field** further inverts them. These operations fundamentally change the stochastic field and the shape of the structures that appear after applying the threshold. See the Field Post-Processing in GrainGeo's Stochastic Field Thresholding command.

☒ Square Random Field

☒ Invert Squared Field

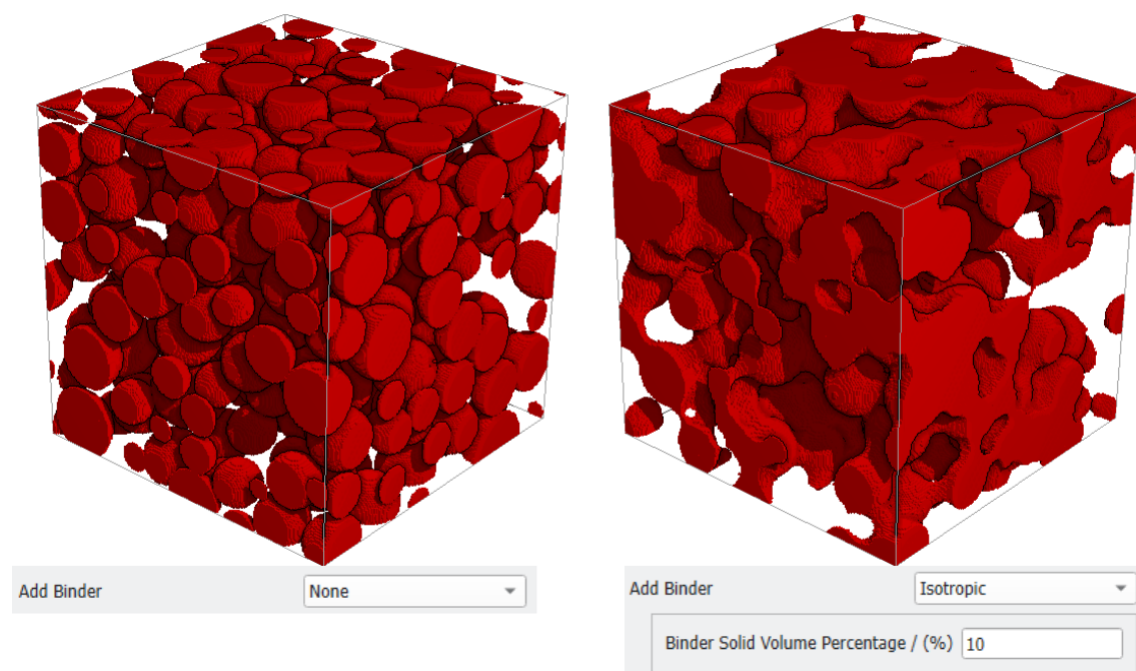
✓ Add Binder

It is possible to use GrainGeo - Add Binder as an additional structure generation step. Select **Isotropic** and enter the desired **Binder Solid Volume Percentage**.

Add Binder Isotropic

Binder Solid Volume Percentage / (%) 5

This function does not add another 'binder' material to the structure. Instead, it fills the small pores between the generated grains with the same material, thus creating a well-connected solid phase from unconnected objects. The added material is isotropic and homogeneously distributed inside the structure.



✓ Domain Size: NX, NY, NZ and Voxel Length

Define the domain size and resolution of the created 3D structure model. When changing the **Voxel Length**, be aware that the parameters of the [Random Field](#)⁷¹ and the [Grain Generator](#)⁷⁰ are given in units of the voxel length.

✓ Total Solid Volume Percentage, Pore and Solid Materials

The **Total Solid Volume Percentage** defines the percentage of grid cells filled with the **Solid Material**.

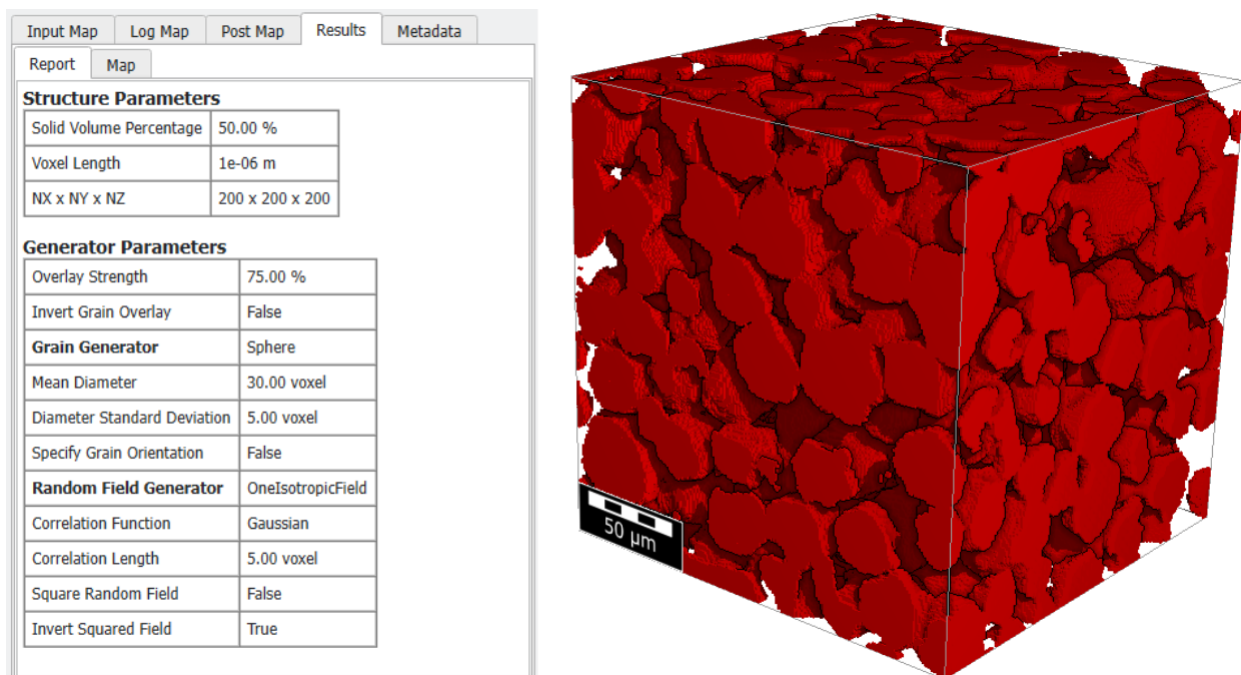
You can select one material for the solid part and one fluid material to fill the pores.

✓ Random Seed

The random seed is used for the grain structure generation with GrainGeo - Create and to create the random field(s).

Results

The default settings create a sphere packing overlaid with a random field of short correlation length.



Generate Granular Twin From 2D

The **Generate Granular Twin From 2D** uses the [Generate Granular Structure](#)^[69] app to generate a digital twin of a 2D reference structure, combined with an optimization algorithm to iterate the twin to the target.



Know how! The Nelder–Mead method is a direct search method (based on function comparison) to find the minimum of an objective function in a multidimensional space. The method approximates a local optimum of a problem with n variables when the objective function varies smoothly and is unimodal. The method uses the concept of a simplex, which is a special polytope of $n + 1$ vertices in n dimensions. In each iteration, it extrapolates the behavior of the objective function measured at each test point in order to find a new test point and to replace one of the old test points with the new one. See the [Wikipedia](#) page and [Brownlee, 2021](#)^[240] for further details.

In each iteration step of the optimization method, a structure is generated based on the optimization parameters and a scalar-valued error function is evaluated. For this,

the generated structure is analyzed, and the results are compared with reference values from the reference structure.



Modules needed to run this GeoApp:

GrainGeo, PoroDict+MatDict, GeoApp-2Dto3D

Clicking **Edit...** opens the **Generate Granular Twin From 2D** dialog. At the top, define a **Result File Name** for the result file and the result folder containing the generated structure.

The image displays two side-by-side screenshots of the 'GeoApp - Generate Granular Twin From 2D' dialog box. The left screenshot shows the 'Initial Parameter Values' section, where 'GlobalOptimizer' is selected under 'Initial Parameter Values'. The right screenshot shows the 'Optimization Components' section, where four checkboxes are checked: 'Optimize Overlay Strength', 'Optimize Grain Generator Parameters', 'Optimize Random Field Parameters', and 'Optimize Binder Parameters'. Both screenshots show the 'Result File Name' as 'StatisticalDigitalTwin2D' and the 'Grain Generator' as 'Sphere'.

Initial Parameter Values

Select **UseManual** to use the structure generation parameters given in the [Overlay Grains and Random Field Settings](#)^[76], [Grain Generator](#)^[76], and [Random Field](#)^[77] panels as starting point for the local optimization.

Select **GlobalOptimizer** to run a global optimization to find good initial parameters for the local optimizer. In this case, only the selections made in the **Grain Generator**, **Random Field** and **Add Binder** drop-down menus are complied with. The parameter values entered in the [Overlay Grains and Random Field Settings](#)^[76], [Grain Generator](#)^[76], [Random Field](#)^[77] and [Add Binder](#)^[78] panels, e.g., for diameters and

correlation lengths are not taken into account. Rather, the global optimizer tries to find good values for these parameters.

✓ Overlay Grains and Random Field Settings

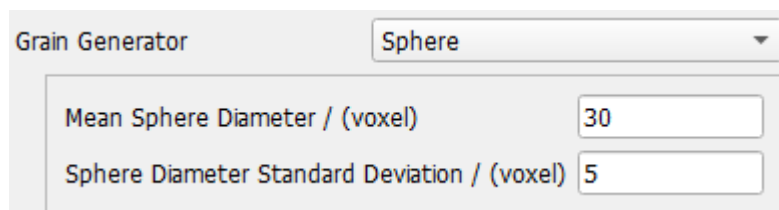
In this panel you setup the initial structure for the local optimization.

The **Overlay Strength** is the field overlay strength in percentage. At 100% overlay strength the result will only show the grain package, while at 0% overlay strength the result will show only the Gaussian random field. If no **Random Field** is used, this value is automatically set to 100%. If no **Grain Generator** is used, this value is automatically set to 0%.

✓ Grain Generator

Select the basic shape used to generate the 3D structure. Select **None** as **Grain Generator** to use only the **Random Field** for the structure generation. The app uses the GrainGeo - Create Grains command to create the grain structure. Be aware that all lengths are given in the unit voxel.

For the **Sphere** shape, the diameters are Gaussian distributed. Select the mean diameter and the standard deviation.

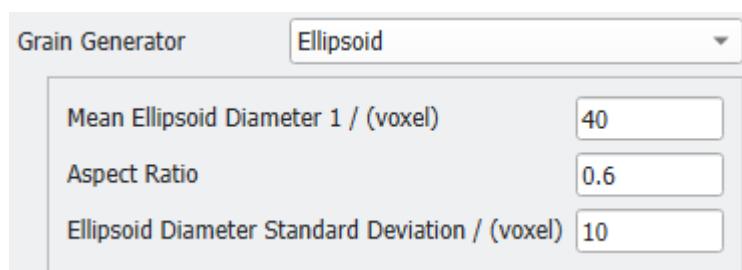


Grain Generator: Sphere

Mean Sphere Diameter / (voxel): 30

Sphere Diameter Standard Deviation / (voxel): 5

For the **Ellipsoid** shape, the first diameter is Gaussian distributed. Select the mean diameter and the standard deviation. For the other two diameters, the same fixed aspect ratio is used. The selected aspect ratio must be between 0.25 and 1. Therefore, only prolate spheroid shapes are possible here.



Grain Generator: Ellipsoid

Mean Ellipsoid Diameter 1 / (voxel): 40

Aspect Ratio: 0.6

Ellipsoid Diameter Standard Deviation / (voxel): 10

For the **Convex Polyhedron** shape, an (prolate spheroid) ellipsoid is used as enclosing object with matching Enclosing Object Volume (see the GrainGeo user guide for details). Select the mean diameter and the standard deviation. For the other two diameters, the same fixed aspect ratio is used. Again, the selected aspect ratio must be between 0.25 and 1.

Grain Generator
ConvexPolyhedron

Mean Polyhedron Diameter 1 / (voxel)
40

Aspect Ratio
0.6

Polyhedron Diameter Standard Deviation / (voxel)
10



The values entered for diameters, standard deviations and aspect ratios define the initial structure for the local optimization. They are only used if **UseManual** was selected for [Initial Parameter Values](#)

Random Field

Select **None** as **Random Field** to use only the **Grain Generator** for the structure generation.

Select **OneIsotropicField** to use the GrainGeo - Stochastic Field Thresholding command to create a random field. With the **Correlation Function**, you can switch between the Isotropic Squared Exponential (Gaussian) generation mode and the Isotropic Exponential (Laplacian) generation mode.

Enter the **Correlation Length** for the selected random field

Random Field
OneIsotropicField

Correlation Function
Gaussian

Correlation Length / (voxel)
5

Select **TwoIsotropicFields** to use the GrainGeo - Stochastic Field Thresholding command to create a random field with the Custom Generation Option using two kernels. You can define the **Relative Influence** of the first kernel, select a **Correlation Function** for each kernel and give both **Correlation Lengths**.

Random Field
TwoIsotropicFields

Correlation Function 1
Gaussian

Correlation Length 1 / (voxel)
5

Relative Influence / (%)
50

Correlation Function 2
Gaussian

Correlation Length 2 / (voxel)
5



The values entered for correlation length(s) and relative influence define the initial structure for the local optimization. They are only used if **UseManual** was selected for [Initial Parameter Values](#) ⁷⁵.

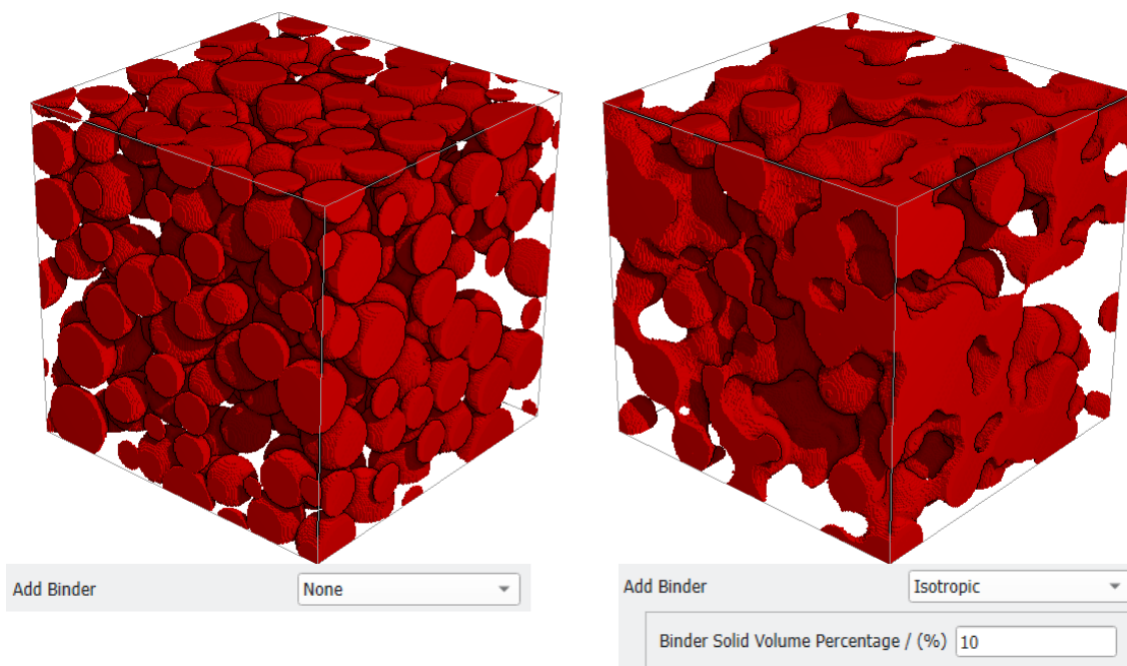
✓ Add Binder

It is possible to use GrainGeo - Add Binder as an additional structure generation step. Select **Isotropic** and enter the desired **Binder Solid Volume Percentage**.

Add Binder Isotropic

Binder Solid Volume Percentage / (%)

This function does not add another 'binder' material to the structure. Instead, it fills the small pores between the generated grains with the same material, thus creating a well-connected solid phase from unconnected objects. The added material is isotropic and homogeneously distributed inside the structure.



✓ Criteria to Match

The error function is a combination of several components. Define the error function components from the list of physical properties. These structure properties will be matched by the twin as good as possible.

Criteria to Match

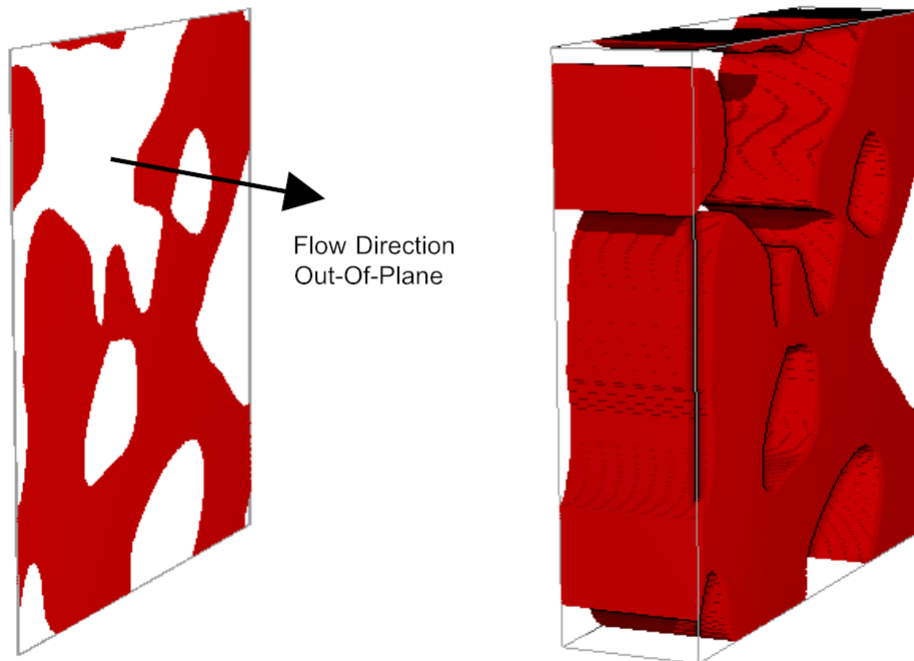
- ☒ Pore and Solid Granulometry (PoroDict/MatDict)
- ☒ Pore and Solid Chord Length (PoroDict/MatDict)
- ☒ Specific Surface Area (PoroDict/MatDict)
- ☒ Out-Of-Plane 2D Permeability (FlowDict)

Select **Pore and Solid Granulometry** to use the PoroDict - Pore Size Distribution (Granulometry) and MatDict - Solid Size Distribution commands to compare the digital twin with the original 2D image.

Select **Pore and Solid Chord Length** to use the PoroDict - Chord Length Distribution and MatDict - Chord Length Distribution commands to compare the digital twin with the original 2D image.

Select **Specific Surface Area** to use the MatDict - Estimate Surface Area command to compare the digital twin with the original 2D image.

Select **Out-Of-Plane 2D Permeability** to use the FlowDict - Stokes command to compare flow simulation results on a 2D slice with the original 2D image. The flow is computed in orthogonal (normal) direction to the 2D image plane with periodic boundary conditions. This corresponds to a 3D structure with parallel channels as illustrated below. Be aware that the computed 2D permeability is not comparable to the permeability of the 3D structure. This criteria is well suited as a supplementary matching criteria, because it alone exhibits a quadratic relationship on the pore radius size.



You must select at least one of these criteria, otherwise the optimizer will fail with an error message during the first optimization step.

✓ Optimization Components

Select the sets of parameters to be used as optimization variables for fitting the reference structure. If not selected, the according parameters from the Digital Twin Setup will stay constant during the optimization.

Optimization Components

- ☒ Optimize Overlay Strength
- ☒ Optimize Grain Generator Parameters
- ☒ Optimize Random Field Parameters
- ☒ Optimize Binder Parameters

Select **Optimize Overlay Strength** to vary the [Overlay Strength](#)⁷⁶.

Select **Optimize Grain Generator Parameters** to vary the diameter, standard deviation and aspect ratio parameters of the [Grain Generator](#)⁷⁶. Note that the optimizer does not optimize the generator type, i.e., does not vary between **Sphere**, **Ellipsoid** and **ConvexPolyhedron** shapes.

Select **Optimize Random Field Parameters** to vary the correlation length(s) and the relative influence parameters of the [Random Field](#)^[77]. Note that the optimizer does not vary between the **OnIsotropicField** and **TwoIsotropicFields** models.

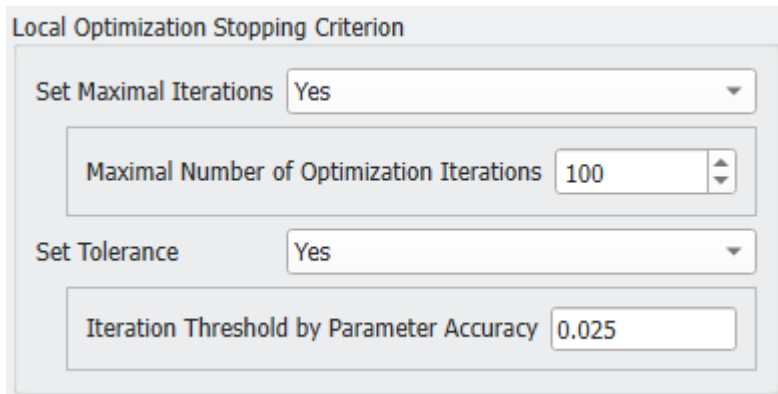
Select **Optimize Binder Parameters** to vary the solid volume percentage of the binder.

You must select at least one of these options, otherwise the optimizer will fail with an error message.

✓ Local Optimization Stopping Criterion

Set the stopping criterion by choosing a maximal number of iterations or set a tolerance accuracy to reach. Note that choosing none or setting the **Maximal Number of Optimization Iterations** to 0 will perform one single iteration step only.

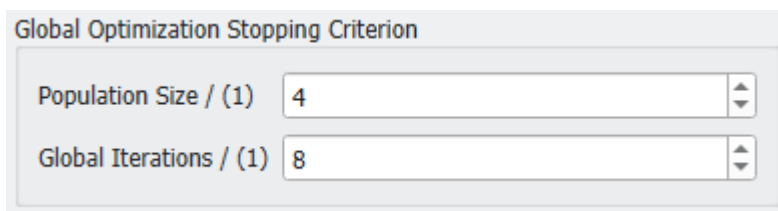
The selected tolerance applies to the structure generation parameters varied in each iteration step. If the change in these parameters becomes smaller than the selected tolerance, the optimizer stops. The tolerance does not set a limit value for the resulting [error function](#)^[78] of the found digital twin.



The dialog box titled "Local Optimization Stopping Criterion" contains four settings:

- Set Maximal Iterations:** A dropdown menu with "Yes" selected.
- Maximal Number of Optimization Iterations:** A numeric input field with the value "100".
- Set Tolerance:** A dropdown menu with "Yes" selected.
- Iteration Threshold by Parameter Accuracy:** A numeric input field with the value "0.025".

✓ Global Optimization Stopping Criterion



The dialog box titled "Global Optimization Stopping Criterion" contains two settings:

- Population Size / (1):** A numeric input field with the value "4".
- Global Iterations / (1):** A numeric input field with the value "8".

The **Population Size** is the number of random samples taken per parameter within the parameter bounds. A large value improves the exploration but increases the runtime for the Differential Evolution. The minimal value allowed is 2.

Global Iterations are the maximum number of generations to evolve the population in the Differential Evolution. Higher values refine the results but require more evaluations. The minimal value allowed is 2.

In total, the number of function evaluations can be up to **Population Size** times **Global**

Iterations times the number of parameters. The number of parameters is defined by the selected **Optimization Components**.

✓ Set Geometry Size

Check the box to set the size of the structure model used during the optimization.

☒ Set Geometry Size

NX	200	↕
NY	200	↕
NZ	200	↕

If the box is not checked, the app chooses a size automatically.



Important! The numbers given for **NX**, **NY**, **NZ** must be even! The generation fails when uneven numbers are entered here.

✓ Clean up after completion

If checked, all intermediate results are deleted.

✓ Set Expert Structure Generation Settings

Activating the check box enables to set several additional parameter.

☒ Invert Grains for Overlay

Check **Invert Grains for Overlay** to switch pore and solid material. In this case, the grain generator creates the pore space, and the background becomes the solid material.

Each granular object is created with a random orientation. By default, the orientation is isotropic, and every direction has the same probability. Check the **Specify the Grain Orientation** box to define an anisotropic distribution of the object's orientation.

Define the orientation tensor as described for the Object Options of the GrainGeo - Create Grains command. The three **Orientation Tensor** parameters entered here correspond to the diagonal entries of the orientation tensor.

The tensor describes the distribution of the grain's main direction, which corresponds to the long axis of the prolate spheroid.

☒ Specify the Grain Orientation

Orientation Tensor XX	0.7
Orientation Tensor YY	0.2
Orientation Tensor ZZ	0.1

The created random field contains values distributed around mean value 0. Check **Square Random Field** to square these values, thus turning all values positive. Checking **Invert Squared Field** further inverts them. These operations fundamentally change the stochastic field and the shape of the structures that appear after applying the threshold. See the Field Post-Processing in GrainGeo's Stochastic Field Thresholding command.

☒ Square Random Field

☒ Invert Squared Field

✓ Set Expert Local Optimization Settings

☒ Set Expert Local Optimization Settings

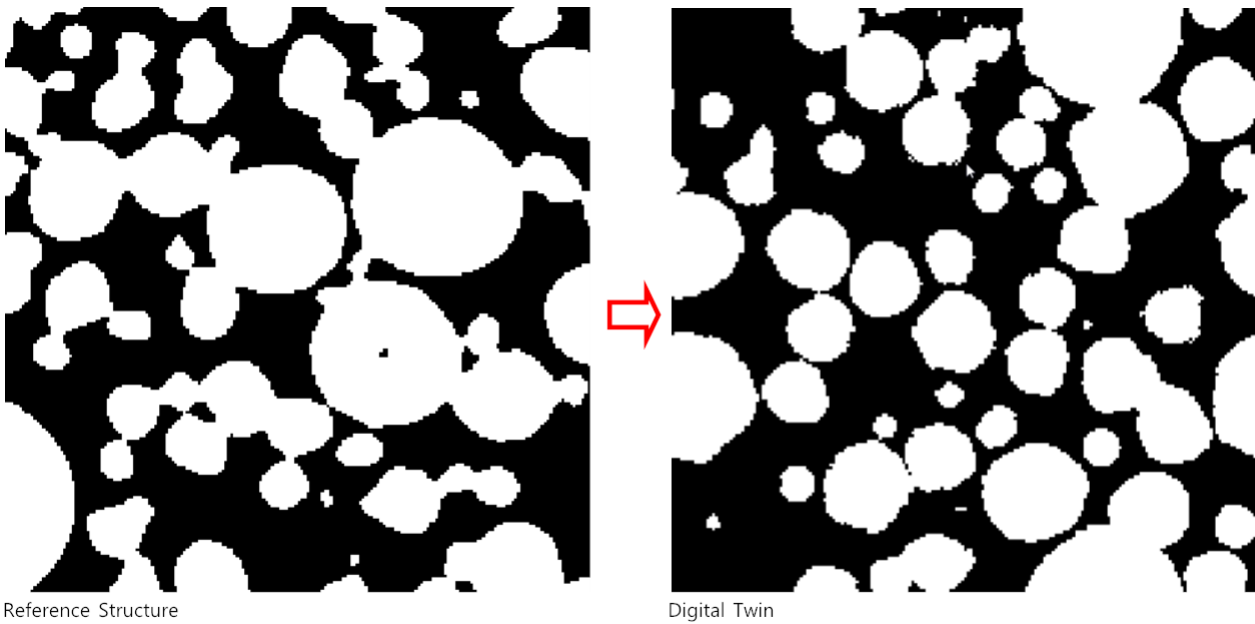
Initial Simplex Scaling Factor

Increasing the step size of the local optimization may improve the results of the optimizer.

The structure generation is a stochastic process, therefore each test structure is not only dependent on the parameters to optimize, but also on a random number. The computed matching criteria are therefore dependent on the random number, too. If the dependency on the random number is larger than the dependency on the structure generation parameters, the local optimization may become stuck and cannot find the correct direction for the parameter search. Therefore, it may help to enlarge the step size to increase the effect of the parameter choice on the result and to help the algorithm find the new search direction.

Results

Click OK to input the entered parameters, and then click Run in the GeoApp section to start the app. The results are immediately shown in the opening Result Viewer after the process is finished.



Report tab

The **Structure Details** table reports the grid size, voxel length and solid volume percentage of the reference structure and the digital twin. The **Digital Optimization Twin** is the structure used for the comparison with the reference structure, the **Digital Twin** the created 3D structure.

Structure Details						
Type	Location	Size x	Size y	Size z	VL / μm	SVP / (%)
Reference Structure	Reference Structure/Structure.gdt	1	200	200	1.00	52.87
Digital Optimization Twin	Digital Optimization Twin/Structure.gdt	1	400	400	1.00	52.44
Digital Twin	Digital Twin/Structure.gdt	200	200	200	1.00	52.90

The **Structure Generation Parameters** table shows the found optimal structure generation parameters. You can use these parameters as input in the [Generate Structure app](#) ⁶⁹ to create multiple digital twin models.

Structure Generation Parameters		
Description	Value	Length / μm
Dia Mean	20.87	20.87
Dia SD	10.01	10.01
Sigma1	5.01	5.01

The **Structure Comparison** table compares the computed measures of the reference structure and the digital twin and states the error in the respective measure.

Structure Comparison			
Name	Reference Structure	Dig Twin Structure	Error
Pore Size Distribution	8.15 µm 13.73 µm 18.82 µm 23.44 µm 29.62 µm	6.96 µm 12.82 µm 17.63 µm 23.39 µm 29.61 µm	5.56 %
Solid Granulometry	11.04 µm 18.2 µm 24.86 µm 30.87 µm 52.16 µm	12.08 µm 18.85 µm 26.48 µm 34.04 µm 46.74 µm	8.06 %
Specific Surface Area	7.15e+04	7.92e+04	10.73 %
Chord Length Distribution Pore Y Dir	3.91 µm 8.37 µm 13.72 µm 23.34 µm 38.97 µm	2.22 µm 6.52 µm 11.61 µm 20.61 µm 38.03 µm	18.97 %
Chord Length Distribution Pore Z Dir	3.61 µm 8.13 µm 13.82 µm 21.31 µm 38.62 µm	1.88 µm 5.78 µm 10.98 µm 19.59 µm 38.83 µm	21.19 %
Chord Length Distribution Solid Y Dir	5.04 µm 10.79 µm 16.04 µm 21.88 µm 46.38 µm	3.91 µm 10.57 µm 16.13 µm 22.89 µm 37.57 µm	9.75 %
Chord Length Distribution Solid Z Dir	4.22 µm 9.79 µm 15.71 µm 24.63 µm 41.84 µm	3.71 µm 10.83 µm 16.39 µm 23.42 µm 37.01 µm	8.70 %
Permeability X Dir	1.37e-11	1.39e-11	1.82 %
Permeability Solid X Dir	2.27e-11	1.97e-11	13.15 %
Weighted Average Error			7.63 %

Distributions are given as Percentiles P10, P30, P50, P70 and P90.

The **Optimization** table report the number of iterations and function evaluations needed. Below, the total runtime of the optimization is reported.

Optimization	
Local Optimization Results	
Number of Iterations	33
Number of Function Evaluations	79
Result Message	Optimization terminated successfully.

Plots tab

The **Parameters by Evaluation** and **Parameters by Iteration** plots show the evolution and convergence of the structure generation parameters in each step.

The **Target Errors by Evaluation / Iteration** plots show the results of the structure comparison in each step.

Data Visualization

Digital Optimization Twin	Load Digital Optimization Twin/Structure.gdt
Digital Twin	Load Digital Twin/Structure.gdt
Reference Structure	Load Reference Structure/Structure.gdt

In this tab, you can load the 2D reference structure, the 2D **Digital Optimization Twin** used to compute the matching criteria and the created 3D **Digital Twin**.

Generate Granular Twin From 3D

The **Generate Granular Twin From 3D** uses the [Generate Granular Structure](#)^[69] app to generate a digital twin of a 3D reference structure, combined with an optimization algorithm to iterate the twin to the target.



Modules needed to run this GeoApp:

GrainGeo, PoroDict+MatDict

Depending on the settings: FlowDict, DiffuDict

Clicking **Edit...** opens the **Generate Granular Twin From 3D** dialog. At the top, define a **Result File Name** for the result file and the result folder containing the generated structure.

The dialog box is titled "GeoApp - Generate Granular Twin From 3D". It contains the following sections:

- Result File Name (*.gdr)**: Text field with "StatisticalDigitalTwin3D".
- Initial Parameter Values**: Dropdown menu with "GlobalOptimizer".
- Overlay Grains and Random Field Settings**:
 - Overlay Strength / (%)**: Text field with "75".
 - Grain Generator**: Dropdown menu with "Sphere".
 - Mean Sphere Diameter / (voxel)**: Text field with "30".
 - Sphere Diameter Standard Deviation / (voxel)**: Text field with "10".
 - Random Field**: Dropdown menu with "OneIsotropicField".
 - Correlation Function**: Dropdown menu with "Gaussian".
 - Correlation Length / (voxel)**: Text field with "5".
- Add Binder**: Dropdown menu with "None".
- Criteria to Match**:
 - ☒ Pore and Solid Granulometry (PoroDict/MatDict)
 - ☐ Porosimetry (PoroDict/MatDict)
 - ☒ Pore and Solid Chord Length (PoroDict/MatDict)
 - ☒ Specific Surface Area (PoroDict/MatDict)
 - ☐ Permeability (FlowDict)
 - ☐ Diffusivity (DiffuDict)
- Optimization Components**:
 - ☒ Optimize Overlay Strength
 - ☒ Optimize Grain Generator Parameters
 - ☒ Optimize Random Field Parameters
 - ☒ Optimize Binder Parameters
- Local Optimization Stopping Criterion**:
 - Set Maximal Iterations**: Dropdown menu with "No".
 - Set Tolerance**: Dropdown menu with "Yes".
 - Iteration Threshold by Parameter Accuracy**: Text field with "0.025".
- Global Optimization Stopping Criterion**:
 - Population Size / (1)**: Text field with "4".
 - Global Iterations / (1)**: Text field with "8".
 - ☐ Set Geometry Size
 - ☒ Clean up after completion
 - ☐ Set Expert Structure Generation Settings
 - ☐ Set Expert Local Optimization Settings

At the bottom, there are icons for saving, undo, redo, and a "Reset" button, followed by "OK" and "Cancel" buttons.

Initial Parameter Values

Select **UseManual** to use the structure generation parameters given in the [Overlay Grains and Random Field Settings](#)^[87], [Grain Generator](#)^[87], and [Random Field](#)^[88] panels as starting point for the optimization.

Select **GlobalOptimizer** to run a global optimization to find good initial parameters for the local optimizer. In this case the values selected in the [Overlay Grains and Random Field Settings](#)^[87], [Grain Generator](#)^[87], and [Random Field](#)^[88] panels are not used.

✓ Overlay Grains and Random Field Settings

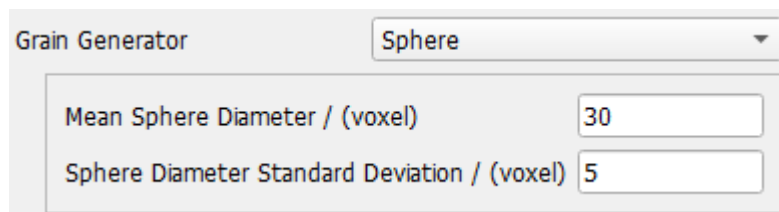
In this panel you setup the initial structure for the local optimization.

The **Overlay Strength** is the field overlay strength in percentage. At 100% overlay strength the result will only show the grain package, while at 0% overlay strength the result will show only the Gaussian random field. If no **Random Field** is used, this value is automatically set to 100%. If no **Grain Generator** is used, this value is automatically set to 0%.

✓ Grain Generator

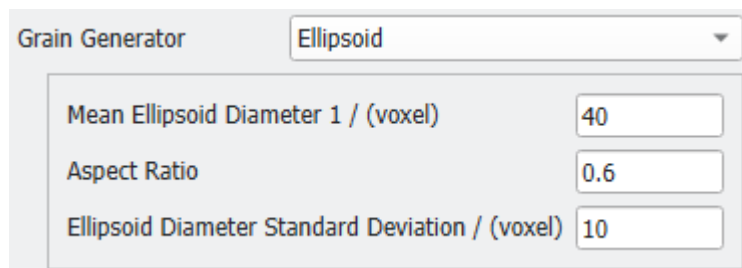
Select the basic shape used to generate the 3D structure. Select **None** as **Grain Generator** to use only the **Random Field** for the structure generation. The app uses the GrainGeo - Create Grains command to create the grain structure. Be aware that all lengths are given in the unit voxel.

For the **Sphere** shape, the diameters are Gaussian distributed. Select the mean diameter and the standard deviation.



The screenshot shows the 'Grain Generator' panel with a dropdown menu set to 'Sphere'. Below the dropdown, there are two input fields: 'Mean Sphere Diameter / (voxel)' with a value of 30, and 'Sphere Diameter Standard Deviation / (voxel)' with a value of 5.

For the **Ellipsoid** shape, the first diameter is Gaussian distributed. Select the mean diameter and the standard deviation. For the other two diameters, the same fixed aspect ratio is used. The selected aspect ratio must be between 0.25 and 1. Therefore, only prolate spheroid shapes are possible here.



The screenshot shows the 'Grain Generator' panel with a dropdown menu set to 'Ellipsoid'. Below the dropdown, there are three input fields: 'Mean Ellipsoid Diameter 1 / (voxel)' with a value of 40, 'Aspect Ratio' with a value of 0.6, and 'Ellipsoid Diameter Standard Deviation / (voxel)' with a value of 10.

For the **Convex Polyhedron** shape, an (prolate spheroid) ellipsoid is used as enclosing object with matching Enclosing Object Volume (see the GrainGeo user guide for details). Select the mean diameter and the standard deviation. For the other two

diameters, the same fixed aspect ratio is used. Again, the selected aspect ratio must be between 0.25 and 1.

Grain Generator	ConvexPolyhedron
Mean Polyhedron Diameter 1 / (voxel)	40
Aspect Ratio	0.6
Polyhedron Diameter Standard Deviation / (voxel)	10



The values entered for diameters, standard deviations and aspect ratios define the initial structure for the local optimization. They are only used if **UseManual** was selected for [Initial Parameter Values](#) ⁸⁶

✓ Random Field

Select **None** as **Random Field** to use only the **Grain Generator** for the structure generation.

Select **OneIsotropicField** to use the GrainGeo - Stochastic Field Thresholding command to create a random field. With the **Correlation Function**, you can switch between the Isotropic Squared Exponential (Gaussian) generation mode and the Isotropic Exponential (Laplacian) generation mode.

Enter the **Correlation Length** for the selected random field

Random Field	OneIsotropicField
Correlation Function	Gaussian
Correlation Length / (voxel)	5

Select **TwoIsotropicFields** to use the GrainGeo - Stochastic Field Thresholding command to create a random field with the Custom Generation Option using two kernels. You can define the **Relative Influence** of the first kernel, select a **Correlation Function** for each kernel and give both **Correlation Lengths**.

Random Field
TwoIsotropicFields

Correlation Function 1
Gaussian

Correlation Length 1 / (voxel)
5

Relative Influence / (%)
50

Correlation Function 2
Gaussian

Correlation Length 2 / (voxel)
5


The values entered for correlation length(s) and relative influence define the initial structure for the local optimization. They are only used if **UseManual** was selected for [Initial Parameter Values](#).

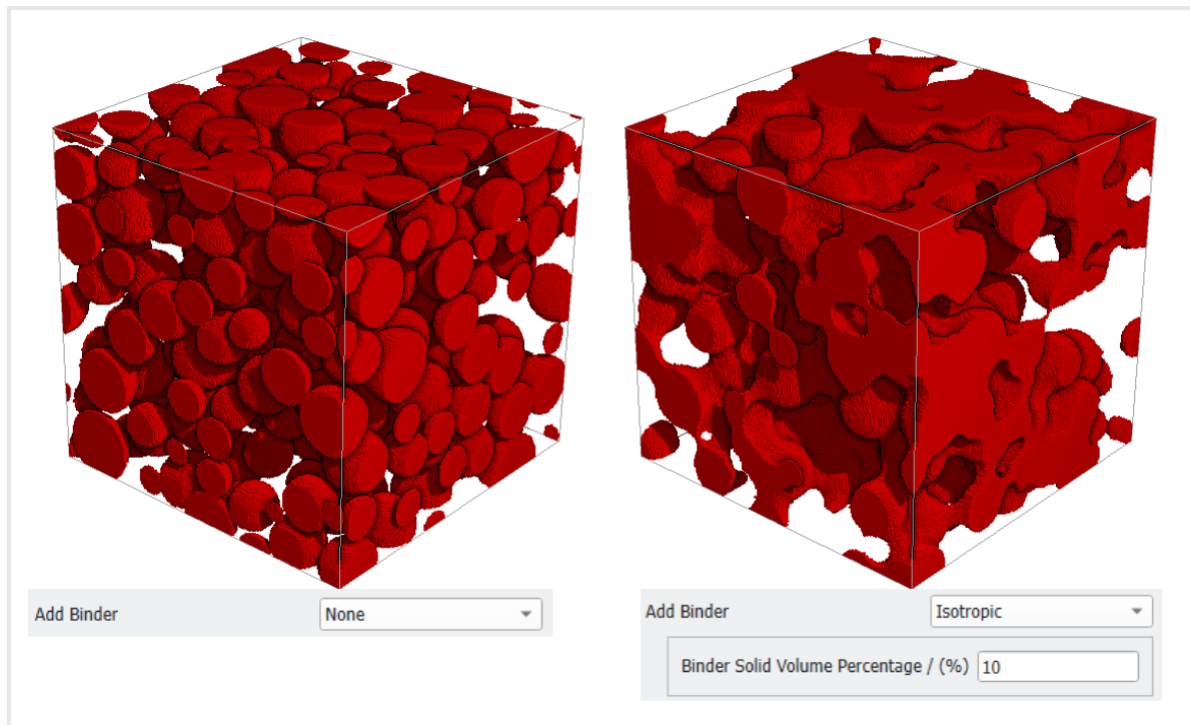
Add Binder

It is possible to use GrainGeo - Add Binder as an additional structure generation step. Select **Isotropic** and enter the desired **Binder Solid Volume Percentage**.

Add Binder
Isotropic

Binder Solid Volume Percentage / (%)
5

This function does not add another 'binder' material to the structure. Instead, it fills the small pores between the generated grains with the same material, thus creating a well-connected solid phase from unconnected objects. The added material isotropic and homogeneously distributed inside the structure.



✓ Criteria to Match

The error function is a combination of several components. Define the error function components from the list of physical properties. These structure properties will be matched by the twin as good as possible.

Criteria to Match

- ☒ Pore and Solid Granulometry (PoroDict/MatDict)
- ☒ Porosimetry (PoroDict/MatDict)
- ☒ Pore and Solid Chord Length (PoroDict/MatDict)
- ☒ Specific Surface Area (PoroDict/MatDict)
- ☒ Permeability (FlowDict)
 - ☒ Permeability in X-Direction
 - ☒ Permeability in Y-Direction
 - ☒ Permeability in Z-Direction
- ☒ Diffusivity (DiffuDict)
 - ☒ Diffusivity in X-Direction
 - ☒ Diffusivity in Y-Direction
 - ☒ Diffusivity in Z-Direction

Select **Pore and Solid Granulometry** to use the PoroDict - Pore Size Distribution (Granulometry) and MatDict - Solid Size Distribution commands to compare the digital twin with the original 3D image.

Select **Porosimetry** to use the PoroDict - Pore Size Distribution (Porosimetry) command to compare the digital twin with the original 3D image.

Select **Pore and Solid Chord Length** to use the PoroDict - Chord Length Distribution and MatDict - Chord Length Distribution commands to compare the digital twin with the original 3D image.

Select **Specific Surface Area** to use the MatDict - Estimate Surface Area command to compare the digital twin with the original 3D image.

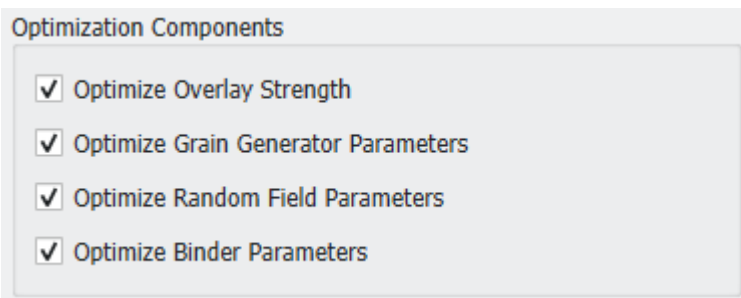
Select **Permeability** to use the FlowDict-Stokes command to determine the permeability. Select the space directions used to compare the digital twin with the original 3D structure. To use this option, a FlowDict license is required.

Select **Diffusivity** to use the DiffuDict - Bulk Diffusion command to determine the diffusivity. Select the space directions used to compare the digital twin with the original 3D structure. To use this option, a DiffuDict license is required.

You must select at least one of these criteria, otherwise the optimizer will fail with an error message.

✓ Optimization Components

Select the sets of parameters to be used as optimization variables for fitting the reference structure. If not selected, the according parameters from the Digital Twin Setup will stay constant during the optimization.



Select **Optimize Overlay Strength** to vary the [Overlay Strength](#)^[87].

Select **Optimize Grain Generator Parameters** to vary the diameter, standard deviation and aspect ratio parameters of the [Grain Generator](#)^[87]. Note that the optimizer does not optimize the generator type, i.e., does not vary between **Sphere**, **Ellipsoid** and **ConvexPolyhedron** shapes.

Select **Optimize Random Field Parameters** to vary the correlation length(s) and the relative influence parameters of the [Random Field](#)^[88]. Note that the optimizer does not vary between the **OnIsotropicField** and **TwoIsotropicFields** models.

Select **Optimize Binder Parameters** to vary the solid volume percentage of the binder. You must select at least one of these options, otherwise the optimizer will fail with an error message.

✓ Local Optimization Stopping Criterion

Set the stopping criterion by choosing a maximal number of iterations or set a tolerance accuracy to reach. Note that choosing none or setting the **Maximal Number of Optimization Iterations** to 0 will perform one single iteration step only.

The selected tolerance applies to the structure generation parameters varied in each iteration step. If the change in these parameters becomes smaller than the selected tolerance, the optimizer stops. The tolerance does not set a limit value for the resulting [error function](#) of the found digital twin.

Local Optimization Stopping Criterion

Set Maximal Iterations

Maximal Number of Optimization Iterations

Set Tolerance

Iteration Threshold by Parameter Accuracy

✓ Global Optimization Stopping Criterion

Global Optimization Stopping Criterion

Population Size / (1)

Global Iterations / (1)

The **Population Size** is the number of random samples taken per parameter within the parameter bounds. A large value improves the exploration but increases the runtime for the Differential Evolution. The minimal value allowed is 2.

Global Iterations are the maximum number of generations to evolve the population in the Differential Evolution. Higher values refine the results but require more evaluations. The minimal value allowed is 2.

In total, the number of function evaluations can be up to **Population Size** times **Global Iterations** times the number of parameters. The number of parameters is defined by the selected **Optimization Components**.

✓ Set Geometry Size

Check the box to set the size of the structure model used during the optimization.

☒ Set Geometry Size

NX	200
NY	200
NZ	200

If the box is not checked, the app chooses a size automatically.



Important! The numbers given for **NX**, **NY**, **NZ** must be even! The generation fails when uneven numbers are entered here.

☒ Clean up after completion

If checked, all intermediate results are deleted.

☒ Set Expert Structure Generation Settings

Activating the check box enables to set several additional parameter.

Check **Invert Grains for Overlay** to switch pore and solid material. In this case, the grain generator creates the pore space, and the background becomes the solid material.

☒ Invert Grains for Overlay

Each granular object is created with a random orientation. By default, the orientation is isotropic, and every direction has the same probability. Check the **Specify the Grain Orientation** box to define an anisotropic distribution of the object's orientation.

Define the orientation tensor as described for the Object Options of the GrainGeo - Create Grains command. The three **Orientation Tensor** parameters entered here correspond to the diagonal entries of the orientation tensor.

The tensor describes the distribution of the grain's main direction, which corresponds to the long axis of the prolate spheroid.

☒ Specify the Grain Orientation

Orientation Tensor XX	0.7
Orientation Tensor YY	0.2
Orientation Tensor ZZ	0.1

The created random field contains values distributed around mean value 0. Check

Square Random Field to square these values, thus turning all values positive. Checking **Invert Squared Field** further inverts them. These operations fundamentally change the stochastic field and the shape of the structures that appear after applying the threshold. See the Field Post-Processing in GrainGeo's Stochastic Field Thresholding command.

☒ Square Random Field

☒ Invert Squared Field

✓ Set Expert Local Optimization Settings

☒ Set Expert Local Optimization Settings

Initial Simplex Scaling Factor

1

Increasing the step size of the local optimization may improve the results of the optimizer.

The structure generation is a stochastic process, therefore each test structure is not only dependent on the parameters to optimize, but also on a random number. The computed matching criteria are therefore dependent on the random number, too. If the dependency on the random number is larger than the dependency on the structure generation parameters, the local optimization may become stuck and cannot find the correct direction for the parameter search. Therefore, it may help to enlarge the step size to increase the effect of the parameter choice on the result and to help the algorithm find the new search direction.

Results

After the generation is finished, the corresponding result file is opened in the **Result Viewer**.

The Report tab

The **Structure Details** table reports the grid size, voxel length and solid volume percentage of the reference structure and the digital twin. The **Digital Optimization Twin** is the structure used for the comparison with the reference structure, the **Digital Twin** the created 3D structure.

Structure Details

Type	Location	Size x	Size y	Size z	VL / μm	SVP / (%)
Reference Structure	Reference Structure/Structure.gdt	200	200	200	1.00	52.65
Digital Optimization Twin	Digital Optimization Twin/Structure.gdt	400	400	400	1.00	52.68
Digital Twin	Digital Twin/Structure.gdt	200	200	200	1.00	52.67

The **Structure Generation Parameters** table shows the found optimal structure generation parameters. You can use these parameters as input in the [Generate Structure app](#) to create multiple digital twin models.

Structure Generation Parameters

Description	Value	Length / μm
Dia Mean	23.31	23.31
Dia SD	6.83	6.83
Sigma1	18.28	18.28

The **Structure Comparison** table compares the computed measures of the reference structure and the digital twin and states the error in the respective measure.

Structure Comparison

Name	Reference Structure	Dig Twin Structure	Error
Pore Size Distribution	7.31 μm 10.87 μm 13.78 μm 17.1 μm 23.41 μm	5.88 μm 10.45 μm 14.04 μm 17.6 μm 23.5 μm	5.72 %
Solid Granulometry	11.9 μm 18.65 μm 26.2 μm 40.36 μm 65.11 μm	16.56 μm 22.06 μm 26.52 μm 31.54 μm 39.01 μm	24.11 %
Specific Surface Area	9.17e+04	1.01e+05	10.32 %
Permeability Z Dir	1.93e-12	1.97e-12	1.92 %
Tortuosity Z Dir	1.57	1.58	0.13 %
Weighted Average Error			8.44 %

Distributions are given as Percentiles P10, P30, P50, P70 and P90.

The **Optimization** table report the number of iterations and function evaluations needed. Iterations and Evaluations needed for the global optimization and for the local optimization are reported separately. Below, the total runtime of the optimization is reported.

Optimization

Global Optimization Results

Number of Iterations	8
Number of Function Evaluations	54
Result Message	Maximum number of iterations has been exceeded.

Local Optimization Results

Number of Iterations	27
Number of Function Evaluations	66
Result Message	Optimization terminated successfully.

-- Total Runtime: 39840.40s

Plots tab

The **Parameters by Evaluation** and **Parameters by Iteration** plots show the evolution and convergence of the structure generation parameters in each step.

The **Target Errors by Evaluation / Iteration** plots show the results of the structure comparison in each step.

Data Visualization

Digital Optimization Twin	Load Digital Optimization Twin/Structure.gdt
Digital Twin	Load Digital Twin/Structure.gdt
Reference Structure	Load Reference Structure/Structure.gdt

In this tab, you can load the 2D reference structure, the 2D **Digital Optimization Twin** used to compute the matching criteria and the created 3D **Digital Twin**.

Result folder content

In the result folder, find the following:

- The analysis results of the reference structure is stored in the **Reference Structure** folder.
- The analysis results of the found digital twin is stored in the **Digital Twin** folder.
- The intermediate evaluation results, if **Clean up after completion** is not checked.
- The used parameters, the corresponding simulation results and the error function evaluation of every step are contained in the **DigitalTwinGlobal.csv** and **DigitalTwin.csv** files.
- The final statistical digital twin **Structure.gdt**.

Generate Nonwoven Twin

The **Generate Nonwoven Twin** app creates a **Statistical Digital Twin** of a non-woven micro-structure, resembling defined stochastic geometrical properties of the original. Ensure to have a representative cutout of your original structure, since otherwise the resulting twin structure cannot match all properties sufficiently. The app optimizes for curvature and, if selected, for density distribution in Z-direction

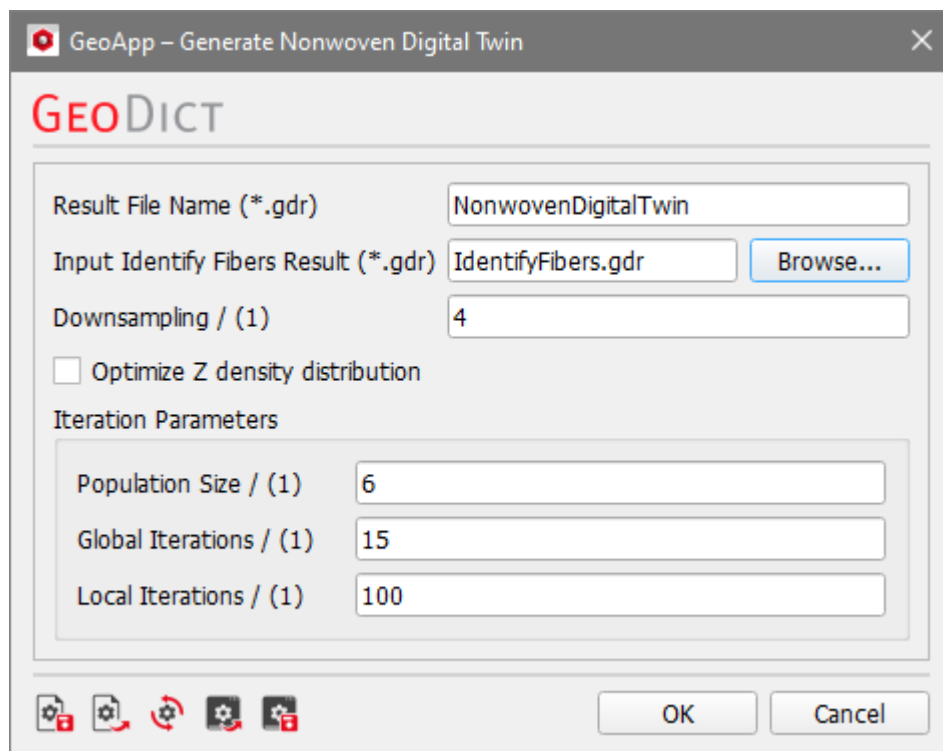


Modules needed to run this GeoApp:

FiberGeo, FiberFind

Optional: MatDict

A 3D structure and the corresponding result file (*.gdr) from FiberFind - Identify Fibers (AI) is required as input, providing necessary information for the target structure.



Clicking **Edit** opens the **GeoApp - Generate Nonwoven Digital Twin** dialog.

Enter a **Result File Name** and **Browse** for the **Input Identify Fibers Result** generated with FiberFind - Identify Fibers (AI).

The **Downsampling factor** determines the downsampling for the optimization to reduce runtime. The numbers of voxels in Z-direction must be dividable by this value. A higher value leads to a faster optimization, but reduces the accuracy. The final digital twin has the same resolution as the original structure.

Check **Optimize Z Density Distribution** if also the density distribution in Z-direction should be optimized. For this option a MatDict license is required. If selected, browse for an Thickness Estimation result file computed for the same structure as used for the Identify Fibers result.

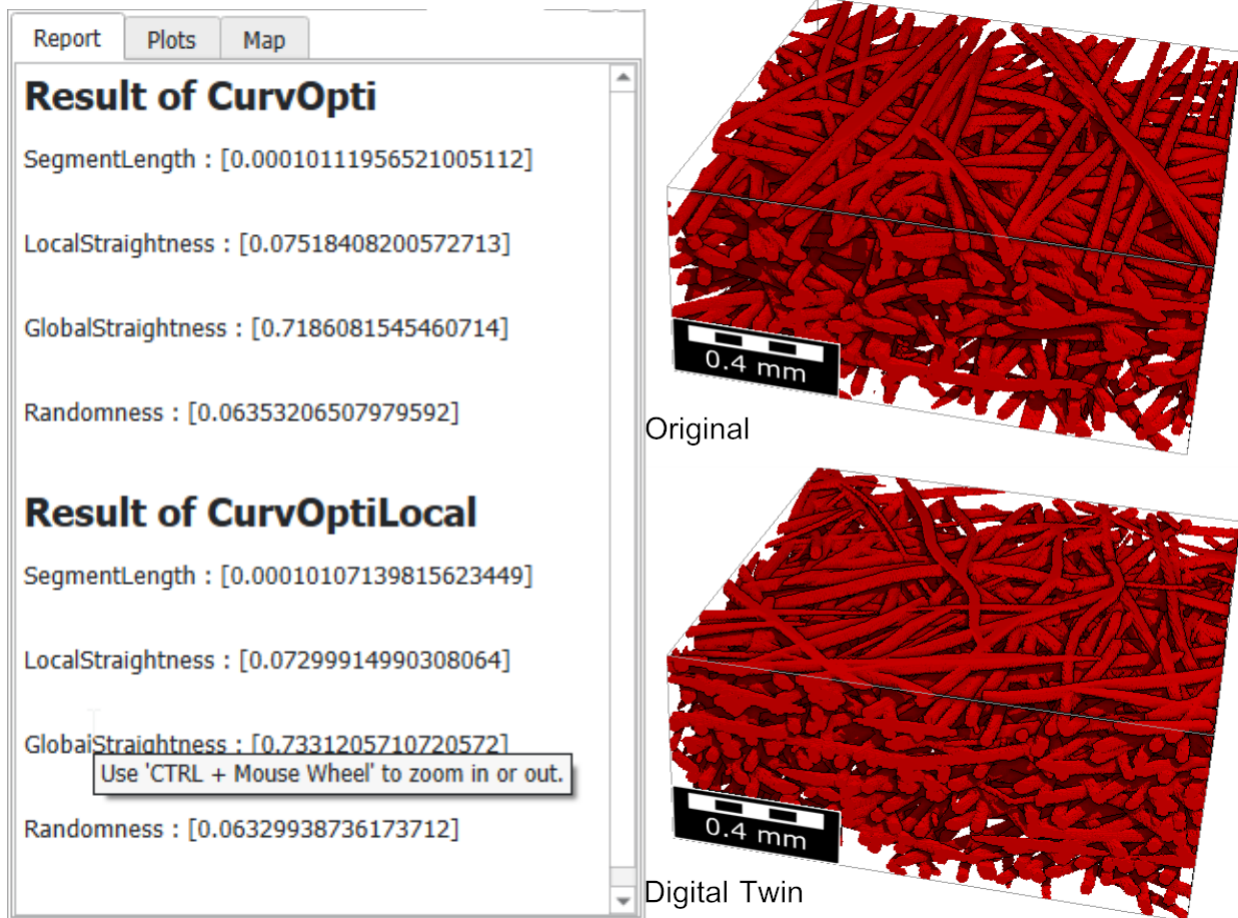
The statistical digital twin is optimized using a differential evolution method. This optimization method mutates a population of nonwoven structures iteratively trying to improve them in every evolution to match the Identify Fibers result (and the 1D statistics result, if selected) finding a statistical digital twin.

Three iteration parameters can be edited. First, define the **Population Size** (PS) for one evolution. Then, set the **Global Iterations** (GI) of one differential evolution. For the local optimizer then set the number of **Local Iterations** (LI). The total number of iterations for the global optimizer is $PS \times GI \times LI$.

Clicking **Run** starts the twin generation.

Results

The result file is opened in the **Result Viewer** when the generation is finished, and the **Report** tab provides information about the structure generation and the resulting twin structure can be viewed in GeoDict. The algorithm optimizes for curvature and, if selected, for density distribution in Z-direction. In the **Plots** subtab of the **Results** tab find the convergence plots for the different parameters to optimize.



In the result folder find the intermediate results for the different optimization targets, created with FiberGeo.

The resulting twin structure is the `structure.gdt` file. Additionally, the according FiberGeo result file `Result.gdr` can be opened in GeoDict, e.g., to view the input parameters.

1.3 Battery GeoApps

The **GeoApp - Battery** group contains GeoApps to create realistic anodes and cathodes for a battery.



New in GeoDict 2026

- The app [Battery Capacity Test](#)^[110] is new in GeoDict 2026 and calculates the accessible capacity of a battery for different charge rates.
- The app [Electrochemical Impedance Spectroscopy](#)^[117] is new in GeoDict 2026 and simulates an EIS experiment while charging a battery or electrode. In the BatteryDict result file the Nyquist and Bode plots are added.
- The apps Bimodal Anode and Bimodal Cathode are merged into one GeoApp: [Bimodal Electrode](#)^[99]
- The apps ElectrodeGeo - Anode and ElectrodeGeo - Cathode are merged into one GeoApp: [ElectrodeGeo](#)^[107]
- The app [ElectrodeGeo](#)^[107] now also writes a result file and saves the structure in a result folder.

Find the following Battery GeoApp groups:

- [Structure Generation](#)^[99]
Create anode and cathode structures for a battery.
- [Physical Properties](#)^[109]
Calculate physical properties of your battery and electrode structures.

1.3.1 Structure Generation

Several **GeoApps** to create anodes and cathodes for battery structures are available.

The following Electrode Generation GeoApps are shipped with GeoDict:

- [Bimodal Electrode](#)^[99]
Generates anode and cathode structures, which consist of one or two types of solid spherical, elliptical or polyhedron particles. Define grain size distributions, solid carbon black and binder domain (CBD) and fluid electrolyte.
- [ElectrodeGeo](#)^[107]
Generates an anode or cathode structure from different materials.

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/cm^2) of the electrode.



Modules needed to run this GeoApp:

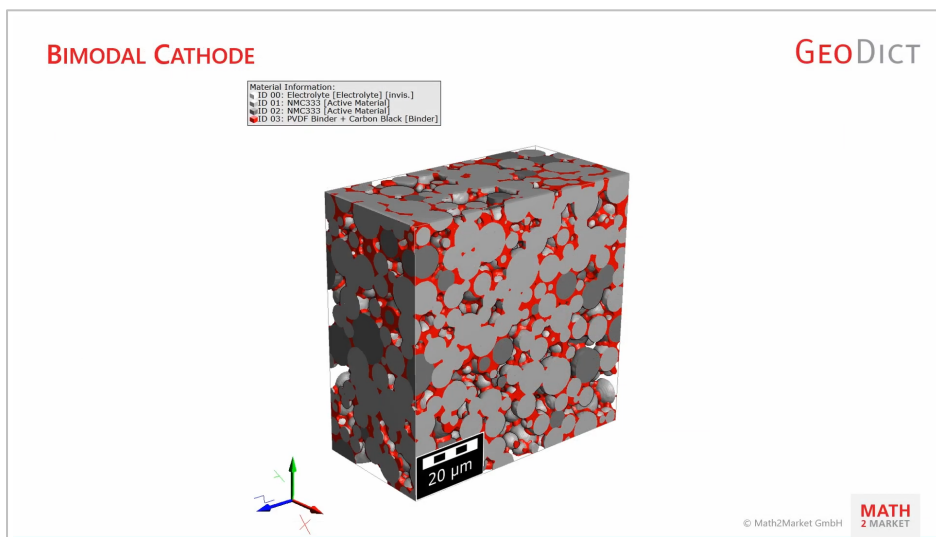
GrainGeo



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.

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

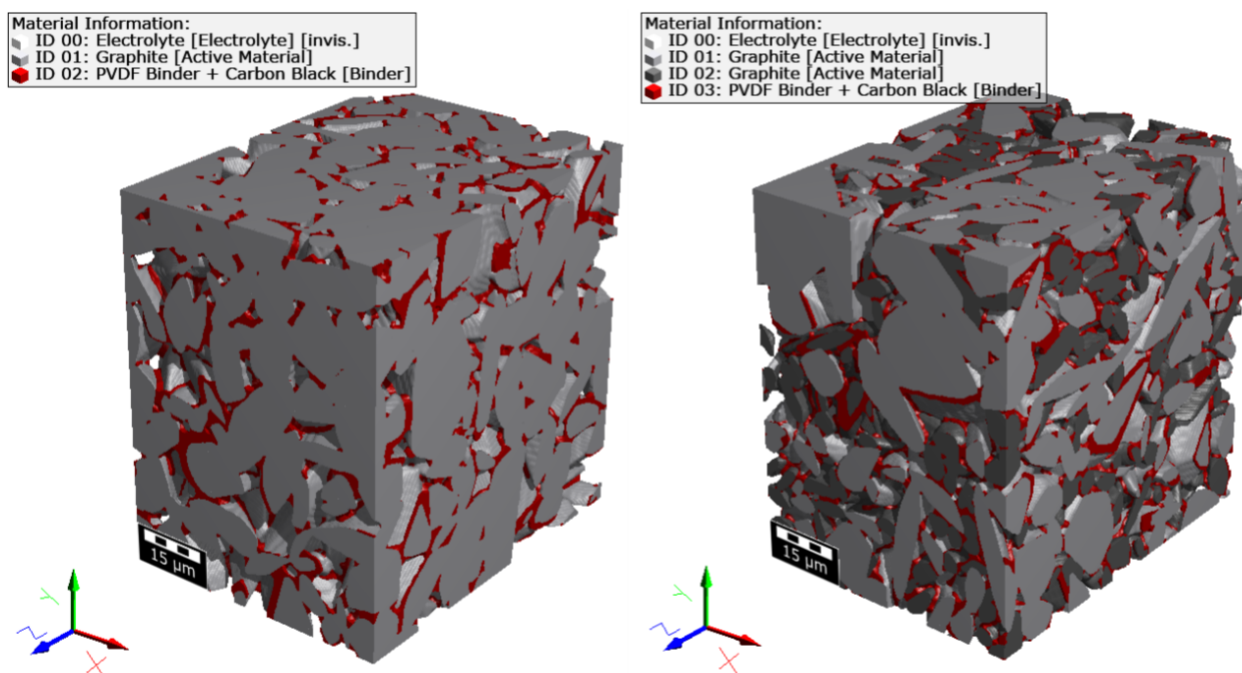
Target Particle Overlap / (%)
1

Iterations
100

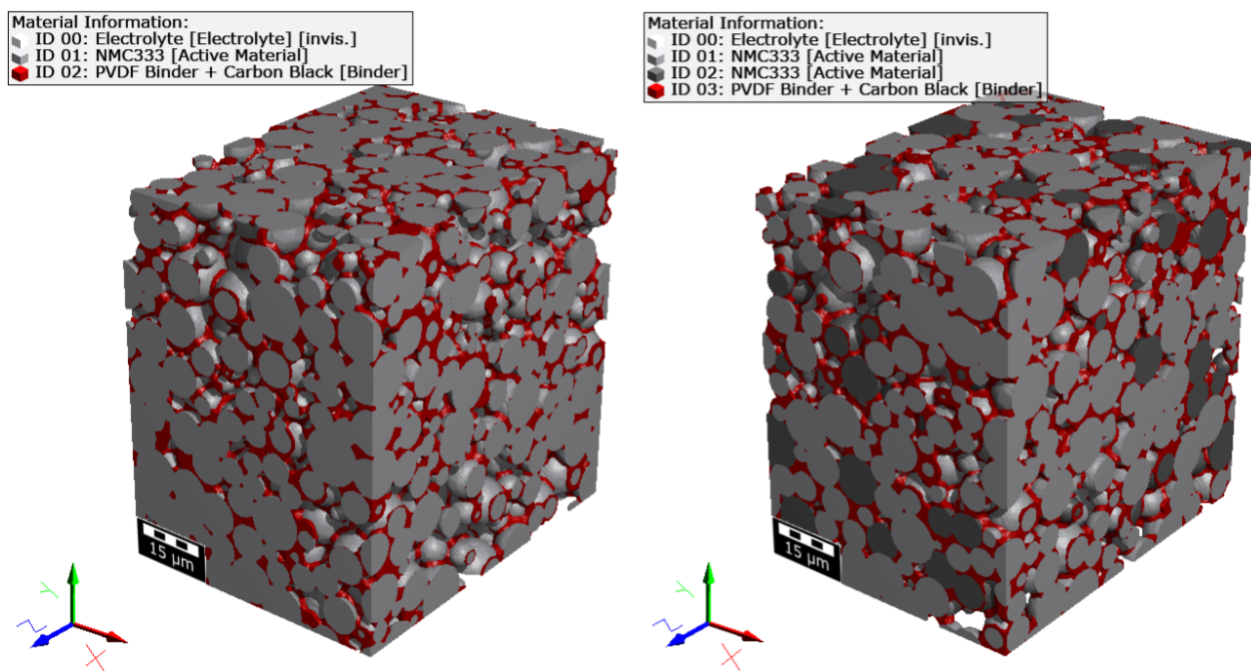
Maximum Generation Time / (hours)
6

Results

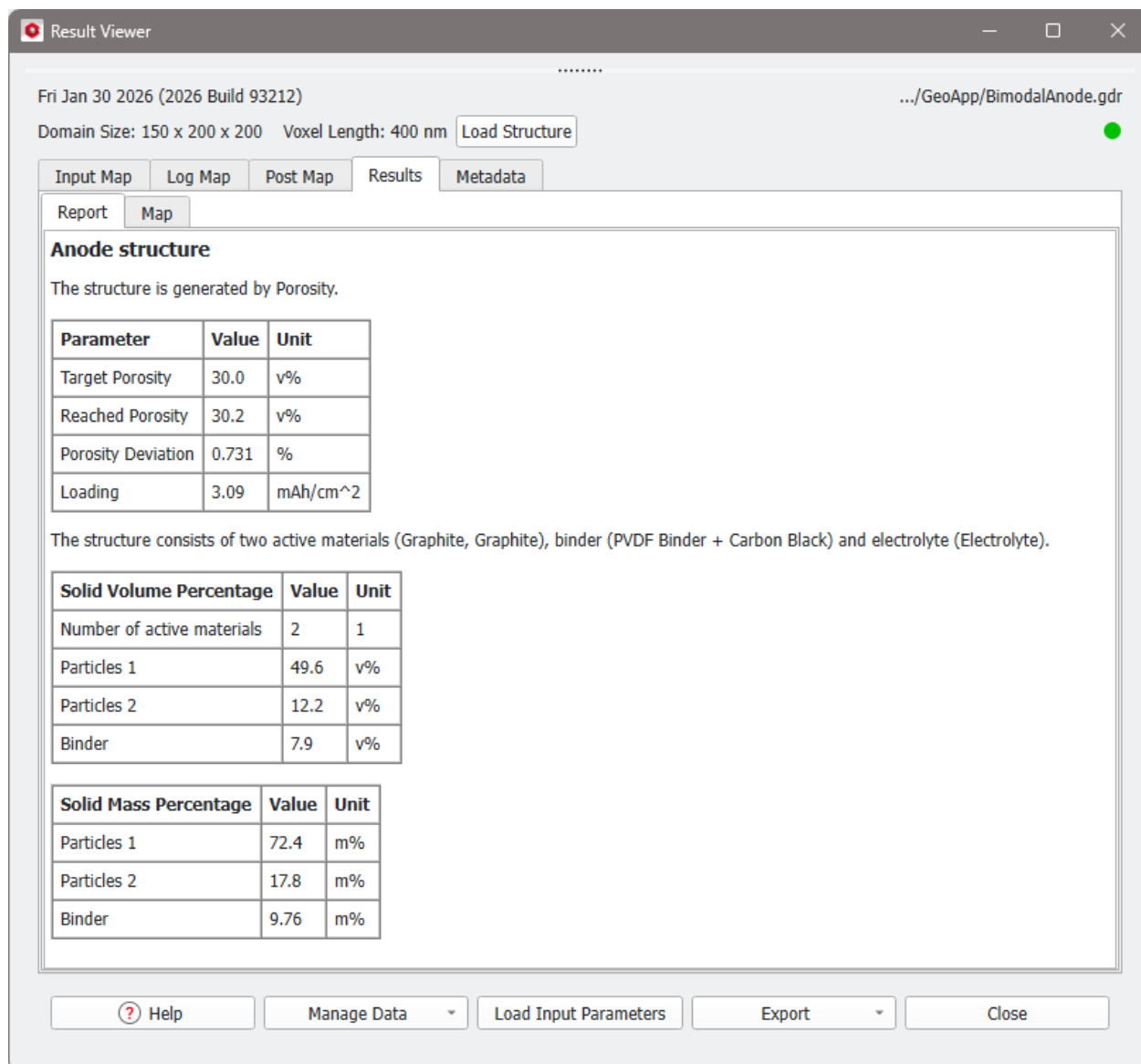
In the figure below, on the left, a monomodal battery anode is shown and on the right, a bimodal battery anode is shown. Both are generated with the respective default settings. Of course, the half cell type must be set to anode and for the bimodal anode, the second particle type was enabled. For comparability, 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.



The result file is opened in the **Result Viewer** when the generation is finished, and the Report tab provides information about the structure generation.



ElectrodeGeo

The **ElectrodeGeo** app generates an anode according to the given materials and solid volume percentages.

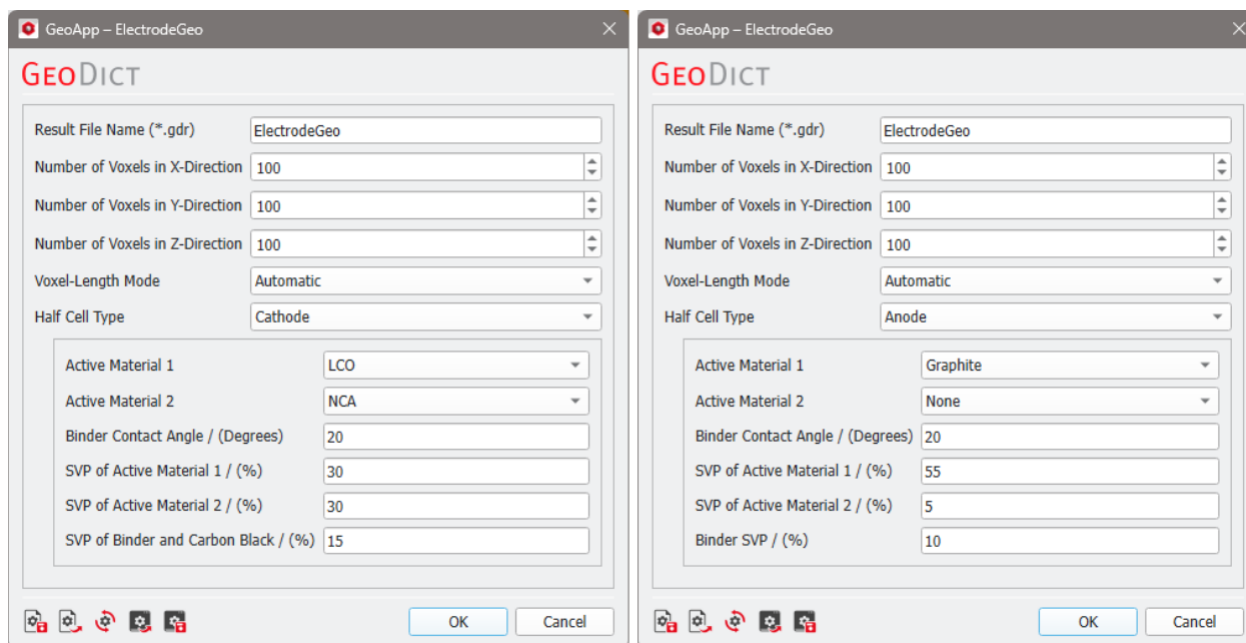


Modules needed to run this GeoApp:

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.

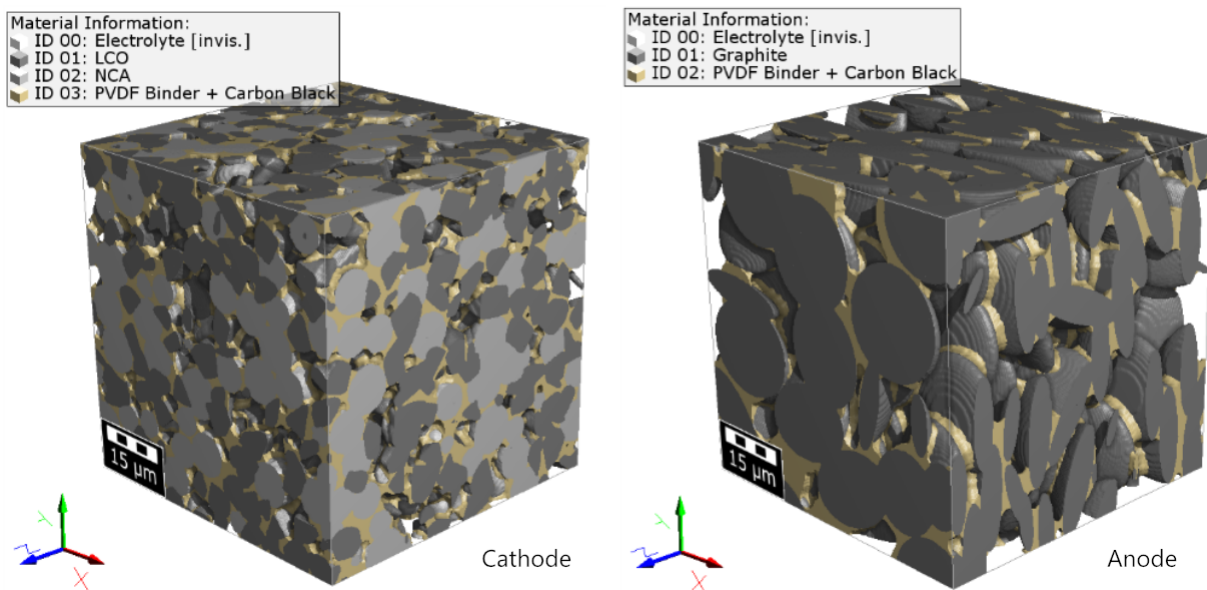
Determine the solid volume percentages (**SVP**) for the active materials and the binder.

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**.

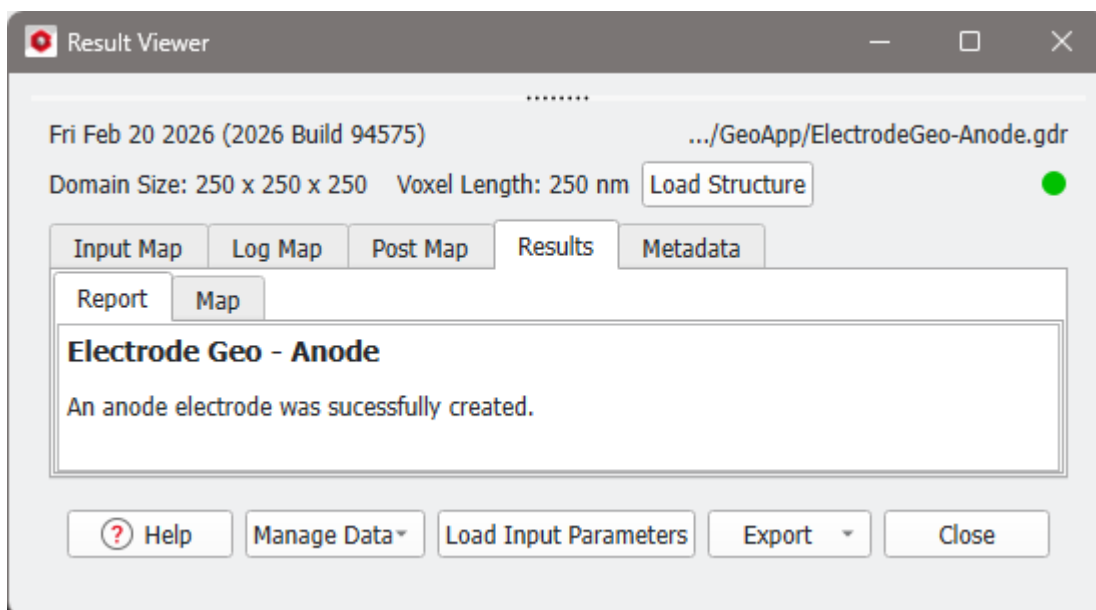
Results

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.



1.3.2 Physical Properties

Several **GeoApps** to compute physical properties in battery and electrode structures are available.

The following GeoApps to compute physical properties in batteries are shipped with GeoDict:

- [Battery Capacity Test](#)^[110]
Fast charging of batteries reduces the accessible cell capacity. The GeoApp Battery Capacity Test allows prediction of accessible cell capacity for different charge rates.
- [Electrochemical Impedance Spectroscopy](#)^[117]

The following GeoApps to compute physical properties in batteries are shipped with GeoDict:

Calculate the complex -valued resistance called "impedance".

Battery Capacity Test

Fast charging of batteries reduces the accessible cell capacity. The GeoApp **Battery Capacity Test** allows prediction and easy comparison of accessible cell capacity for different charge rates. A voltage window can be defined in the same way as it is defined in experiments for a battery or electrode.

A charging profile, consisting of 4 steps is computed for each charge rate:

1. Charging (delithiation) with constant charge rate until a defined maximum voltage
2. Charging (delithiation) with constant voltage until a limiting C-rate or maximum time
3. Relaxation to equilibrium
4. Discharging (lithiation) with constant charge rate until a defined minimum voltage



Needed Modules:

BatteryDict



Note! Also have a look at our [website](#) for more information.

Parameters

Clicking **Edit...** opens the **Battery Capacity Test** dialog. At the top, define a **Result File Name** for the result file and the result folder containing the generated structure and volume fields.

GeoApp – Battery Capacity Test

GEODICT

Result File Name (*.gdr)

Structure, Materials and Simulation Settings

Result File of a Charge Battery Simulation (*.gdr)

Minimum Voltage / (V)

Maximum Voltage / (V)

Step 1 and 4, Charging/Delithiation and Discharging/Lithiation with Constant Current

Boundary Conditions in Through Direction

Charging/Discharging Type

Constant Current: Charge Rates

Charge Rates Charging/Delithiation and Discharging/Lithiation / (1)	
1	

Step 2, Charging with Constant Voltage

☒ Run Step 2, Charging with Constant Voltage

Constant Voltage: Stopping Criterion at Boundary

Charge Rate Limit / (1)

Constant Voltage: Time Limit / (s)

Step 3, Relaxation

☒ Use Perfect Relaxation



✓ Structure, Materials and Simulation Settings

Browse for the **Result File of a Charge Battery Simulation**. This result file is created by successfully running the BatteryDict commands Charge Battery or Charge Electrode. It contains all the necessary parameters. The parameters from the Constituent Materials,

Solver and Output Options tab as well as the Boundary Conditions in Tangential Directions defined under the Experiment tab are used for the simulations in the GeoApp Battery Capacity Test. The other settings under the Experiment tab are replaced by a charging profile set according to the input parameters defined in the GeoApp dialog.

Define the voltage range for the battery capacity test by entering **Minimum Voltage** and **Maximum Voltage**. Below the settings for the [example](#)¹¹⁴ are entered.

Structure, Materials and Simulation Settings

Result File of a Charge Battery Simulation (*.gdr)

Minimum Voltage / (V)

Maximum Voltage / (V)

✓ Step 1 and 4, Charging / Delithiation and Discharging / Lithiation with Constant Current

Choose the **Boundary Conditions in Through Direction**.

- **Charge Rate:** Specify a charge rate. The necessary current density for the given charge rate will be calculated by the solver.
- **Current Density:** Specify a current density.
- **Current:** Specify a current. Please note, that the current in the microstructure is very small.

Below, the settings for the [example](#)¹¹⁴ are entered.

Step 1 and 4, Charging/Delithiation and Discharging/Lithiation with Constant Current

Boundary Conditions in Through Direction

Charging/Discharging Type

Constant Current: Charge Rates

Charge Rates Charging/Delithiation and Discharging/Lithiation / (1)	
1	1
2	3
3	5
4	7

Decide whether the values for the selected **Charging / Discharging Type** should be the same for both processes or different. Enter the values in the table. As soon, as you enter a value, another row appears in the table. Fill in as many rows as desired. A simulation will be run for each row, and the accessible capacities for all simulations will be compared in the GeoApp's [Result File](#)¹¹⁴.

✓ Step 2, Charging with Constant Voltage

Uncheck **Run Step 2, Charging with Constant Voltage**, if this step should be omitted.

If checked, select which **Stopping Criterion at Boundary** should be used and enter the respective limiting value for the second simulation step.

You can provide a **Time Limit** that defines the simulated-time-threshold after which the step will end, regardless of whether previous stopping criteria were reached.

Below the settings for the [example](#)¹¹⁴ are entered.

Step 2, Charging with Constant Voltage
☒ **Run Step 2, Charging with Constant Voltage**
Constant Voltage: Stopping Criterion at Boundary CRate
Charge Rate Limit / (1) 0.1
Constant Voltage: Time Limit / (s) 1800

✓ Step 3, Relaxation

Check **Use Perfect Relaxation**, if a perfect relaxation to equilibrium after charging/delithiation should be assumed.

Step 3, Relaxation
☒ **Use Perfect Relaxation**

Otherwise, define a **Relaxation Time** for defining the time after that the relaxation of the cell is stopped.

Below, the settings for the [example](#)¹¹⁴ are entered.

Step 3, Relaxation

☐ Use Perfect Relaxation

Relaxation Time / (s)

Results

After successfully running the command, the result file created is opened in the GeoDict Result Viewer.

Under the **Results-Report** subtab, the file names of all simulations run, and saved in the project folder, are listed. The accessible area-normalized and mass-normalized cell capacities are shown in separate tables for the charging/delithiation and discharging/lithiation.

Input MapLog MapPost MapResultsMetadata

ReportPlotsMap

Battery Capacity Test Results

4 simulations were run successfully. 10 result plots were created.

Results were created using the following files:

Battery_C_1.0.gdr

Battery_C_3.0.gdr

Battery_C_5.0.gdr

Battery_C_7.0.gdr

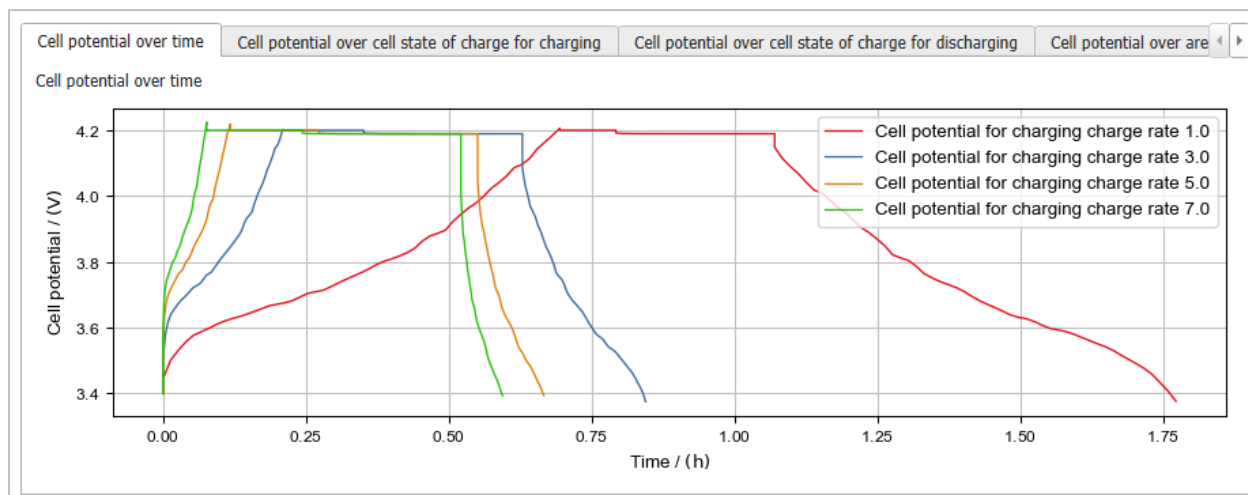
Accessible cell capacity for charging

ChargeRate	Accessible area-normalized cell capacity for charging with constant current / (mAh/cm ²)	Accessible area-normalized cell capacity for charging with constant current and constant voltage / (mAh/cm ²)	Accessible mass-normalized cell capacity for charging with constant current / (mAh/g)	Accessible mass-normalized cell capacity for charging with constant current and constant voltage / (mAh/g)
1.0	1.553	1.627	65.37	68.46
3.0	1.404	1.627	59.08	68.45
5.0	1.314	1.627	55.31	68.44
7.0	1.195	1.626	50.28	68.44

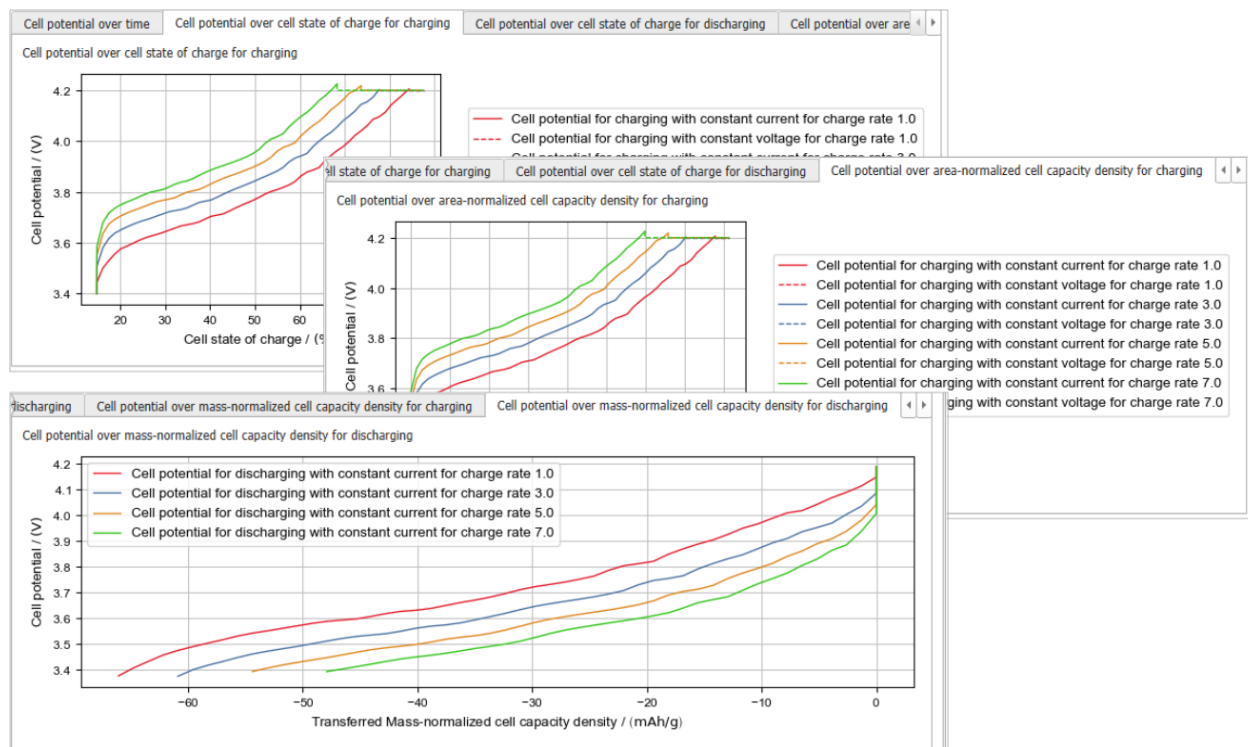
Accessible cell capacity for discharging

ChargeRate	Accessible area-normalized cell capacity for discharging with constant current / (mAh/cm ²)	Accessible mass-normalized cell capacity for discharging with constant current / (mAh/g)
1.0	1.57	66.08
3.0	1.447	60.89
5.0	1.293	54.4
7.0	1.139	47.92

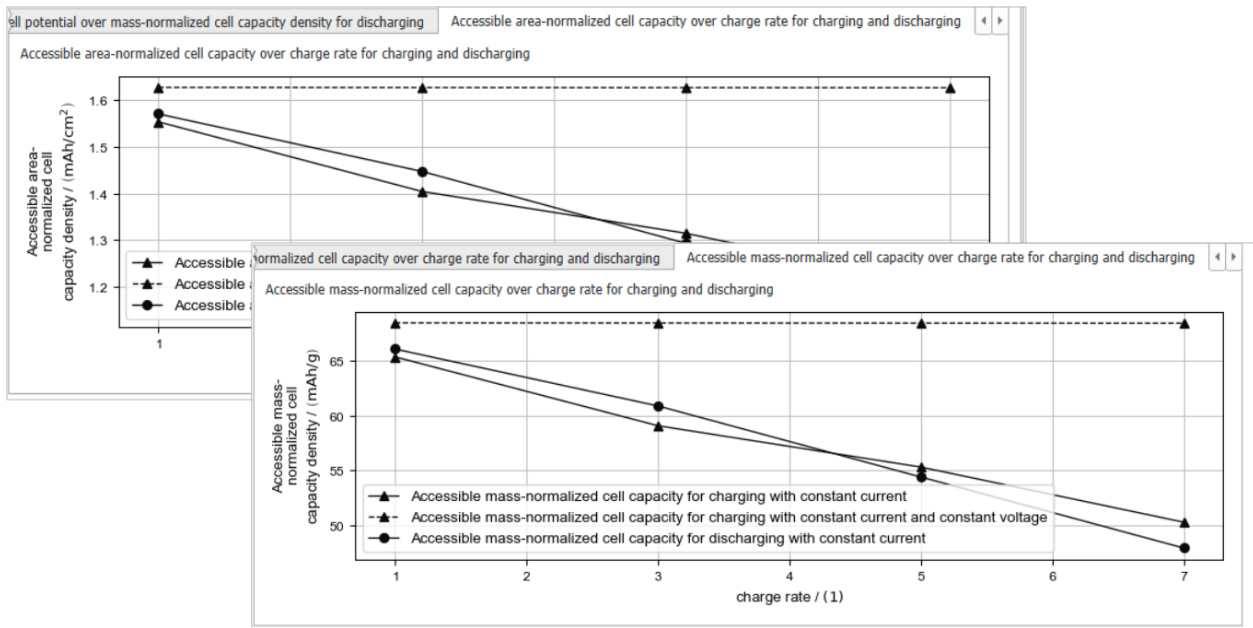
Under the **Results - Plots** subtab, the results of the simulations are compared in different ways. The whole charge curve for all simulations is shown as **Cell potential over time**.



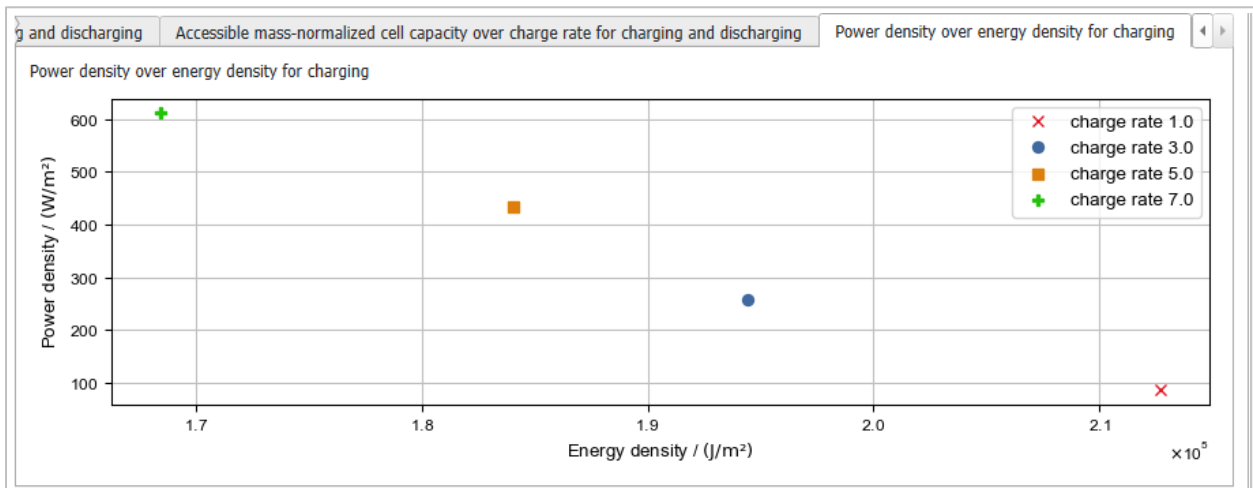
Under the following tabs, the cell potential of all simulations is shown for charging / delithiation and discharging / lithiation separately. First as **cell potential over the cell state of charge**, and then over the **area-normalized** and **mass-normalized cell capacity density**.



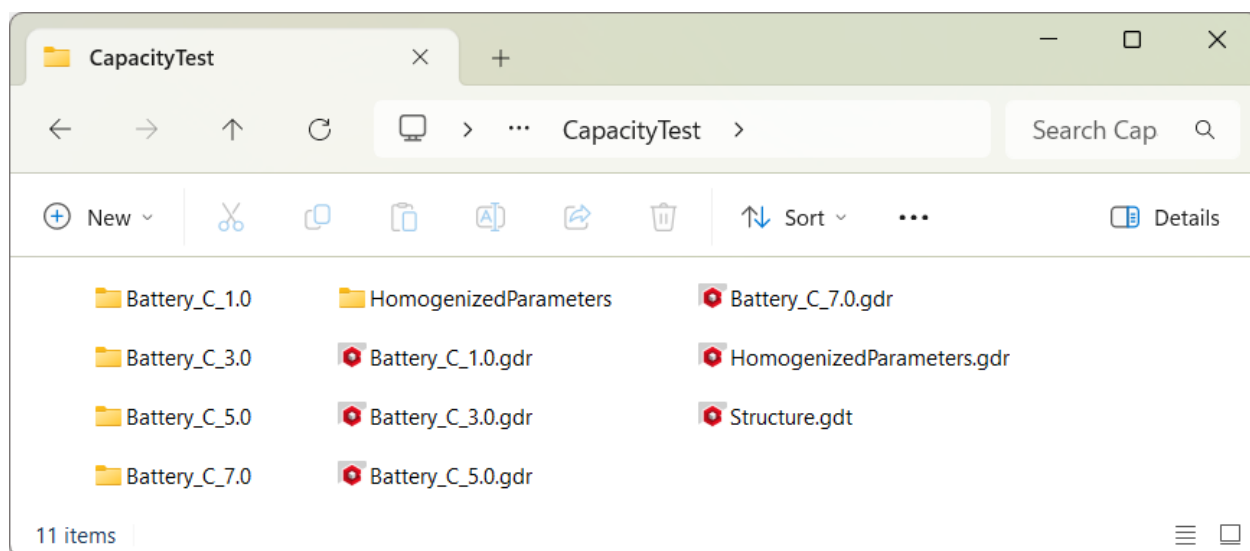
The two tabs **Accessible area-normalized cell capacity** and **Accessible mass-normalized cell capacity over charge rate for charging and discharging**, compare the accessible capacities for the different simulations. These values are also listed in the **Report**.



Finally, the plot under the last tab shows the **Power density over the energy density** computed for the charging step 1, charging with constant charge rate.



In the **Result Folder** find the intermediate results from the charging simulations for the different charging steps:



Electrochemical Impedance Spectroscopy

Calculate the complex-valued resistance called "impedance" that many battery developers and scientists use to understand the behavior of electrical components like resistors, capacitors, inductors and batteries.

Technically, this GeoApp sets expert settings for Electrochemical Impedance Spectroscopy (EIS) simulation and runs a charging simulation using the current settings in Charge Battery, Charge Electrode, Charge Homogenized Battery, or Charge Homogenized Electrode in BatteryDict.



Needed Modules:

BatteryDict, BatteryDict-BEST, BatteryDict-EIS

Theoretical Background

Performing an EIS simulation is currently only possible with the BEST solvers. The simulation by itself does not modify the underlying model equations, it only activates an additional double layer model for the interface active material - electrolyte.

The electrochemical double layer describes an effect at the interface of liquid electrolytes and active materials. Due to the polarization of the electrodes, the ions in the electrolyte arrange in a layered structure close to the active material surface, which imposes charge separation and acts as a capacitor. This takes place on the molecular scale. The double layer stores charges based on the voltage at the interface, releasing charges as the voltage drops or accumulating them as voltage increases, similar to a capacitor. Since the capacity of the double layer is comparatively small relative to the overall cell capacity, it equilibrates fast with voltage changes and has minimal impact during regular cell operation in the field. Only when studying

higher frequency dynamics, the double layer becomes crucial to consider. An example for this is the characteristic semi-circle in EIS, which is the result of the intercalation and double layer acting similar to a resistor-capacitor pair.

The double layer model is based on [Hein, 2020](#)^[240] and introduces an additional interface current density between active material and electrolyte that is connected in parallel with the intercalation model resulting in a total interface current $i_{se,EIS}$ of

$$i_{se,EIS} = i_{se} + i_{DL} \quad (6)$$

where i_{se} is the Butler-Volmer interface current and i_{DL} is the double layer current.

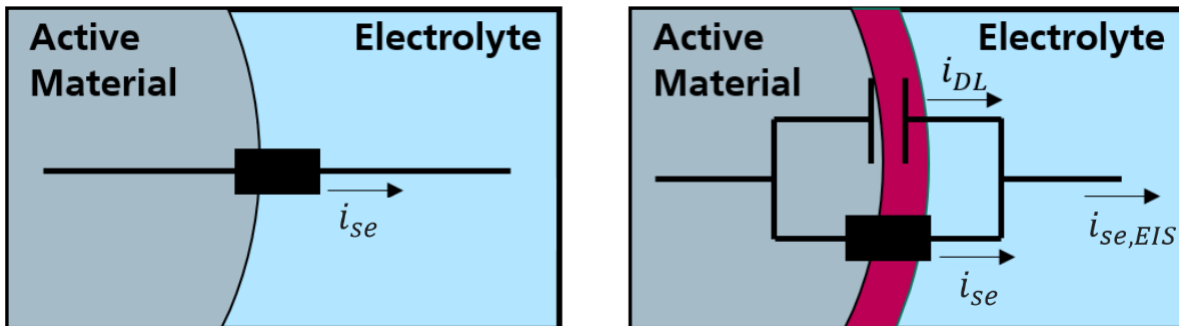
For a comparison the usual equations for the interface between electrolyte and active material are given in the Fully Resolved Simulation and Homogenized Simulation topics of the BatteryDict User Guide.

The double layer is modeled as an effective interface property between active material and electrolyte acting as ideal capacitor. The current density flowing across the double layer is given by

$$i_{DL} = C_{DL} \frac{\partial}{\partial t} (\varphi_s - \varphi_e) \quad (7)$$

using the areal capacitance C_{DL} , the local Maxwell potential of the electrode φ_s , and the local electrochemical potential in the electrolyte φ_e .

The figure below shows the different configurations that can be achieved with the intercalation and double layer model. It visualizes the different settings that are considered with the double layer model. The circuit drawings provide some information on how these settings would translate if the interface conditions of the continuum scale modeling approach would be transferred to an equivalent circuit model. On the left, the active material-electrolyte interface as modeled in Charge Battery and Charge Electrode is shown. Only the Butler-Volmer exchange current density is considered, resulting in an interface resistance. On the right, the model used in EIS-simulations is shown. Double layer and intercalation kinetics are both active and connected in parallel acting as a resistor-capacitor pair.



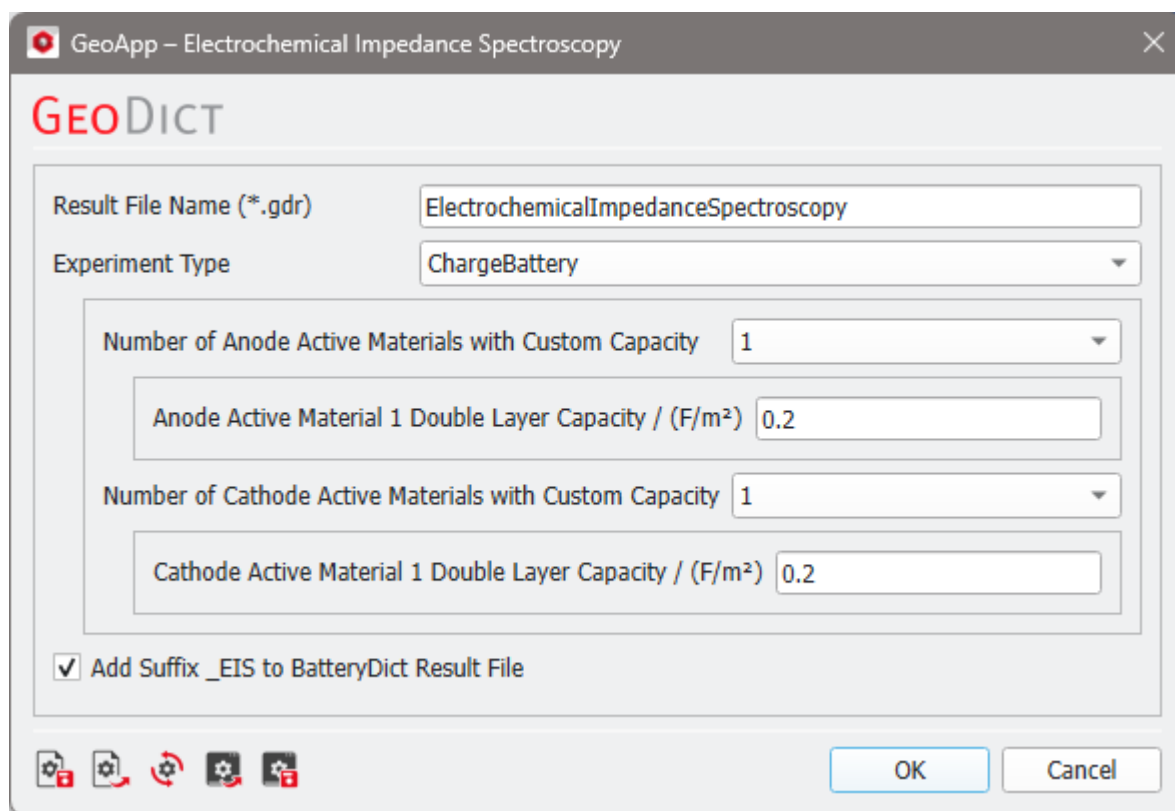
Finally, a specific predefined voltage operation protocol with Amplitude 10mV is executed including the double layer model to get the time transient current response of the cell.

Afterward, the time, current and voltage information can be post-processed to translate the information to the frequency domain and evaluate the complex impedance.

Parameters

Clicking **Edit...** opens the **Electrochemical Impedance Spectroscopy** dialog. At the top, define a **Result File Name** for the result file and the result folder containing the BatteryDict charging simulation run with the EIS plots.

To automatically add the suffix "_EIS" to this result file name, check **Add Suffix _EIS to BatteryDict Result File**.



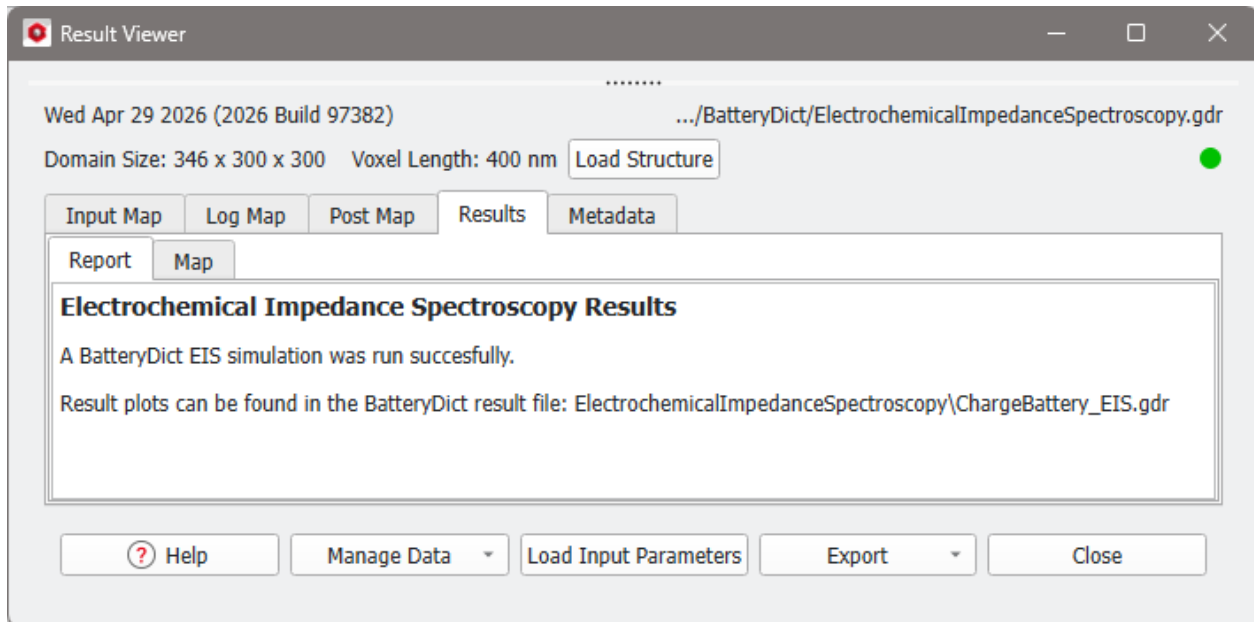
Choose the experiment type (Charge Battery, Charge Electrode, Charge Homogenized Battery or Charge Homogenized Electrode) and optionally the custom double layer capacities of the active materials.

Subsequently, when choosing Charge Battery or Charge Electrode for the simulation, you can use either BESTmeso (homogenized simulation) or BESTmicro (fully resolved simulation) as a solver. Charge Homogenized Battery or Charge Homogenized Electrode are always run with the BESTmeso solver.

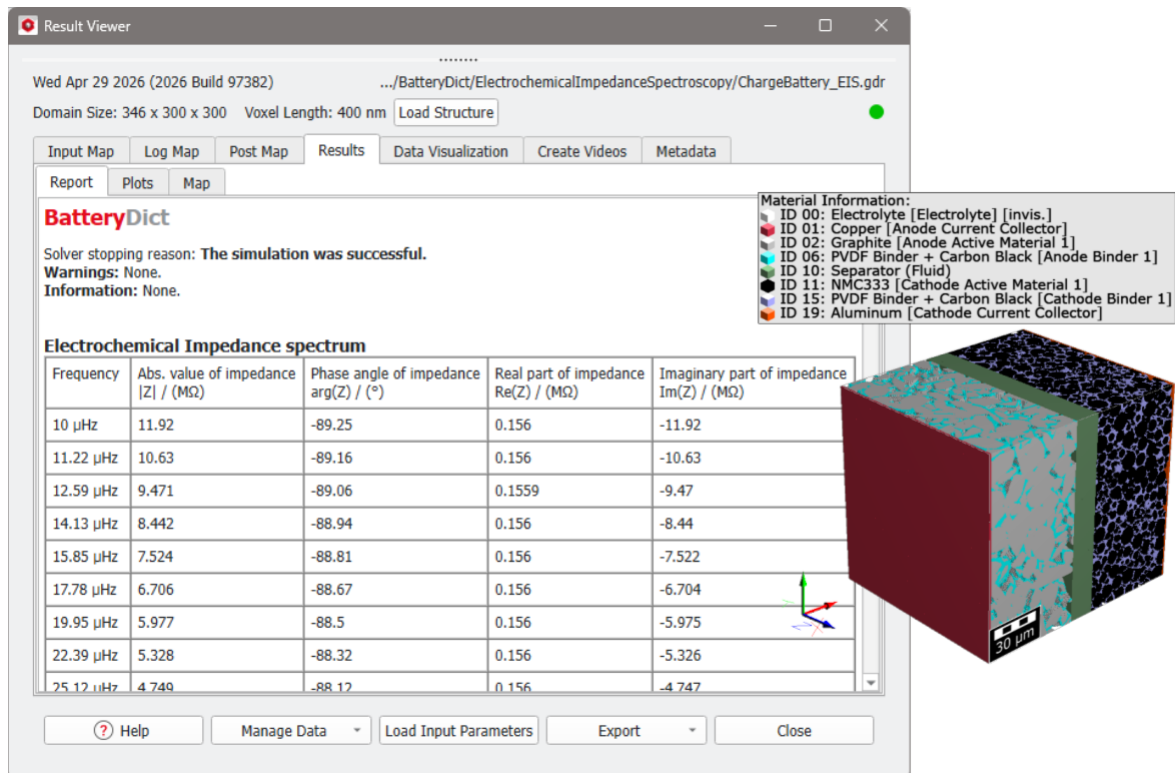
The start condition of the **Experiment** tab of the selected experiment type will be used. However, instead of a (dis)charging / (de)lithation experiment, the EIS experiment at this start condition is simulated.

Results

After the BatteryDict simulation is finished the result file is opened in the Result Viewer.

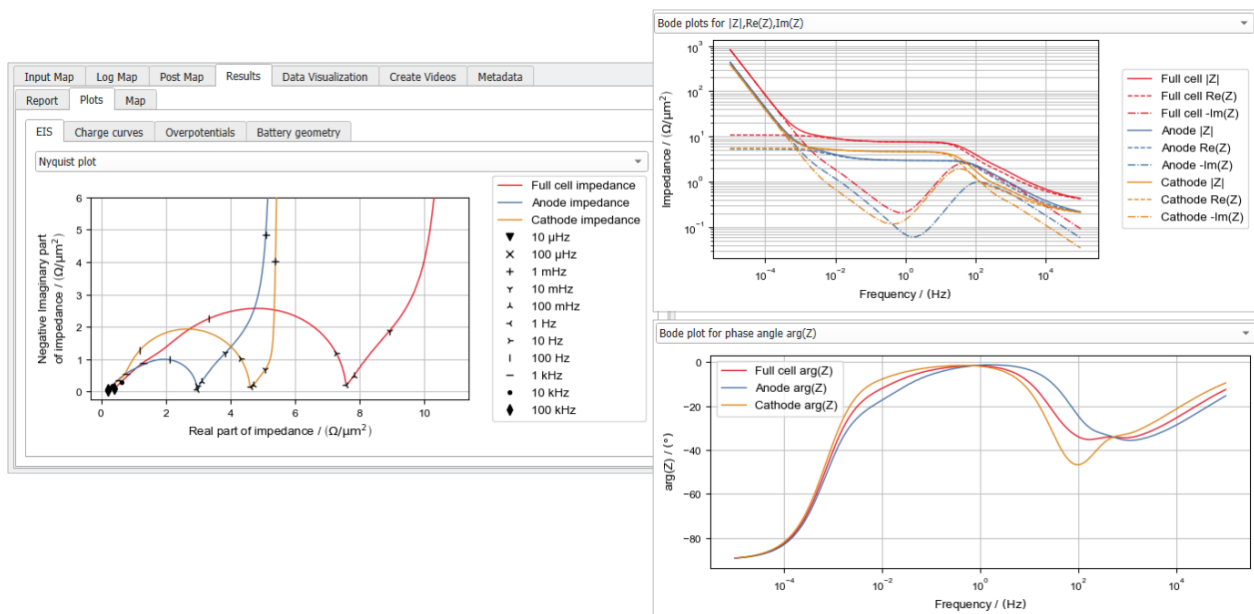


The report tells you where to look for the results. Load the BatteryDict result file from the result folder (**File** → **Open Results (*.gdr)**) Additionally to the usual BatteryDict results, the report shows the **Electrochemical impedance spectrum** table. In the example, we used Charge Battery with the BESTmeso solver.



Under the **Plots** tab you find three **EIS** plots selectable from the pull-down menu: One Nyquist plot and two Bode plots.

The Bode plots visualize the real and imaginary part of the frequency response as well as the phase angle. All plots are shown for the full cell as well as for cathode and anode separately.



1.4 Composites GeoApps

Create composite structures with the **Composite** GeoApps.



New in GeoDict 2026

- The [LamiGeo \(Create Laminates\)](#)¹²² GeoApp now directly offers the possibility to edit the fiber angles for the different layers instead of opening a new dialog for this.

Find the following Composites GeoApp groups:

- [Structure Generation](#)¹²²
Create structures as glass-fiber enforced plastic and laminates.

1.4.1 Structure Generation

Create structures as glass-fiber enforced plastic and laminates with the **Structure Generation** GeoApps.

The following Structure Generation GeoApps are shipped with GeoDict:

- [LamiGeo \(Create Laminates\)](#)¹²²
Generates a model of a multi-layer laminate composite.
- [Short Fiber Reinforced Plastic](#)¹²⁴
Generates a predefined fiber structure.

LamiGeo (Create Laminates)

The **LamiGeo** app generates a laminate structure.



Modules needed to run this GeoApp:

FiberGeo

Parameters

Clicking **Edit** opens the **LamiGeo Parameters** dialog.

GeoApp – LamiGeo (Create Laminates)

GeoDict

Result File Name (*.gdr)

Voxel Length / (μm)

Domain Width / Length / (μm)

Materials

Matrix Material

Fiber Material

Fibers

Diameter / (μm)

Solid Volume Percentage / (%)

Waviness / (Deg)

☒ No Fiber Overlap

Isolation Distance / (μm)

Layers

Layer Height / (μm)

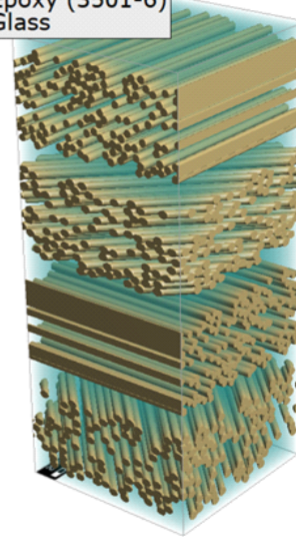
Layer Coating / (μm)

Number of Layers with Fiber Angle in Layer

	Fiber Angle in Layer / (Deg)
1	0
2	45
3	90
4	135
5	

OK Cancel

Material Information:
 ID 00: Epoxy (3501-6)
 ID 01: Glass



Enter a **Result File Name** for the generated result file (*.gdr) and the corresponding result folder.

Define **Voxel Length** and the **Domain Width / Length** in X- and Y-direction.

In the **Materials** panel select the **Matrix Material** and the **Fiber Material** from the GeoDict material database.

Below, in the **Fibers** panel, define the parameters for the generated circular fibers:

- Define **Diameter** of the fibers in μm.
- Select a **Solid Volume Percentage** to define the fibers volume percentage for each layer.
- Enter the fiber **Waviness** as angle around the fiber orientation direction, where positive values lead to slightly curved fibers.
- Choose, if the overlap should be removed (**No Fiber Overlap**) or not.
- Set an **Isolation Distance**, in case the overlap is removed.

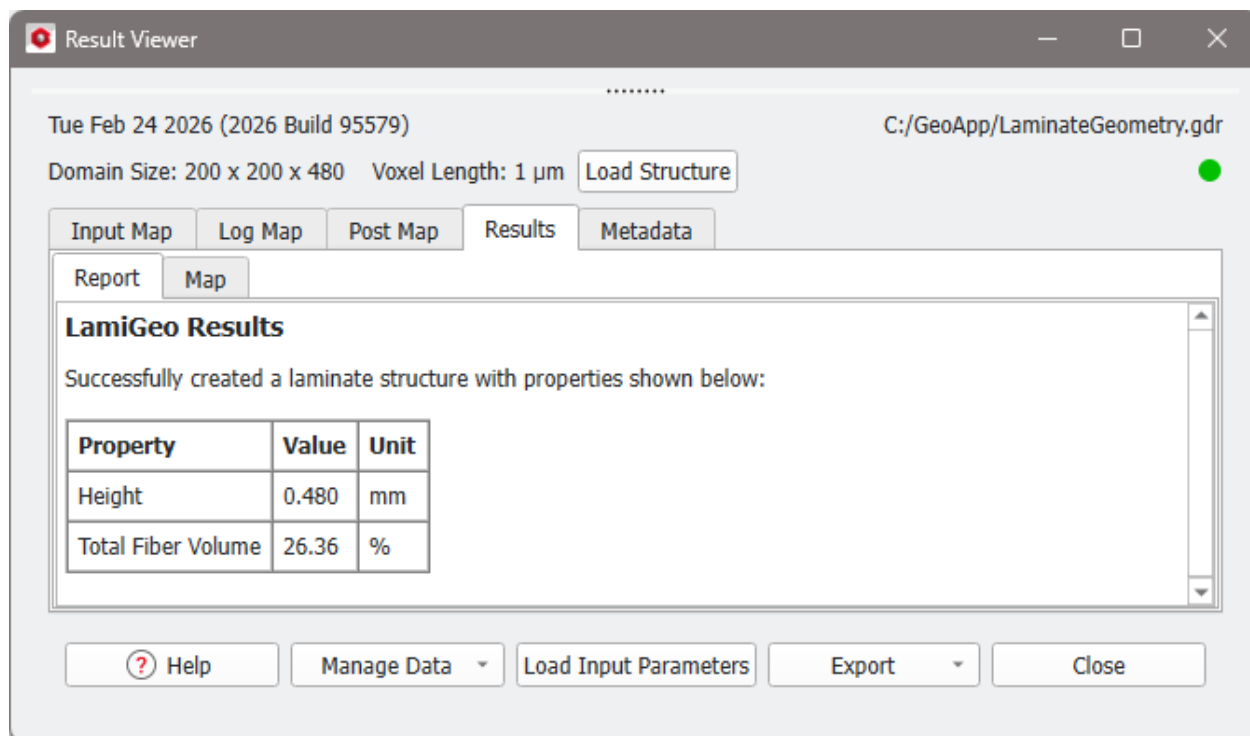
In the **Layers** panel enter the desired **Layer Height** for each layer and how much **Layer Coating** should be generated around the fibers in Z-direction. In the table, enter the **Fiber Angle in Layer**. Entering a value in the last row adds another row below, while deleting an entry, deletes the row. The generated structure will have as many layers as values are entered in this table.

Clicking on **OK** closes the dialog and clicking on **Run** creates the plastic structure.

When the structure generation is finished, the **Result Viewer** of the result file (*.gdr) opens automatically.

Results

The **Results - Report** tab displays a short report about the resulting structure. Note, that the total fiber volume is lower than the given Solid Volume Percentage because of the added layers of coating material.



Short Fiber Reinforced Plastic

The **Short Fiber Reinforced Plastic** app generates a predefined fibrous structure.

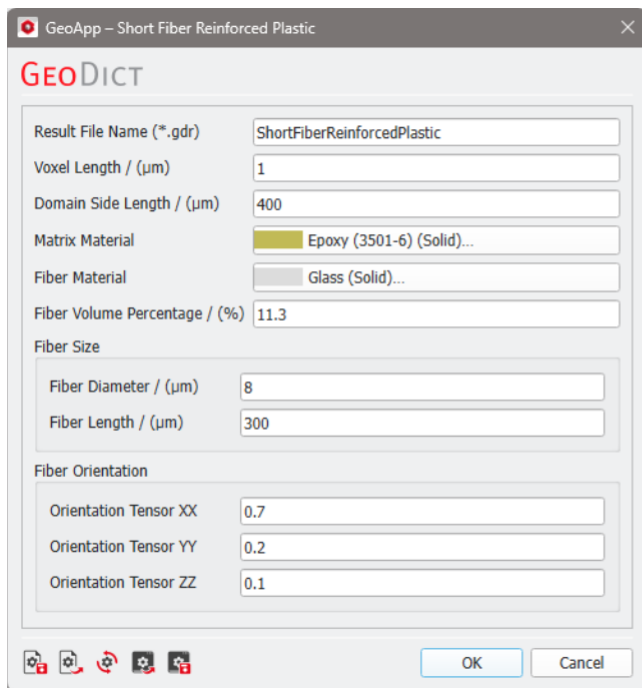


Modules needed to run this GeoApp:

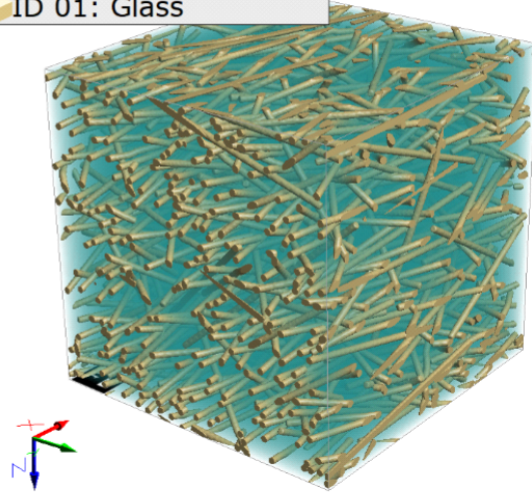
FiberGeo

Parameters

Clicking **Edit** opens the **Short Fiber Reinforced Plastic** parameters dialog.



Material Information:
 ID 00: Epoxy (3501-6)
 ID 01: Glass



Enter a **Result File Name** for the generated result file (*.gdr) and the corresponding result folder.

Define **Voxel Length** and the **Domain Side Length** in X- and Y-direction.

Select the **Matrix Material** and the **Fiber Material** from the GeoDict material database.

Set the **Fiber Volume Percentage** to define how many fibers should be generated.

In the **Fiber Size** panel, enter the **Fiber Diameter** and the **Fiber Length** of the generated curved circular fibers.

Below, in the **Fiber Orientation** panel, define the entries on the diagonal of the **Orientation Tensor**. Please note that the sum of the three orientation values **XX**, **YY**, and **ZZ** has to be 1.

Clicking on **OK** closes the dialog and clicking on **Run** creates the plastic structure.

Results

When the structure generation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically. The resulting structure has no overlap. For more information on this result file refer to the **FiberGeo** User Guide.

Result Viewer

Mon Feb 23 2026 (2026 Build 94575) .../GeoApp/ShortFiberReinforcedPlastic.gdr

Domain Size: 400 x 400 x 400 Voxel Length: 1 μm Load Structure

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: 480 target: --- error: ---	realized: 11.31 target: 11.30 error: 0.01	realized: 560.16 target: --- error: ---	realized: 1.4004 target: --- error: ---	realized: 20.83 target: --- error: ---
Object type 1	realized: 480 target: --- error: ---	realized: 11.31 target: --- error: ---	realized: 560.16 target: --- error: ---	realized: 1.4004 target: --- error: ---	realized: 20.83 target: --- error: ---

Stopping criterion error: 0.076 %

Relative object distribution:

	Count / (%)	Volume / (%)	Weight / (%)
Object type 1	realized: 100.00 target: --- error: ---	realized: 100.00 target: --- error: ---	realized: 100.00 target: 100.00 error: 0.00%

Maximal probability error: 0%

Help Manage Data Load Input Parameters Export Close

1.5 Digital Rock Physics (DRP) GeoApps

Analyze and modify digital rocks with the **Digital Rock Physics** GeoApps.



New in GeoDict 2026

- The Quantitative Seismic Interpretation GeoApp was renamed to [Acoustic Rock Properties](#)^[163].
- The MICP for Rocks GeoApps is no longer available. Instead, use the MICP command in SatuDict.

Find the following Digital Rock Physics (DRP) GeoApp groups:

- [Geometric Properties](#)^[127]
Run a quality control on a sandstone.
- [Physical Properties](#)^[132]
Determine Physical Properties of your digital rock structure.
- [Structure Generation](#)^[167]
Prepare your structure for further simulations.

1.5.1 Geometric Properties

Determine **Geometric Properties** of your structure.

The following Geometric Properties GeoApps are shipped with GeoDict:

- [Sandstone Quality Control](#)^[127]
Run a quality control on the current sandstone structure.

Sandstone Quality Control

Segmented 3D digital images require a quality check. Therefore, we implemented the **Sandstone Quality Control** app to offer a user-friendly tool to perform a Quality Control specifically for segmented digital sandstone rocks based on methods and findings published by [Saxena et al. \(2017\)](#)^[241] and [Saxena et al. \(2018\)](#)^[241]. These recommendations aim at the determination of the suitability of the sample under investigation for single-phase flow computations.

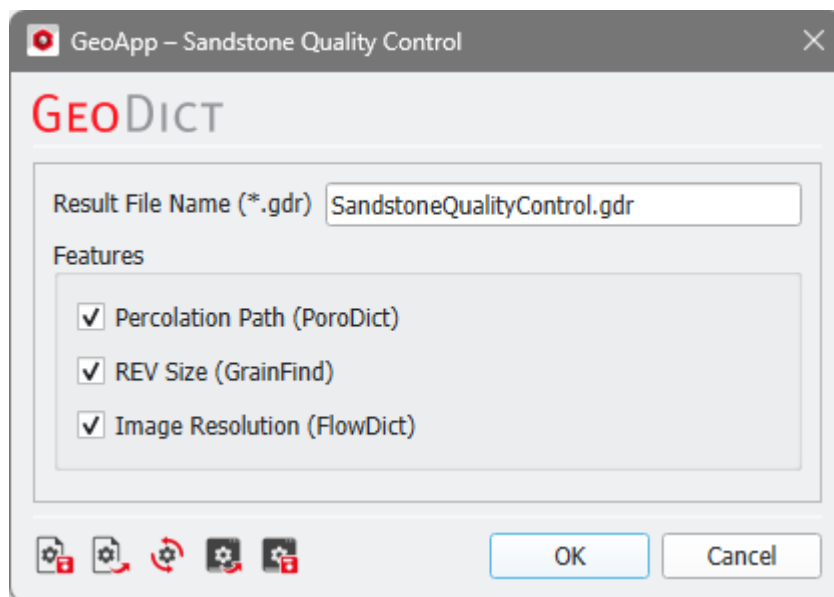


Modules needed to run this GeoApp (depending on the selected options):

PorDict, GrainFind, FlowDict

Parts of the following quality control recommendations may also be considered for other rock types and further samples.

After loading a 3D structure, click **Edit** open the **Sandstone Quality Control Parameters** dialog.



An online workshop for this feature (amongst others) is available [here](#).

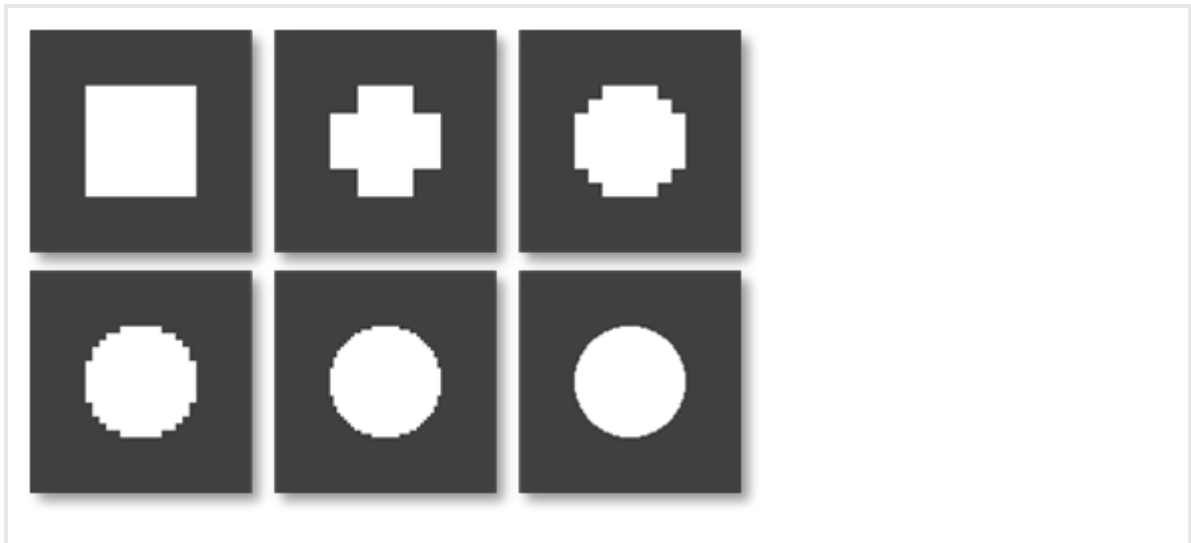
After choosing a project name and which properties should be computed click **OK** to close the dialog. Go back to GeoApp GUI and click **Run**.

The usage of all the three available features is recommended (as long as the required modules are available):

✓ Percolation Path

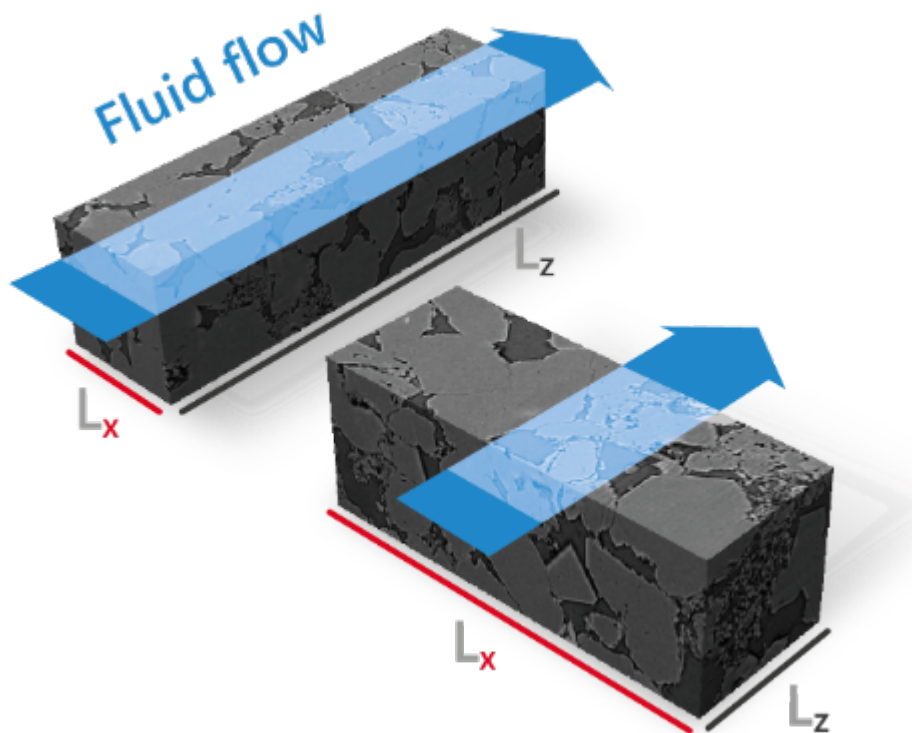
The **Percolation Path** feature investigates the pore throat resolution, which affects the computed permeability. [Saxena et al. \(2018\)](#)^[241] recommend a resolution of 10 voxels to sufficiently resolve pore throats for single-phase flow computations that predict the absolute permeability. For the usage of our flow solvers, we recommend a resolution of at least 4 voxels. Below 4 voxels, the runtime might increase significantly, and the permeability prediction may become inaccurate.

In the following figure find a schematic representation of tubes resolved at varying voxel diameter highlighting the significant effect of the pore throat resolution on the permeability that may be predicted by numerical solvers.



✓ REV Size

The **REV Size** considers the Representative Elementary Volume that is required to compute an absolute permeability that is representative for the rock formation under investigation. In general, an REV may be defined as a rock volume large enough that properties under investigation are insensitive to changes in rock volume and in boundary conditions of numerical tools. [Saxena et al. \(2018\)](#)^[24] recommend considering the ratio of the (smallest) structure length to the effective grain diameter:

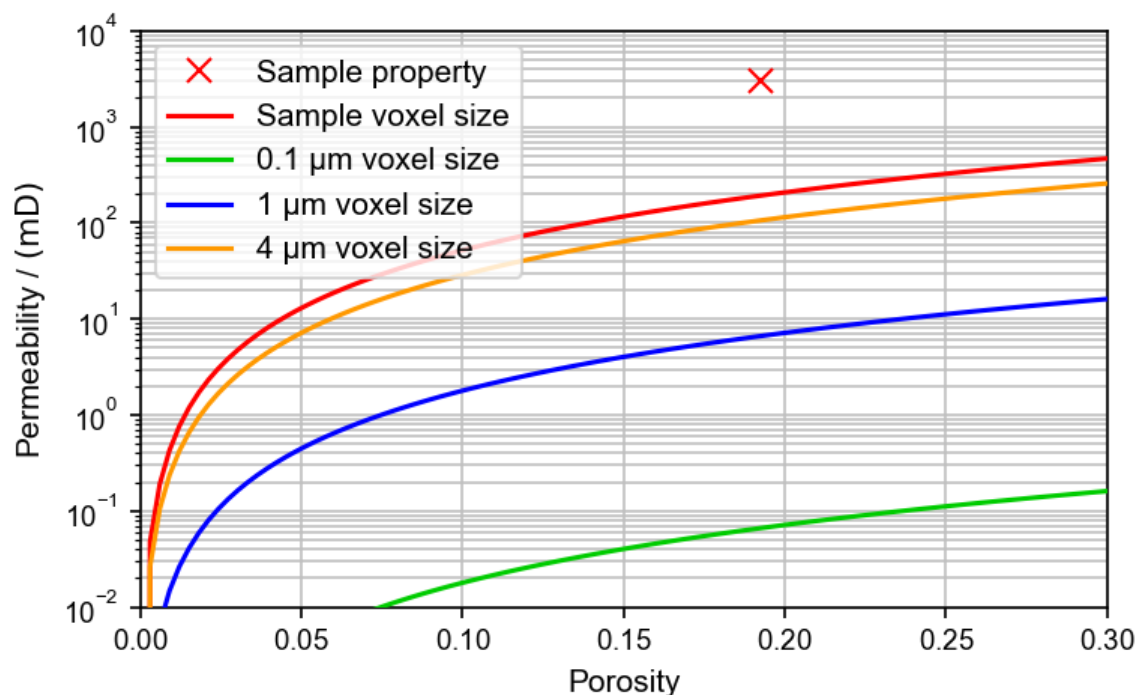


$$L_{structure} > 5 \cdot d_{Grains} \quad (8)$$

✓ Image Resolution

The **Image Resolution** feature applies sample porosity and roughly approximated permeability (with a short computational runtime) to check if the acquired image resolution is suitable for single-phase flow computations. The applied workflow is based on findings published by [Saxena et al. \(2018\)](#)^[241] upon consideration of a large sandstone database.

The following figure shows the result for a workshop geometry (dimensions: 256^3). The red curve shows the minimum permeability computable for this sample. The red cross shows a computed permeability, which is far above the numerical minimum (red curve) and thus the image resolution is fine, from this perspective.

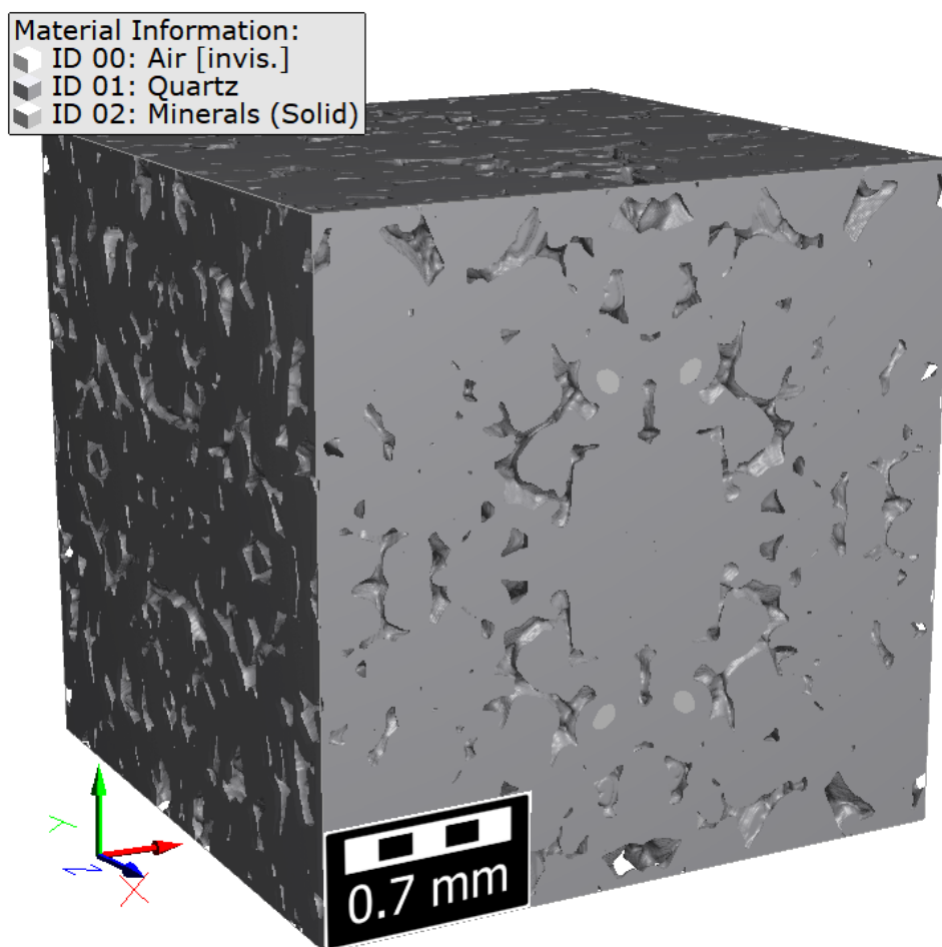


The curves depict the permeability that can be computed by Stokes solvers – at minimum – based on segmented porosity, image voxel size, and numerics. The permeability of the sample (red cross) should be above the numerical minimum (red curve). Otherwise, we recommend acquiring an image of higher resolution.

If porosity and permeability are known a priori, we recommend using the additional curves as a suggestion for a suitable image resolution.

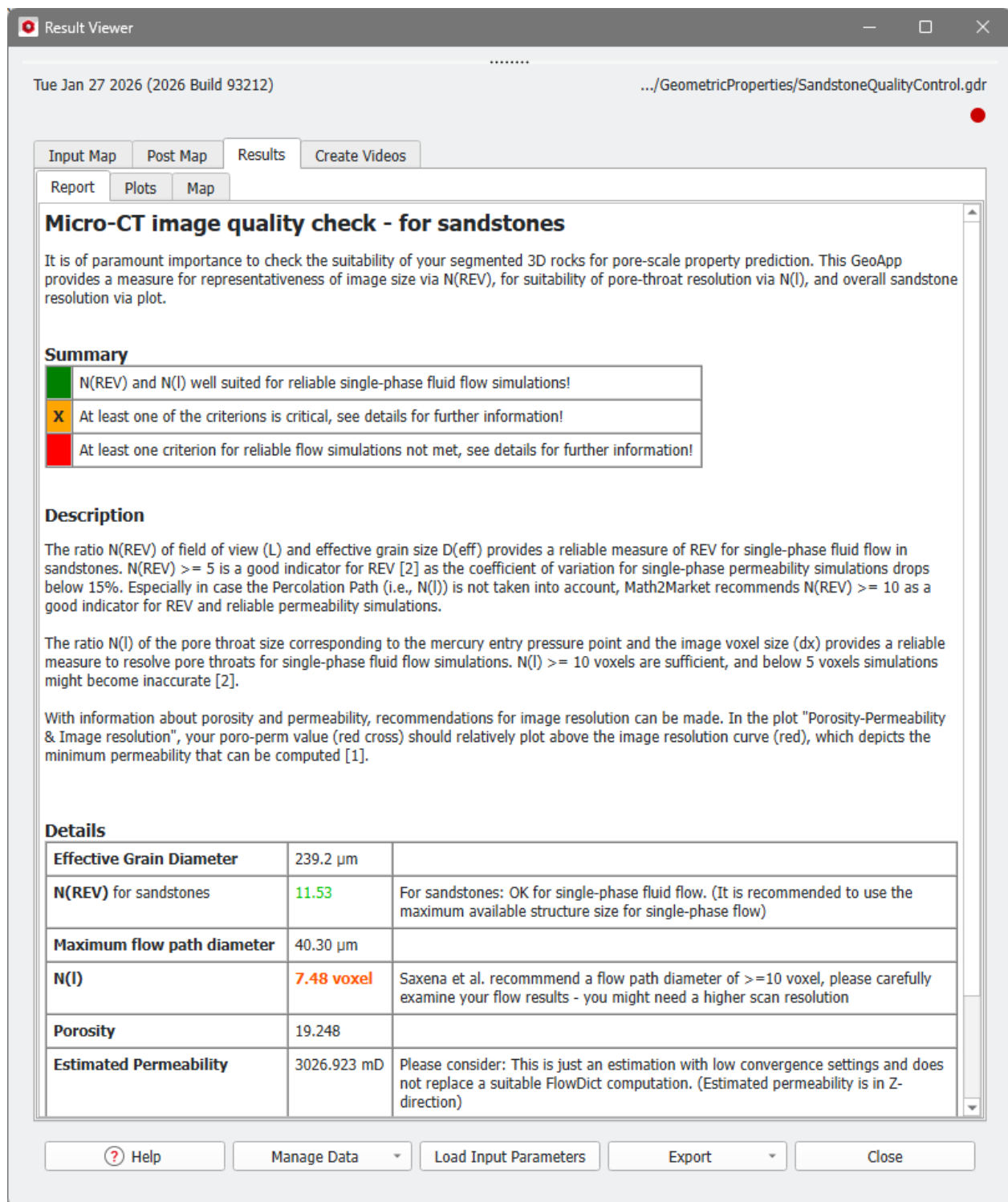
Results

When the simulation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically. The results for the rock sample shown below are presented here.



The **Results - Report** subtab of the **Result Viewer** shows the results of the quality control.

The resolution is displayed in orange in the table, but the plot under the **Results - Plots** tab shows, that in this case, the image resolution is fine, as explained in the [Image Resolution](#)¹³⁰ section.



1.5.2 Physical Properties

Determine **Physical Properties** of your digital rock structure.

The following Physical Properties GeoApps are shipped with GeoDict:

- [Digital Routine Core Analysis](#)^[133]

Run an entire digital routine core analysis workflow.

The following Physical Properties GeoApps are shipped with GeoDict:

- [Hysteresis for Oil-Water Setups](#)¹³⁶
Predict a Capillary Pressure Hysteresis Cycle in an oil-water setup.
- [Porous Plate Capillary Pressure](#)¹⁴¹
Run a Porous Plate Capillary Pressure (PPCP) simulation.
- [Trapping Curve](#)¹⁴³
Create a trapping curve for the currently loaded structure and given contact angle.
- [Reactive Flow](#)¹⁴⁷
Simulate reactive flow by executing mineral dissolution and/or precipitation.
- [NMR](#)¹⁵⁹
Run nuclear magnetic resonance (NMR) experiments on rock structures.
- [Acoustic Rock Properties](#)¹⁶³
Compute seismic rock properties based on a prediction of elastic properties by solving the static problem.

Digital Routine Core Analysis

The **Digital Routine Core Analysis** app runs an entire digital routine core analysis workflow with the chosen properties. Additionally, a PowerPoint presentation is saved which contains images and data from the structure and the selected properties.



Modules needed to run this GeoApp (depending on the selected options):

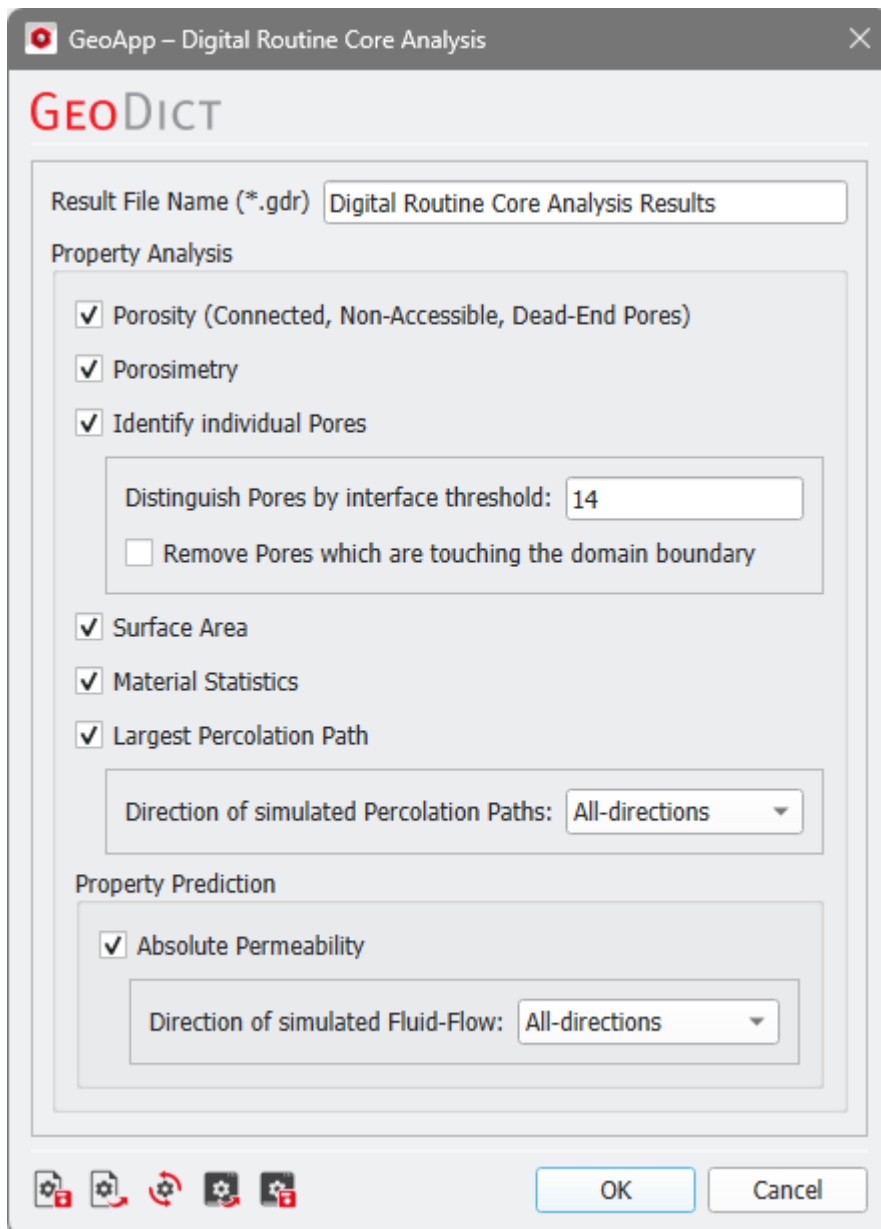
PorDict, FlowDict

Click **Edit** to open the **Digital Routine Core Analysis** parameters dialog.

Define the **Result File Name** for the result file and the result folder where all results will be stored.

Decide if the app should:

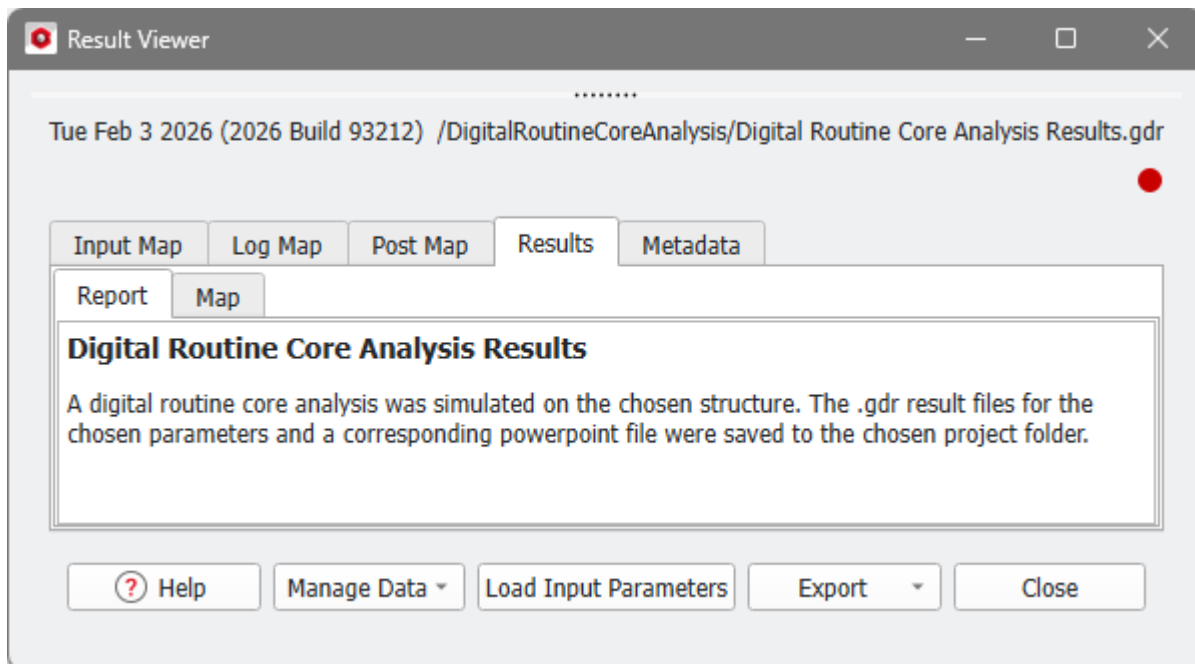
- compute the **Porosity** with PorDict - Open and Closed Porosity
- determine the **Porosimetry** with PorDict - Pore Size Distribution (Porosimetry)
- identify individual **Pores** with PorDict - Identify Pores
- estimate the **Surface Area** with MatDict - Estimate Surface Area
- compute the **Material Statistics** with MatDict - Material Statistics
- determine the **Largest Percolation Path** in the chosen direction (X-, Y-, Z-, or All-directions) with PorDict - Percolation Path
- compute the **Absolute Permeability** with FlowDict - Solve Stokes in the chosen direction (X-, Y-, Z-, or All-directions).



After selecting the desired options, click **Run** to start the digital routine core analysis.

Results

When the simulation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically.

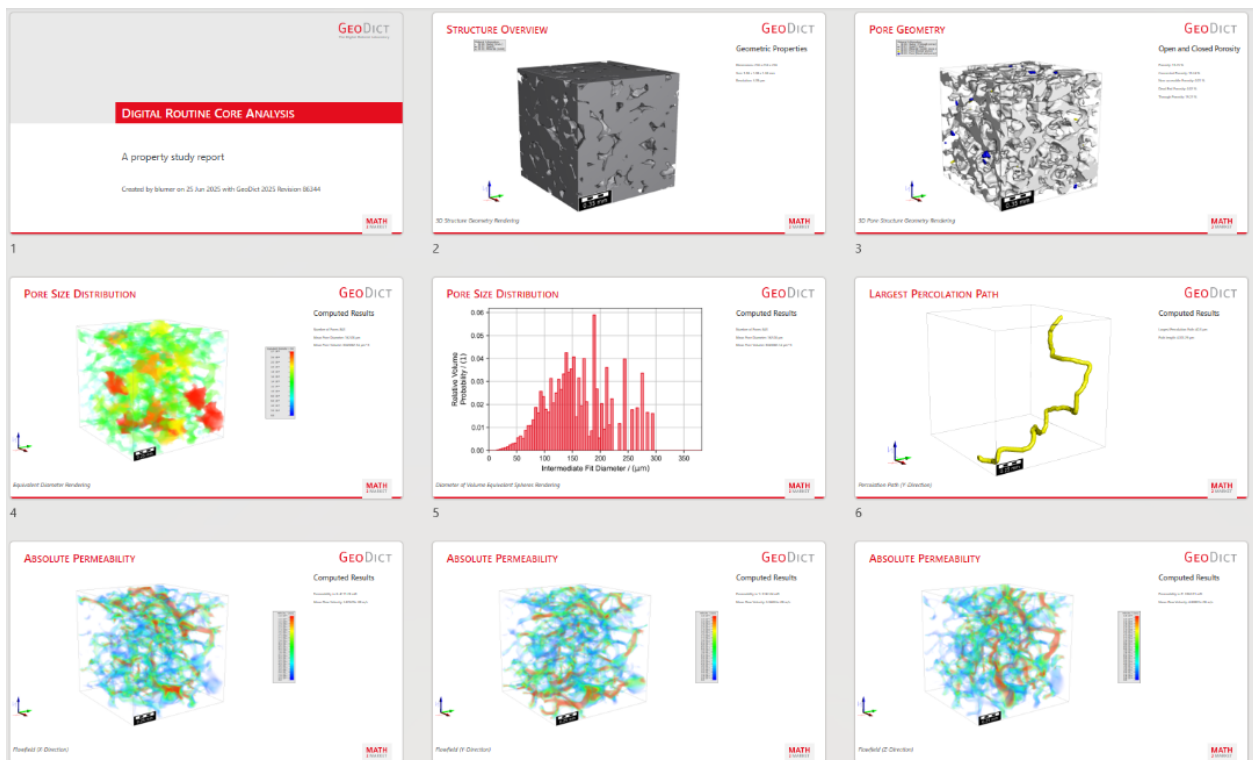


The result files of the chosen property computations are saved in the corresponding folder. Up to nine different result files are available:

- OpenAndClosedPorosity.gdr
- Porosimetry.gdr
- IdentifyPores.gdr
- SurfaceArea.gdr
- 1DStatistics.gdr
- PercolationPath_x.gdr
- PercolationPath_y.gdr
- PercolationPath_z.gdr
- StokesResult_xyz

Additionally, a PowerPoint report can be found in the result folder.

Depending on the selected options, the PowerPoint report shows a structure overview, the pore geometry, the pore size distribution, the largest percolation path and the absolute permeability in the selected directions.



Hysteresis for Oil-Water Setups

The **Hysteresis for Oil-Water Setups** GeoApp predicts a capillary pressure hysteresis cycle in an oil-water setup with primary drainage, spontaneous and forced imbibition, and, if selected, secondary drainage.



Modules needed to run this GeoApp:

SatuDict

Click **Edit** to open the **Hysteresis for Oil-Water Setups Parameters** dialog.

Select a **Result File Name** fitting to the current project.

The parameters are organized into three groups:

✓ Properties of Hysteresis Cycle

Define the **Properties of Hysteresis Cycle**.

Select a material for the **Drainage – Invading Phase** and set the **Primary Drainage – Invading Side**. Choose an **Imbibition – Invading Phase** and set the **Imbibition – Invading Side**.

Properties of Hysteresis Cycle

Drainage - Invading Phase	 Oil...
Primary Drainage - Invading Side	z- ▼
Imbibition - Invading Phase	 Water (Brine)...
Imbibition - Invading Side	z+ ▼
☐ Compute Secondary Drainage	

Select if also **Secondary Drainage** should be considered in the computation and choose the invading phase boundary for it.

☒ Compute Secondary Drainage

Secondary Drainage - Invading Side z- ▼

✓ Two-Phase Flow Properties

Set the **Two-Phase Flow Properties**.

Define the **Interfacial / Surface Tension** in N/m between the two material phases, e.g., water and oil. At the beginning the structure is filled with water and all solids are water-wet. For up to four solid materials the **Water Contact Angle** can be set. During the primary drainage simulation oil enters the structure. The contact angle of the solids to the oil is $180^\circ - \theta_w$, where θ_w is the Water Contact Angle.

Two-Phase Flow Properties

Interfacial / Surface Tension / (N/m)	0.03
Water Contact Angle for Material ID 1 / (°)	40
Water Contact Angle for Material ID 2 / (°)	40
Water Contact Angle for Material ID 3 / (°)	40
Water Contact Angle for Material ID 4 / (°)	40
Wettability during imbibition	WaterWet ▼

After the primary drainage, the wettability of the solids may change for the imbibition and secondary drainage. The **Wettability during imbibition** can be selected from the pull-down menu.

- If **WaterWet** is chosen, nothing changes after the primary drainage and all solid surfaces remain water-wet.
- For **MixedWet** the wettability only changes locally after the primary drainage.

- If **OilWet** is selected, the wettability changes globally after primary drainage. All solid surfaces that are covered by oil change from water-wet surfaces to oil-wet surfaces. They are then non-wetting against water.

In the case of a changing wettability, the new contact angles for the oil-rock contacts must be defined. Again, for up to four solid material IDs the **Oil-Wet Contact Angles** can be defined.

Wettability during imbibition OilWet

Turn local Oil-Rock Contacts into non-wetting Phase (after Drainage - before Imbibition)

Oil-Wet Contact Angle for Material ID 1 / (°)	140
Oil-Wet Contact Angle for Material ID 2 / (°)	140
Oil-Wet Contact Angle for Material ID 3 / (°)	140
Oil-Wet Contact Angle for Material ID 4 / (°)	140

For a **MixedWet** set-up additionally the distribution of the oil-wet solids must be specified. First, select an **Aging Method** and then set the corresponding parameters. The aging method introduces which surfaces change their wettability after the primary drainage and before the imbibition.

For a **Deterministic** aging method, the wettability is changed at surfaces in large pores and in contact with the invading oil. The **Pore volume considered for "aging"** defines the limit for the material reassignments to oil-rock surfaces in large pores. A geometric pore size distribution is applied to determine the pore space that allows consideration of oil-wet surfaces with adjusted contact angles. For example, a value of 70% means that the largest 70% of the pores are changed from water-wet to oil-wet. A higher percentage leads to more contact material changes and an increased saturation change during forced imbibition, while the saturation changes during spontaneous imbibition are decreased.

Wettability during imbibition MixedWet

Turn local Oil-Rock Contacts into non-wetting Phase (after Drainage - before Imbibition)

Oil-Wet Contact Angle for Material ID 1 / (°)

Oil-Wet Contact Angle for Material ID 2 / (°)

Oil-Wet Contact Angle for Material ID 3 / (°)

Oil-Wet Contact Angle for Material ID 4 / (°)

Aging Method Deterministic

Distribute Contact Angles by Volume Percentage of largest Pores

Pore volume considered for "aging" / (%)

A **Stochastic** aging method distributes the wettability changes using Gaussian random fields. Define the **Desired Oil-Wet Region Size**, representing the standard deviation for the applied Gaussian distribution. Additionally, enter the **Desired Oil-Wet Solid Volume Percentage**.

Aging Method Stochastic

Distribute Contact Angles by Gaussian Random Fields

Desired Oil-Wet Region Size / (μm)

Desired Oil-Wet Solid Volume Percentage / (%)

Find out more about the aging methods in the [Simulate Aging GeoApp](#)¹⁷⁰ chapter.

✓ Others

To compute the relative permeability during the imbibition check **Compute Relative Permeability for the Imbibition Process**. Define the **Number of Saturations** for which to compute the relative permeability. The default number of 7 means that for seven different saturations of the structure the permeability is computed. Increase the number to obtain more data points on the relative permeability curve.

☒ Compute Relative Permeability for the Imbibition Process

Number of Saturations

☐ Expert Settings

Finally, determine the **Expert Settings**. Here, define the **Dynamic Pore Morphology Method** parameters and the **Parallelization**.

The **Fluid Interface Step Size** defines how many voxels the computed fluid interface can move in each step. Lower values might increase the runtime significantly.

The imbibition starts with the spontaneous imbibition part. At some point, defined by the **Transition Radius**, the imbibition changes from spontaneous to forced:

- For the **Transition Radius Setting Automatic** this point is determined automatically.
- For a **Manual Transition Radius**, you define the sphere radius in voxel at which the dynamic transition from spontaneous to forced occurs. The meniscus of the water-front can be interpreted as a part of a circle. If this circle has a radius larger than the transition radius, the meniscus flips over, and the forced imbibition applies. This parameter is experimental. Examine the results carefully, especially if contact angles close to 90° are chosen.

For the **Parallelization** of the execution either use the **Maximum** number of cores or enter a **Manual** value.

☒ Expert Settings

Dynamic Pore Morphology Method

Fluid Interface Step Size / (voxel)

Transition Radius Setting

Parallelization

Click **OK** to save the settings. Click **Run** to perform the hysteresis simulation.

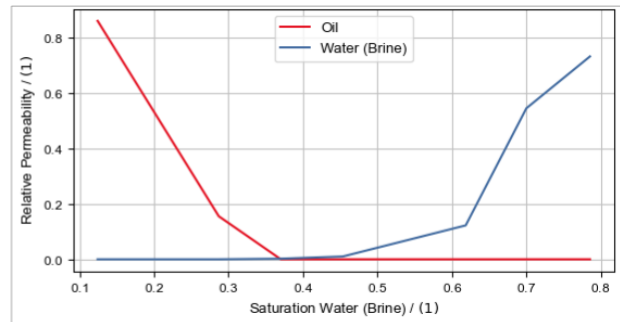
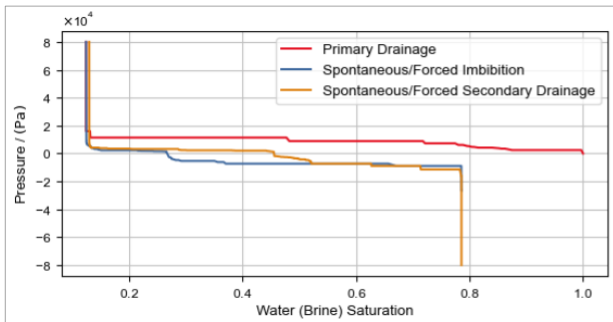
Results

When the simulation is finished, the result file automatically opens in the **Result Viewer**.

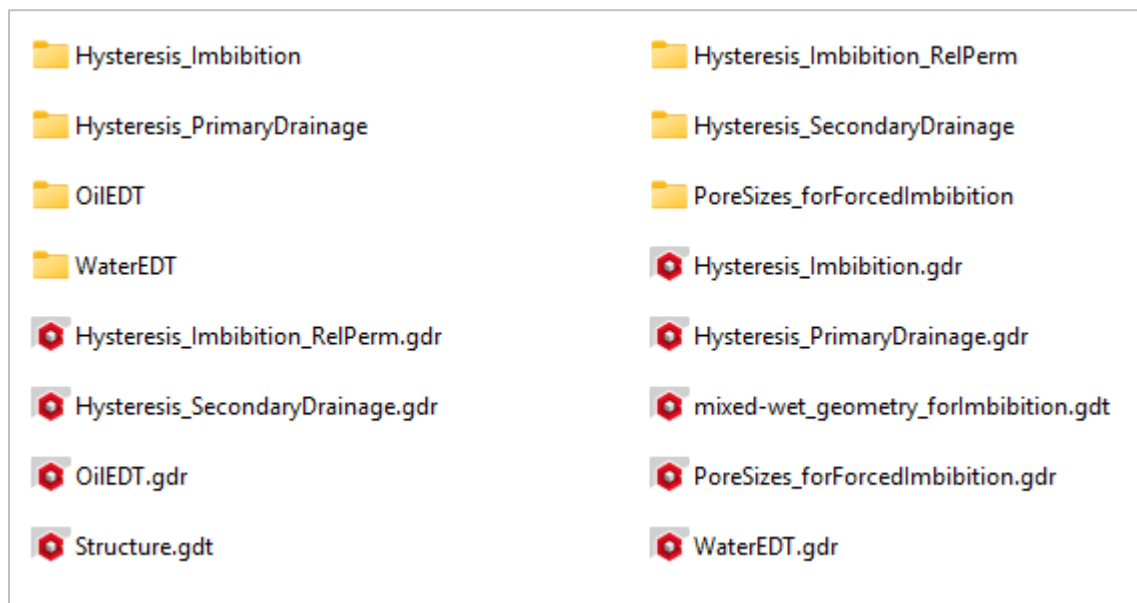
The **Results - Plots** tab contains plots for **Hysteresis**, **Relative Permeability**, and **Relative Permeability at irreducible Water (Brine) Saturation**.

To obtain the **Relative Permeability** values, the permeabilities of the different saturation steps are divided by the absolute permeability.

For the **Relative Permeability at irreducible Water (Brine) Saturation** the effective permeability of the state with irreducible water saturation (at the end of the primary drainage) is used for normalization.



Several result files and result folders are generated and can be found in the project folder. The prefix is based on the chosen **Result File Name** (default is Hysteresis).



Porous Plate Capillary Pressure

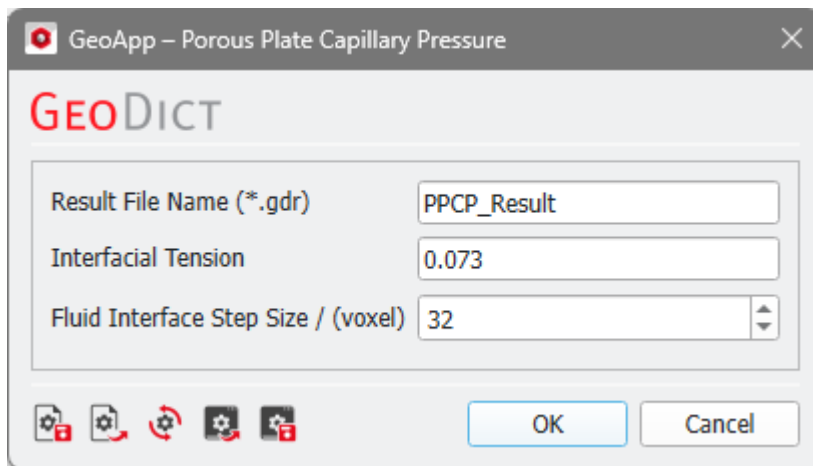
The **Porous Plate Capillary Pressure** GeoApp fills the pore space of the current structure with water. Then, air invades the structure from all but one side. The face in Z- direction is connected to a porous plate. The **Porous Plate Capillary Pressure** app is similar to the MICP command, but here air displaces water.



Modules needed to run this GeoApp:

SatuDict

Click **Edit** to open the **Porous Plate Capillary Pressure Parameters** dialog.



Enter the **Result File Name** for the generated GeoDict result file (*.gdr) and the corresponding result folder.

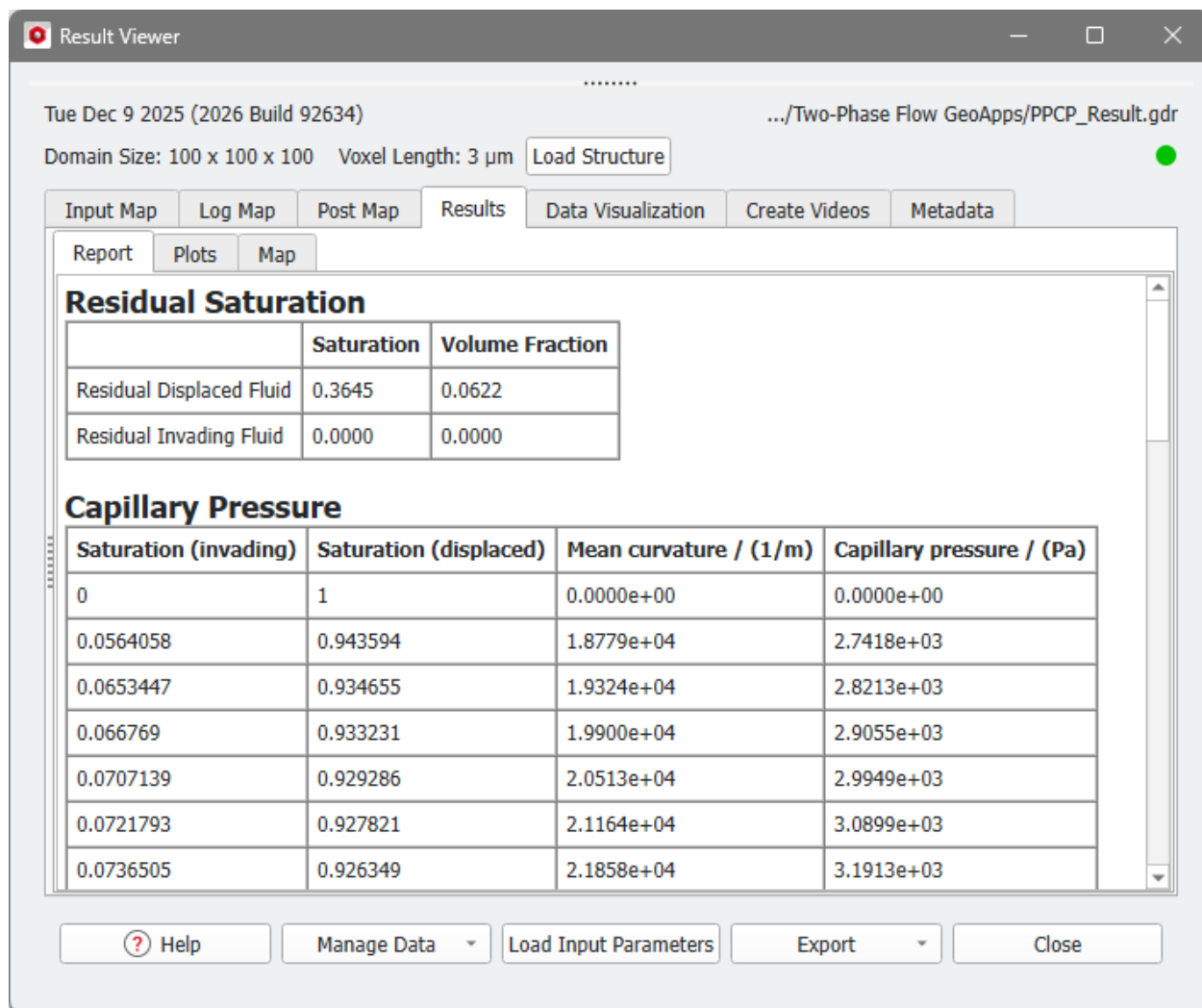
Two parameters can be defined:

- Set the **Interfacial Tension** in N/m between water and air. The given default value refers to the value at 20°C for an air contact angle of 140°. The air contact angle cannot be changed.
- The **Fluid Interface Step Size** determines the range of voxels that can be maximally saturated within one pressure step. Lower values might increase the runtime and the number of saturation steps significantly, but give a more realistic development of the saturation process.

Click **Run** to perform the porous plate capillary pressure simulation. The pore space is filled with water, then air invades the structure from all sides except for Z-.

Results

After the simulation is finished, the result file is opened in the Result Viewer. Refer to the Capillary Pressure Curve Results chapter for more details regarding the results.



Trapping Curve

The **Trapping Curve** GeoApp predicts a capillary pressure hysteresis cycle and creates a trapping curve for the currently loaded structure and given contact angle. Initially, the pore space is filled with water. Then, a primary drainage with a selected invading fluid is computed. For a chosen number of saturation steps a secondary imbibition with water is computed.



Modules needed to run this GeoApp:

SatuDict

Click **Edit** to open the **Trapping Curve Parameters** dialog.

GeoApp – Trapping Curve

GEODICT

Result File Name (*.gdr)

Trapping curve parameters

Minimum Initial (Gas) Saturation

Number Of Saturations

Capillary Pressure Computation

Fluid Interface Step Size / (voxel)

Interfacial / Surface Tension / (N/m)

☐ Adjust expert settings

Primary Drainage Settings

Water Contact Angle / (°)

Invading Fluid (Drainage)

Imbibition Settings

Wettability during Imbibition

OK Cancel

The parameters are organized in four groups:

✓ Trapping curve parameters

Set the **Minimum Initial (Gas) Saturation** to determine the trapping curve from fully gas-saturated pore volume down to the given value between 0 and 1.

Define the **Number Of Saturations**, i.e., the number of imbibitions calculated for the trapping curve.

The starting saturations of the invading fluid for the imbibition are distributed between the value entered in Minimum Initial Saturation and 1.

Trapping curve parameters

Minimum Initial (Gas) Saturation

0.5

Number Of Saturations

4

Capillary Pressure Computation

Define the **Fluid Interface Step Size** for the corresponding capillary pressure method. The **Fluid Interface Step Size** determines the range of voxels that can be maximally saturated within one pressure step. Lower values might increase the runtime and the number of saturation steps significantly, but give a more realistic development of the saturation process.

Set the **Interfacial / Surface Tension** between the invading and the displaced fluid.

Capillary Pressure Computation

Fluid Interface Step Size / (voxel)

32

Interfacial / Surface Tension / (N/m)

0.05

☐ Adjust expert settings

The available **expert settings** include **Parallelization**, **Transition Radius**, and whether **Thin Wetting Layers** and/or **Non-Monotonic Capillary Pressure** should be applied. Refer to the Capillary Pressure Curve chapter for a detailed explanation of these saturation experiment parameters.

☒ Adjust expert settings

Parallelization

maximum

Transition Radius / (voxel)

1000

☐ Use Thin Wetting Layers

☐ Non-Monotonic Capillary Pressure

Primary Drainage Settings

By default, the initial pore fluid is water. Enter the **Water Contact Angle** that is used for the primary drainage computation. Select the **Invading Fluid** for the primary drainage from the Material Database.

Primary Drainage Settings

Water Contact Angle / (°)

0

Invading Fluid (Drainage)

Oil...

✓ Imbibition Settings

Set the **Wettability during Imbibition** as explained for the Hysteresis for Oil-Water Setups GeoApp. Note, that here oil-wet means that the solid surfaces covered with the invading fluid (not necessarily oil) change their wettability.

Imbibition Settings

Wettability during Imbibition

WaterWet

WaterWet

MixedWet

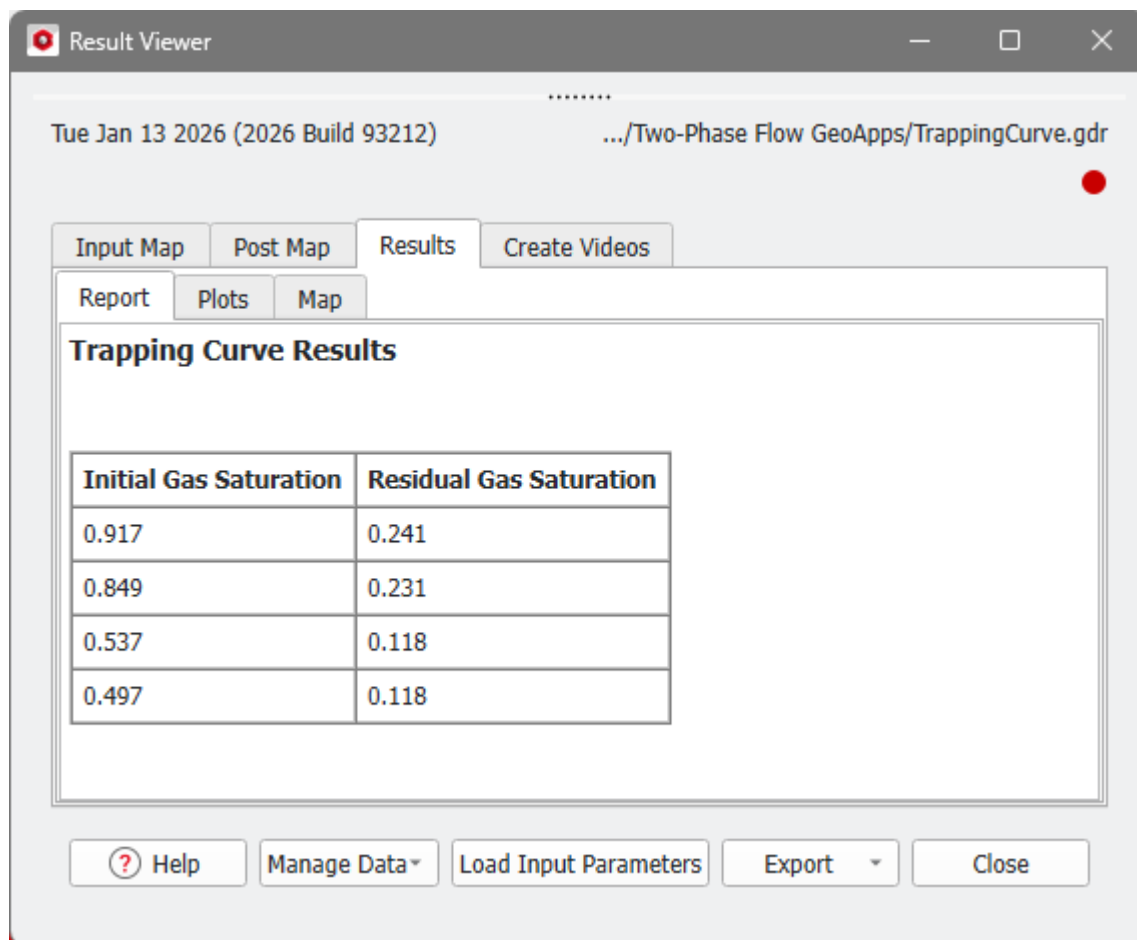
OilWet

Click **Run** to create the trapping curve.

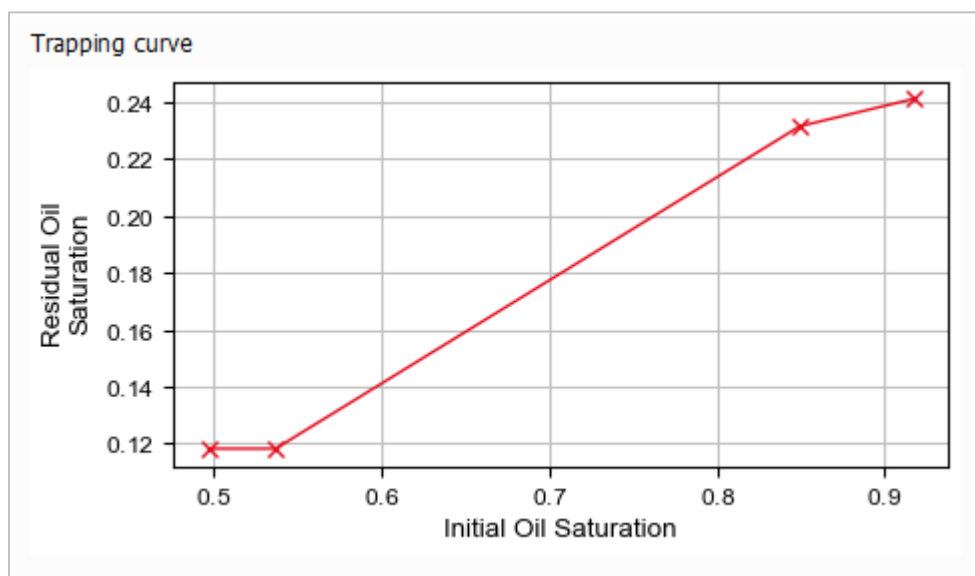
Results

When the simulation is finished, the result file opens in the **Result Viewer** automatically.

The **Results - Report** subtab of the **Result Viewer** shows a table with the saturation of the invading fluid at the beginning of the imbibition (**Initial Gas Saturation**) and after the imbibition (**Residual Gas Saturation**).



These values are also plotted in a **Trapping curve** available in the **Plots** subtab.



Reactive Flow

Simulate **Reactive Flow** by executing mineral dissolution and/or precipitation.

Additionally, a pH-based model is available. This reactive flow model computes mineral dissolution due to acid injection. The reactivity is controlled by a user-defined pH value and

particle-rock collisions based on the approach of [Nunes et al. \(2016\)](#)^[240]. See also our dedicated technical report: [Cvijetkovic et al. \(2018\)](#)^[240]

These GeoApps are applicable to many different research and business topics such as CO₂ sequestration, Acidizing treatments, and further applications such as Nuclear Waste Storage, Environmental Remediation, and Hydrogen Underground Storage.

Learn how to set up and run both GeoApps in our tutorial [Reactive flow GeoApp for CO2 sequestration](#).

The following Reactive Flow GeoApps are shipped with GeoDict:

- [Reactive Flow - Reaction Rate Model](#)^[148]
Execute mineral-specific dissolution and precipitation reactions based on particle-mineral collisions.
- [Reactive Flow - iPhreeqC Model](#)^[151]
Simulate mineral dissolution and/or precipitation based on transport of aqueous solutions.

Reactive Flow - Reaction Rate Model

The **Reactive Flow – reaction rate model** GeoApp computes dissolution and precipitation of mineral phases during continuous inflow of reactants (e.g., acid) and predicts:

- Permeability reduction & enhancement (porosity-permeability relationship)
- 4D rock alteration: automated generation of animations that enable visual determination of the precipitation and dissolution patterns in addition to the analysis via various plots that are generated automatically
- Chemical transport in the geometry, determined on the voxel scale



Modules needed to run this GeoApp:

AddiDict

Optional: FlowDict, PoroDict

Click **Edit** to open the **Reactive Flow - reaction rate model** parameters dialog.

The parameters are organized into five groups:

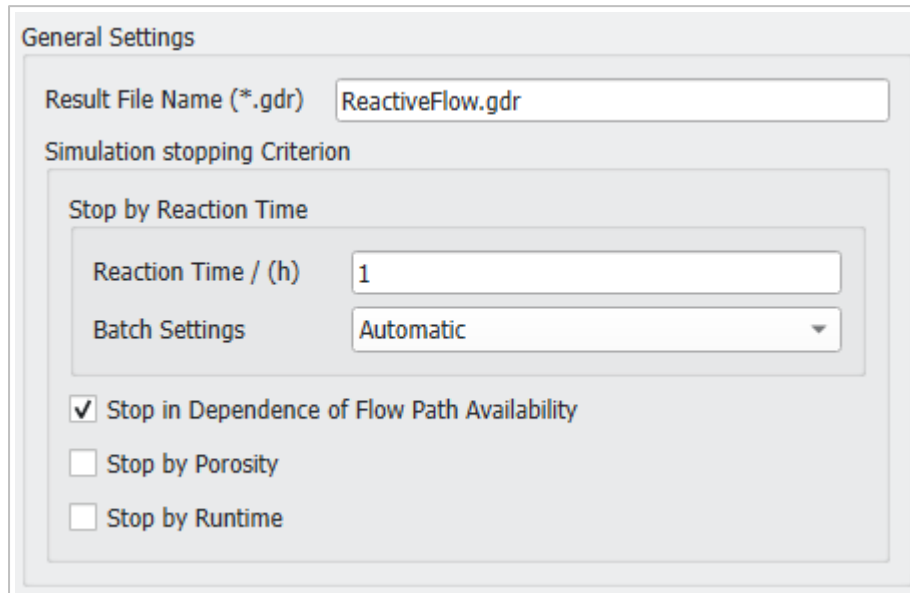
✓ General Settings

Choose a **Result File Name** for the GeoDict result file (*.gdr) and the corresponding result folder.

Enter the **Reaction Time** after which the simulation stops and choose the desired **Batch Settings** from the pull-down menu. **Automatic** is based on reaction time and geometry. If selected, the number of times steps (batches) and particles are chosen dynamically. For **Manual** batch settings the number of **Particles per Batch** and the

Number of Batches from which the time per batch is calculated must be defined manually.

Additional stopping criteria are **Stop in Dependence of Flow Path Availability**, after reaching a given **Porosity**, and/or reaching a given **Runtime**.



General Settings

Result File Name (*.gdr)

Simulation stopping Criterion

Stop by Reaction Time

Reaction Time / (h)

Batch Settings

☒ Stop in Dependence of Flow Path Availability

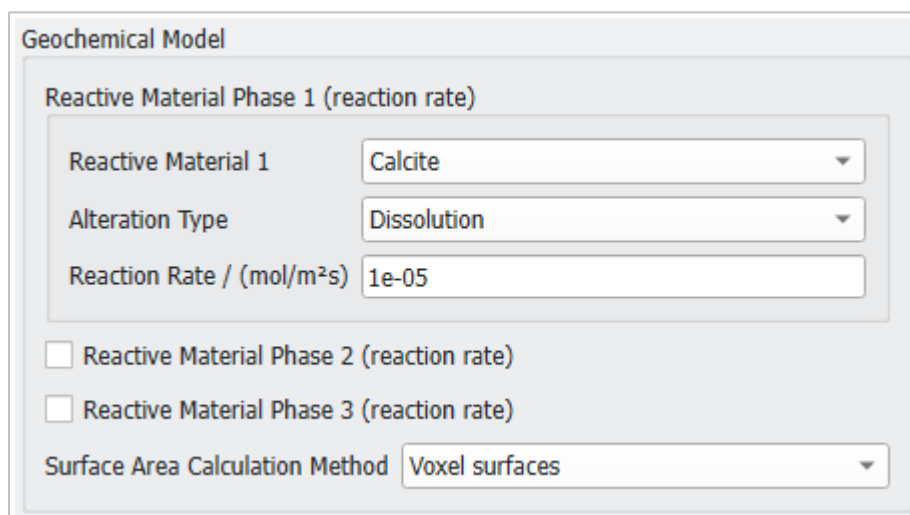
☐ Stop by Porosity

☐ Stop by Runtime

✓ Geochemical Model

Select a **Reactive Material** from the pull-down menu and set the **Alteration Type** to **Dissolution** or **Precipitation**.

Define the global **Reaction Rate** of the reactive material phase. This reaction rate is a prerequisite for each batch.



Geochemical Model

Reactive Material Phase 1 (reaction rate)

Reactive Material 1

Alteration Type

Reaction Rate / (mol/m²s)

☐ Reactive Material Phase 2 (reaction rate)

☐ Reactive Material Phase 3 (reaction rate)

Surface Area Calculation Method

Up to three material phases can be defined here. For materials 2 and 3 the alteration type is always **Dissolution**.

The surface area is calculated as in MatDICT - Estimate Surface Area. You can choose which of the two algorithms is used.

✓ Transport Settings

Select the **Material ID of Reactive Fluid** and enter a **Diffusion Coefficient** as described for the [iPhreeqc Model](#) ¹⁵² GeoApp.

If the transport should be computed from **Pure Diffusion**, select the corresponding checkbox. Otherwise, depending on the **Experiment Setup** or reservoir system select **Mean Velocity**, **Pressure Drop**, or **Flow Rate** as input parameter. Enter the according value below. Alternatively, a **Previous Flow Simulation** can be used as input, which is especially beneficial in case of restarting simulations in large geometries.

The screenshot shows the 'Transport Settings' panel. It contains the following fields and options:

- Material ID of Reactive Fluid:** A text input field with the value '0'.
- Diffusion Coefficient / (m²/s):** A text input field with the value '2.299e-09'.
- Pure Diffusion (Non-Advective Transport):** An unchecked checkbox.
- Experiment Setup:** A dropdown menu currently showing 'MeanVelocity'.
- Mean Velocity / (m/s):** A text input field with the value '0.001', which is nested within the 'Experiment Setup' dropdown's content area.
- Use a Previous Flow Simulation as Input:** An unchecked checkbox.

✓ Post-Processing Settings

If **Create video showing Reaction Spots** is selected, the structure changes are animated with dissolution and precipitation locations highlighted in red, while the solid matrix is made invisible in the front half.

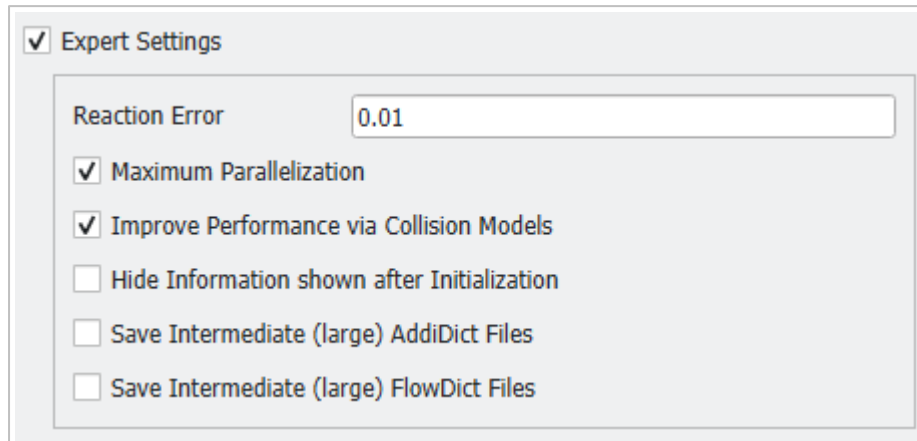
For the animation select if the structure should be rendered with the **Box** or **Smooth** renderer.

The screenshot shows the 'Post-Processing Settings' panel. It contains the following fields and options:

- Create Video showing Reaction Spots:** A checked checkbox.
- Structure Rendering Mode:** A dropdown menu currently showing 'Box'.

✓ Expert Settings

The **Expert settings** include **Reaction Error**, **Parallelization**, **Improve Performance via Collision Models**, **Hide Information shown after Initialization**, and **Save Intermediate AddiDict** and **FlowDict Files**.



☒ Expert Settings

Reaction Error

☒ Maximum Parallelization

☒ Improve Performance via Collision Models

☐ Hide Information shown after Initialization

☐ Save Intermediate (large) AddiDict Files

☐ Save Intermediate (large) FlowDict Files

You can find more details on the setup of a Reactive Flow - Reaction Rate Model simulation in our tutorial [Reactive flow GeoApp for CO2 sequestration](#).

Reactive Flow - iPhreeqC Model

The **Reactive Flow – iPhreeqC model** GeoApp computes dissolution and precipitation of mineral phases during continuous inflow of reactants (e.g., acid) and predicts:

- Permeability reduction & enhancement (porosity-permeability relationship)
- 4D rock alteration: automated generation of animations that enable visual determination of the precipitation and dissolution patterns in addition to the analysis via various plots that are generated automatically
- Chemical transport in the geometry, determined on the voxel scale

For solving Reactive Flow for the various application areas, the geochemical calculator [PhreeqC](#) (USGS) is coupled to GeoDict to compute geochemical transport and mineral dissolution / precipitation based on the Lagrangian Transport method.



Modules needed to run this GeoApp:

AddiDict

Optional: FlowDict, PoroDict

Click **Edit** to open the **Reactive Flow – iPhreeqC model** parameters dialog.

Choose a **Result File Name** for the resulting GeoDict result file (*.gdr) and the corresponding result folder.

The parameters are organized into five groups:

☒ General Settings

Under the **General Settings** define the **Total Simulation Time**, the **Number Of Batches** and the **Particles Per Batch** for the reaction rate simulation. During each batch first the flow is computed if the current and relative porosity change is larger than 1%. Then, the transport is computed and finally the reactions at water-rock interfaces are computed. Fewer particles decrease the accuracy of the simulation. Using more particles increases the accuracy while leading to longer runtimes. As a rule of thumb, it is sufficient to use the number of pore voxels at the inflow boundary (approx. $n_x \cdot n_y \cdot \text{porosity}$). Feel free to decrease that number for ~linearly improved performance at a relatively lower cost of accuracy.

General Settings

Total Simulation Time / (h) 0.01

Number Of Batches 10

Particles Per Batch 200

✓ Transport Settings

The Reactive transport experiment is based on advection-diffusion-reaction or diffusion-reaction. In both cases the transport is computed along the Z-axis.

Select the **Material ID of Pore Space** and set the **Diffusion Coefficient**. This coefficient affects the inflow fluid transport paths according to the Brownian motion. The default value is the self-diffusion coefficient of pure water at 25°C.

Select **Compute Flow** if a reactive flow experiment should be performed by computing the flow field regularly. This requires a FlowDict license. For this, define the **Mean Velocity**. Alternatively, a **previous Flow Simulation** can be used as input, which is especially beneficial in case of restarting simulations in large geometries.

Transport Settings

Material ID of Pore Space 0

Diffusion Coefficient / (m²/s) 2.299e-09

☒ Compute Flow

Mean Velocity / (m/s) 0.001

☐ Use a previous Flow Simulation as Input

✓ Geochemical Model

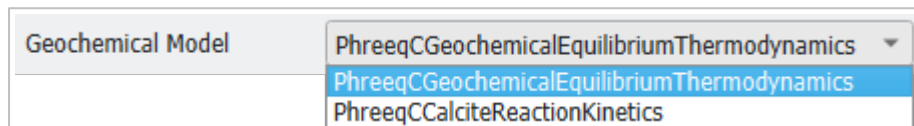
Two **Geochemical Models** can be selected for the simulation.

You do not need a separate PhreeqC installation to run this reactive flow model. But, we recommend to install PhreeqC, get used to the software and set up your geochemistry therein in advance. Please make sure to check your setup for reactive mineral phases and to balance the electrical charge.

Please visit <https://www.usgs.gov/software/phreeqc-version-3> for more information.

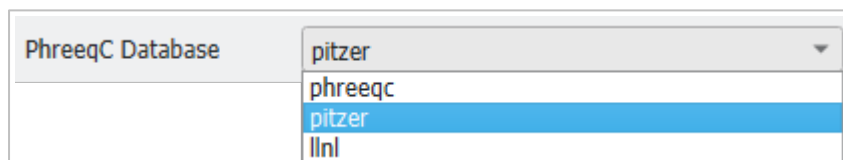
PhreeqC Geochemical Equilibrium Thermodynamics (PGET) calculates reactions based on the input of aqueous fluids by employing the geochemical calculator PhreeqC.

PhreeqC Calcite Reaction Kinetics (PCRK) calculates kinetic reactions with calcite as the reactive mineral phase and is based on the input of aqueous fluids by employing the geochemical calculator PhreeqC. The database (phreeqc.dat) for calcite kinetics is however limited to ambient conditions.



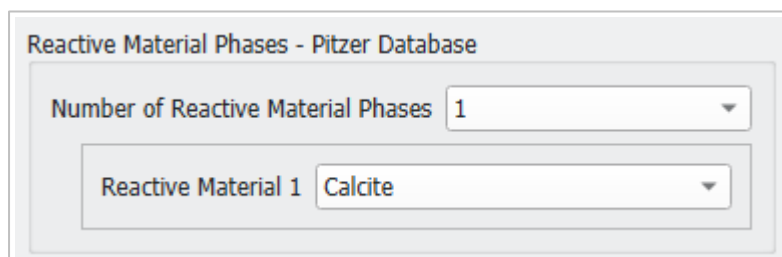
A screenshot of a software interface showing a dropdown menu for 'Geochemical Model'. The menu is open, displaying three options: 'PhreeqCGeochemicalEquilibriumThermodynamics' (selected), 'PhreeqCGeochemicalEquilibriumThermodynamics', and 'PhreeqCCalciteReactionKinetics'.

For PGET select a **PhreeqC Database**. The databases are located in the app folder within the GeoDict installation folder and can be adjusted or replaced. This may require administrator rights. For reservoir conditions with high pressure, temperature, and salinity the **pitzer** database is recommended. For most other setups the **phreeqc** database should work well. Additionally, the **llnl** (Lawrence Livermore National Laboratory) database is available, which contains the highest number of mineral phases. Note that we have not included all of the approx. 2000 mineral phases considered by the llnl database. Feel free to contact us if you are missing a specific mineral phase.



A screenshot of a software interface showing a dropdown menu for 'PhreeqC Database'. The menu is open, displaying four options: 'pitzer' (selected), 'phreeqc', 'pitzer', and 'llnl'.

Define the **Number of Reactive Material Phases** and select each **Reactive Material** from the pull-down menu. The chosen mineral phases will be dissolved and / or precipitated based on the PhreeqC calculations. The available materials depend on the selected database.



A screenshot of a software interface showing the 'Reactive Material Phases - Pitzer Database' settings. It includes a dropdown menu for 'Number of Reactive Material Phases' set to '1', and a dropdown menu for 'Reactive Material 1' set to 'Calcite'.

Set the **Fluid Pressure**, **pH Value**, and **Temperature**. For pressure and temperature, values are limited to the ranges specified for the corresponding database.

Subsequently, set the **Number of Concentrations** for both the pore fluid (formation fluid) and the inflow fluid (injected fluid). For each concentration, select the **Add Element** and enter a **Concentration** value in mol per kg water (mol/kgw), which is the default PhreeqC unit.

PhreeqC calculates using element concentrations and converts them into the respective molecules for further geochemical calculations. This requirement is well in line with hydrogeochemical fluid analysis, so the user interface is designed towards these factors.



Important! Please make sure to equilibrate your fluids in advance (e.g., via PhreeqC). This includes an electric charge balance for both fluids and an equilibrium of the pore fluid with respect to the reactive materials (mineral phases) selected above. Note that future GeoDict developments will aim at a simplified user experience in this context.

Pore Fluid - Pitzer Database

Fluid Pressure / (atm)	200
pH Value	6.021
Temperature / (°C)	100
Number of Concentrations	1
Add Element	C
Concentration / (mol/kgw)	0.001312

✓ Post-Processing Settings

Decide if the structure changes during the reactive flow simulation should be animated in a video by selecting or deselecting **Create Animation(s)**. In case of a geochemical model including PhreeqC calculations pore fluid animations are created as well. Animations have a default length of 10 s each. They are especially smooth in case of a large number of batches.

Note that for an improved visibility of geochemical transport with respect to the inflow fluid a transparency is introduced for the initial pore fluid concentration.

For the animation select if the structure should be rendered with **Box**, **Smooth**, or **GPU** renderer.

Post-Processing Settings

☒ Create Animation(s)

Structure Rendering Mode: Box

✓ Expert Settings

The available **Expert Settings** include **Parallelization**, defining the factor for **Decreased Transport Accuracy** and **Increased Pore Alteration**, selecting to **Keep Particle Trajectory Files** and **Non-Required Flow Fields**, and deciding to **Equilibrate Fluids Arithmetically** or not.

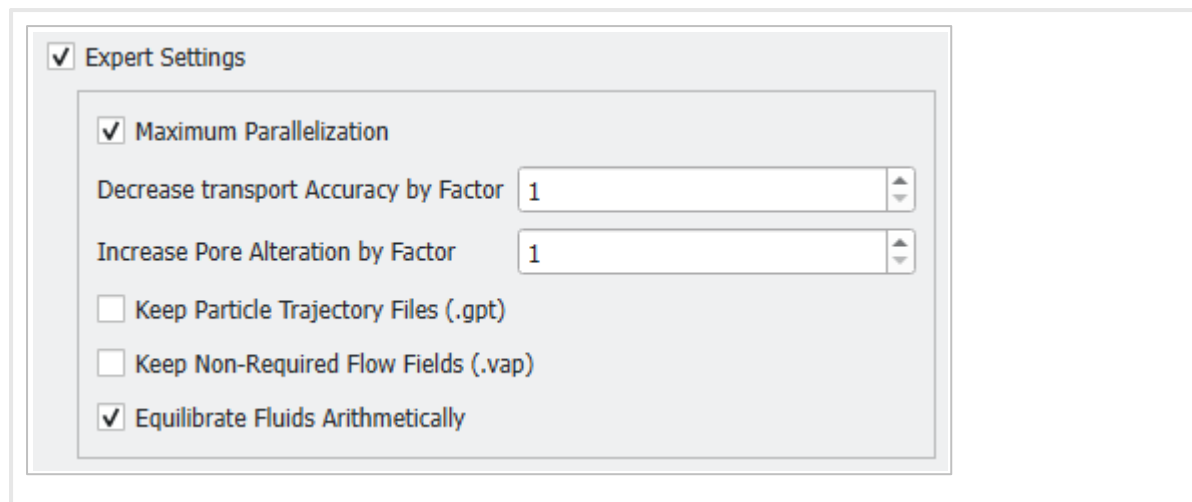
A decreased transport accuracy improves the geochemical performance at the cost of transport accuracy. The value shouldn't be increased above 1 unless there is no other option left.



Note! Increase Pore Alteration increases the reaction time beyond the transport time. This option allows you to compute reactions at time scales beyond s / min / h. Technically, the computed volume of dissolved / precipitated mineral phase is scaled by the given factor. It is thus recommended to first calculate a reasonable value. This could be exercised via PhreeqC. As an alternative, you could run test simulations in small structures and investigate the fraction of minerals altered at voxel surfaces as stored in the corresponding volume file (e.g., SolidFractions01.gvf) in your result folder.

By default, some non-required files are deleted from your result folder during the reactive flow simulation to save disk space. You may deactivate this behavior by checking the **Keep** options.

Finally, **Equilibrate Fluids Arithmetically** significantly improves the performance by reducing the overall amount of PhreeqC calculations for the geochemical transport.



After completing your individual setup, click **OK** to close the dialog. Go back to the GeoApp section and click **Run**.

You can find more details on the setup of a Reactive Flow - iPhreeqC Model simulation in our tutorial [Reactive flow GeoApp for CO2 sequestration](#).

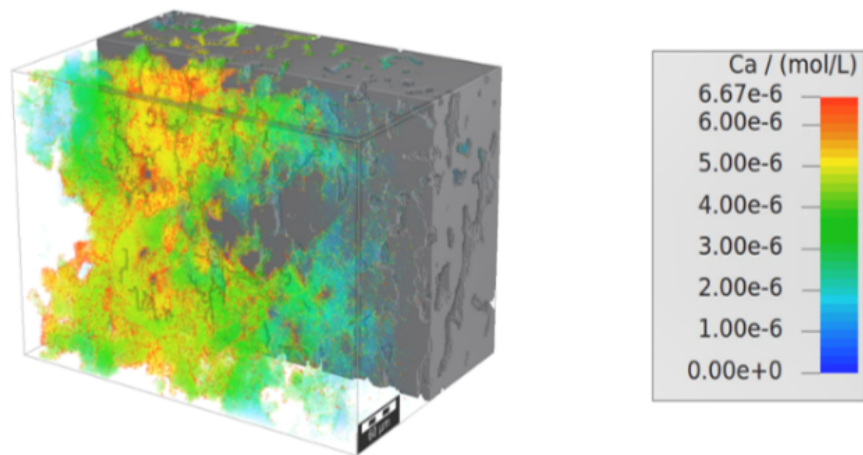
Results

Once the simulation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically. The results show the Number of Batches, Total Simulation Time, Total Reaction Time, and Delta Porosity in the **Results** → **Report** tab.

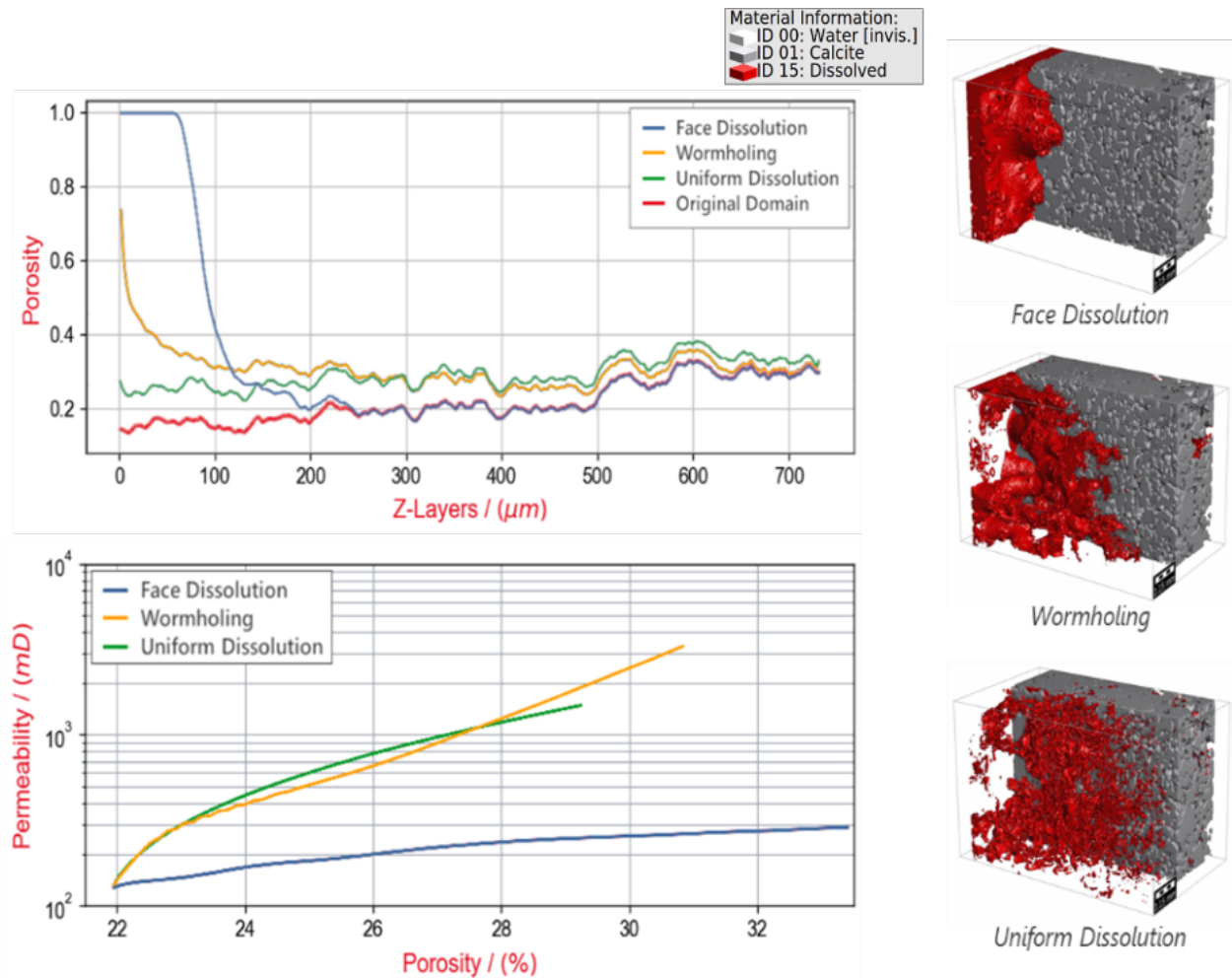
Multiple result plots are found under the **Results** → **Plots** tab, depending on your setup: Porosity-permeability, Porosity, Porosity gradient (in flow direction), Reaction rate, Damkohler number (Da), Péclet number (Pe), and PeDa number (product of Pe and Da).

In the following, see some sample visualizations of the computation on a Grosmont carbonate rock ([Andrä et. al, 2013](#)^[240]) that are generated automatically depending on your post-processing settings and stored in your result folder as images and (*.mp4) animation:

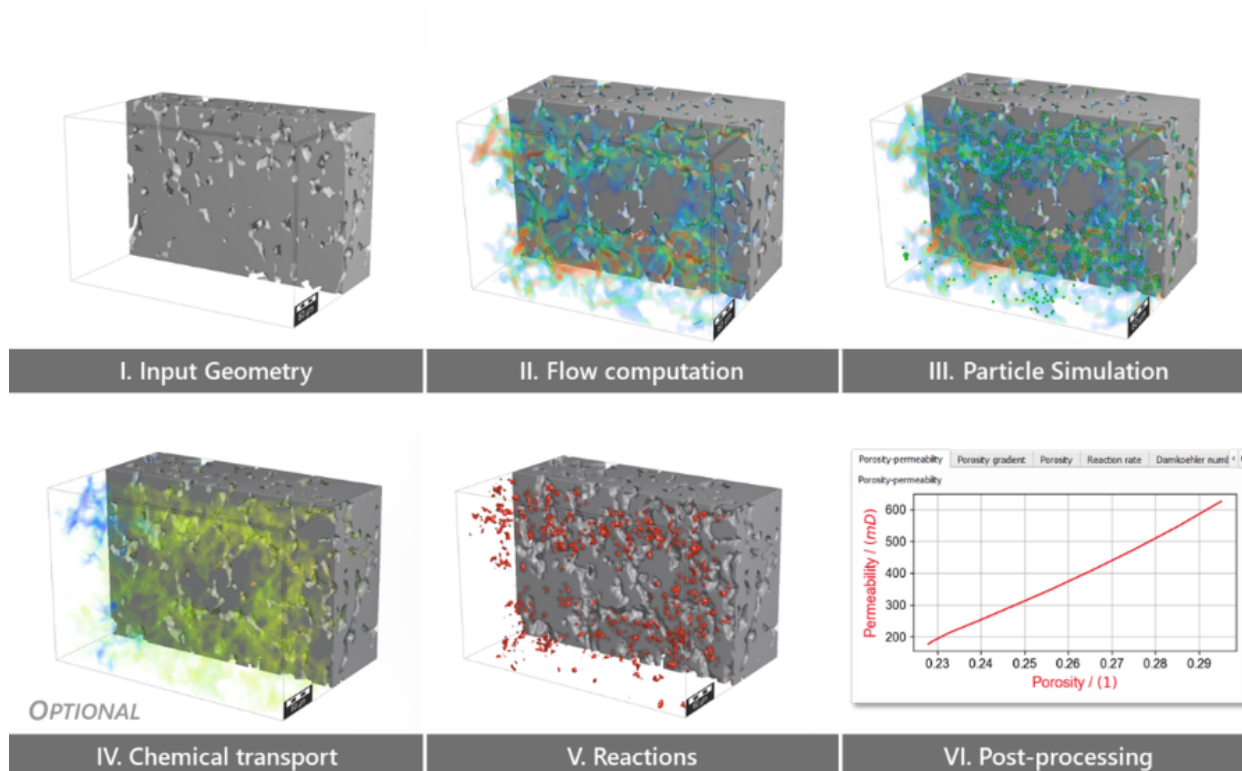
Material Information:
ID 00: Water [invis.]
ID 01: Calcite



Digital Reactive Flow Experiment considering the entire aqueous geochemistry here showing an intermediate result of a digital kinetically-controlled acidizing treatment of a Grosmont carbonate rock upon inflow of a hydrochloric acid at pH 5.5



Simulation of acidizing treatment in the digital Grosmont carbonate rock using different injection velocities and the same geochemical setup, which results in three main different Dissolution regimes upon usage of the reaction-rate model or pH-based model to dissolve the calcite at computed particle-rock collisions.



The general workflow for Reactive Flow modeling in GeoDict.
Step IV is only considered upon usage of the PhreeqC models.

NMR

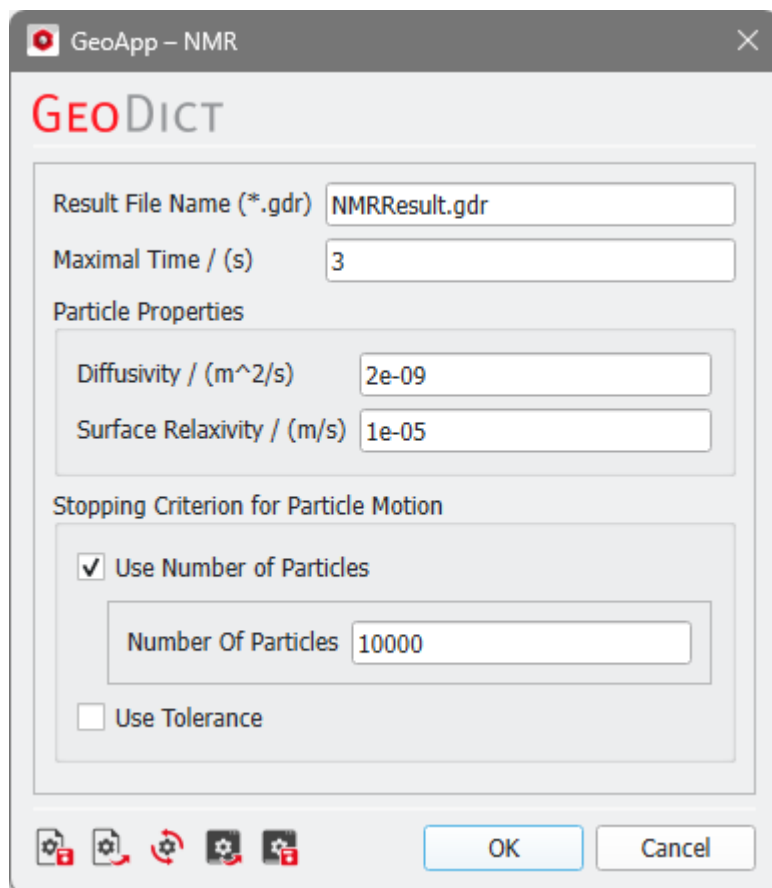
The **NMR** app computes the T2 relaxation curve of a simulated NMR experiment on the current 3D structure.



Modules needed to run this GeoApp:

AddiDict

After loading a structure, click **Edit** to open the **NMR** parameters dialog.



First, define the **Result File Name**.

The **Maximal Time** is the time duration of the particle tracking.

Under **Particle Properties** define the **Diffusivity** of particles in the fluid (the default $2\text{e-}9\text{ m}^2/\text{s}$ refers to the self-diffusion coefficient of water) and the **Surface Relaxivity** of the pore wall material.

As **Stopping Criterion for Particle Motion** either choose **Use Number of Particles** (the number of walkers to be simulated) or **Use Tolerance** (give the result deviation tolerance, then particles are added until the tolerance is reached).

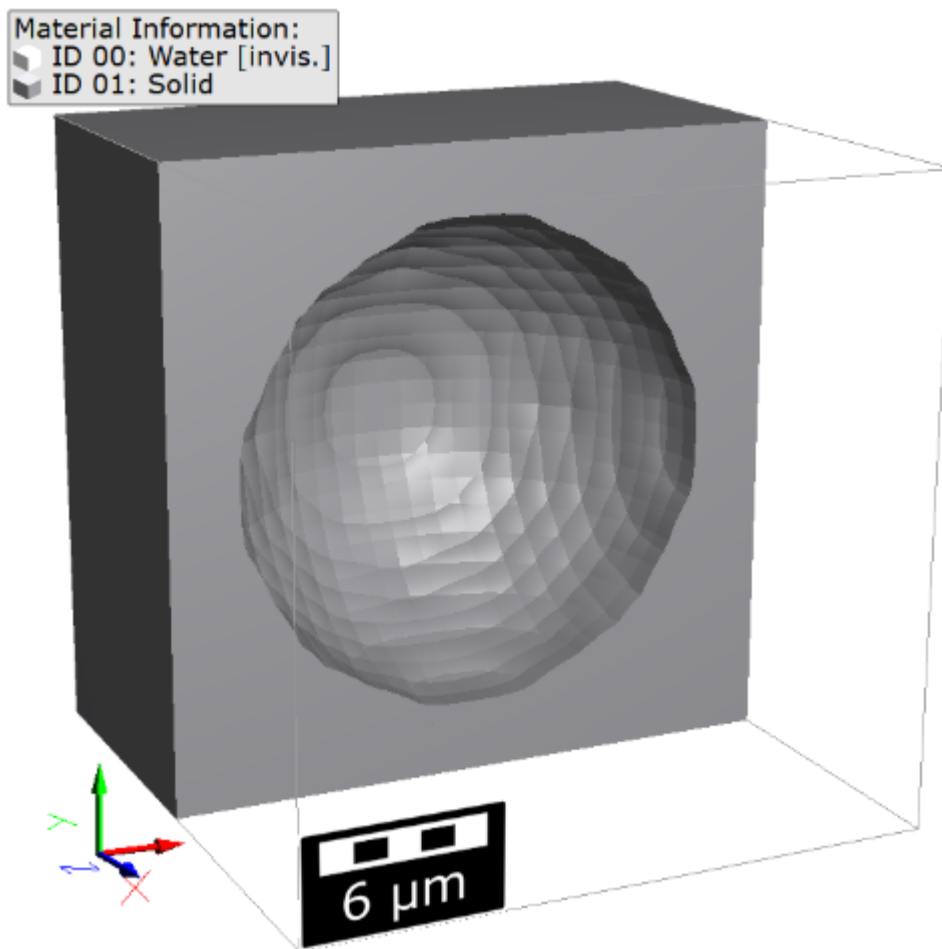
Two NMR simulation examples, one for a Bentheim sandstone and the other for an Obernkirchen sandstone are found in the tutorial [Random-walk method to simulate T2 of NMR](#).

Click **OK** to close the dialog, go back to the GeoApp section, and click **Run**.

Results

When the simulation finishes, the **Result Viewer** of the result file (*.gdr) opens automatically.

In the example, an NMR experiment was run on a cube with one spherical pore; here clipped in Z-direction.



The **Results - Report** subtab of the **Result Viewer** shows the table for the number of **Active particles** and the resulting relative ratio vs. the simulation time.

Result Viewer

Tue Feb 3 2026 (2026 Build 93212) .../NMR/NMRResult.gdr

Domain Size: 24 x 24 x 24 Voxel Length: 1 μm Load Structure

Input Map Log Map Post Map Results Data Visualization Metadata

Time Steps

Time / (s) 3

Time Step / (s) 0.01

☒ Time Step in Log Space

T2 Signal

☒ Enable Bulk Relaxation / (s) 2.5

☒ Normalize to Porosity

Max. Iteration 200

Signal Noise Ratio (SNR) 3000

Regularization Parameter lambda 20000

☐ Compute Spatial Particle Distribution (*.num)

Apply

☒ Back-up result file

Plot Options

Report Plots Map

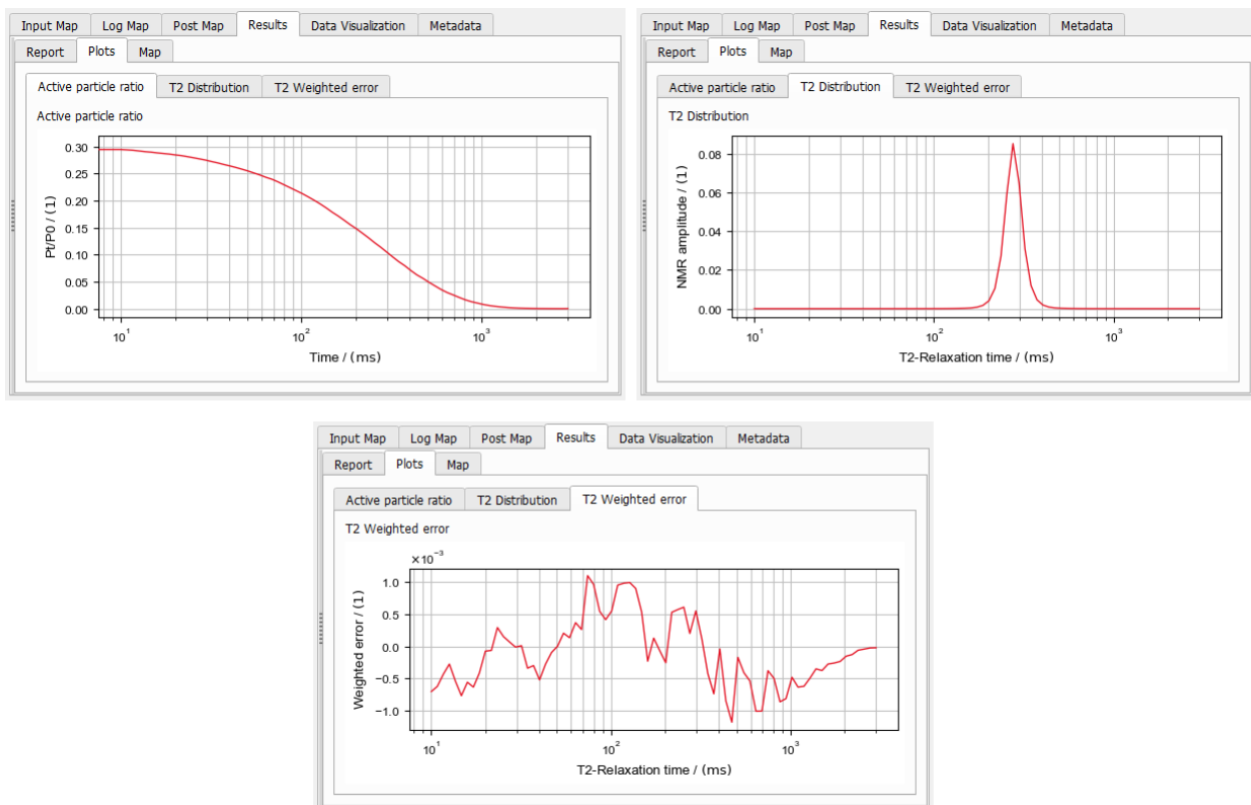
Information

Active particles:

Time / (s)	Active particle number	Relative ratio
0	10000	0.305556
0.01	9682	0.294658
0.0108013	9663	0.293985
0.0116667	9641	0.293215
0.0126015	9603	0.29195
0.0136113	9564	0.290647
0.0147019	9537	0.2897
0.0158799	9498	0.288379
0.0171523	9466	0.287261
0.0185266	9435	0.286163
0.0200111	9390	0.284629
0.0216145	9353	0.283326
0.0233464	9296	0.281404

Help Manage Data Load Input Parameters Export Close

In the **Results - Plots** subtab, the plot of **Active particle ratio**, corresponding to the values of the **Active particles** table, the plot of **T2 Distribution**, and **T2 Weighted error** are shown. For more details on the results, refer to the NMR tutorial linked above.



Acoustic Rock Properties

The **Acoustic Rock Properties** GeoApp computes the p-wave and s-wave velocities of a structure by converting the E-modul to the velocities.



Modules needed to run this GeoApp:

ElastoDict, GrainFind, MatDict (for the Contact Correction)

Click **Edit** to open the **Acoustic Rock Properties** dialog.

GeoApp – Acoustic Rock Properties

GEOdict

Result File Name (*.gdr)

Rock Structure Input

Predict QSI on

Solver Settings

Boundary Condition

Computation Direction

Reconnect Fragmented Grains - Interface Threshold / (%)

Contact Correction Method

Reduce Contact Properties by / (%)

OK Cancel

The **Result File Name** can be changed to fit to your current project.

As **Rock Structure Input** you can select to either use the **current_Structure** or browse for a **Folder_of_Structures** to **Predict QSI** (Quantitative Seismic Interpretation) on multiple structures.

Rock Structure Input

Predict QSI on

Structure Folder



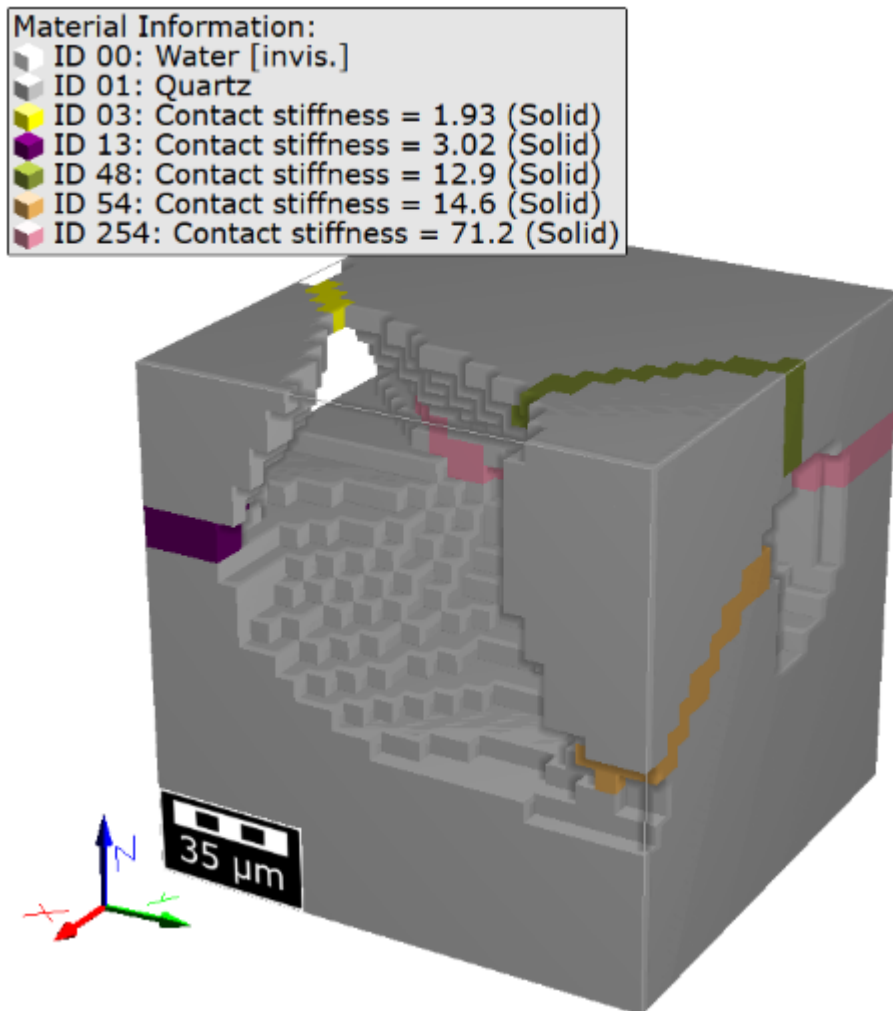
Important! In this case, make sure to select a "Compressible Fluid" law within the mechanical properties constituents for all fluids in all structures.

Under the **Solver Settings** set the **Boundary Condition** used by the ElastoDict solver. Here **Symmetric** and **Periodic** are possible. The **Computation Direction** can be one of the three main computation directions (**X**, **Y**, or **Z**) or select **All** to compute the full tensor.

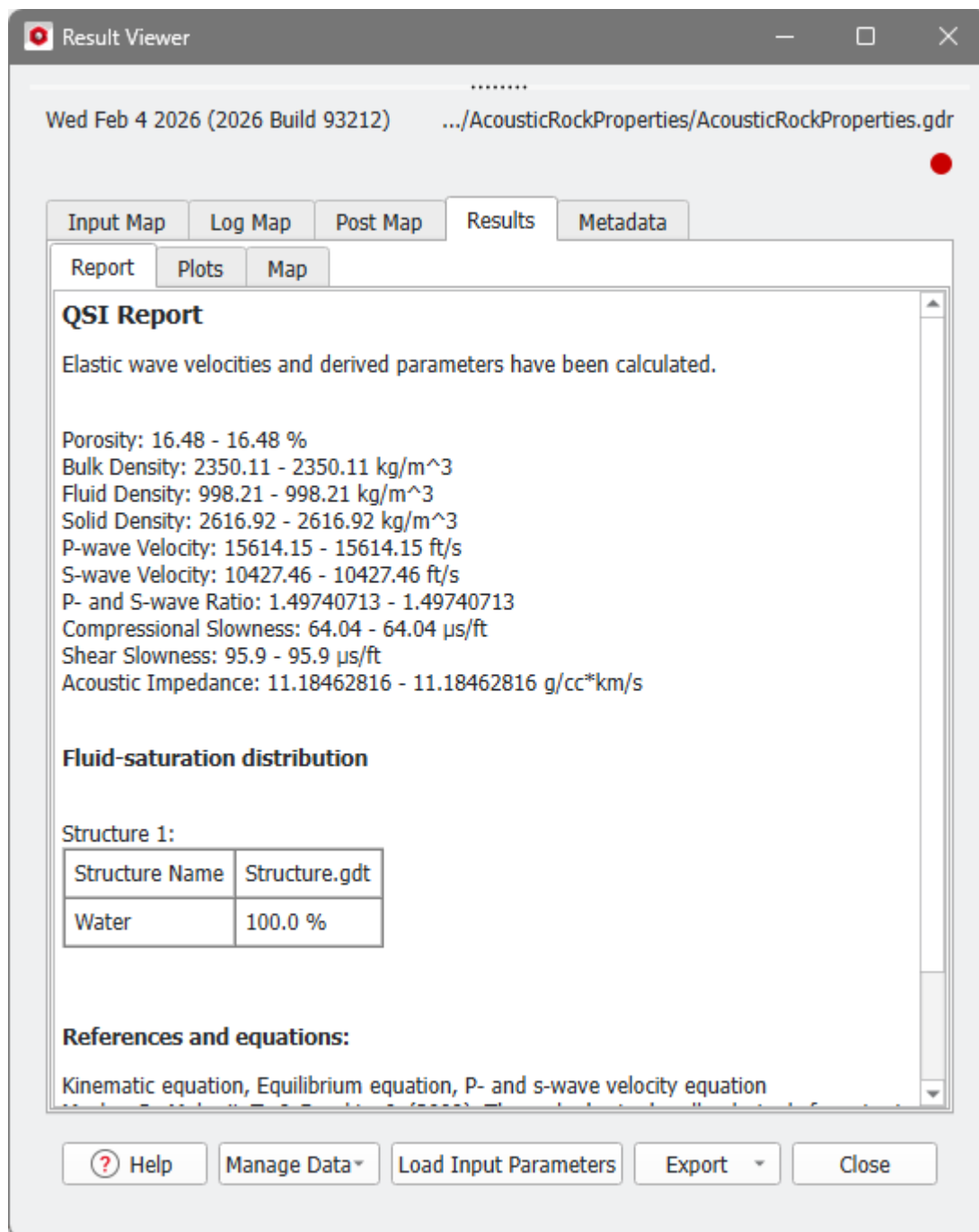
The settings for the parameters **Reconnect Fragmented Grains - Interface Threshold** and the **Contact Correction Method** are the same as for the [Contact Correction GeoApp](#)⁶³ since this app is used to correct the grain-grain contacts.

Results

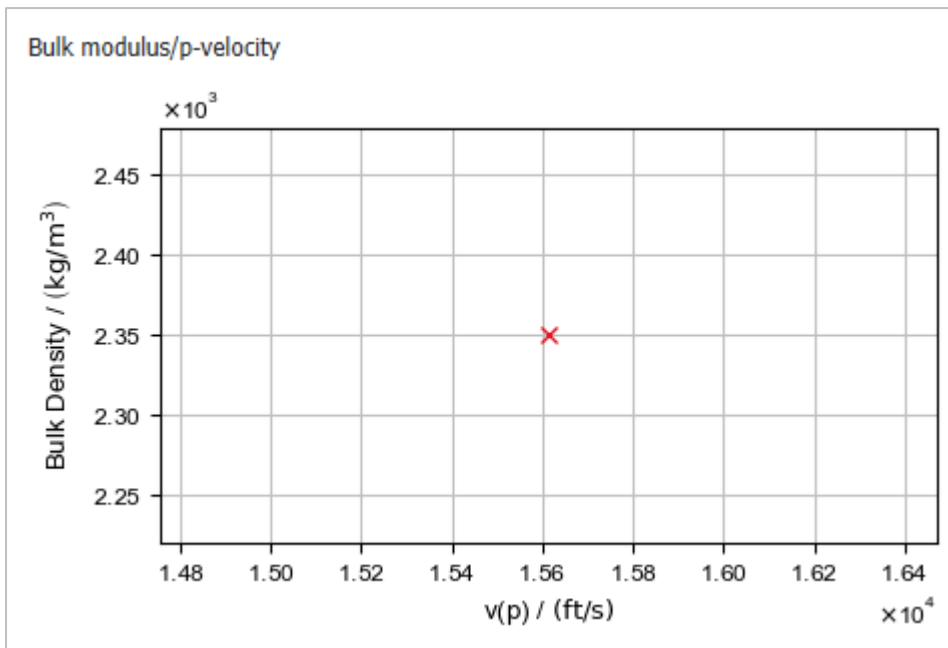
When the simulation finishes, the **Result Viewer** with the result file (*.gdr) opens automatically.



The **Results - Report** subtab of the **Result Viewer** shows the **QSI Report**, which includes the **P-wave Velocity** and the **S-wave Velocity**.



In the **Plots** subtab, the **Bulk Density** for the P-wave velocity is plotted.



1.5.3 Structure Generation

Use **Structure Generation** to prepare your structure for further simulations.

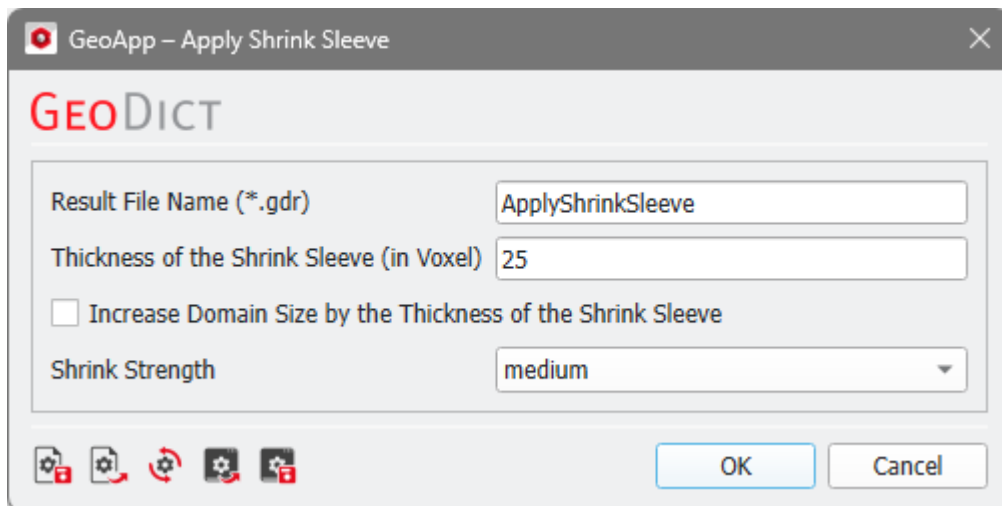
The following Structure Generation GeoApps are shipped with GeoDict:

- [Apply Shrink Sleeve](#)¹⁶⁷
Apply a shrink sleeve around a structure that is oriented in Z-direction.
- [Simulate Aging](#)¹⁷⁰
Simulate the aging of a rock.

Apply Shrink Sleeve

A shrink sleeve is a material that tightens when heat is applied. The **Apply Shrink Sleeve** app simulates this behavior by adding a layer of a different Material ID around a structure. This allows to separate the pore space inside a structure from the pore space on the outside. This is especially helpful when processing cylindrical structures, e.g., core samples. The structure needs to be oriented vertically, i.e., in the Z-direction.

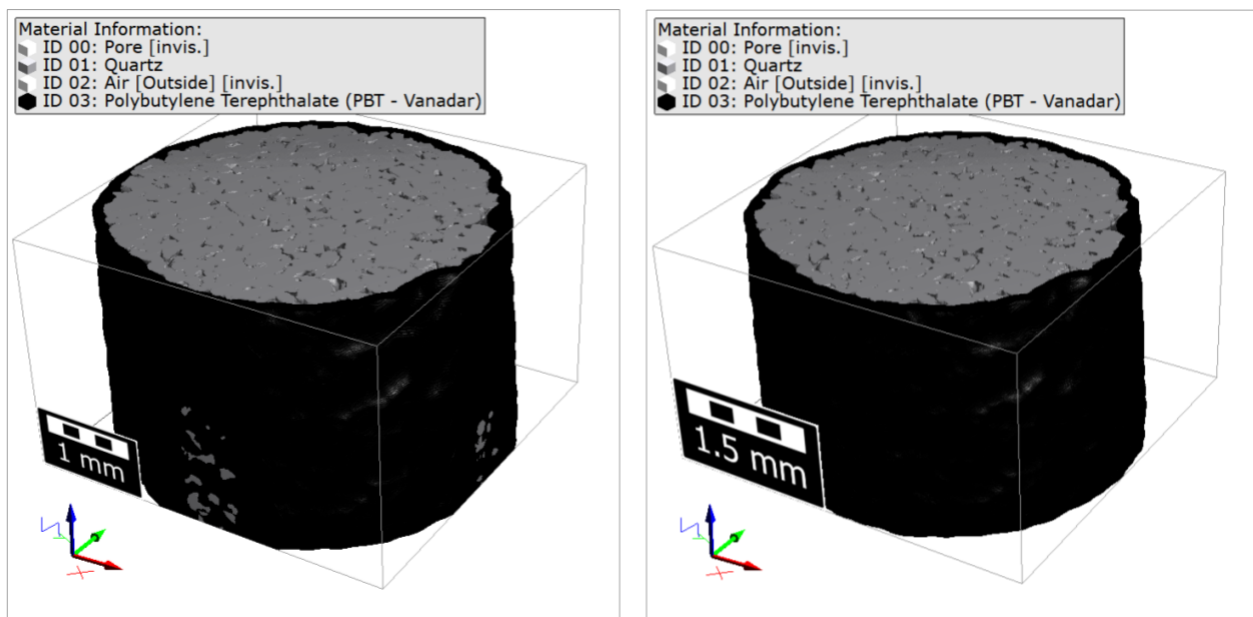
After loading a 3D structure, click **Edit** to open the **Apply Shrink Sleeve Parameters** dialog.



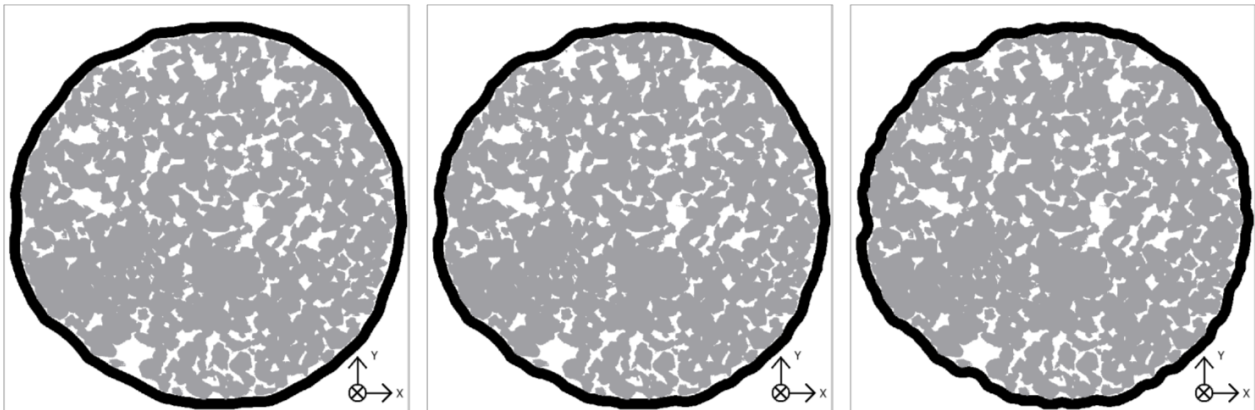
Three parameters can be edited. First enter a **Result File Name**.

The **Thickness of the Shrink Sleeve (in Voxel)** defines the thickness of the applied layer.

Select to **Increase Domain Size by the Thickness of the Shrink Sleeve** in X- and Y-direction. If you check this, the whole shrink sleeve will be contained in the domain. Compare below the result without domain increasing (left) and with increased domain (right).



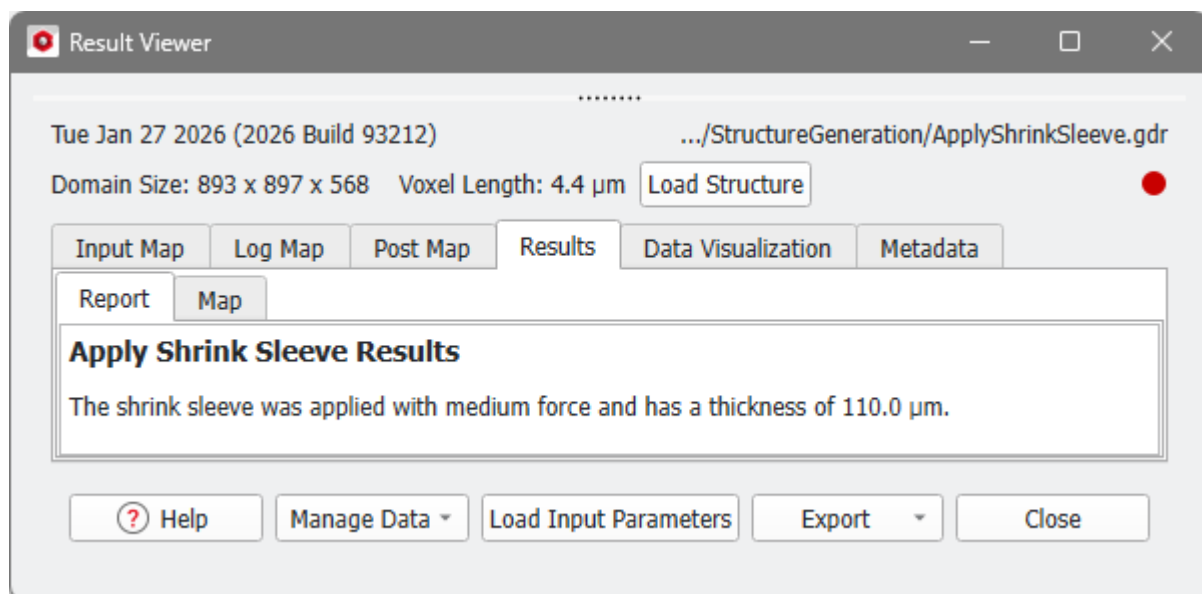
The **Shrink Strength** can be selected as low, medium or high. For a high shrink strength the added shrink sleeve is very tight around the structure. This means that pores at the outside of the solid material might also be filled with the coating material of the shrink sleeve. Observe the influence of the the **Shrink Strength** on the exemplary structure below with low strength on the left, medium strength in the center, and high strength on the right.



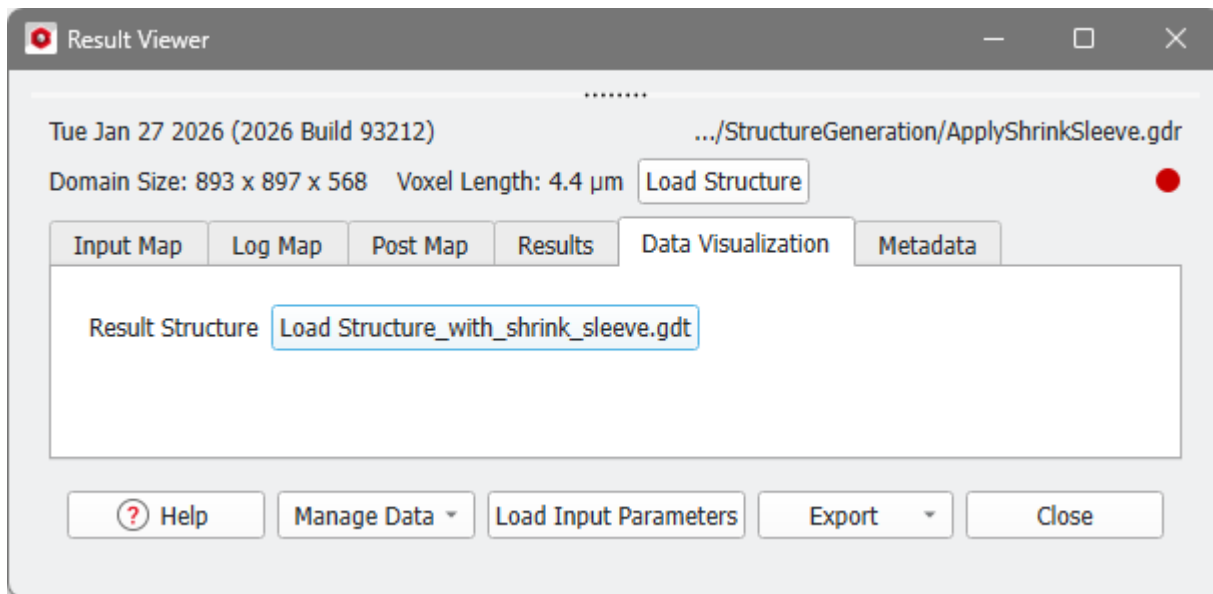
Click **OK** to close the dialog, go back to the GeoApp section, and click **Run**.

Results

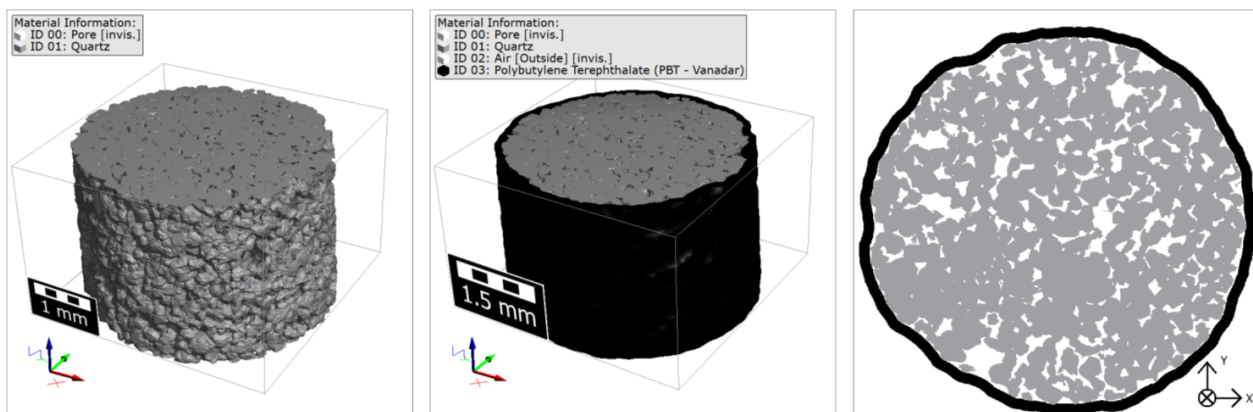
After the run is finished the **Result Viewer** opens automatically.



The structure with the applied shrink sleeve is shown in the visualization area and saved in the result folder as *Structure_with_shrink_sleeve.gdt*. It can also be loaded from the **Data Visualization** tab in the **Result Viewer**.



Below, the result for a medium shrink strength with increased domain size is shown for a Gildehauser sandstone ([Berg et al., 2018](#))^[240] in 3D and 2D visualization.



Simulate Aging

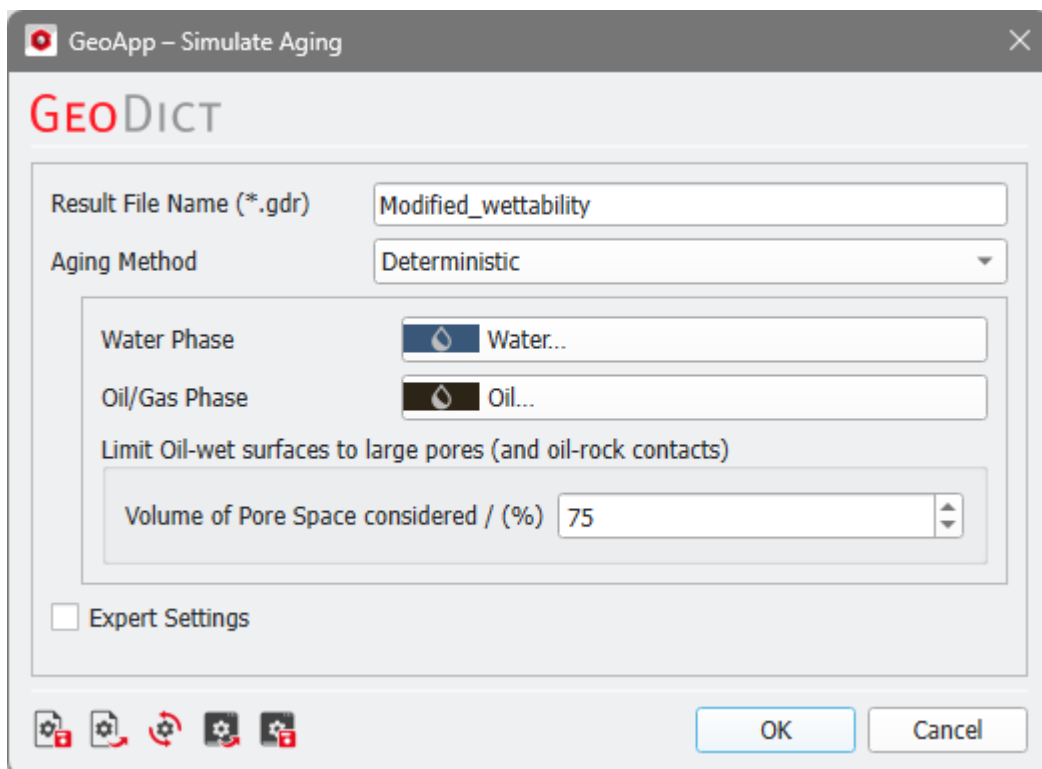
The **Simulate Aging** app simulates the aging process creating a mixed-wet rock structure as shown in [Arnold et al. \(2023\)](#)^[240].



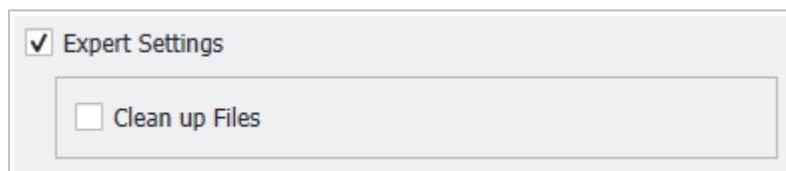
Modules needed to run this GeoApp (depending on the selected options):

PoroDict, GrainGeo

Click **Edit** to open the **Simulate Aging** dialog.



Enter a **Result File Name** and select one of the aging methods. At the bottom of the dialog you can check **Expert Settings** and select to **Clean up files** to delete all intermediate results from the result folder.



There are three different **Aging Methods** selectable: **Deterministic**, **Stochastic**, and **Simple**.

✓ **Deterministic**

For a **Deterministic** aging method, the wettability is changed at surfaces in large pores and in contact with the invading oil/gas. Select materials for the **Water Phase** and the **Oil/Gas Phase**. The **Volume of Pore Space considered** defines the limit for the material reassignments to oil-rock surfaces in large pores. A geometric pore size distribution is applied to determine the pore space that allows consideration of oil-wet surfaces with adjusted contact angles. For example, a value of 75% means that the largest 75% of the pores are changed from water-wet to oil-wet. A higher percentage leads to more contact material changes and an increased saturation change during forced imbibition, while the saturation changes during spontaneous imbibition are decreased.

Aging Method Deterministic

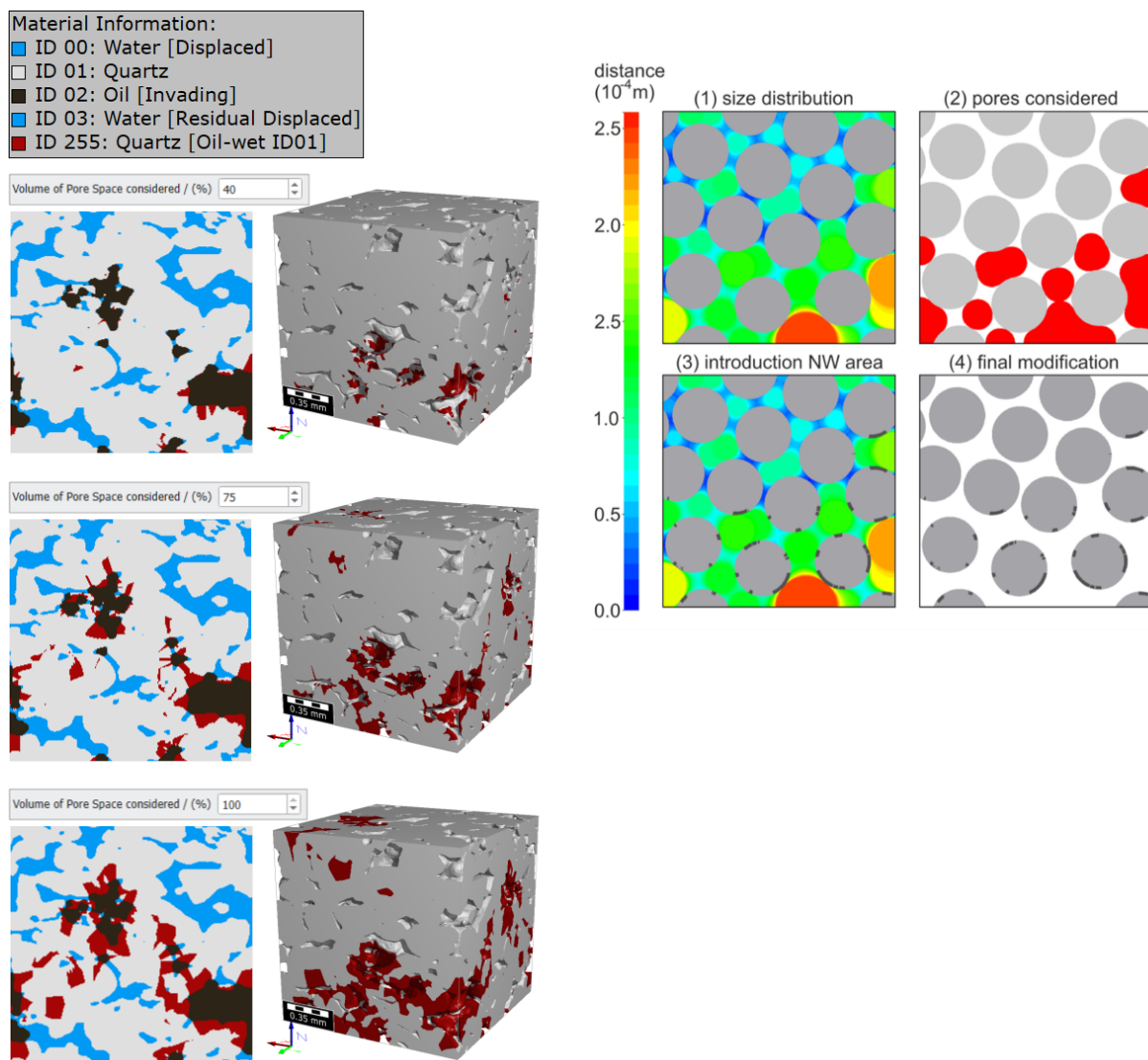
Water Phase Water...

Oil/Gas Phase Oil...

Limit Oil-wet surfaces to large pores (and oil-rock contacts)

Volume of Pore Space considered / (%) 75

The aged material is visualized in red in the example below, where the shown 2D slice is the first slice in X-direction.



☒ Stochastic

The **Stochastic** aging method distributes the wettability using Gaussian random fields in the Stochastic Field Thresholding command in GrainGeo. Select a material for the **Oil/Gas Phase**. It is not necessary to select a water phase for this method, because the result is generated based on a Gaussian random field and not the water phase. Define the **Desired Oil-Wet Region Size** in μm , representing the standard deviation for the applied Gaussian distribution. Additionally, enter the **Desired Oil-Wet Solid Volume Percentage**, which is needed as parameter for the Stochastic Field Thresholding.

Aging Method
Stochastic

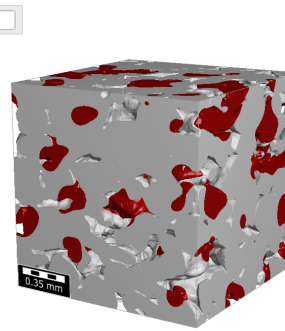
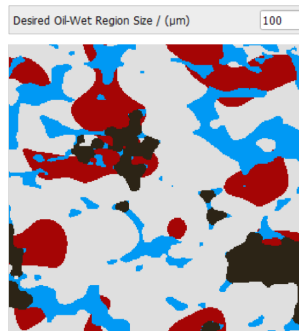
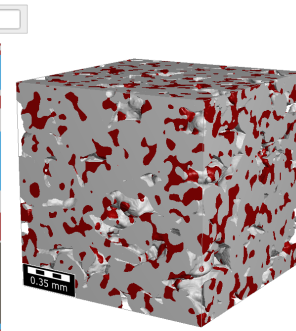
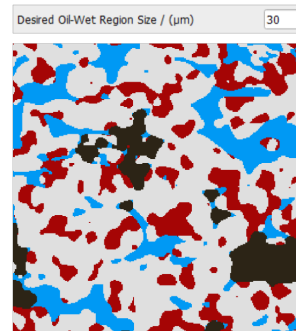
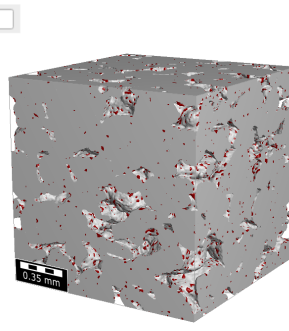
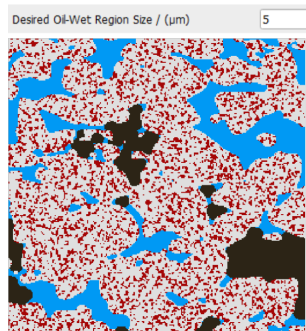
Oil/Gas Phase
Oil...

Distribute Contact Angles by Gaussian Random Fields

Desired Oil-Wet Region Size / (μm)
30

Desired Oil-Wet Solid Volume Percentage / (%)
25

Material Information:
☒ ID 00: Water [Displaced] [invis.]
☐ ID 01: Quartz
☒ ID 02: Oil [Invading] [invis.]
☐ ID 03: Water [Residual Displaced] [invis.]
☒ ID 255: Quartz [Oil-wet ID01]



Simple

The **Simple** aging method reassigns all non-wetting phase contacts with the rock to become non-wetting. Select materials for the **Water Phase** and the **Oil/Gas Phase**.

Choose for which contact phases the surfaces should be aged, Oil/Gas Phase or Water Phase. Enter the **Material ID of the Solid whose Wettability should be changed**.

Aging Method: Simple

Water Phase:  Water...

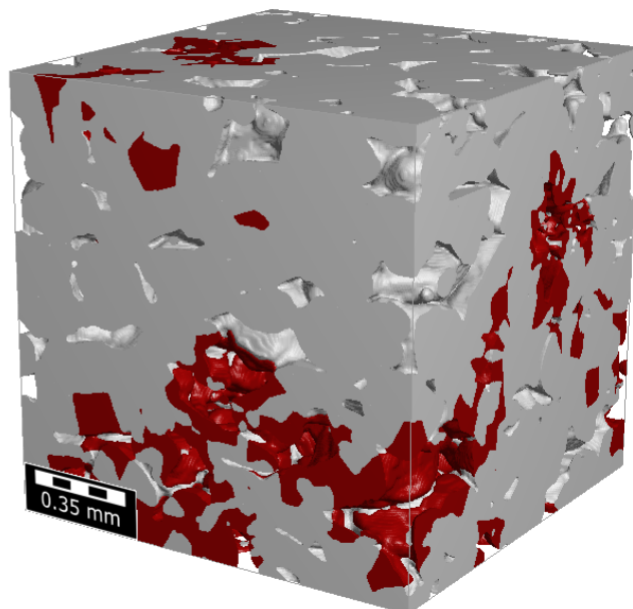
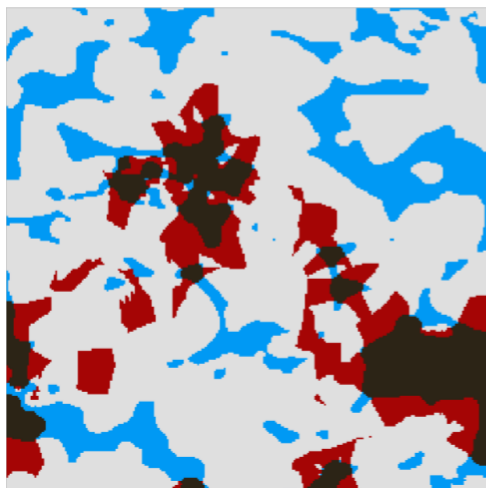
Oil/Gas Phase:  Oil...

Aging of Surfaces with Contact to: Oil/Gas Phase

Material ID of the Solid whose Wettability should be changed: 1

Material Information:

-  ID 00: Water [Displaced]
-  ID 01: Quartz
-  ID 02: Oil [Invading]
-  ID 03: Water [Residual Displaced]
-  ID 255: Quartz [Oil-wet ID01]



The resulting structure is shown in the visualization area after the computations are finished. It is saved as *mixed-wet_geometry.gdt* in the created result folder, which has the same name as the result file (*.gdr). Additionally, you can load it from the **Data Visualization** tab in the **Result Viewer**.

Domain Size: 256 x 256 x 256 Voxel Length: 5.3858 μm Load Structure

Input Map Log Map Post Map Results Data Visualization Metadata

Result File: Load mixed-wet_geometry.gdt

Help Manage Data Load Input Parameters Export Close

1.6 Filtration GeoApps

The **Filtration GeoApps** contain the GeoApps to create 3D structure models of particulate filters and predict physical properties for cross-flow filtration and multi-scale computations.



New in GeoDict 2026

- The apps have been renamed and re-sorted in GeoDict 2026.
- The [Diesel and Gasoline Particulate Filters](#) GeoApps in GeoDict 2025 are now found in the [Structure Generation](#)^[181] sub-menu of the Filtration GeoApps.
- The [2Layer Ceramic Microstructure](#) GeoApp has been moved to **Examples** under **Macro Execution Control**.
- The [Filter and Pleat Optimization](#) GeoApps have been moved to **Examples** under **Macro Execution Control**.
- The Filter GeoApps in FilterDict are accessible also via [Physical Properties](#)^[175] sub-menu of the Filtration GeoApps.

Find the following Filtration GeoApp groups:

- [Physical Properties](#)^[175]
Run filtration-related simulations using predefined scripts.
- [Structure Generation](#)^[181]
Create diesel and gasoline particulate filter structures.

1.6.1 Physical Properties

This sub-menu collects GeoApps which simulate filtration processes. Both apps are also accessible from FilterDict.

The following Physical Properties GeoApps are shipped with GeoDict:

- [Cross-Flow Filtration](#)^[175]
Run cross-flow filtration simulation.
- [Media2Element](#)^[177]
Convert Filter Media Lifetime simulation results to the Filter Element scale.

Cross-Flow Filtration

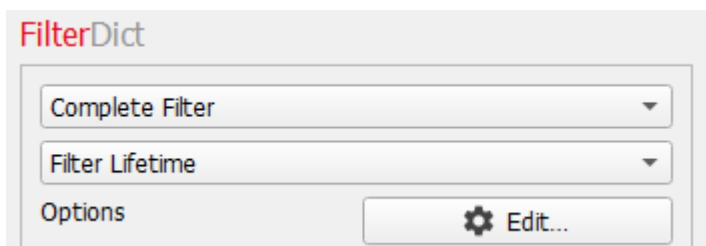
The **Cross-Flow Filtration** GeoApp allows to set up a filtration simulation with one inlet, but with two outlets which have different outlet pressures. In contrast to the Cross Flow command, the app also simulates particle movement and deposition.



Modules needed to run this GeoApp:

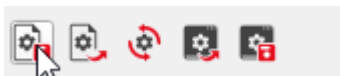
FilterDict, FilterDict-Element

Most of the parameters used are directly loaded from the **Complete Filter - Filter Lifetime** dialog or a corresponding settings file (*.gps). Therefore, in a first step, select **Complete Filter - Filter Lifetime**, open the Complete Filter Lifetime dialog and setup the simulation parameters.

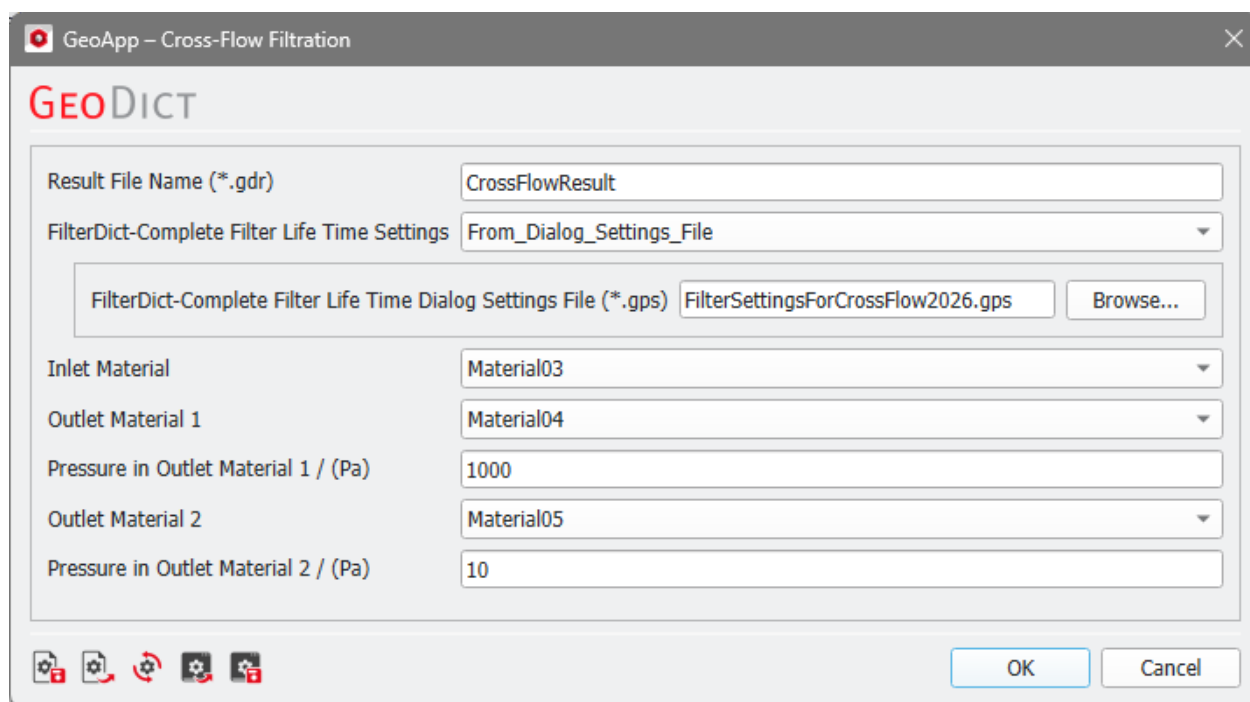


The settings defined in the **Complete Filter - Filter Lifetime** dialog are part of the calculation setup of **Cross-Flow Filtration** GeoApp if you choose to use the current settings. Any changes made during other computations may affect subsequent runs of the **Cross-Flow Filtration** GeoApp. Therefore, unless you are certain that the current configuration is intended, we recommend saving the settings as a *.gps file.

Store the dialog settings in a *.gps file by using the dialog icon. Then close the dialog and return to the Cross-Flow Filtration GeoApp.

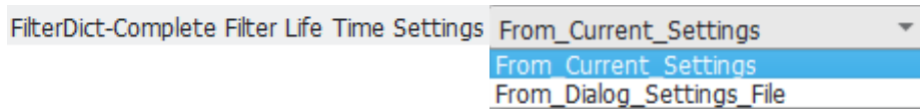


The additional settings for the cross-flow filtration simulation can be defined by clicking the **Edit...** button.



At first, choose a **Result File Name**.

Then, select if the parameters should be taken from the **Complete Filter - Filter Lifetime** dialog (select **From_Current_Settings**) or from a stored settings file (select **From_Dialog_Settings_File**).



Now, the only additional selections that must be made are to define the feed **Inlet Material**, the retentate and permeate **Outlet Materials** and the **Pressure in Outlet Materials**. Two outlets, **Outlet Material 1** and **Outlet Material 2**, and their corresponding pressures, **Pressure in Outlet Material 1** and **Pressure in Outlet Material 2**, can be defined. After these selections are made, close the dialog and click **Run** to start the simulation.

Media2Element

This GeoApp allows to convert Filter Media Lifetime simulations to the Filter Element scale.



Modules needed to run this GeoApp:

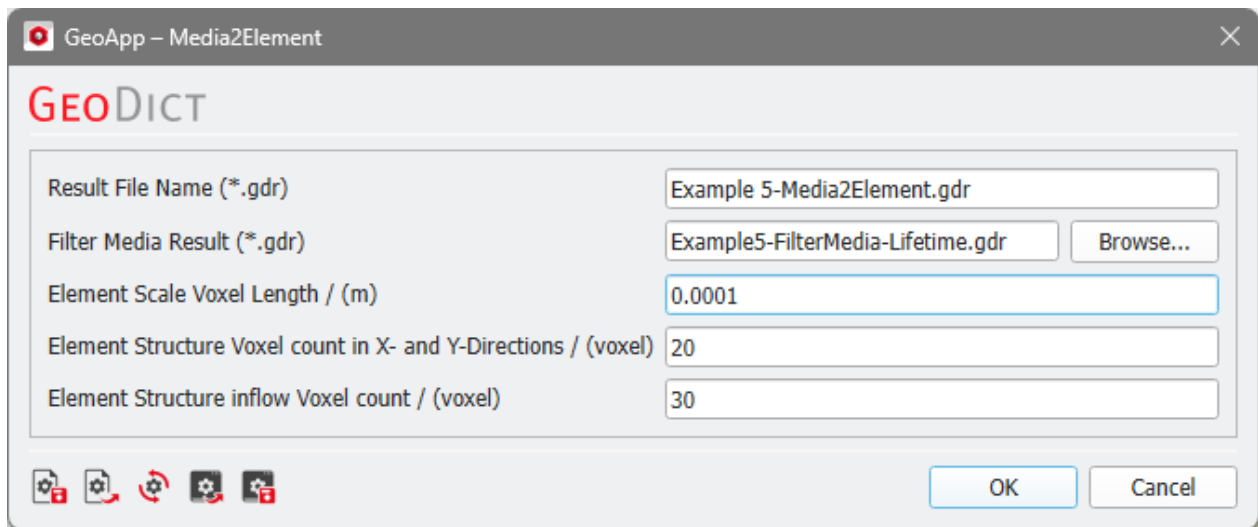
FilterDict, FilterDict-Element, FilterDict-Media

For this, provide a Filter Media Lifetime simulation result (*.gdr file). To be able to create sensible results, the lifetime simulation should

- ... consider a representative part of the filter media (REV),
- ... use a voxel length such that the filter media is well resolved,
- ... run long enough to contain the creation of a filter cake on top of the filter,
- ... simulate a significant number of particles of each size in every batch. This is typically achieved by activating ghost particles.

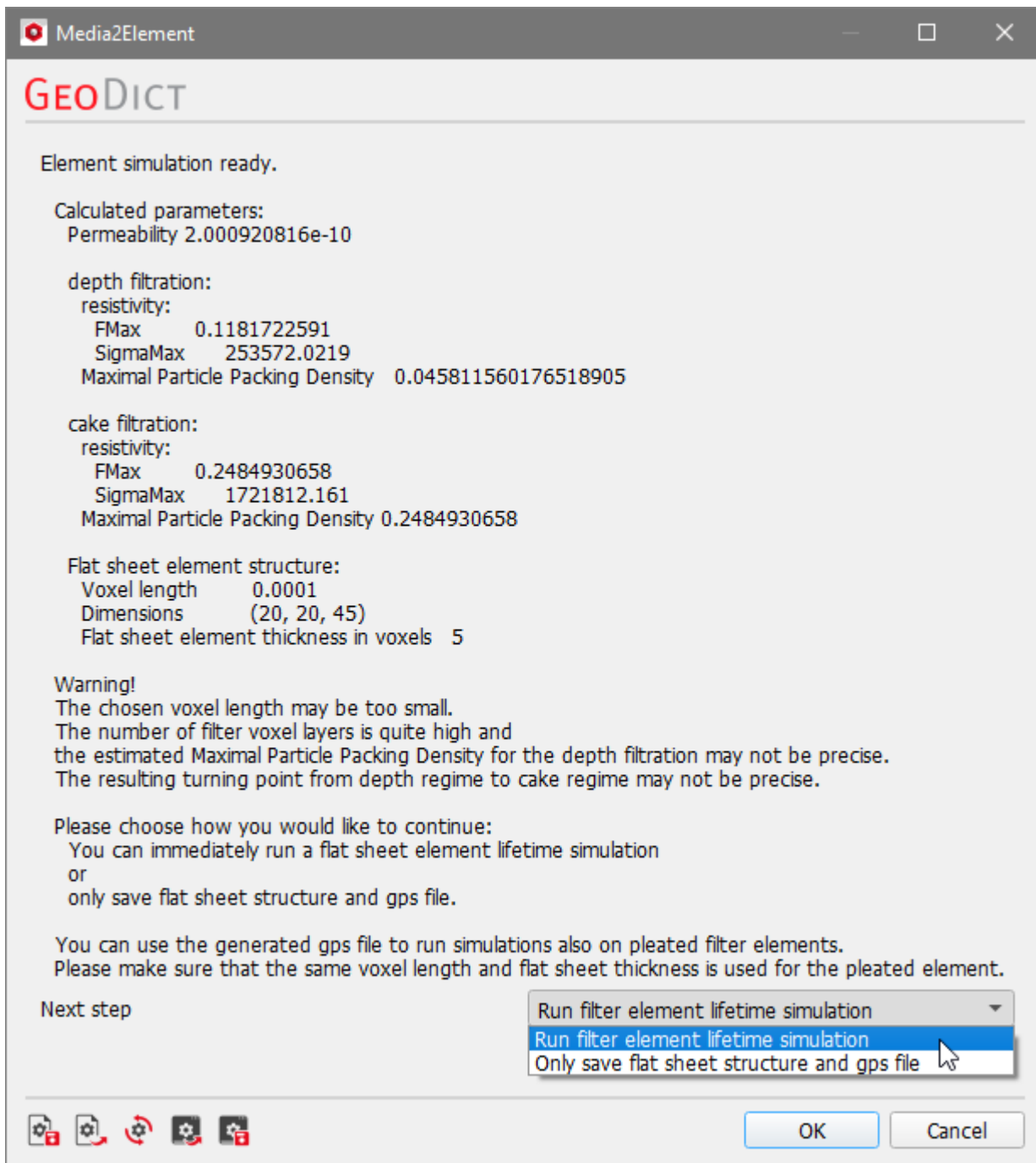
In the app, select a coarser element scale voxel length, such that your filter media thickness is resolved in only a few voxels (the voxel length can even be larger than the media thickness). The app then determines the parameters that describe the filter properties on the coarser scale. It creates a sample structure on the coarser scale and either runs a simulation on it or creates a parameter file to import in Filter Element Lifetime simulations. You can also use the calculated clogging parameters in the Complete Filter scale simulations for the characterization of your pleats.

To run the app, click on the **Options Edit...** button.



In the dialog, select the result file of the high resolution **Filter Media - Filter Lifetime** simulation (**Filter Media Result (*.gdr)**). Select the coarser **Element Scale Voxel Length** that is to be used in the low resolution simulation. The last two parameters describe the size of the element scale sample structure that the app creates as a demo case.

Click **OK** to close the dialog and **Run** to start the app. After a few moments a pop-up dialog appears.



The dialog presents the determined parameters. Clean filter permeability, $f_{\max}$ (FMax) and $\sigma_{\max}$ (SigmaMax) are directly taken from the results of the filter media simulation, i.e., this are the parameters shown in the Filter Clogging Analysis part of the filter media simulation result file:

Filter clogging analysis

	Layer thickness / (mm)	$f_{\max}$	$\sigma_{\max}$ / (kg / m ³ s)
Depth filtration	0.5	0.118714	253997
Cake filtration	0.118	0.248504	1.71516e+06

Clean filter permeability: 2.00092e-10 m²

The Maximal Particle Packing Density is often equal to $f_{\max}$, but may differ in some cases depending on the selected resolution. This is the case, if the resulting filter element is only one voxel in thickness, or if the voxel length is even larger than the filter media height.

In cases where the voxel length selected for the coarse scale simulation is too small, a warning appears.

The dialog asks what should be done as next steps. Two choices exist:

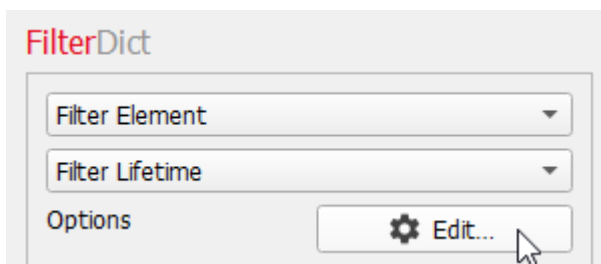
✓ **Only save flat sheet structure and gps file**

This option creates two files in the result folder, named as the selected result file name. A *.gdt file containing the structure and a *.gps file containing the dialog settings:

 Example 5-Media2Element.gdt

 Example 5-Media2Element.gps

To run a simulation on the filter element scale, first load the created *.gdt file into GeoDict. Then, select **Filter Element** and **Filter Lifetime** from the drop-down menus and open the **Options** dialog.

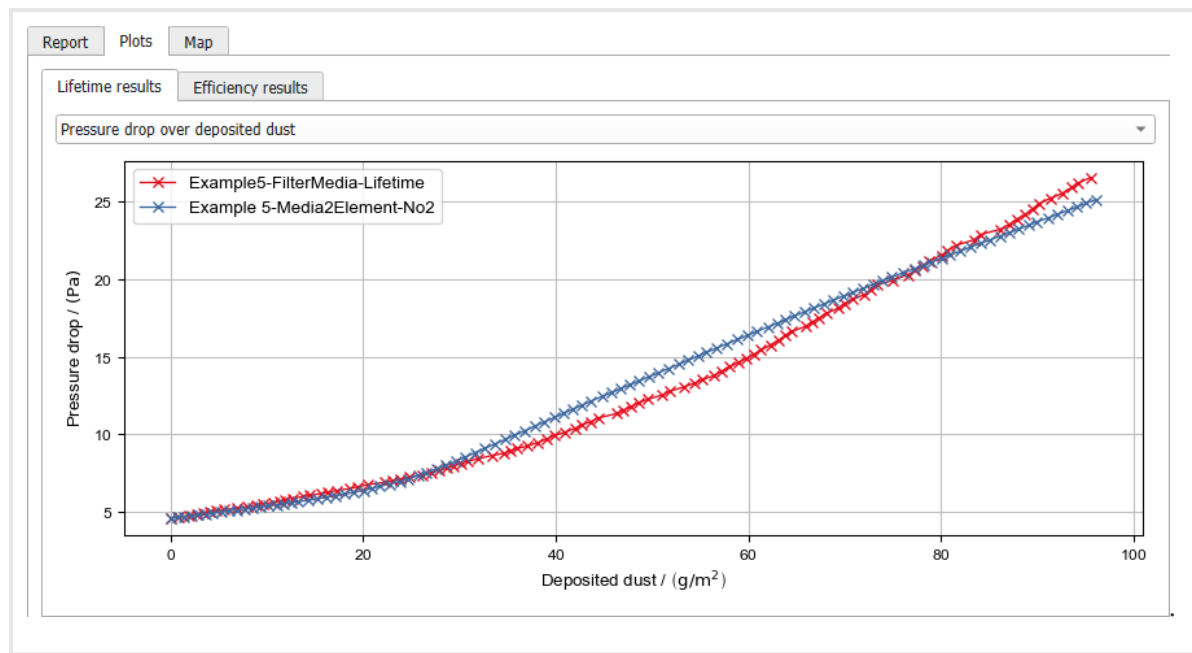


In the dialog, load the setting from the *.gps file. Then run the simulation.

✓ **Run filter element lifetime simulation**

This option runs a simulation on the coarse scale. The sample geometry is a flat sheet media, where the size of the 3D model (in voxels) is determined by the App's input parameters.

Additionally, a second *.gdr result file is created, beginning with **combined_** followed by the result file name. It contains a comparison of the results obtained on the fine scale (the filter media simulation used as input) and the results obtained on the coarse scale (computed now).



1.6.2 Structure Generation

Create diesel and gasoline particulate filter structures.

The following Structure Generation GeoApps are shipped with GeoDict:

- [Honeycomb \(TWC\)](#)^[181]
Create a three-way catalyst monolith with hexagonal combs.
- [Rectangular Monolith \(DPF-GPF\)](#)^[182]
Create a diesel particulate filter / gasoline particulate filter with rectangular combs, which are partly closed.
- [Rectangular Monolith \(TWC\)](#)^[184]
Create a three-way catalyst monolith with rectangular combs with open channels
- [Triangular Monolith \(DPF-GPF\)](#)^[185]
Create a diesel particulate filter / gasoline particulate filter with triangular combs, which are partly closed.
- [Triangular Monolith \(TWC\)](#)^[187]
Create a three-way catalyst monolith with triangular combs with open channels.

Honeycomb (TWC)

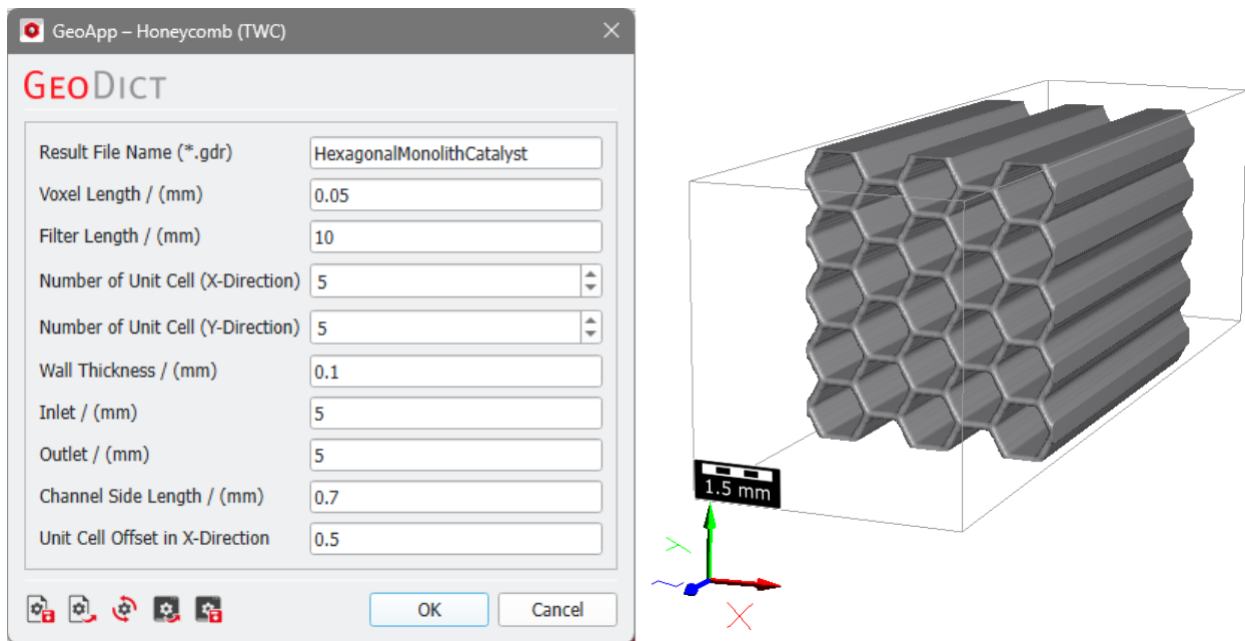
The **Honeycomb (TWC)** app generates a three-way catalyst monolith with hexagonal combs.



Modules needed to run this GeoApp:

GridGeo

Clicking **Edit** opens the **Honeycomb (TWC) Parameters** dialog.



Define the following parameters:

- **Result File Name**,
- the **Voxel Length**,
- the **Filter Length** in Z-Direction without inflow and outflow region,
- the **Number of Unit Cells** in X- and Y-direction,
- the **Wall Thickness**,
- the **Inlet**, defining an inflow region,
- the **Outlet**, defining the outflow region,
- the **Channel Side Length**, for the hexahedron sides,
- and the **Unit Cell Offset in X-Direction** defining the cell positions in X-direction.

Close the dialog with **OK** and then click **Run** to create the honeycomb.

Rectangular Monolith (DPF-GPF)

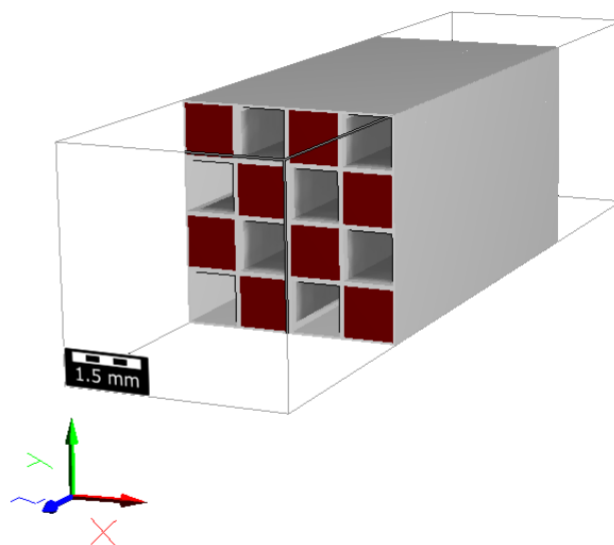
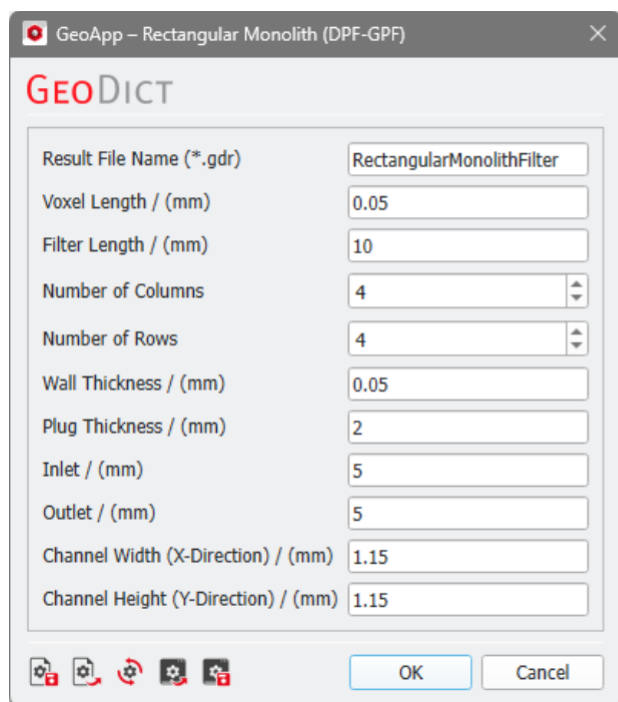
The **Rectangular Monolith (DPF-GPF)** app generates a Diesel Particulate Filter / Gasoline Particulate Filter consisting of rectangular combs. Every channels is plugged on one end in an alternating pattern.



Modules needed to run this GeoApp:

GridGeo

Clicking **Edit...** opens the **Rectangular Monolith (DPF-GPF) Parameters** dialog.



Define the **Result File Name**, the **Voxel Length**, the **Filter Length**, the **Number of Columns** and **Rows**, the **Wall Thickness**, the **Inlet** length, the **Outlet** length, the **Channel Width** and **Height**.

Close the dialog with **OK** and then click **Run** to create the rectangular monolith.

The structure generated using the **Rectangular Monolith (DPF-GPF)** app is identical to that of the **Rectangular Monolith (TWC)** app, except that the former has every channel sealed on one end to create a wall-flow configuration, while the latter keeps all channels open to form a flow-through structure.

GeoApp – Rectangular Monolith (DPF-GPF)

GEODICT

Result File Name (*.gdr)

Voxel Length / (mm)

Filter Length / (mm)

Number of Columns

Number of Rows

Wall Thickness / (mm)

Plug Thickness / (mm)

Inlet / (mm)

Outlet / (mm)

Channel Width (X-Direction) / (mm)

Channel Height (Y-Direction) / (mm)

GeoApp – Rectangular Monolith (TWC)

GEODICT

Result File Name (*.gdr)

Voxel Length / (mm)

Filter Length / (mm)

Number of Columns

Number of Rows

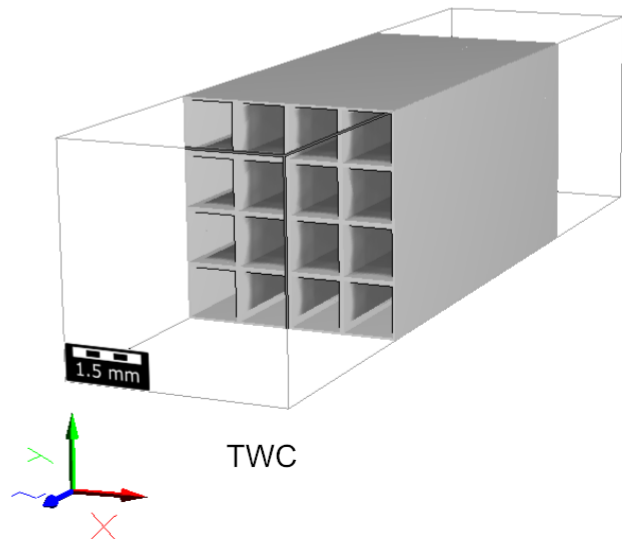
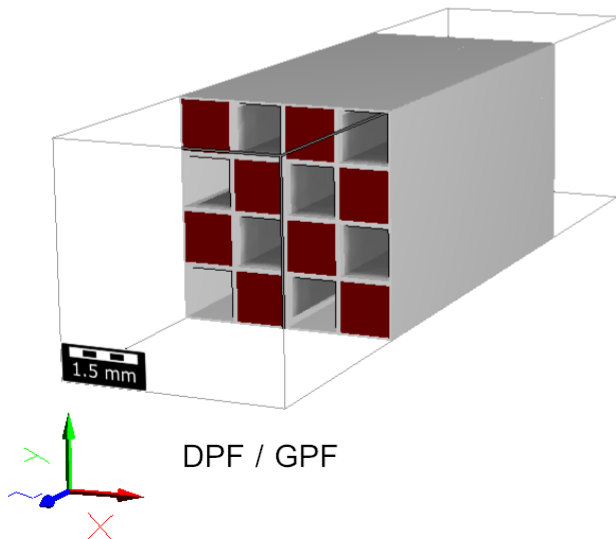
Wall Thickness / (mm)

Inlet / (mm)

Outlet / (mm)

Channel Width (X-Direction) / (mm)

Channel Height (Y-Direction) / (mm)



Rectangular Monolith (TWC)

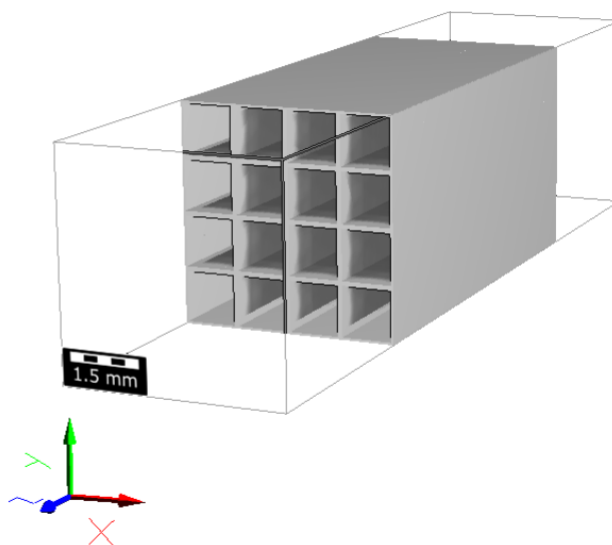
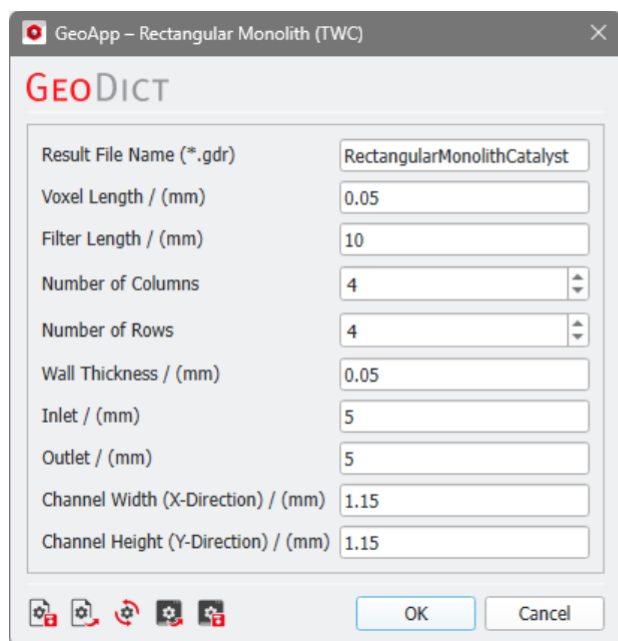
The **Rectangular Monolith (TWC)** app generates a three-way catalyst consisting of rectangular combs with open channels.



Modules needed to run this GeoApp:

GridGeo

Clicking **Edit...** opens the **Rectangular Monolith (TWC) Parameters** dialog.



Define the **Result File Name**, the **Voxel Length**, the **Filter Length**, the **Number of Columns** and **Rows**, the **Wall Thickness**, the **Inlet** length, the **Outlet** length, the **Channel Width** and **Height**.

Close the dialog with **OK** and then click **Run** to create the rectangular monolith.

Compare the structures generated with the **Rectangular Monolith (DPF-GPF)** and the **Rectangular Monolith (TWC)** app in the [Rectangular Monolith \(DPF-GPF\) section](#)¹⁸³.

Triangular Monolith (DPF-GPF)

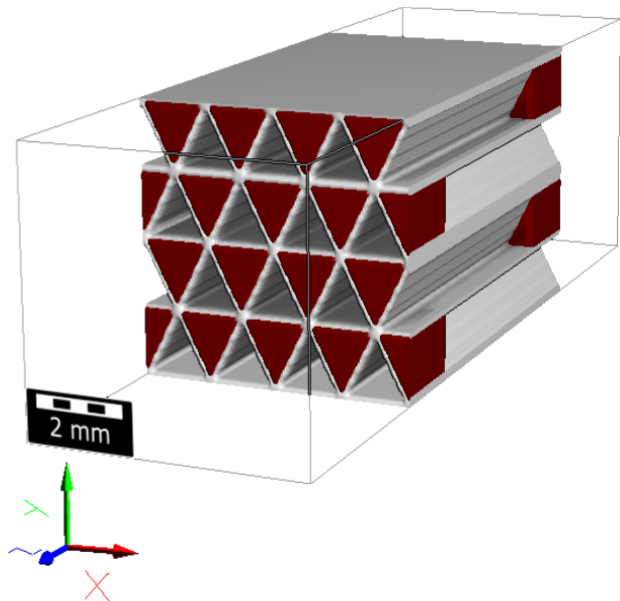
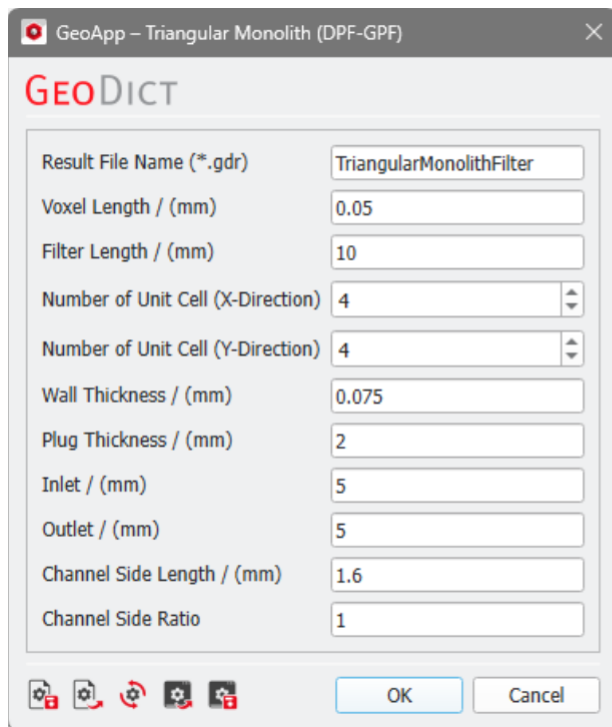
The **Triangular Monolith (DPF-GPF)** app generates a Diesel Particulate Filter / Gasoline Particulate Filter consisting of triangular combs. Every channels is plugged on one end in an alternating pattern.



Modules needed to run this GeoApp:

GridGeo

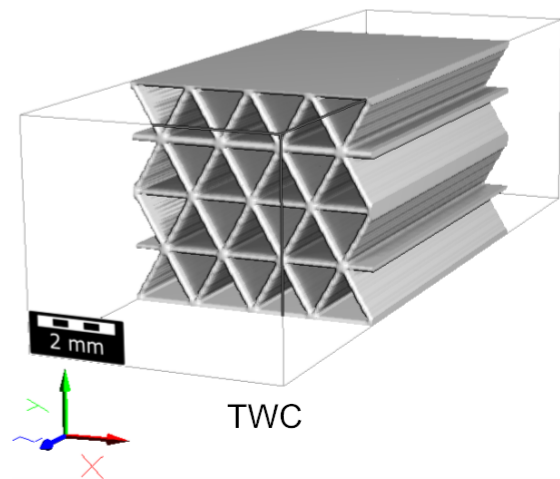
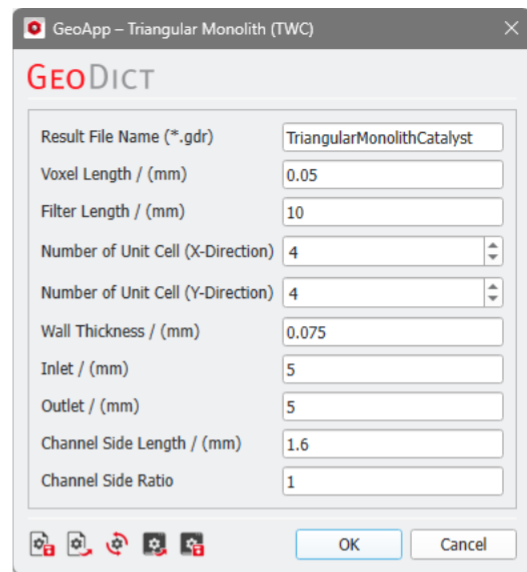
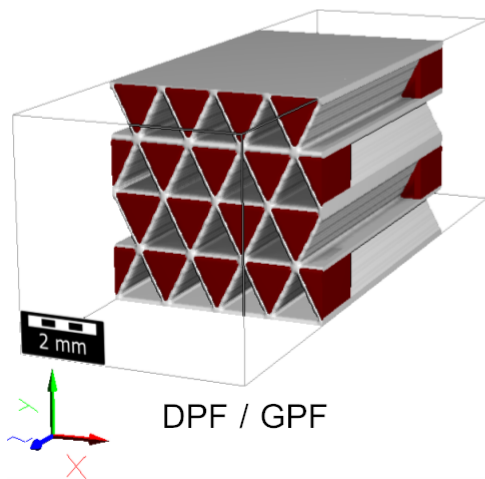
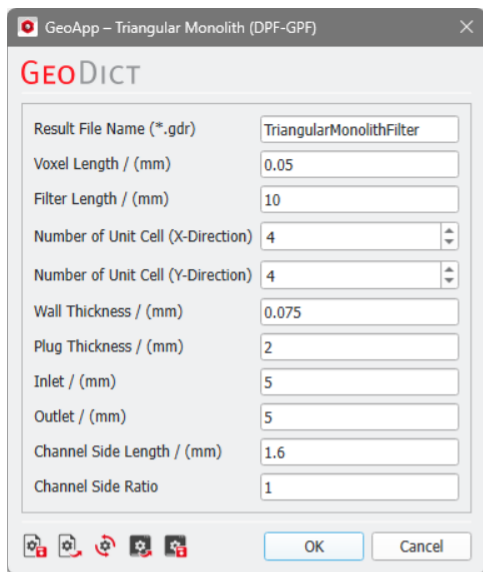
Clicking **Edit** opens the **Triangular Monolith(DPF-GPF) Parameters** dialog.



Define the **Result File Name**, the **Voxel Length**, the **Filter Length**, the **Number of Unit Cells** in X- and Y-direction, the **Wall Thickness**, the **Plug Thickness**, the **Inlet** length, the **Outlet** length, the **Channel Side Length** and **Channel Side Ratio**.

Close the dialog with **OK** and then click **Run** to create the triangular monolith.

The structure generated using the **Triangular Monolith (DPF-GPF)** app is identical to that of the **Triangular Monolith (TWC)** app, except that the former has every channel sealed on one end to create a wall-flow configuration, while the latter keeps all channels open to form a flow-through structure.



Triangular Monolith (TWC)

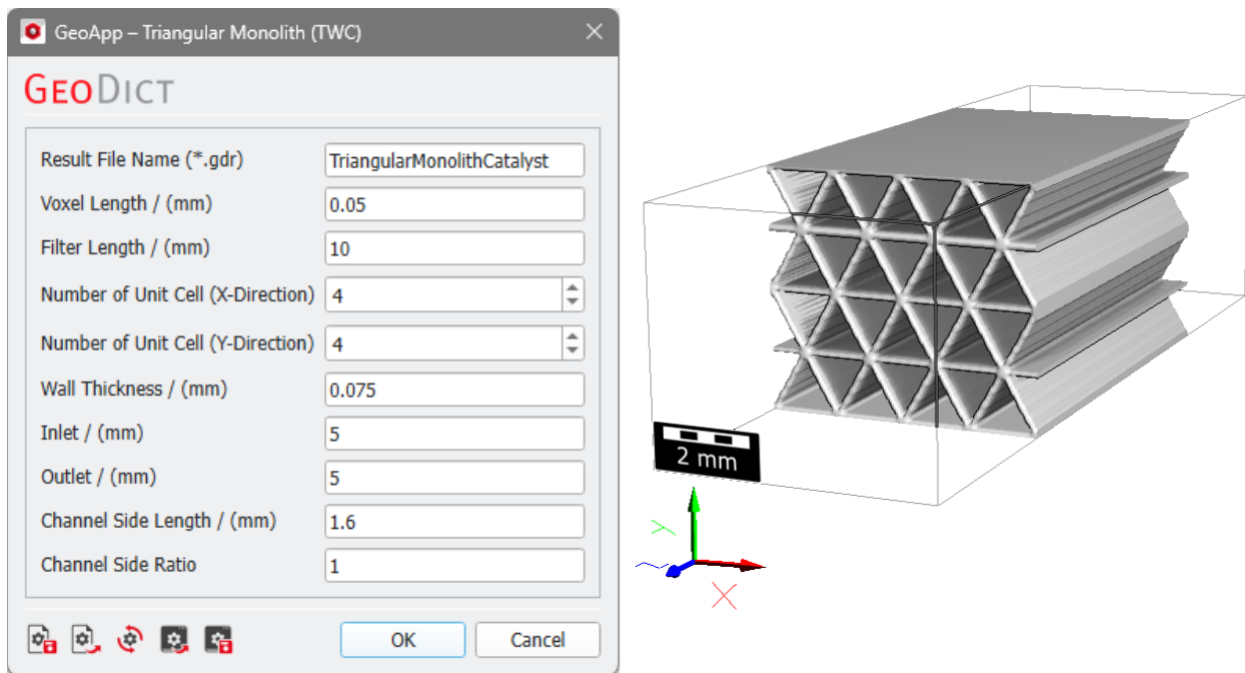
The **Triangular Monolith (TWC)** app generates a three-way catalyst consisting of triangular combs with open channels.



Modules needed to run this GeoApp:

GridGeo

Clicking **Edit** opens the **Triangular Monolith (TWC) Parameters** dialog.



Define the **Result File Name**, the **Voxel Length**, the **Filter Length**, the **Number of Unit Cells** in X- and Y-direction, the **Wall Thickness**, the **Plug Thickness**, the **Inlet** length, the **Outlet** length, the **Channel Side Length** and **Channel Side Ratio**.

Close the dialog with **OK** and then click **Run** to create the triangular monolith.

Compare the structures generated with the **Rectangular Monolith (DPF-GPF)** and the **Rectangular Monolith (TWC)** app in the [Triangular Monolith \(DPF-GPF\) section](#)¹⁸⁶.

1.7 Fuel Cell and Electrolyser GeoApps

Generate components of fuel cells and electrolyzers with the **Fuel Cell and Electrolyser** GeoApps.



New in GeoDict 2026

- For the [solid oxide structure generation](#)^[196] GeoApp you can now also choose exponential correlation functions. Additionally many of the parameters got renamed and reorganized.
- The **Gas Diffusion Layer** GeoApp got some new parameters to choose materials, fiber sizes and orientation.

Find the following Fuel Cell and Electrolyser GeoApp groups:

- [Structure Generation](#)^[189]
Create proton exchange membrane components for fuel cells.

1.7.1 Structure Generation

Create structures for fuel cells or electrolyzers.

The following structure generation GeoApps for Fuel Cells and Electrolyzers are shipped with GeoDict:

- [Catalyst Layer \(PEM Fuel Cell\)](#)^[189]
Create a model of the catalyst layer of a PEM fuel cell.
- [Gas Diffusion Layer](#)^[191]
Create a gas diffusion layer of a PEM fuel cell.
- [Solid Oxide Electrode Generation](#)^[193]
Generate a three-phase microstructures typically observed for SOFC / SOEC electrodes, but also for all-solid-state battery electrodes..

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)

GEODICT

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

OK Cancel

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**.

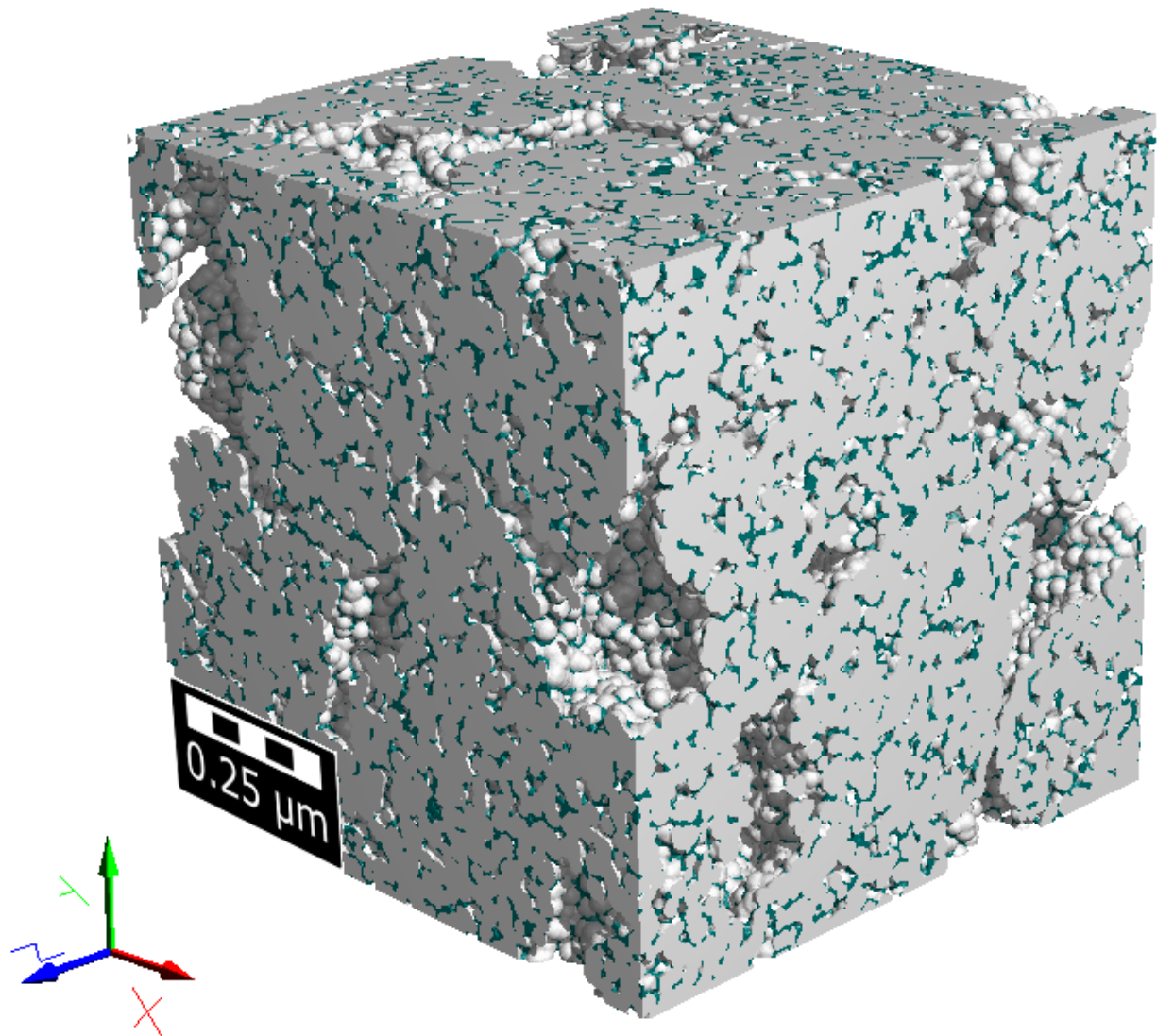
For both materials you can change the material information by editing the **Particle Name** and **Ionomer Name**. The materials will both be set to manual but through the material information they still get individual names.

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)



Gas Diffusion Layer

The **Gas Diffusion Layer** app creates a gas diffusion layer of a PEM fuel cell.



Modules needed to run this GeoApp:

FiberGeo

Parameters

Clicking **Edit** opens the **Gas Diffusion Layer** parameters dialog.

GeoApp – Gas Diffusion Layer

GEODict

Result File Name (*.gdr)

Voxel Length / (μm)

Width (X-Direction) / (μm)

Width (Y-Direction) / (μm)

Height (Z-Direction) / (μm)

Materials

Fiber Material

Binder Material

Create Fibers

Fiber Volume Percentage / (%)

Fiber Size

Fiber Diameter / (μm)

Fiber Length / (μm)

Fiber Orientation

Orientation Tensor XX

Orientation Tensor YY

Orientation Tensor ZZ

Add Binder

Binder Volume Percentage / (%)

Enter a **Result File Name** for the generated result file (*.gdr) and the corresponding result folder.

Set the domain parameters in μm using the parameters **Voxel Length**, **Width (X-Direction)**, **Length (Y-Direction)**, and **Height (Z-Direction)**.

Select **Materials** for the fibers and the binder from the GeoDict material database.

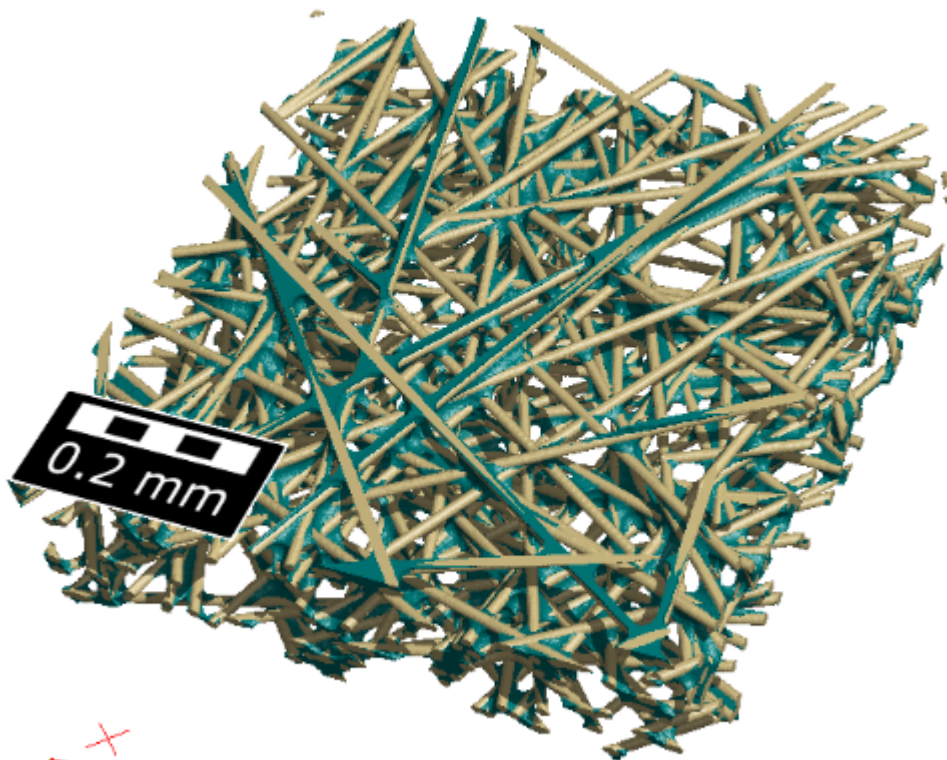
The gas diffusion layer consists of short circular fibers. In the **Create Fibers** panel define the **Fiber Volume Percentage** and set the **Fiber Diameter** and **Fiber Length** of the generated fibers. Define the **Fiber Orientation** by giving the diagonal of the orientation tensor. The three entries are normalized by the GeoApp.

Finally, define the **Binder Volume Percentage**.

Results

Clicking **Run** creates the diffusion layer and saves the structure file in the result folder.

Material Information:	
	ID 00: Pore [invis.]
	ID 01: Carbon Fiber
	ID 02: Binder (Solid)



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. This two-dimensional field is thresholded into three phases according to the specified volume fractions (under [Random Field 1 and 2](#)^[196] and contact angles (under [Change Expert Settings](#))^[196], where the latter determine the wetting behavior of the phases. The approach is based on work of [Marmet et al., 2023](#)^[240].



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 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 ($100 - \text{SVF1} - \text{SVF2}$) 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		Random Field 2	
Material	8YSZ (Solid)...	Material	Nickel (Solid)...
Correlation Function	Gauss	Correlation Function	Gauss
Solid Volume Fraction / (%)	37.5	Solid Volume Fraction / (%)	37.5
Standard Deviation / (voxel)	10	Standard Deviation / (voxel)	10
Random Seed	1	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** ¹⁹⁶.

✓ 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](#) ^[240] 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**

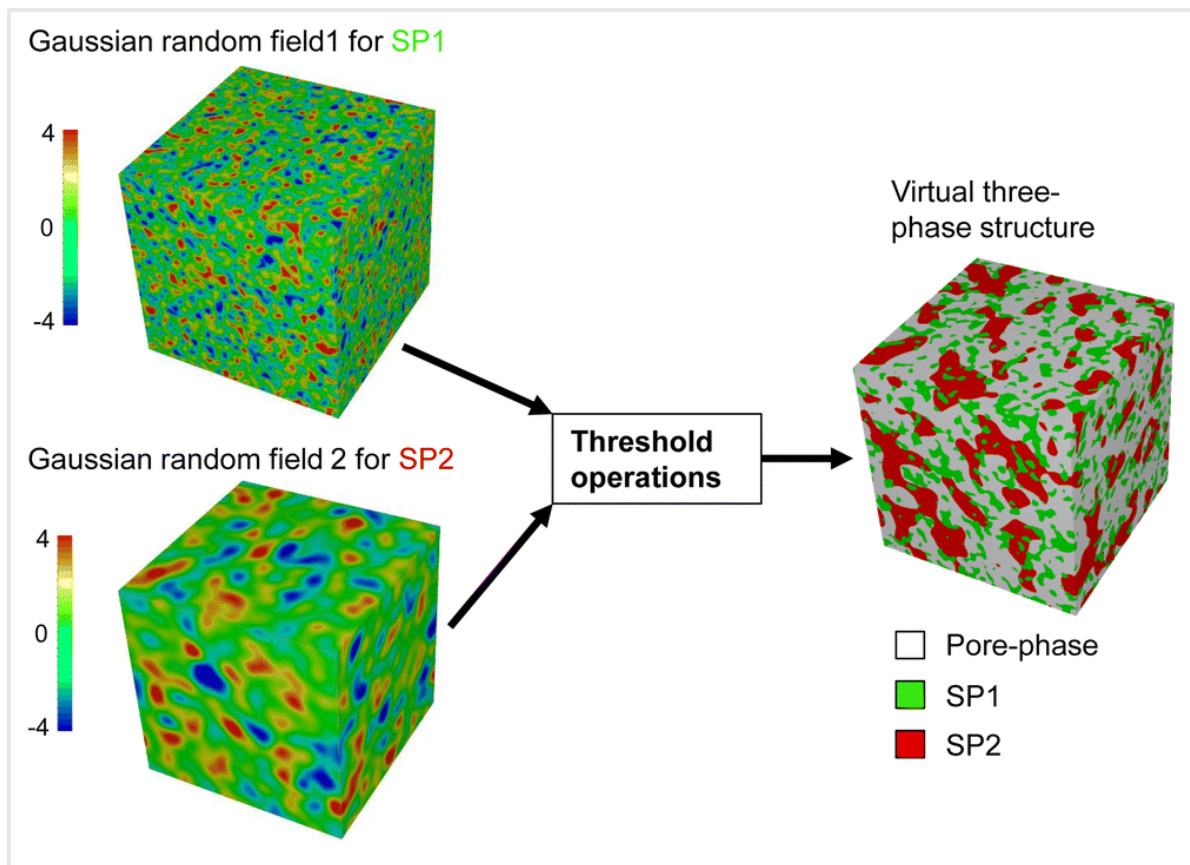
Dilation Radius between Pore and GRF 1 / (voxel)

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](#) ^[240]) 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 Load Structure

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

Help

Manage Data

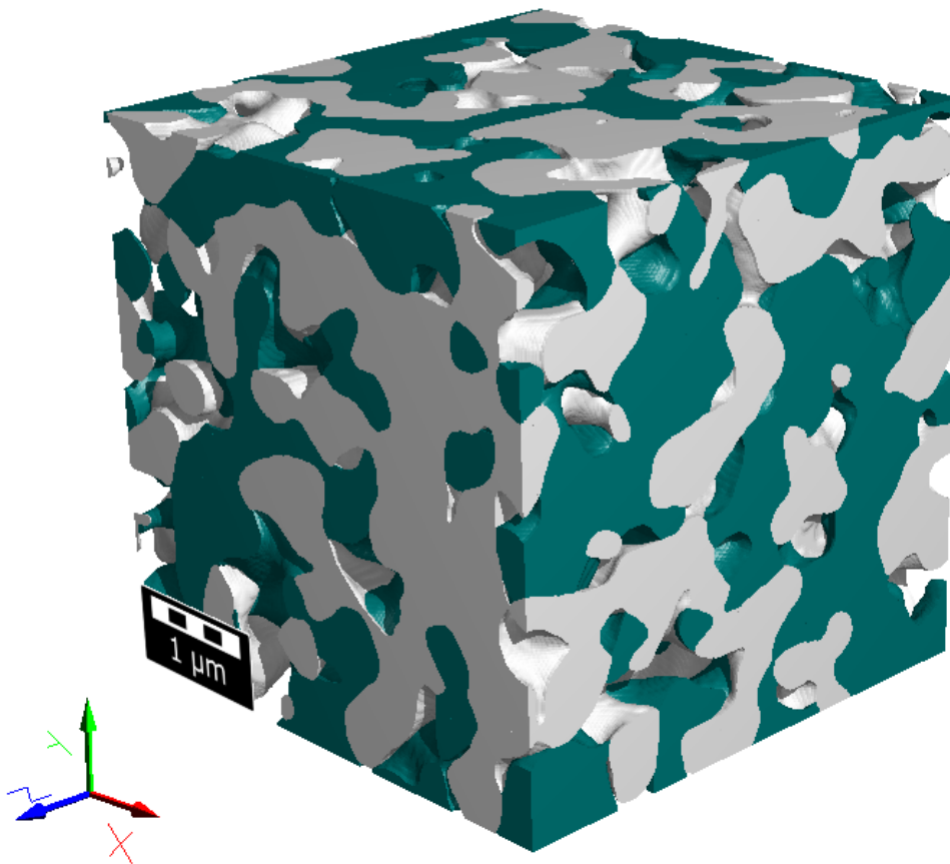
Load Input Parameters

Export

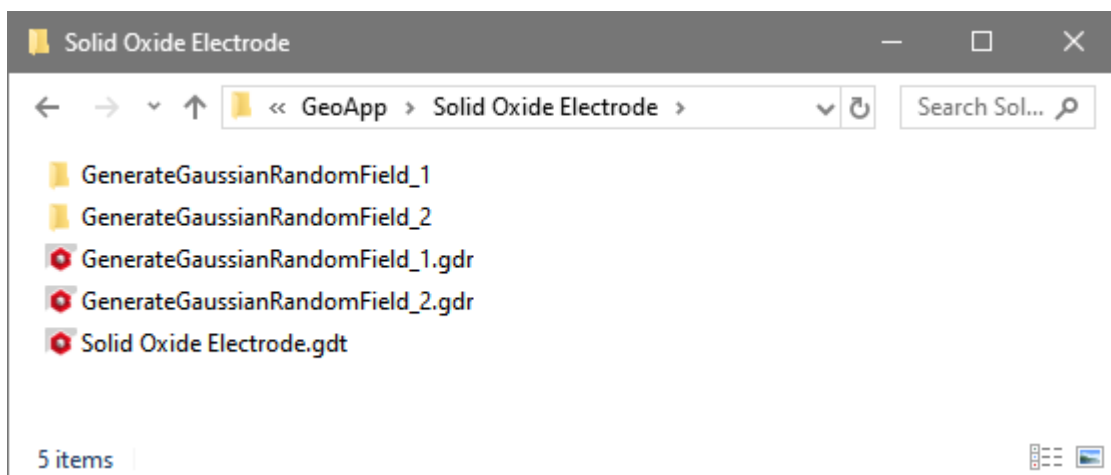
Close

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.



1.8 Additive Manufacturing GeoApps

Generate structures using the **Additive Manufacturing** GeoApps.



New in GeoDict 2026

- The two GeoApps to be found in this GeoApp section are not new in GeoDict. However, it is new that they are also available via the GeoApp menu instead of only via the GridGeo module.

Find the following Additive Manufacturing GeoApp groups:

- [Structure Generation](#)²⁰¹
Create additive manufacturing structures.

1.8.1 Structure Generation

Use the **Structure Generation** GeoApps to create additive manufacturing structures.

The following Structure Generation GeoApps are shipped with GeoDict:

- [Strut-Based Lattices](#)²⁰¹
They are constructed from nodes on the edges or vertices of the unit cell connected via straight beams.
- [Triply Periodic Minimal Surfaces \(TPMS\)](#)²¹⁴
They are mathematically created surfaces which are not self-intersecting or enfolded. They can be packed together in a periodic 3D pattern, locally minimizing the surface area for a given boundary resulting in a mean curvature of zero.

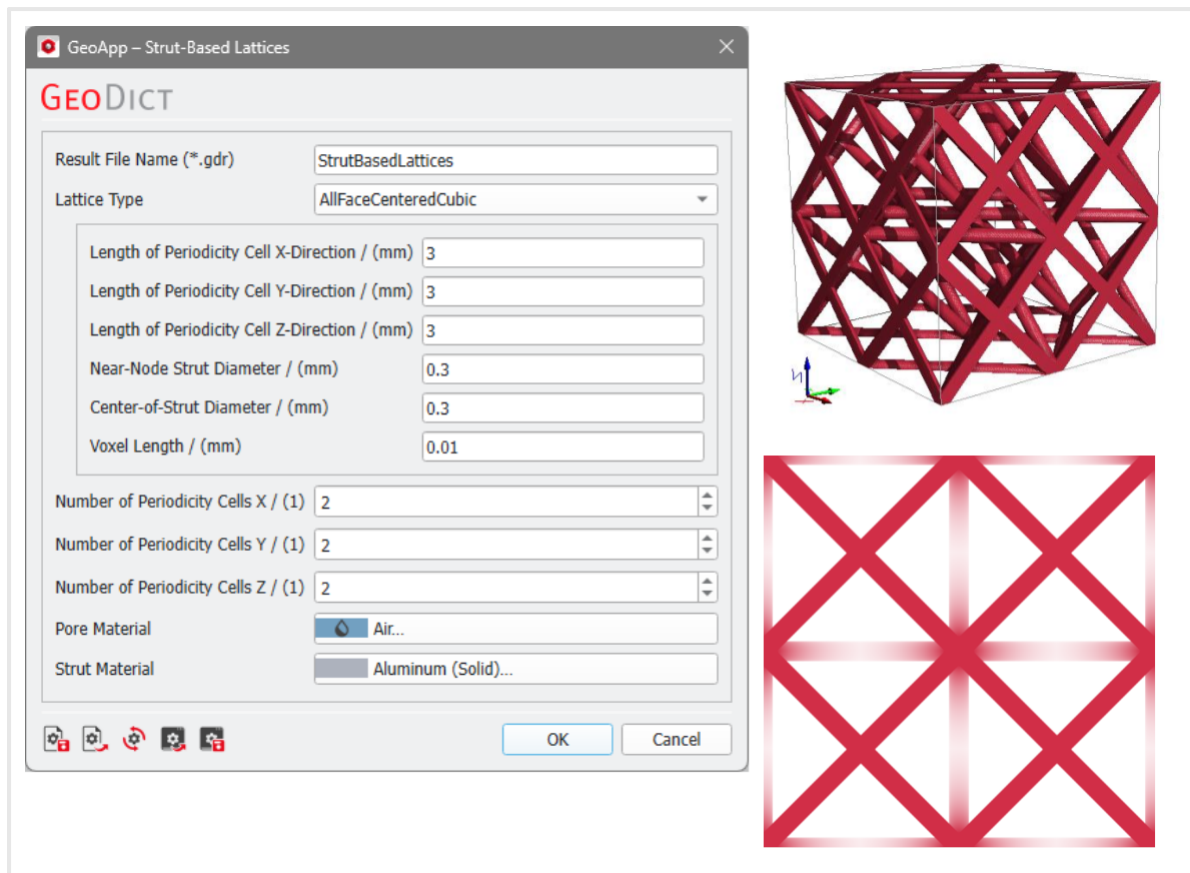
Strut-Based Lattices

In the following, the resulting structures of all **Lattice Types** are shown in both 3D-Rendering and 2D Cross Section View in X-direction together with the default settings for each lattice type.

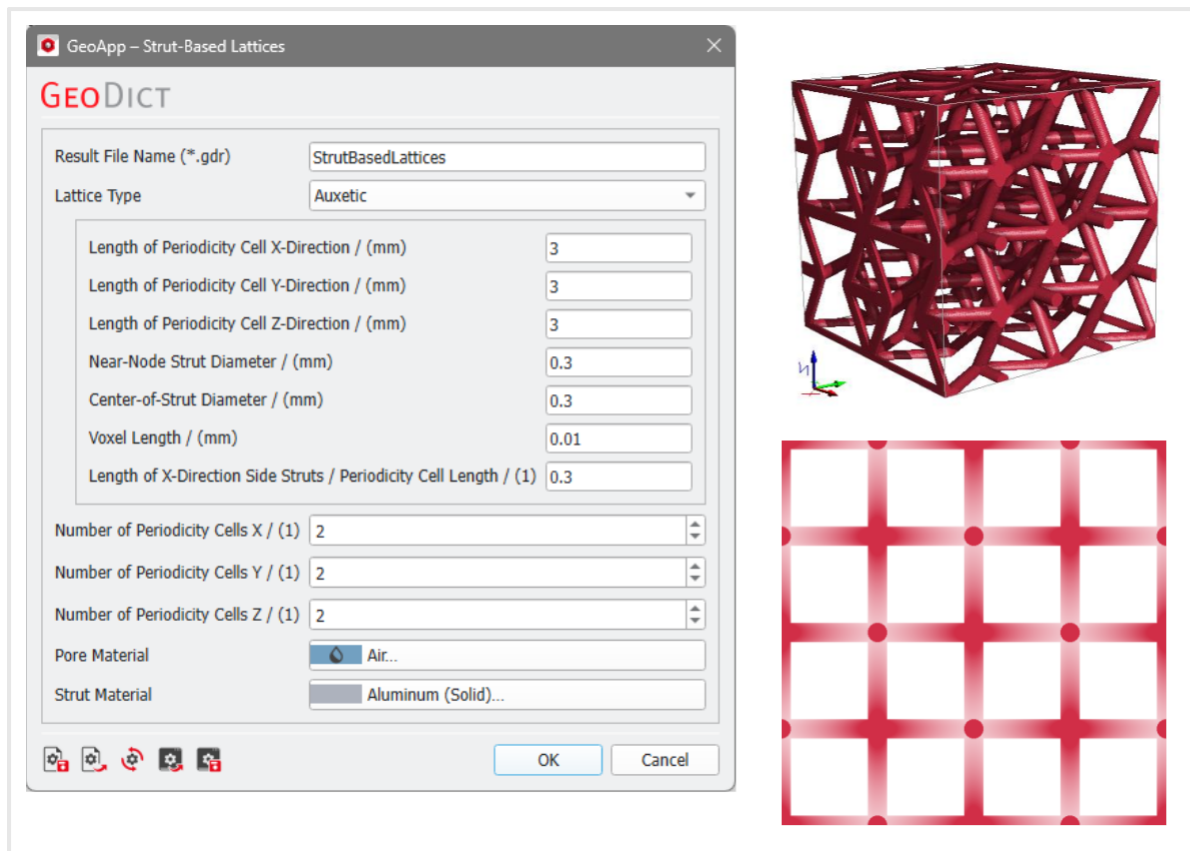


Modules needed to run this GeoApp:
GridGeo

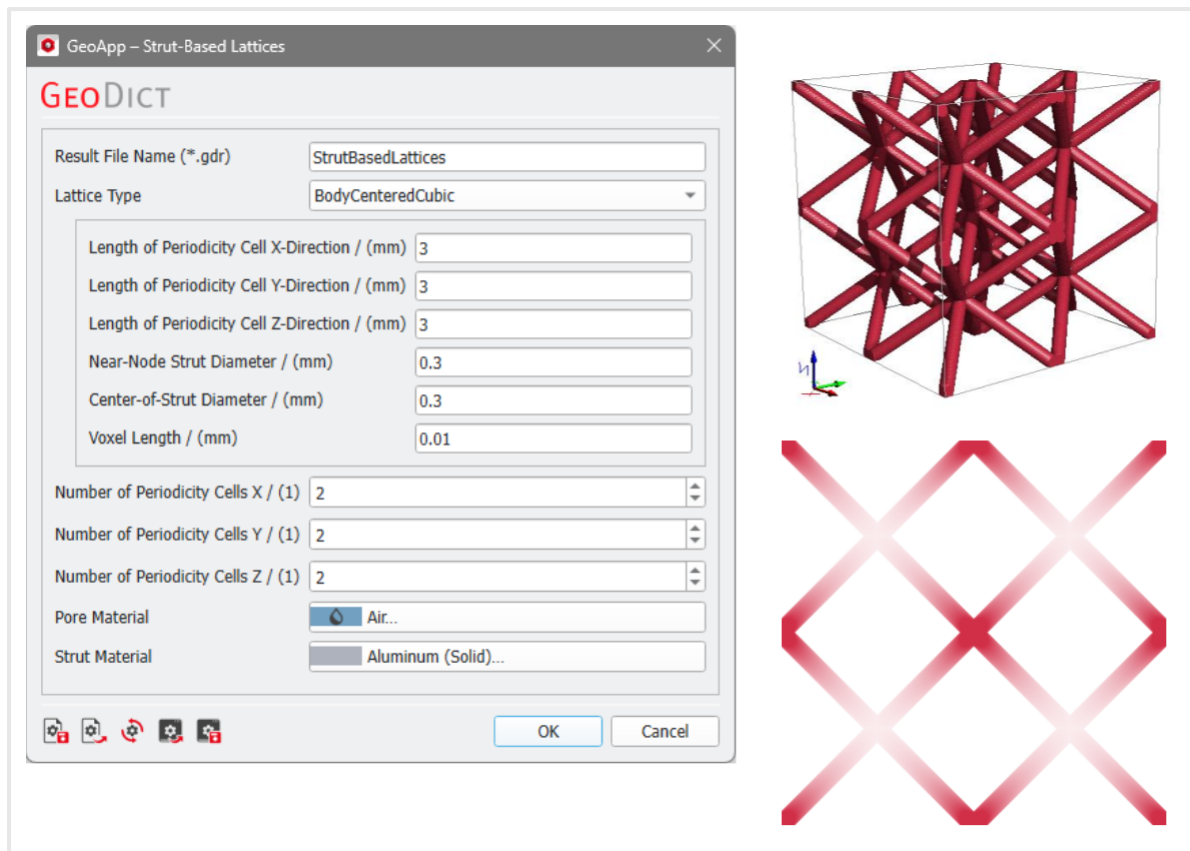
✓ **All-Face-Centered-Cubic-(AFCC)**



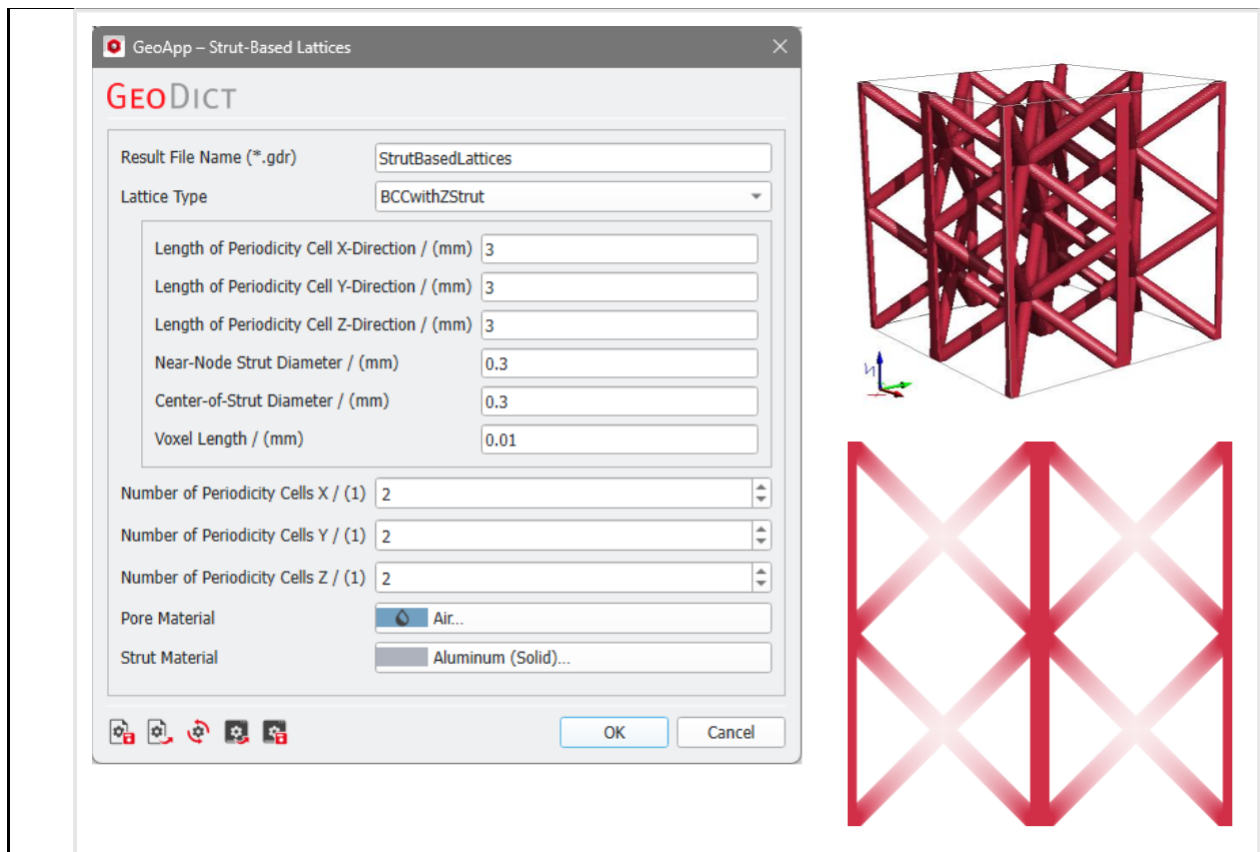
✓ Auxetic



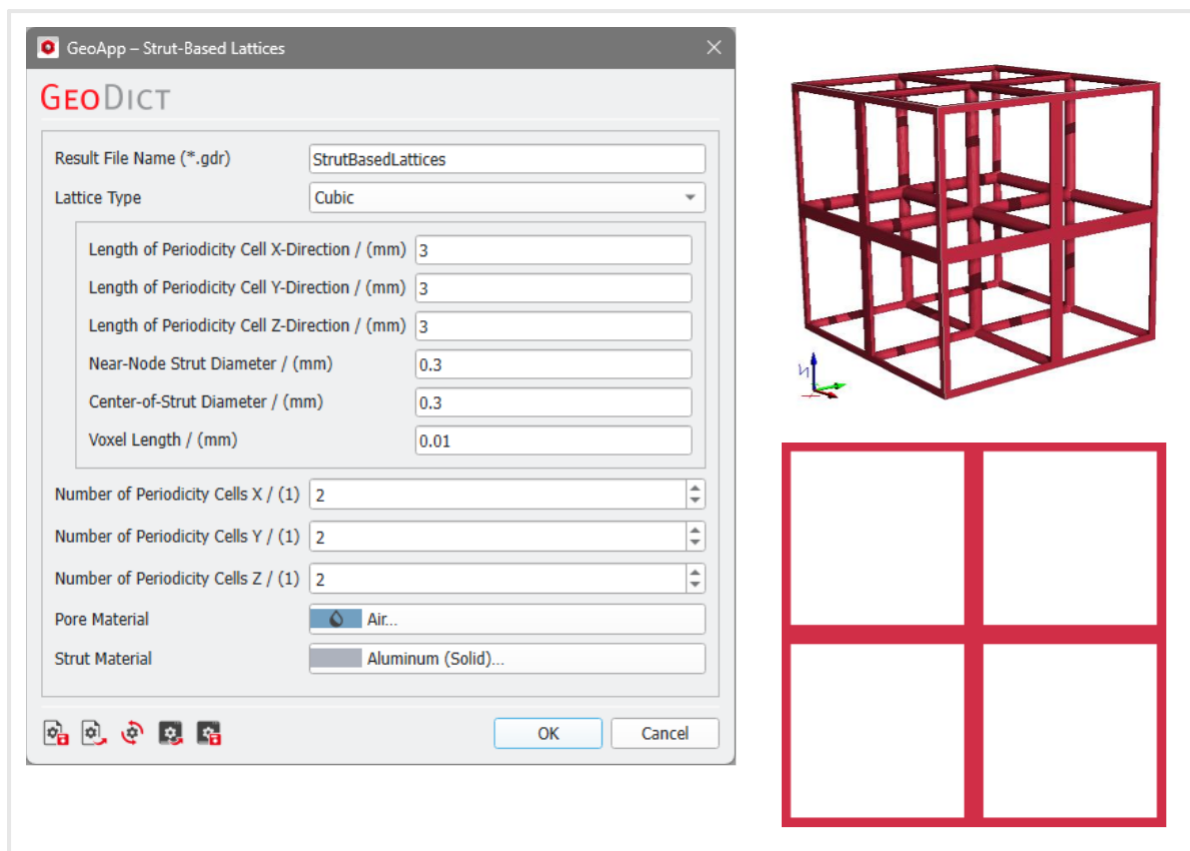
✓ Body-Centered-Cubic-(BCC)



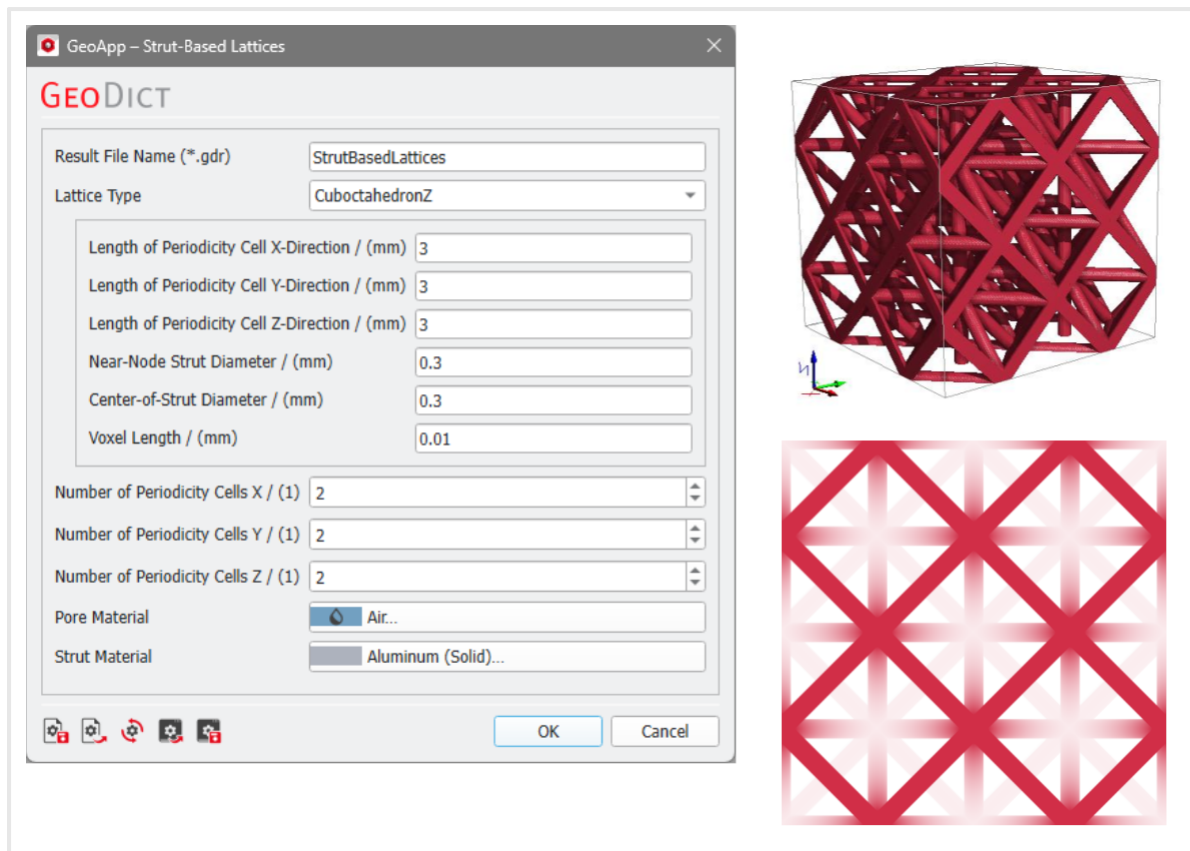
✓ BCC-with-Z-Strut-(BCCZ)



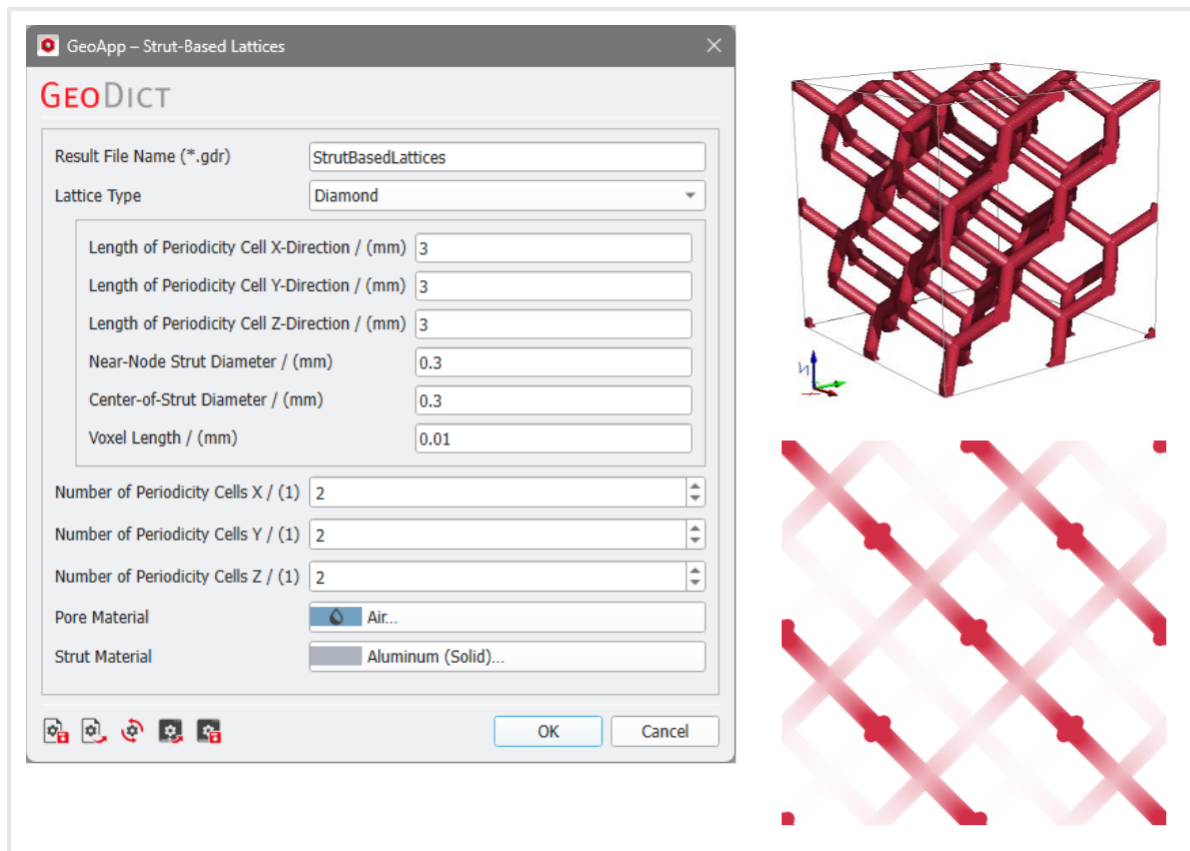
✓Cubic



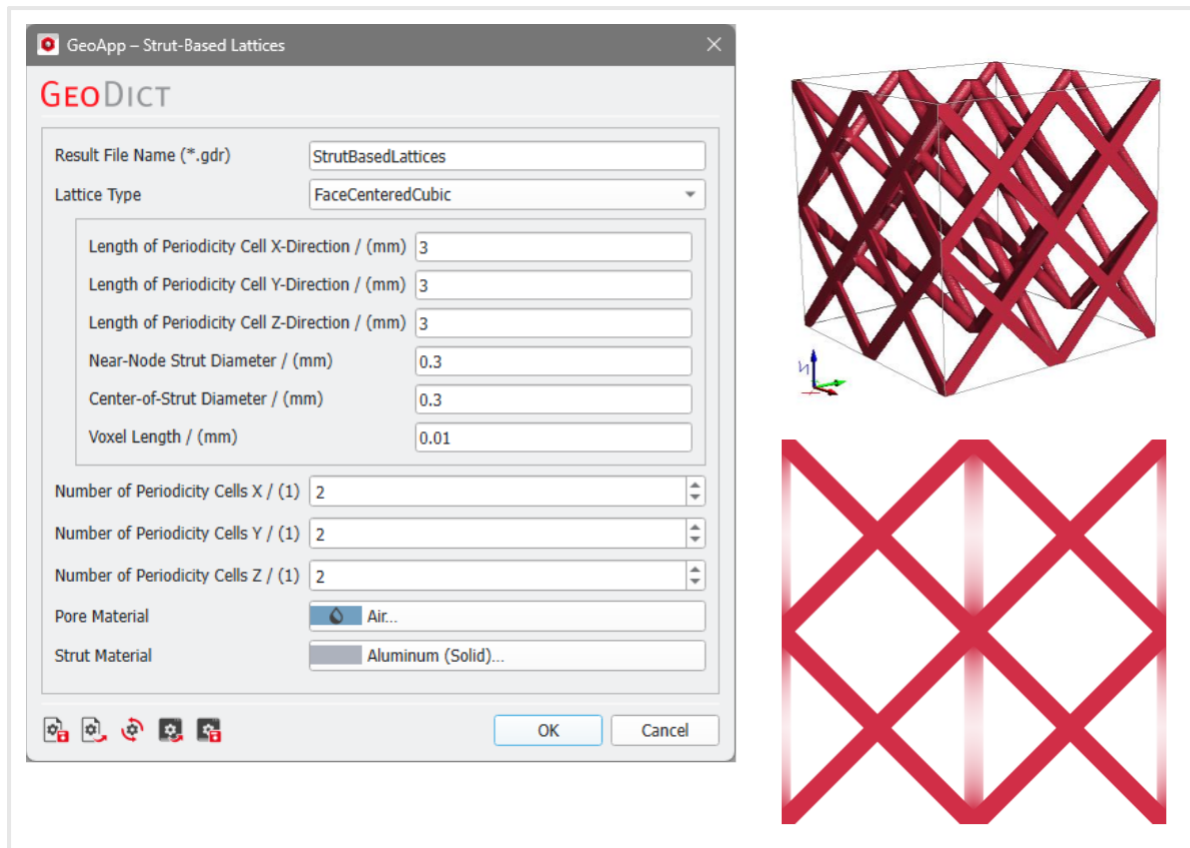
✓Cuboctahedron-Z



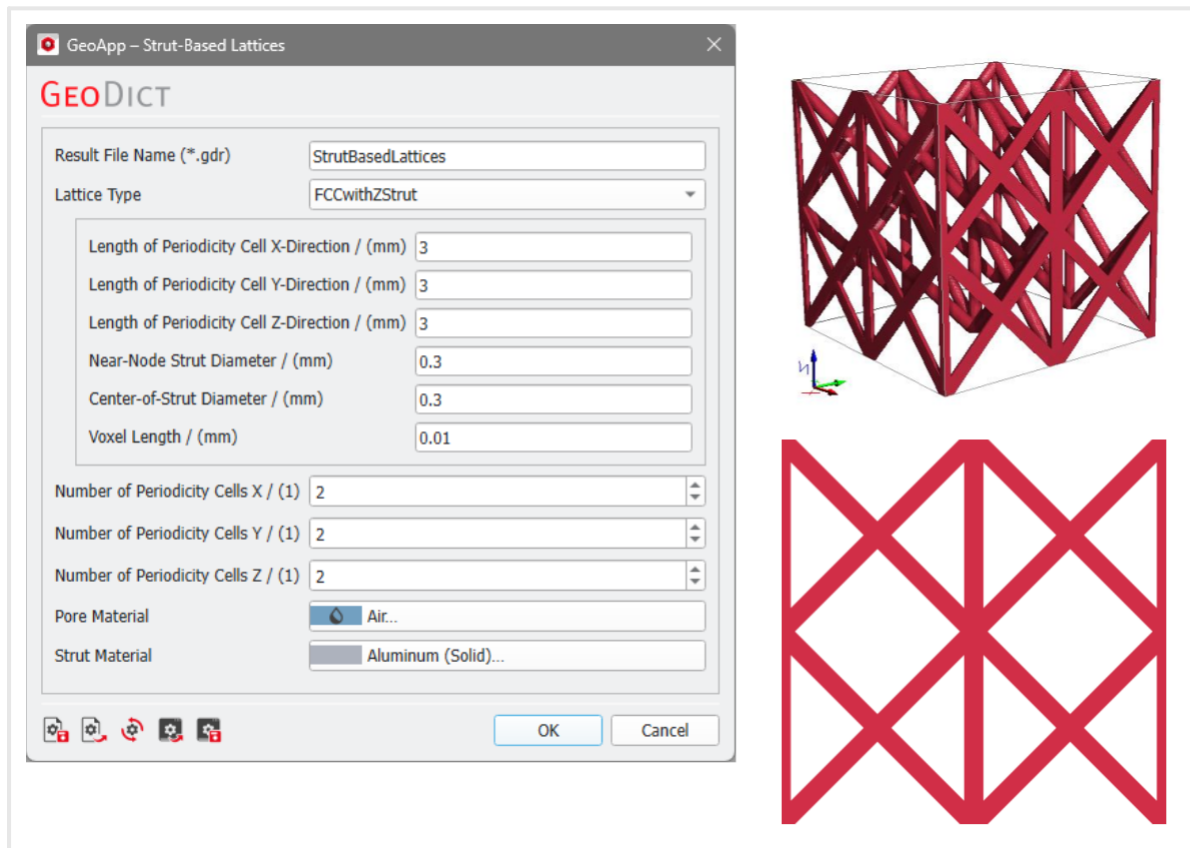
✓ Diamond-(Penta-Mode)



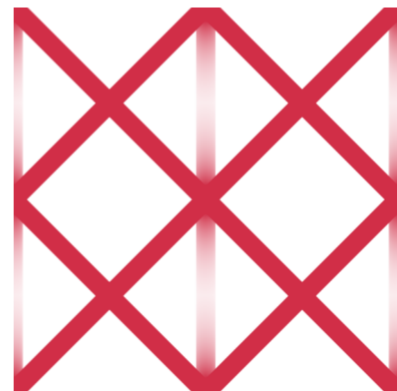
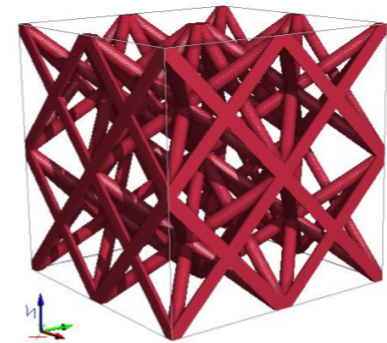
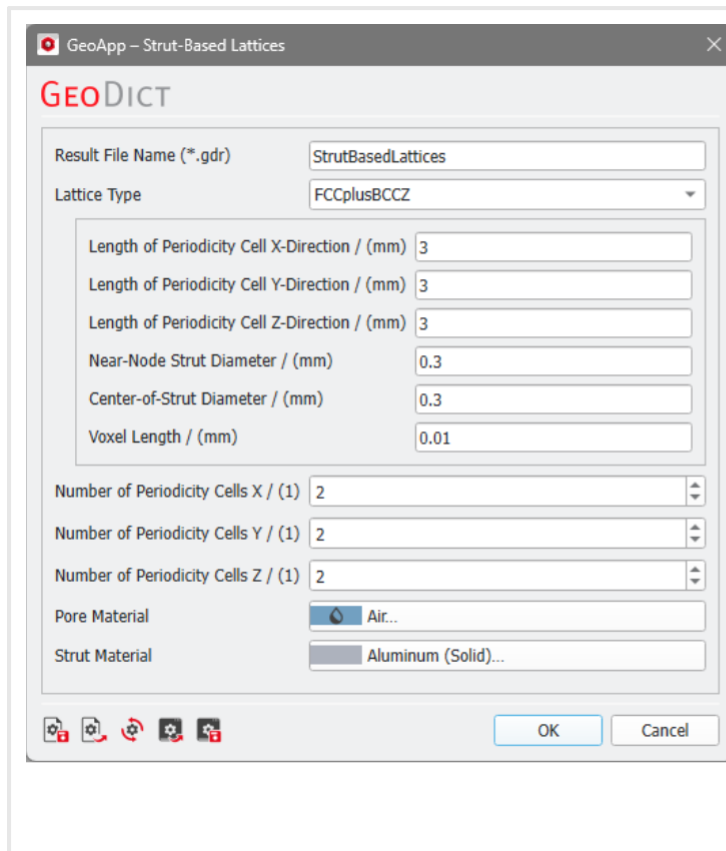
✓ Face-Centered-Cubic-(FCC)



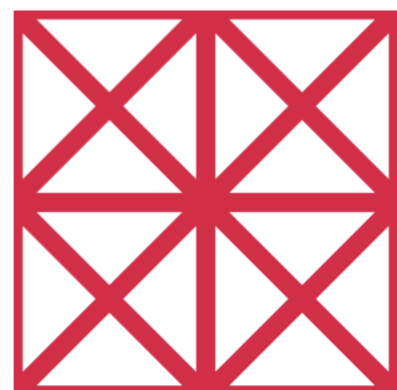
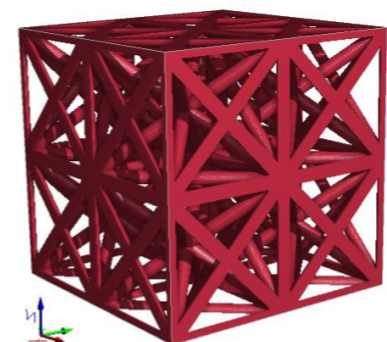
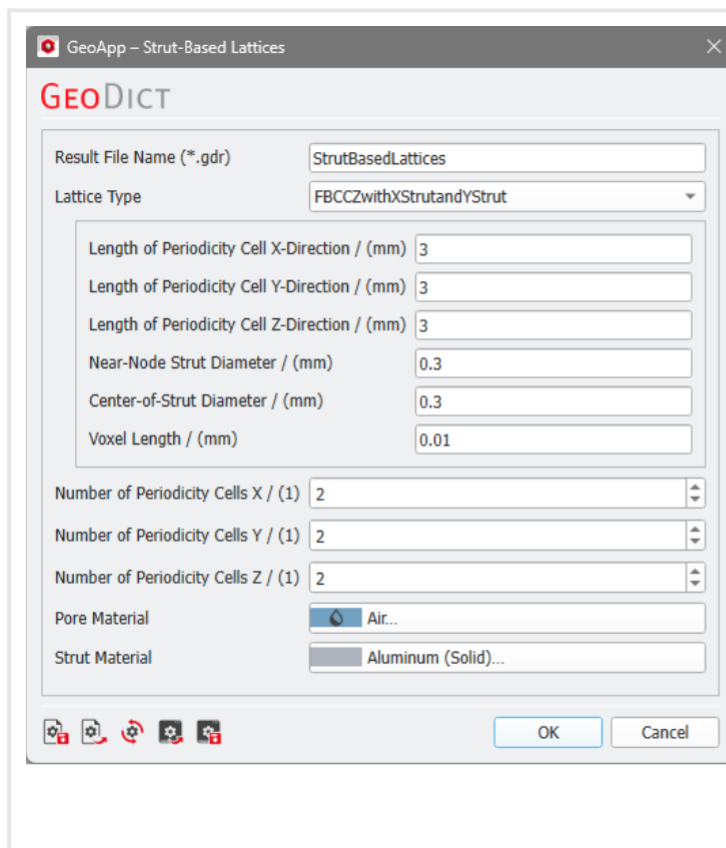
✓ FCC-with-Z-Strut-(FCCZ)



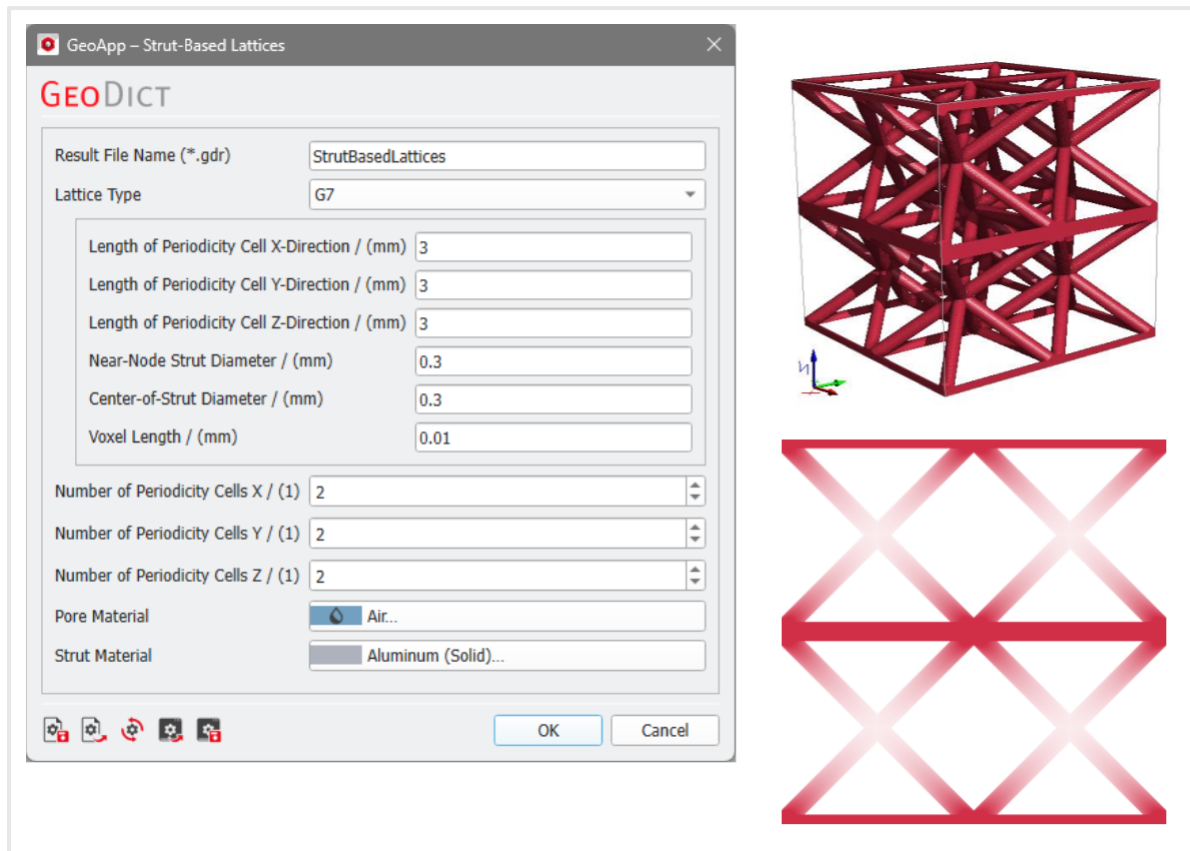
✓FCC-plus-BCCZ-(FBCCZ)



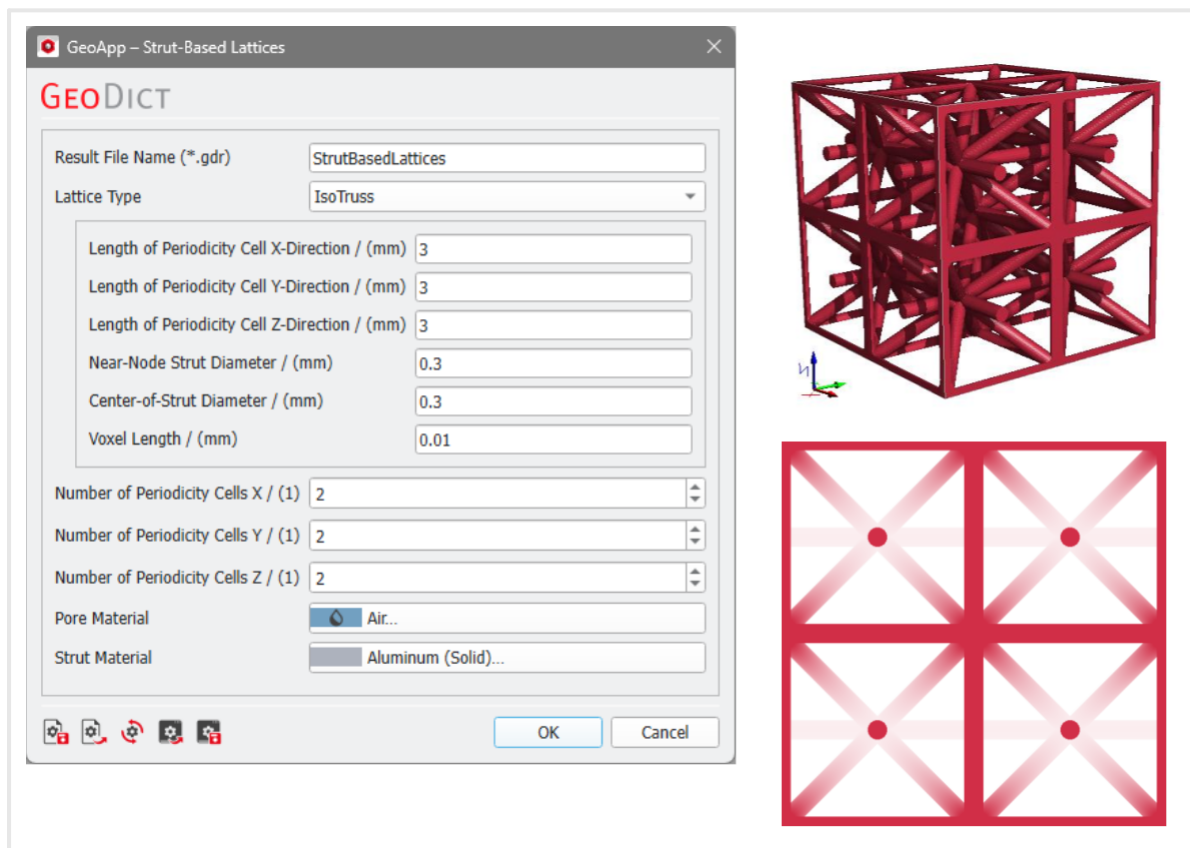
✓FBCCZ-with-X-Strut-and-Y-Strut-(FBCCXYZ)



✓G7



✓Iso-Truss



✓ Kelvin

GeoApp – Strut-Based Lattices

GEODICT

Result File Name (*.gdr)

Lattice Type

Length of Periodicity Cell X-Direction / (mm)

Length of Periodicity Cell Y-Direction / (mm)

Length of Periodicity Cell Z-Direction / (mm)

Near-Node Strut Diameter / (mm)

Center-of-Strut Diameter / (mm)

Voxel Length / (mm)

Diamond Side Length / Periodicity Cell Length / (1)

Number of Periodicity Cells X / (1)

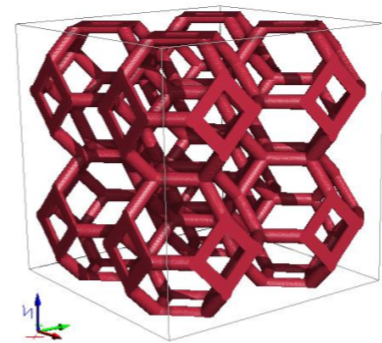
Number of Periodicity Cells Y / (1)

Number of Periodicity Cells Z / (1)

Pore Material

Strut Material

OK Cancel



✓ Octahedron

GeoApp – Strut-Based Lattices

GEODICT

Result File Name (*.gdr)

Lattice Type

Length of Periodicity Cell X-Direction / (mm)

Length of Periodicity Cell Y-Direction / (mm)

Length of Periodicity Cell Z-Direction / (mm)

Near-Node Strut Diameter / (mm)

Center-of-Strut Diameter / (mm)

Voxel Length / (mm)

Number of Periodicity Cells X / (1)

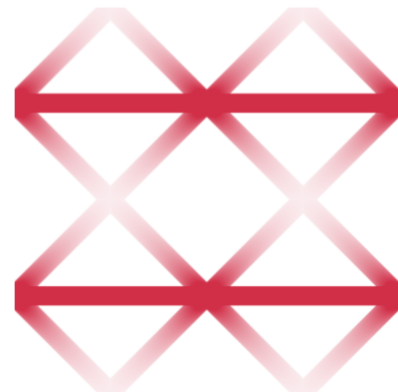
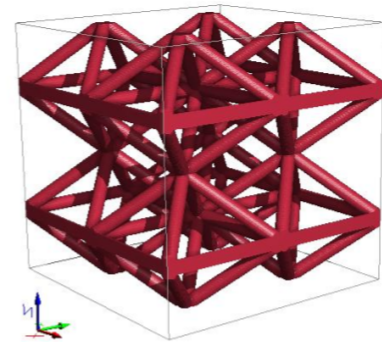
Number of Periodicity Cells Y / (1)

Number of Periodicity Cells Z / (1)

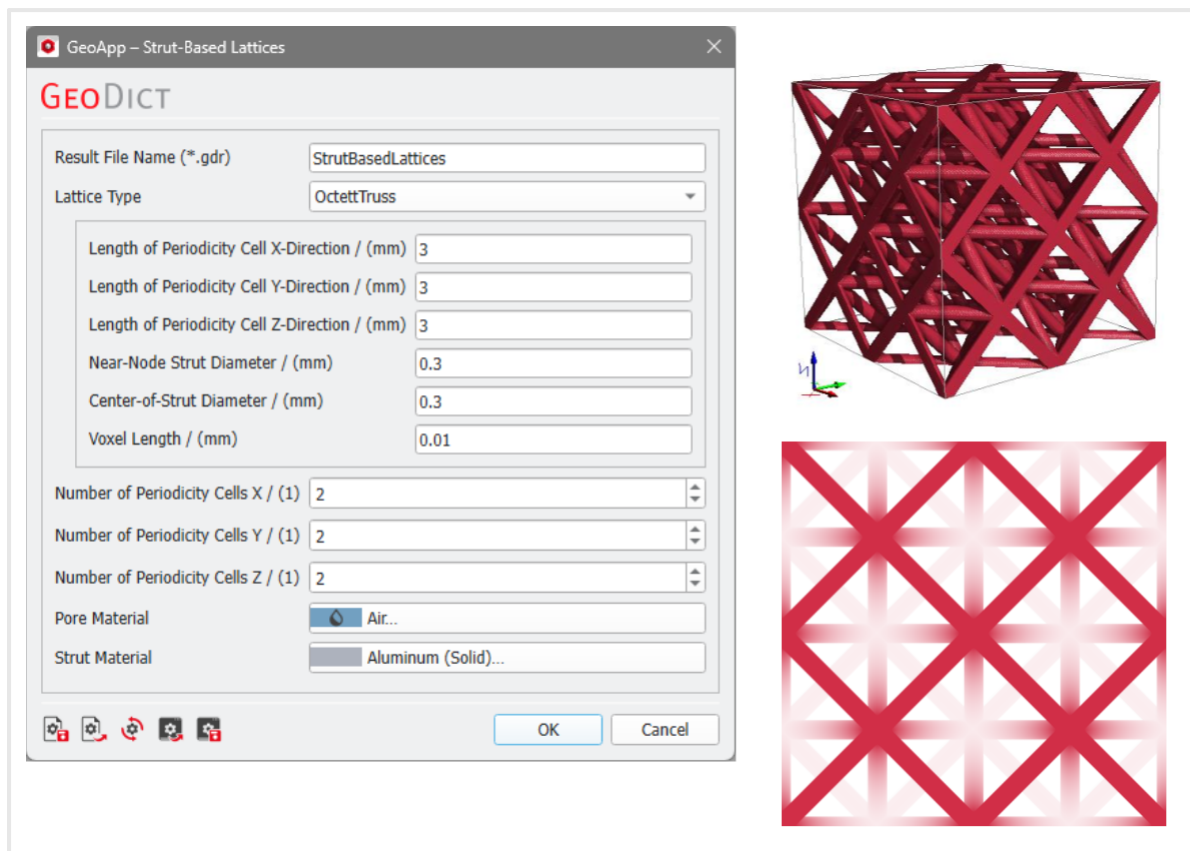
Pore Material

Strut Material

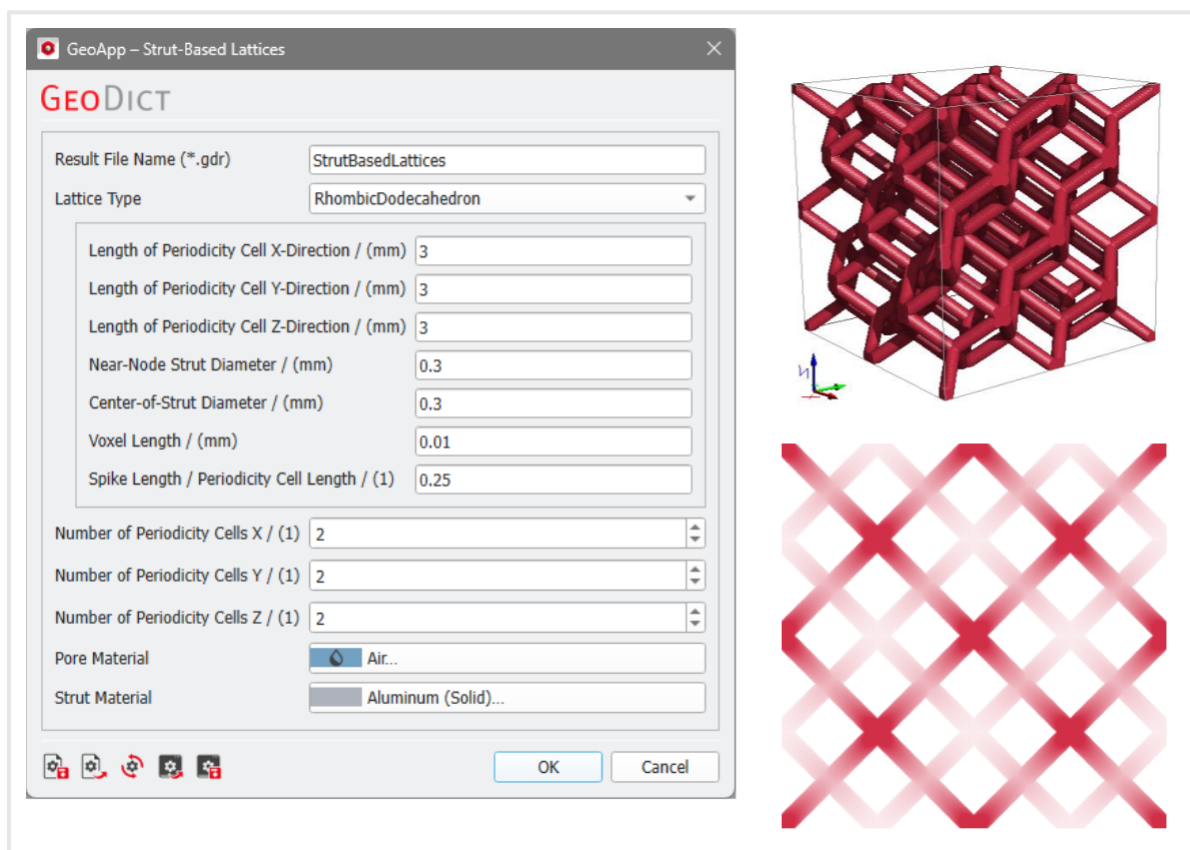
OK Cancel



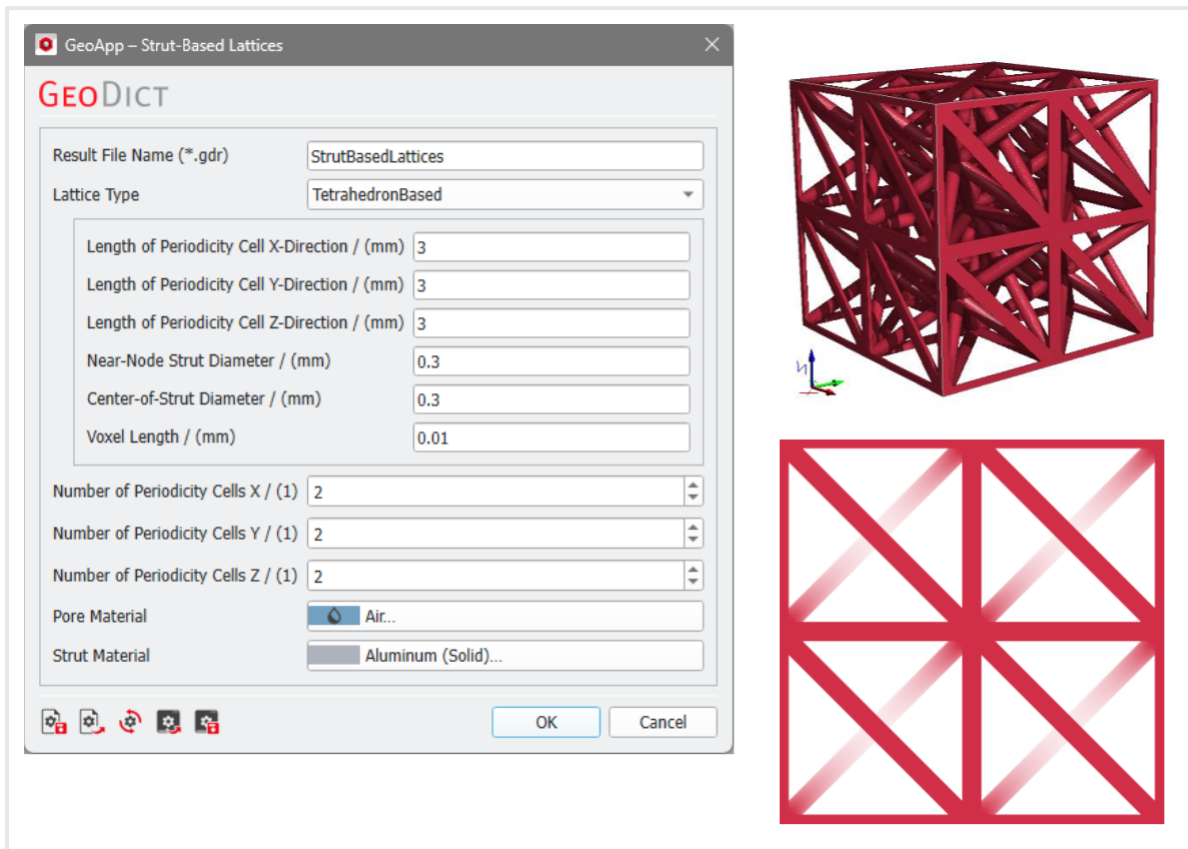
✓ Octett-Truss



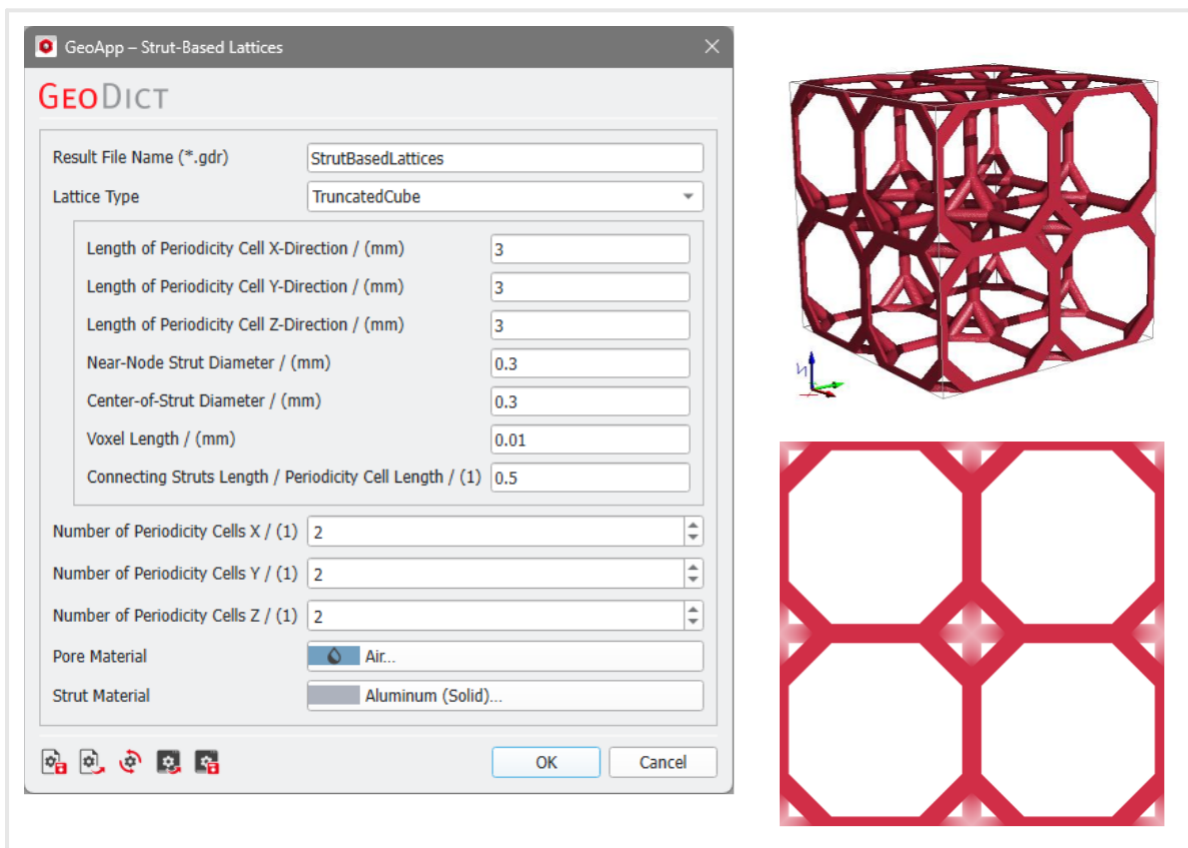
✓ Rhombic-Dodecahedron



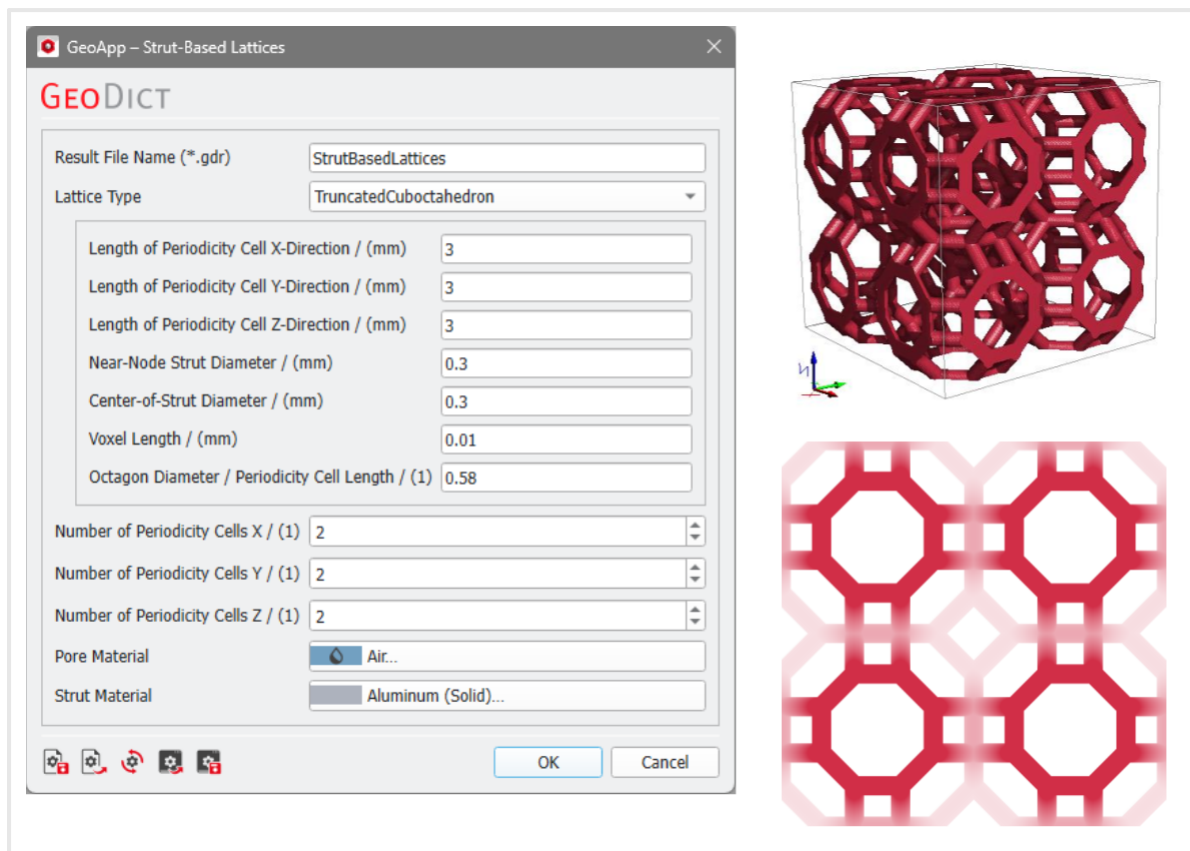
✓ Tetrahedron-Based



✓ Truncated-Cube



✓ Truncated-Cuboctahedron



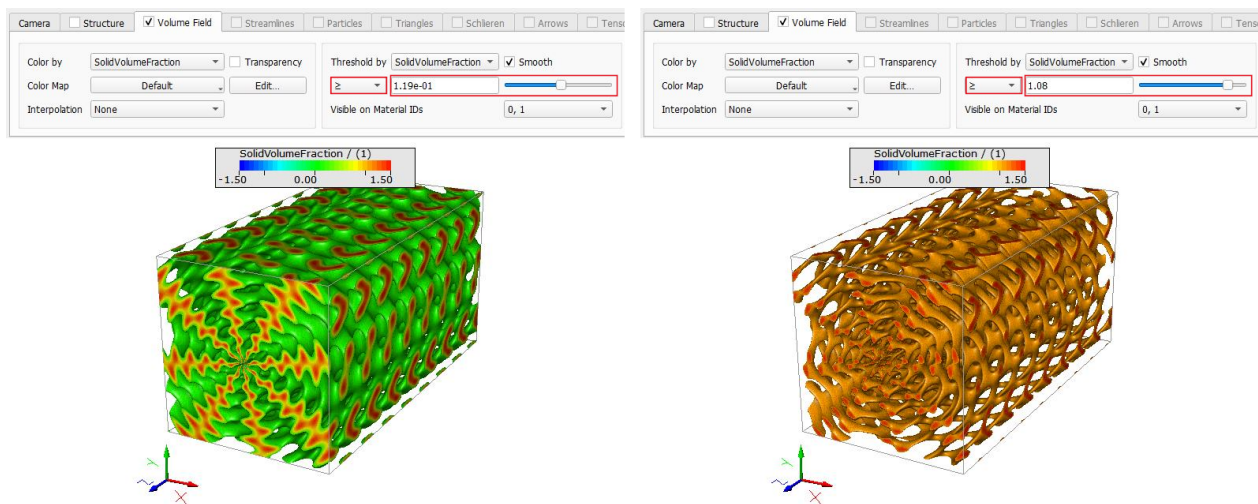
Triply Periodic Minimal Surfaces (TPMS)

What are Triply Periodic Minimal Surfaces (TPMS)?

To generate a TPMS-based structure, a volume field is used. With the threshold mode **SmallerEqual** ($\leq$) the structure is composed of all parts of the volume field that have a solid volume fraction less or equal to the given threshold. If **GreaterEqual** ($\geq$) is chosen, then all parts with a higher solid volume fraction remain for the structure. The third mode **GreaterEqualAndSmallerEqual** ($\leq$ & $\geq$) combines both of the previous mentioned threshold modes and therefore needs a lower and an upper threshold to be defined. Everything between the threshold values is kept for the structure.

You can view the volume field on which the structure is based, by selecting the **Volume Field** tab in the Visualization panel. Uncheck **Structure** to only display the volume field given by the solid volume fraction.

The slider in the threshold section can be used to observe the remaining structure when changing the threshold. Choose between $\geq$, $\leq$, and $=$ mode. For the $=$ mode, only the parts with exactly this threshold value are visible.



More information on how to choose the view settings can be found in the Visualization chapter.

In the following, the resulting structures of all **Shape Modes** are shown in both 3D-Rendering and 2D Cross Section View together with the default settings for each shape mode.



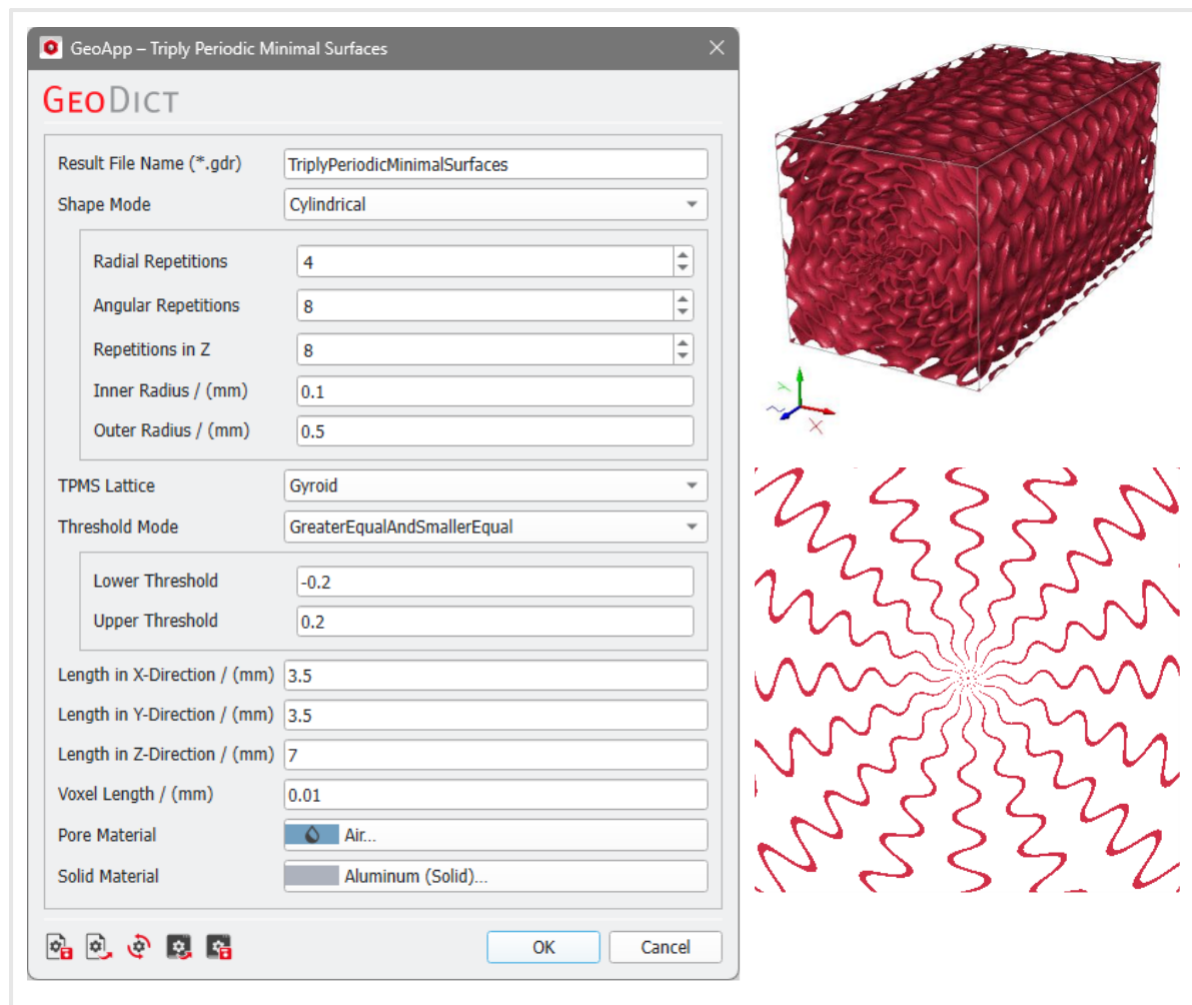
Modules needed to run this GeoApp:

GridGeo

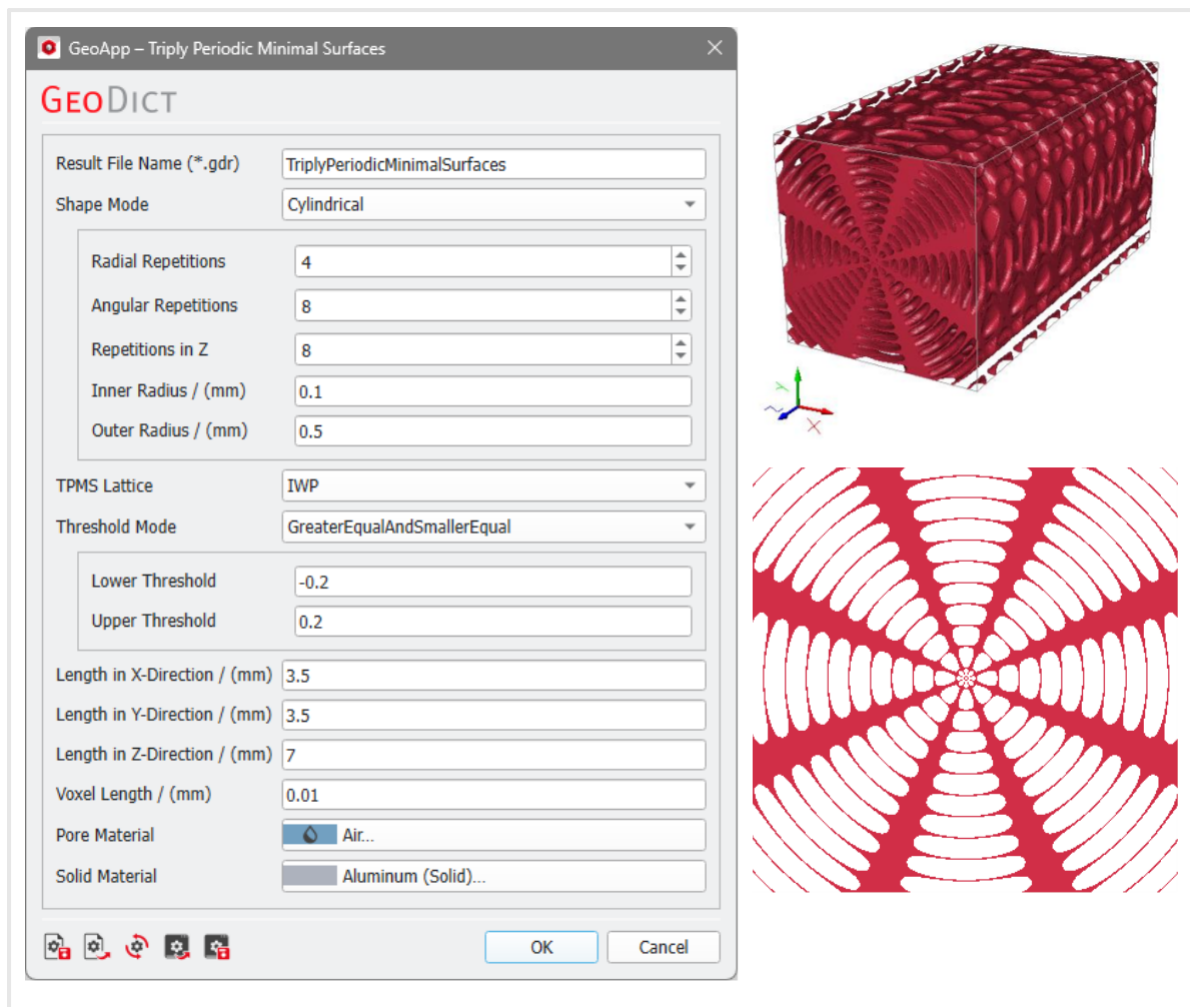
Cylindrical Shape Mode



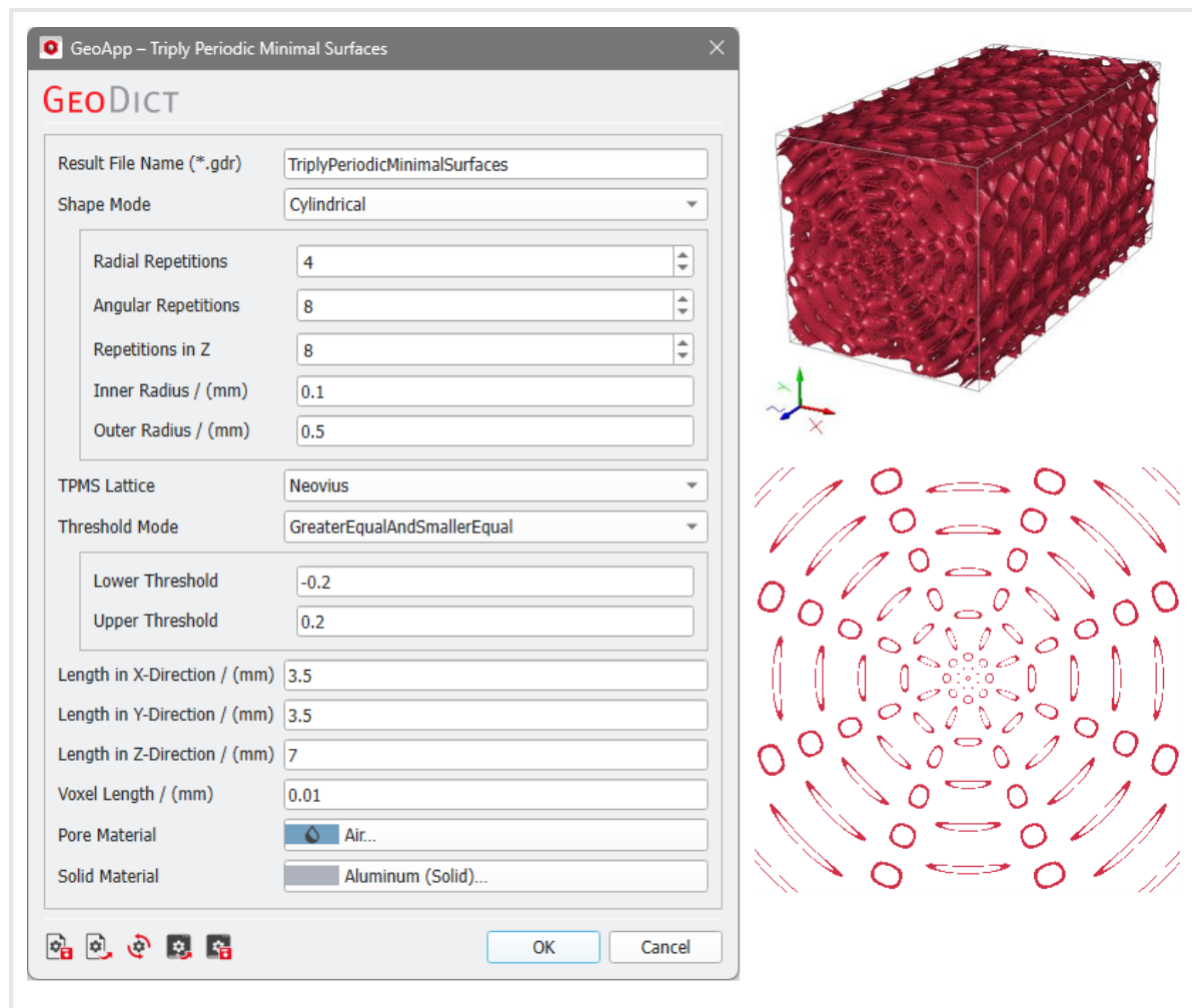
Gyroid



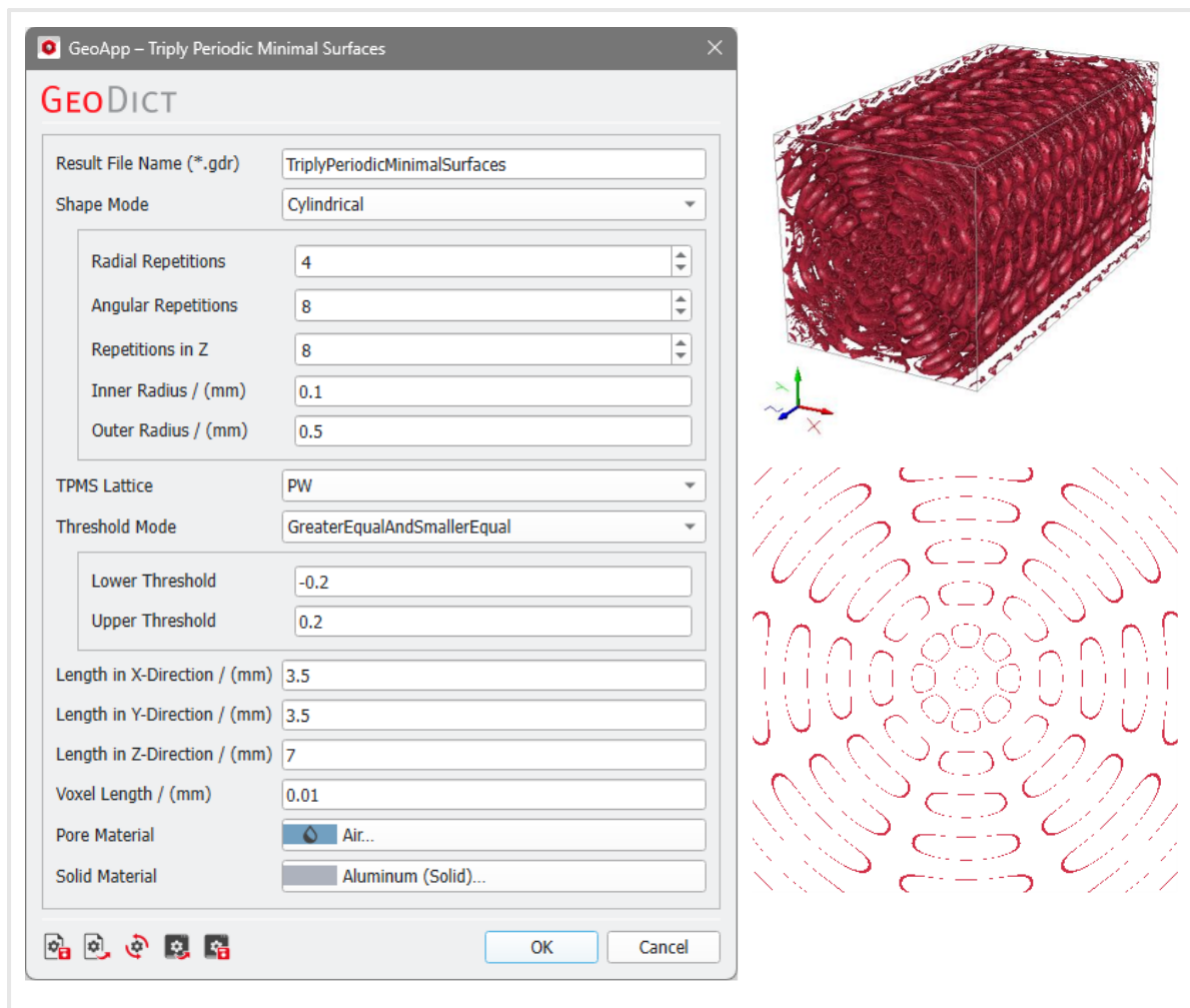
✓ I-WP



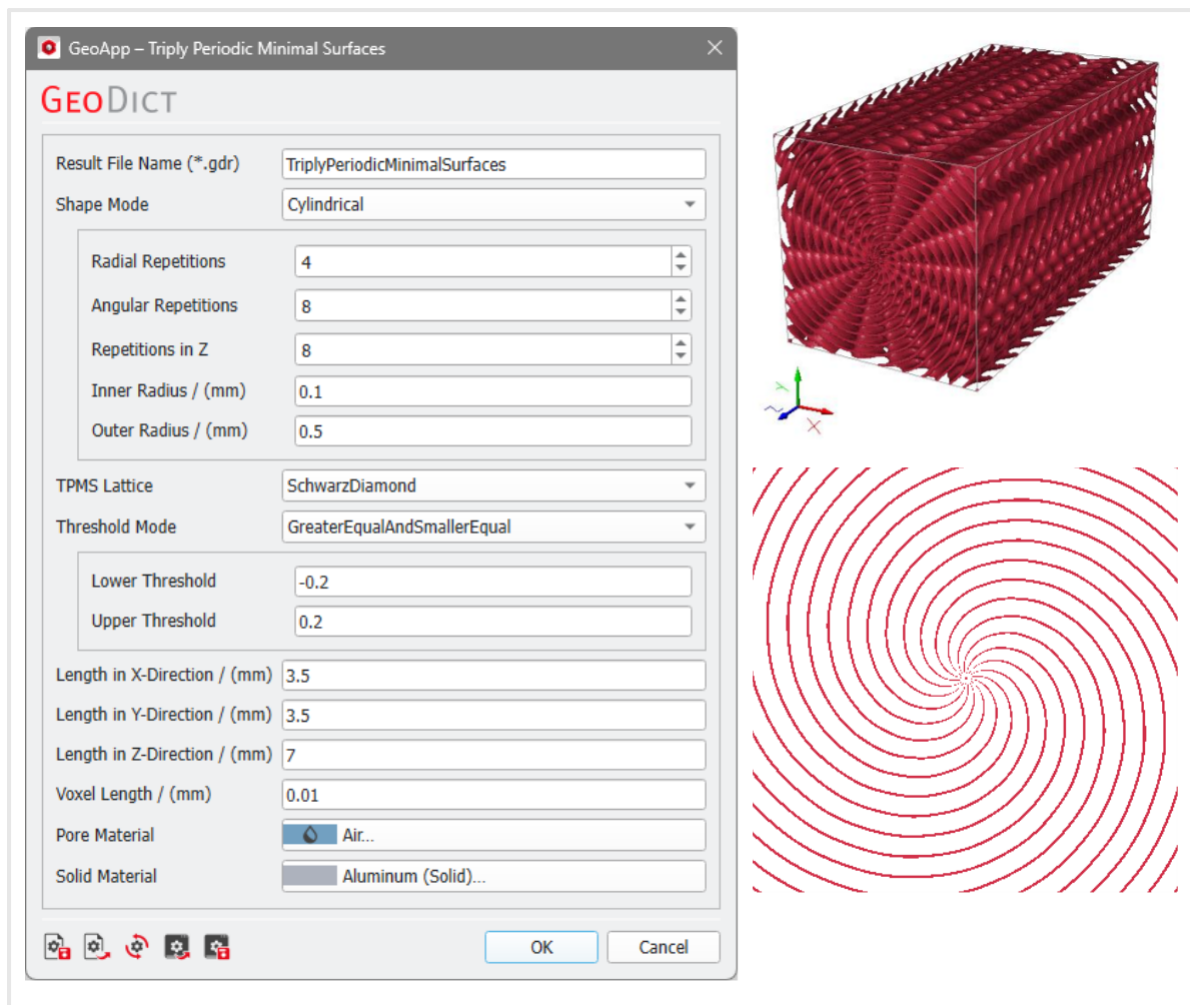
Neovius



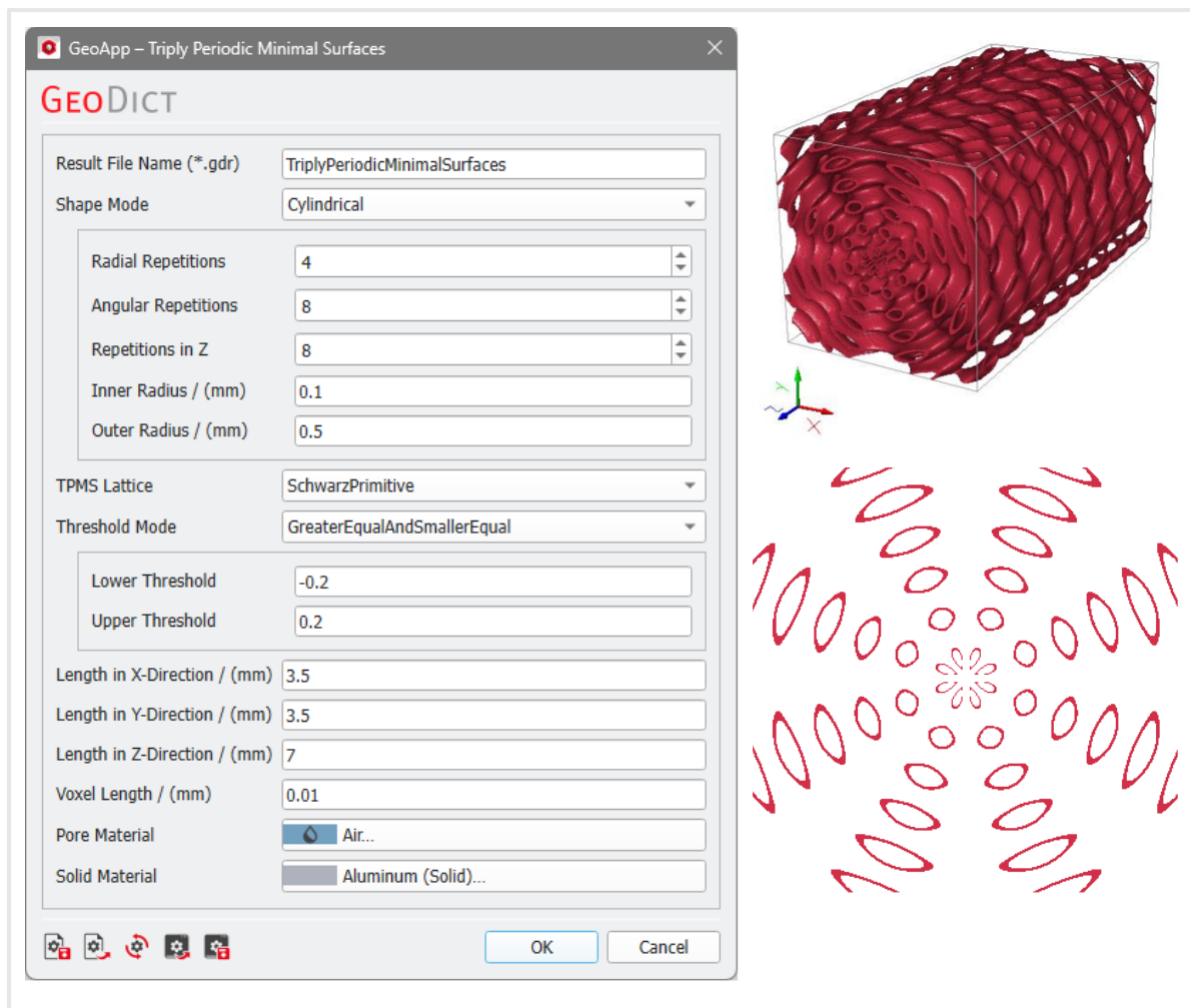
✓ P-W



✓ Schwarz-Diamond

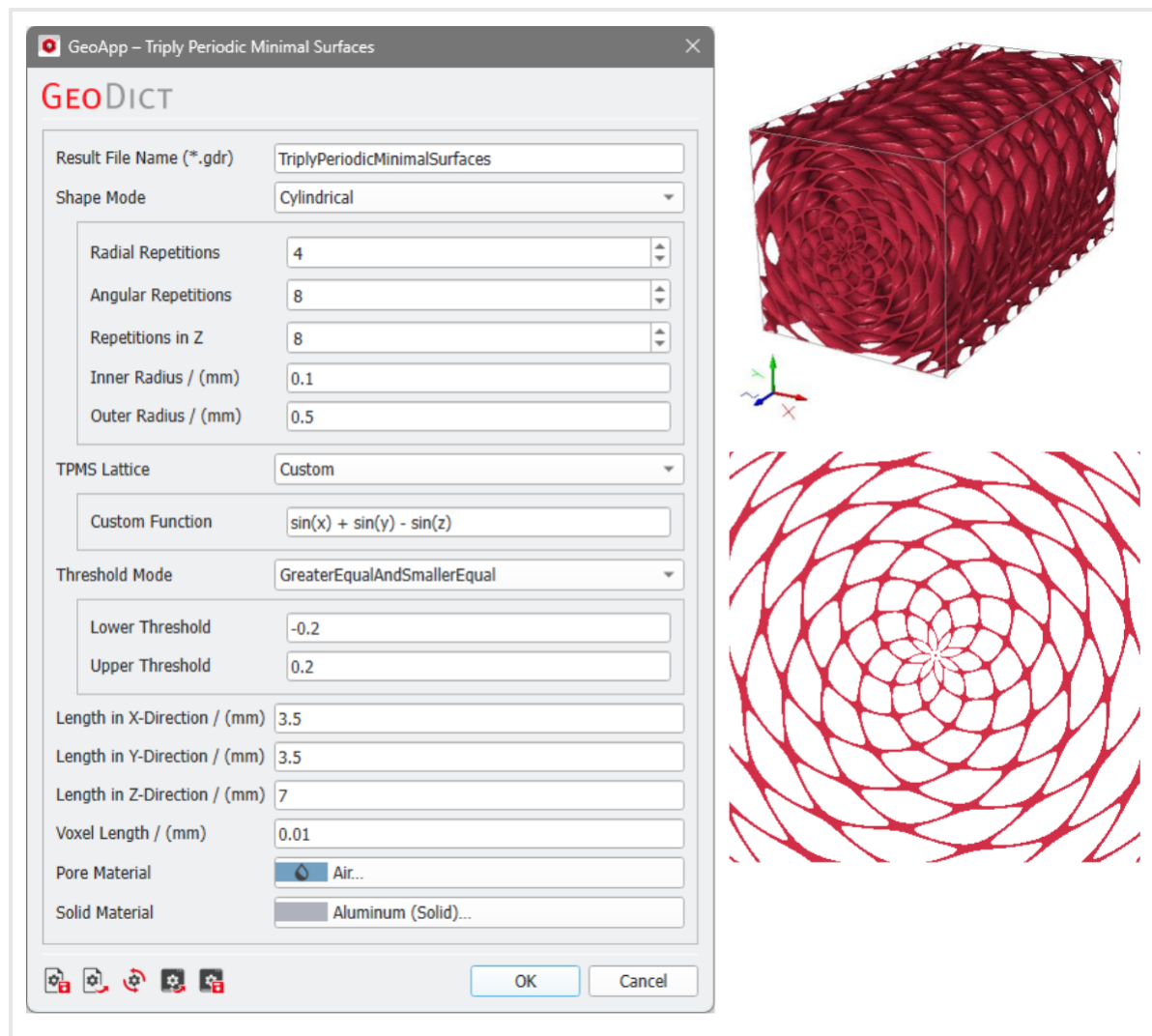


✓ Schwarz-Primitive



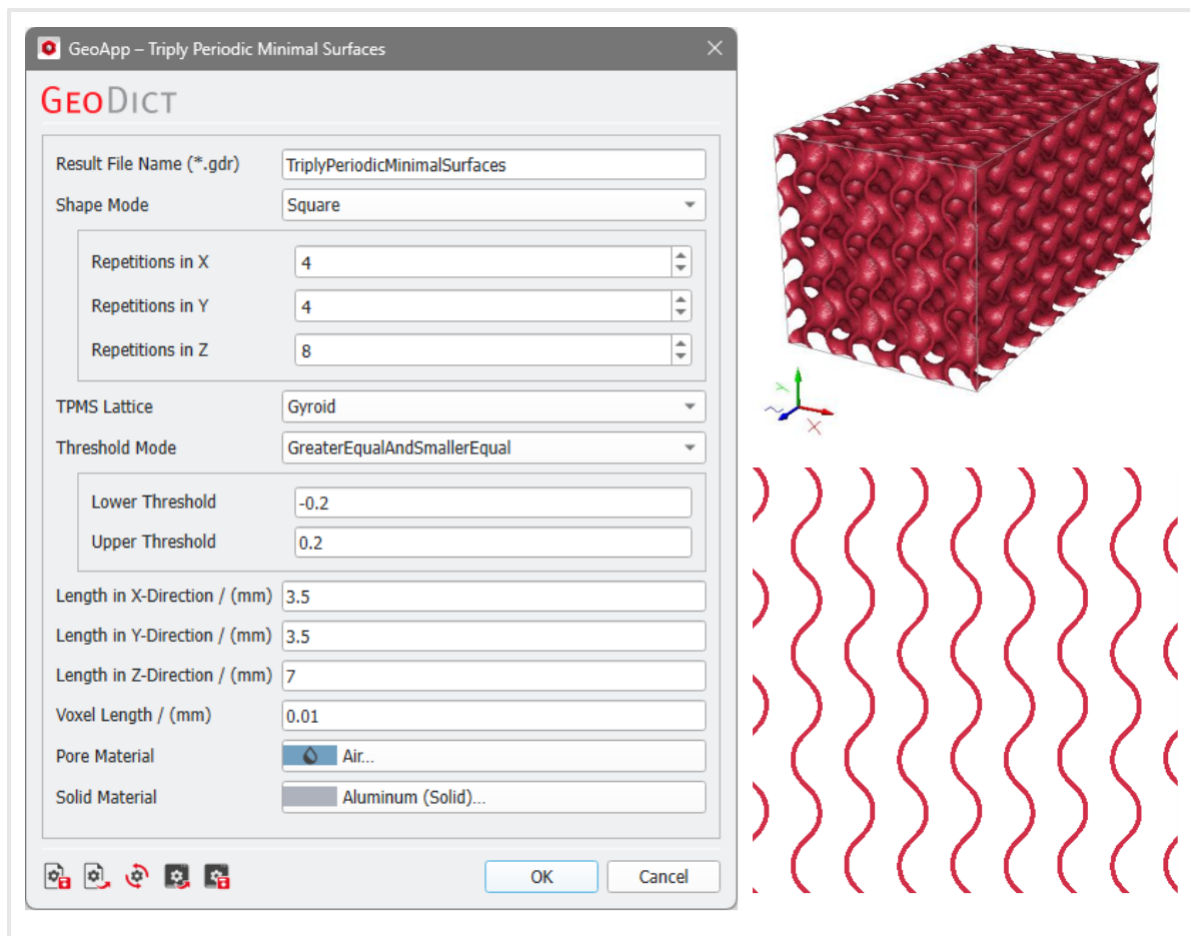
✓ Custom

A custom function in python syntax can be specified to produce a grid of triply periodic minimal surfaces.

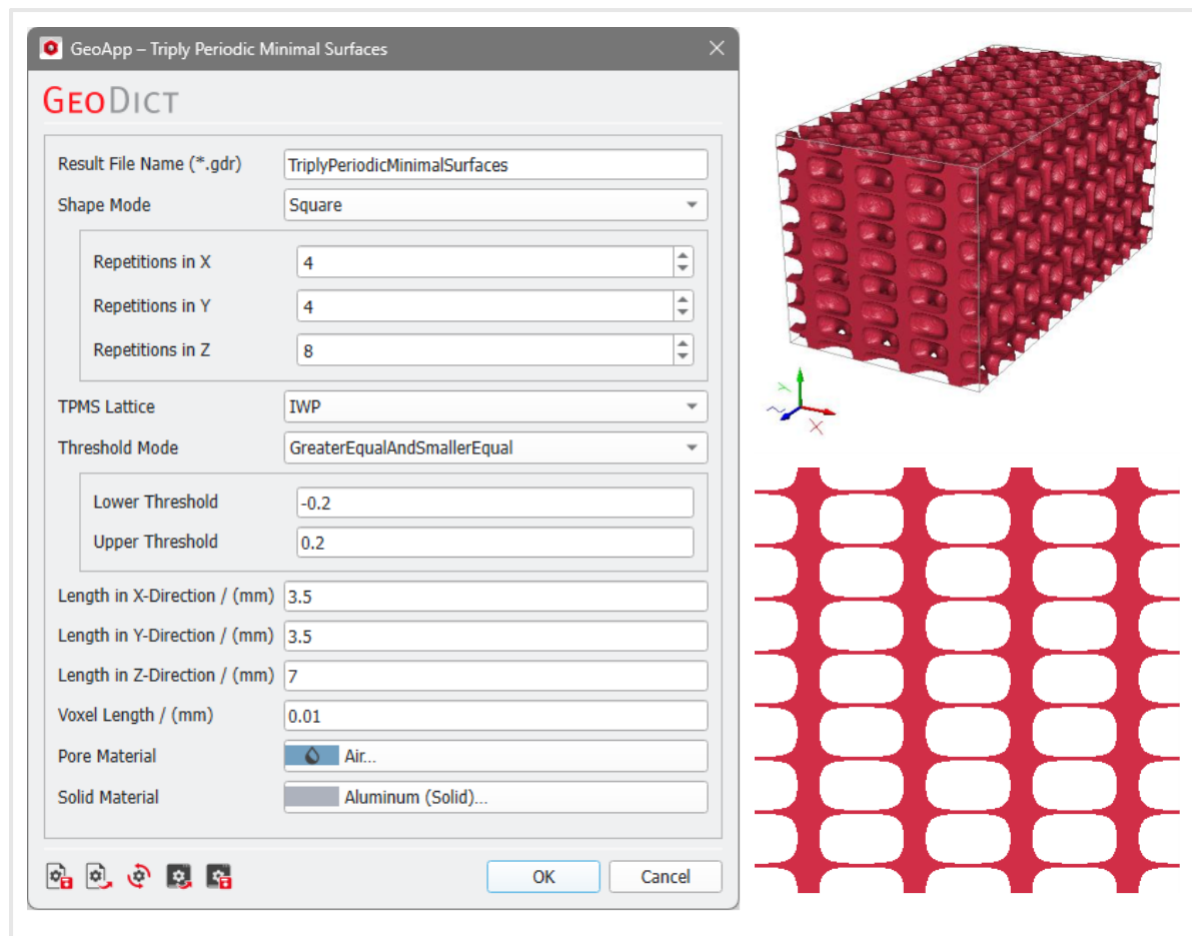


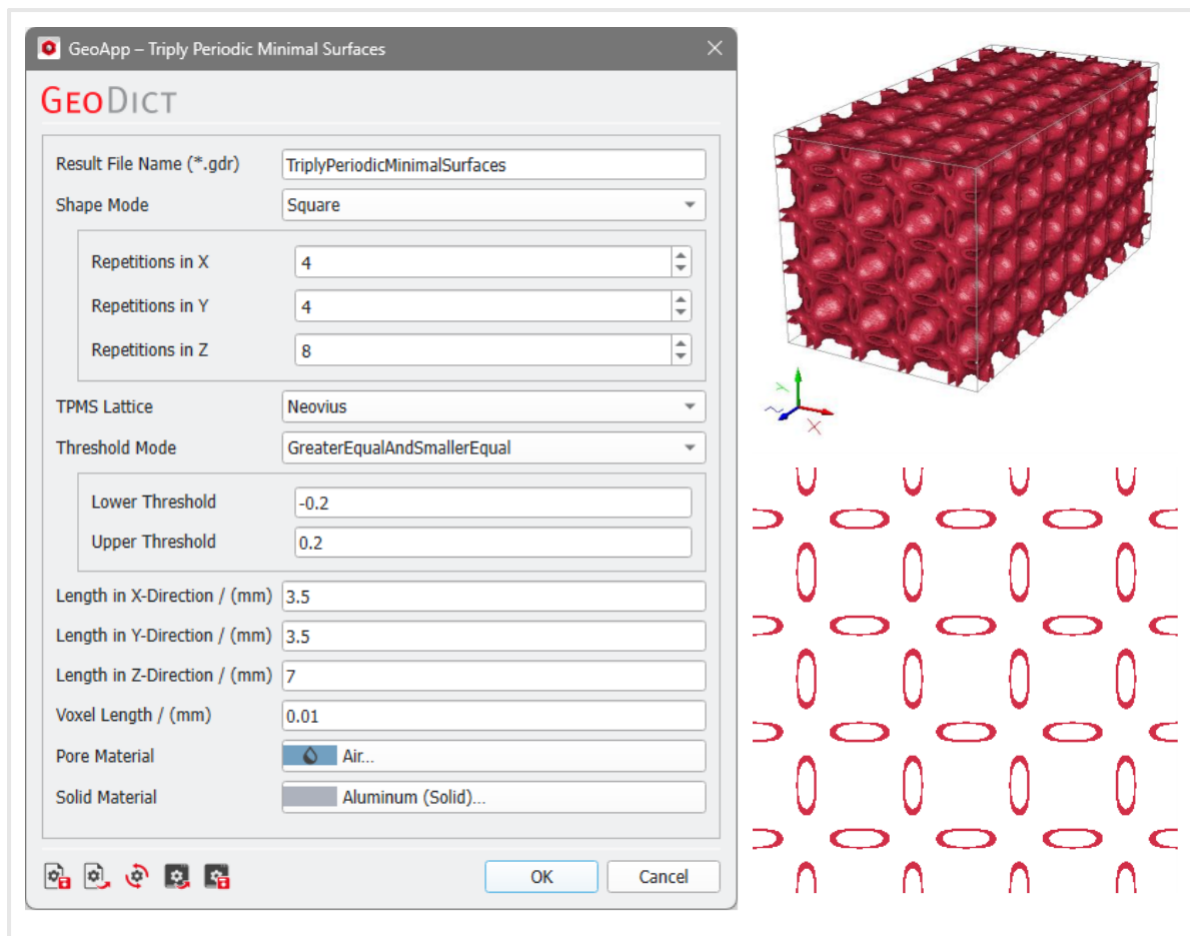
Square Shape mode

✓ Gyroid

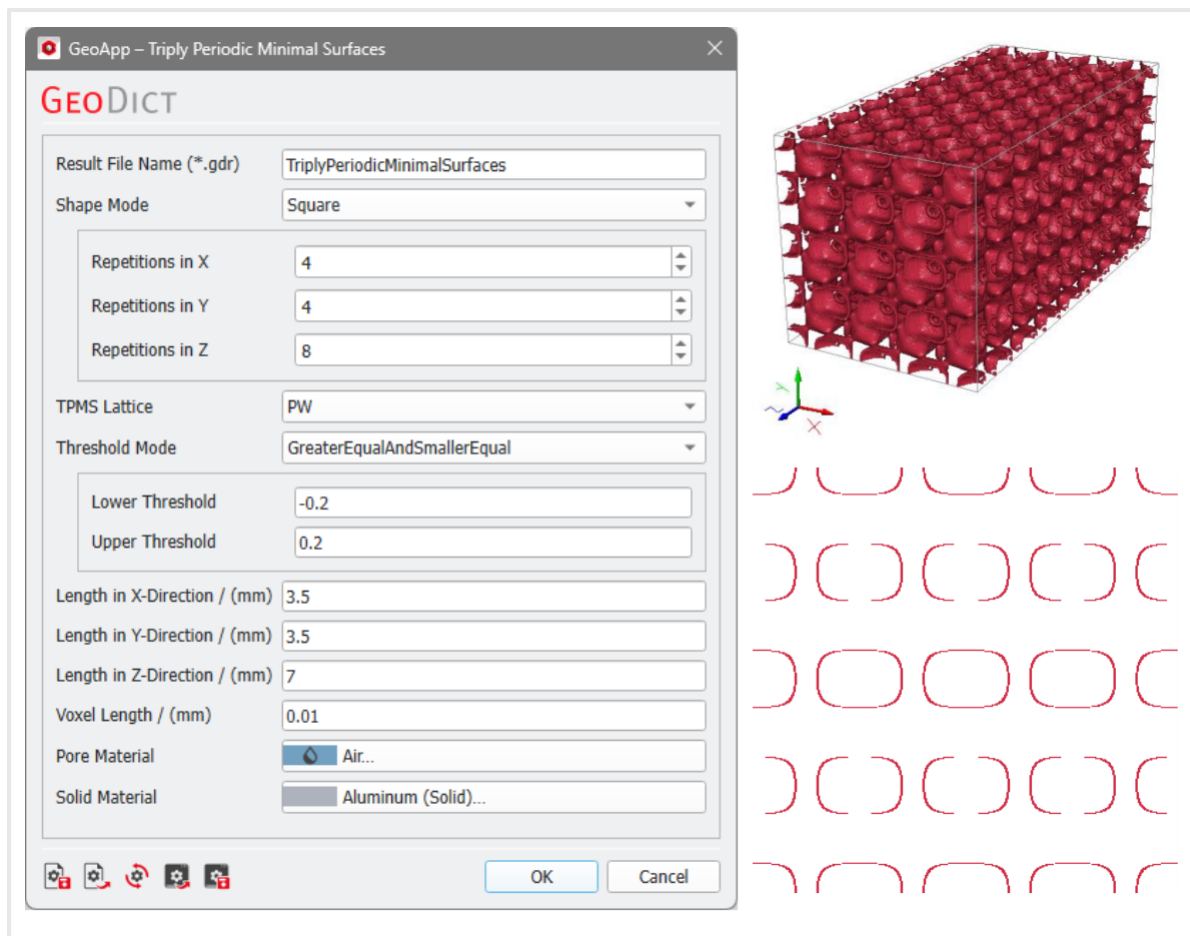


I-WP

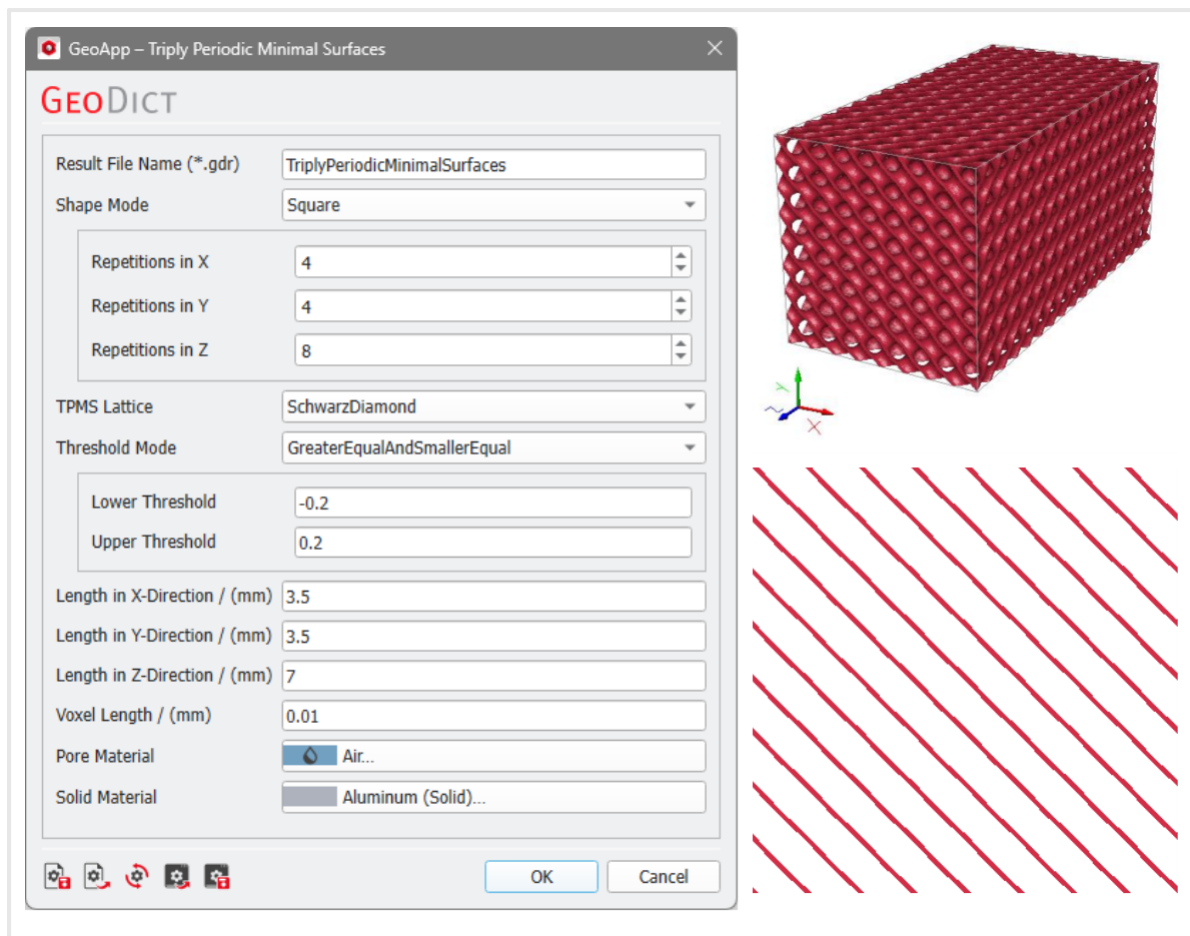




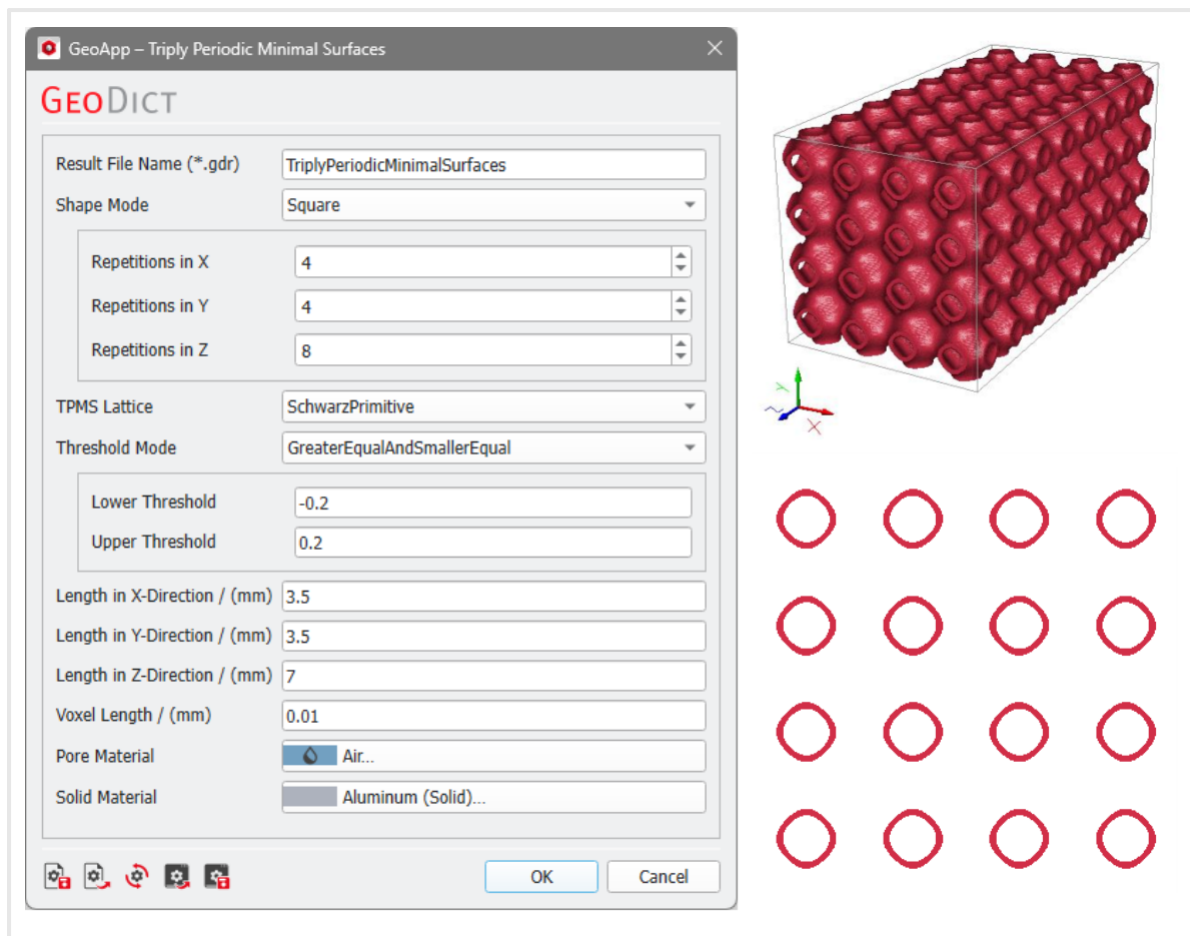
✓ P-W



✓ Schwarz-Diamond

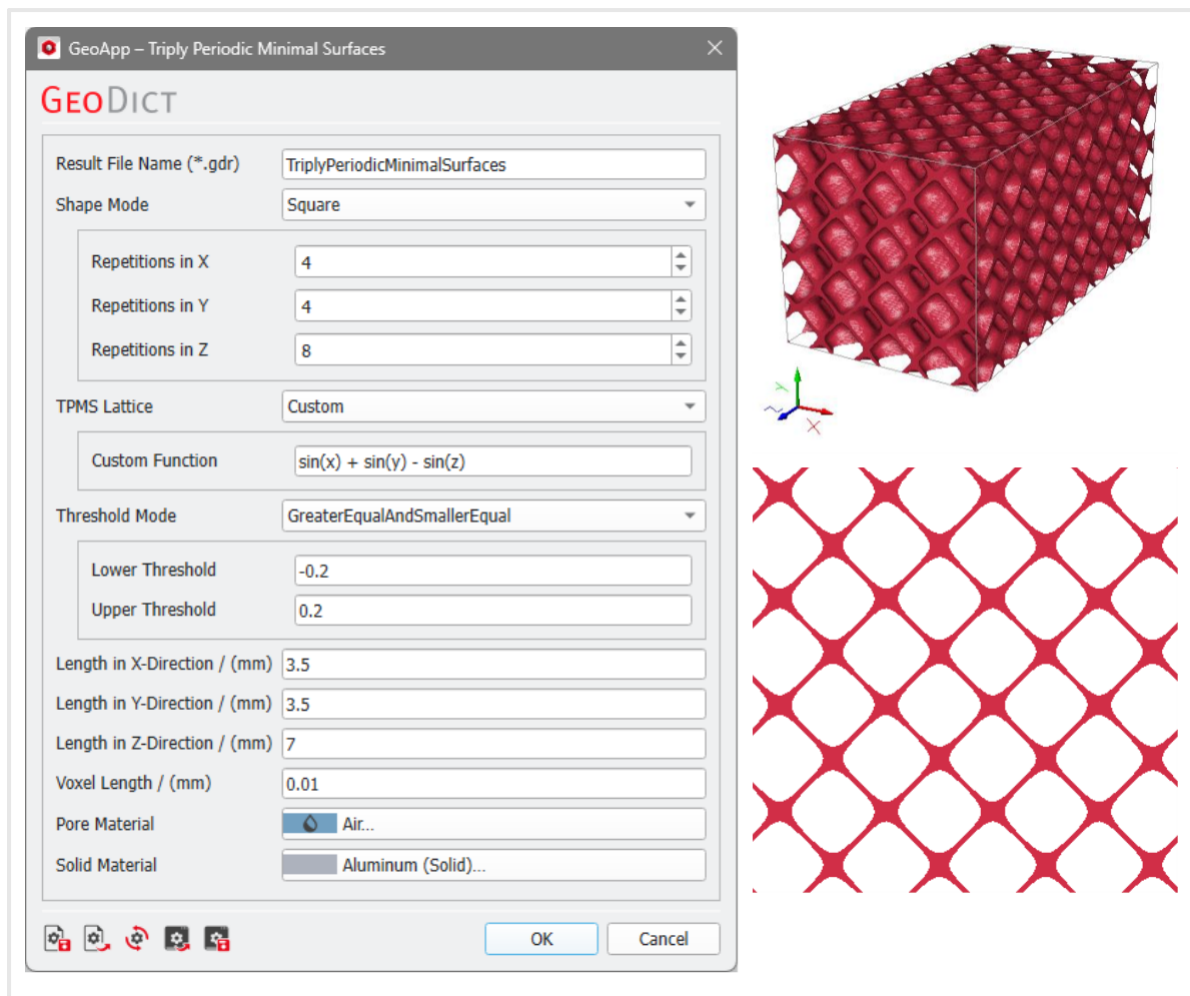


✓ Schwarz-Primitive



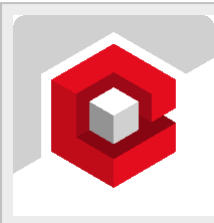
✓ Custom

A custom function in python syntax can be specified to produce a grid of triply periodic minimal surfaces.



1.9 Woven Mesh Materials GeoApps

Generate and analyze woven mesh materials with the **Woven Mesh Materials** GeoApps.



New in GeoDict 2026

- The two GeoApps in this GeoApp section are not new in GeoDict. But it is new that you can also get them from the GeoApp menu.

Find the following **Woven Mesh Materials** GeoApp groups:

- [Geometric Properties](#)^[230]
Compute geometric properties.
- [Structure Generation](#)^[232]
Create Woven Mesh Material structures.

1.9.1 Geometric Properties

Use the **Geometric Properties** GeoApps to analyze woven mesh materials.

Analyze woven mesh materials with the following GeoApps:

- [ASTM Calculation Factor](#)^[230]
Determine the Calculation Factor to convert a test pressure result to a pore size as stated in the ASTM E3278 – 21 norm.

ASTM Calculation Factor

The Pore Analysis GeoApps section contains a GeoApp for the calculation of the ASTM pore size calculation factor according to the ASTM E3278-21 standard.

In this standard, the hydraulic diameter bubble point pressure, percolation path fitting particle diameter, and pore size calculation factor (CF) are generated using the PoroDict module of GeoDict. The CF is used to calculate the pore size of filter cloth from the measured bubble point pressure. These parameters are derived from the non-circular cross-section of the bottleneck through-path of the filter cloth.

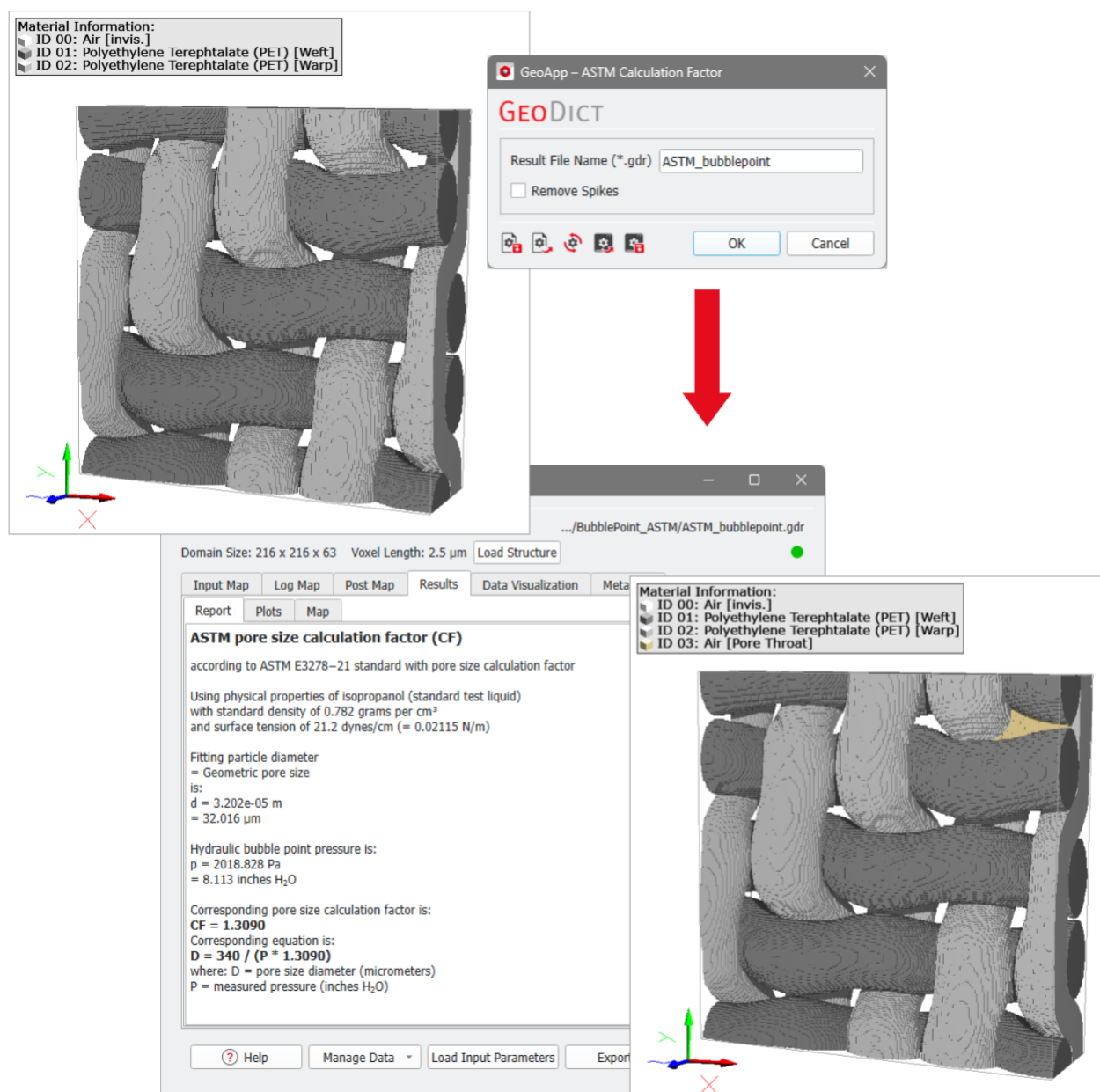
This method employs a capillary flow technique in which air pressure is applied to drive a bubble through a flat specimen of industrial woven wire filter cloth wetted with a liquid of known surface tension. As the required pressure is inversely proportional to the pore size, the measured bubble point pressure is used to determine the pore size. The procedure defines the measurement and standardization of pressure and the calculation of pore size using the CF factor.

For further details, refer to the [GeoDict website](#) and [ASTM E3278-21](#) standard.

The bubble point pressure calculation factor can be determined using only geometric information, i.e., pore throat area and pore throat circumference. To calculate the CF, a

distance map and a percolation path are computed, and local minima in the distance map are used to identify candidate pore throat locations. At each candidate, cutting planes with varying orientations are evaluated using planar ray tracing to determine the cross-sectional area and circumference. The plane with the minimum area defines the effective pore throat, from which the CF is computed. This approach enables accurate bubble point estimation for complex, non-circular pore geometries.

The computation of the ASTM pore size calculation factor was tested and optimized on several metal wire weaves. In the ASTM test, the wire weaves are put in a containment filled with water, while air is injected from below the weave. The bubble point pressure is reached when the first air bubble pushes through the weave layer.



The available result files in the **Data Visualization** tab of the Result Viewer are the same as for the Bubble Point command.

1.9.2 Structure Generation

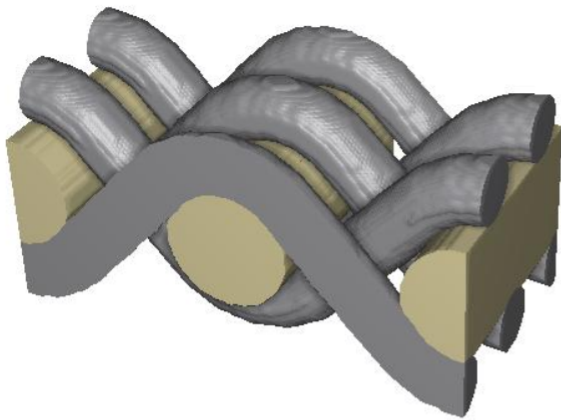
Use the **Structure Generation** GeoApps to create woven mesh materials.

Create woven mesh materials with the following GeoApps:

- [Dutch Weave](#)²³²
Generate Plain Dutch or Twill Dutch Weaves.

Dutch Weave

With this GeoApp, you can generate Plain Dutch Weaves or Twill Dutch Weaves. Please refer to the Plain Weave and Twill Weave section for an explanation of the parameters. The resulting structures for the default parameter sets are displayed below.



GeoApp – Dutch Weave

GEO DICT

Result File Name (*.gdr)

Voxel Length / (μm)

Material

Weaving Pattern

Number of Cells in X/Weft Dir.

Number of Cells in Y/Warp Dir.

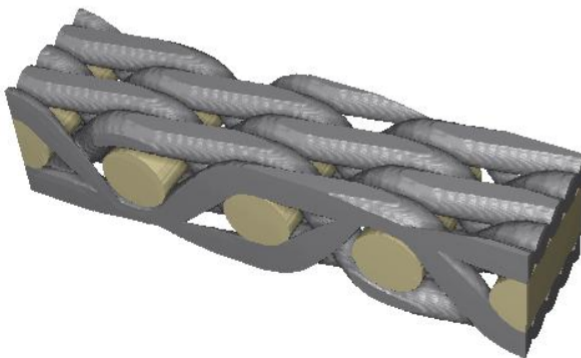
Weft Diameter / (μm)

Weft Broadening

Warp Diameter / (μm)

Warp Pitch / (μm)

OK Cancel



GeoApp – Dutch Weave

GEO DICT

Result File Name (*.gdr)

Voxel Length / (μm)

Material

Weaving Pattern

Float Factor 1

Float Factor 2

Adjust Weft Pitch / (μm)

Number of Cells in X/Weft Dir.

Number of Cells in Y/Warp Dir.

Weft Diameter / (μm)

Weft Broadening

Warp Diameter / (μm)

Warp Pitch / (μm)

OK Cancel

1.10 3rd Party GeoApps

In this GeoApp group **3rd Party** apps can be found, i.e., GeoApps that were not created by Math2Market.

Topics of this section

- [FiberMath](#)  234
This is a special fiber generator for very dense packing in composite materials created by Fraunhofer ITWM.

1.10.1 FiberMath

The **FiberMath** GeoApp is a specialized fiber generator designed for dense packings in composite materials.



Modules needed to run this GeoApp:

GeoApp-FiberMath

FiberMath can generate structures with several fiber types, each with their own set of geometry parameters. Fiber types can either be mixed or separated into layers in the depth direction. This allows, e.g., the generation of structures with a middle layer where the fiber orientation is planar-isotropic, as it is typical for injection-molded components.

Clicking **Run** opens the **Fiber Geometry Generator** parameters dialog.



FiberMath is developed and maintained by Fraunhofer ITWM.

[Open the FiberMath User Guide.](#)

Find more information about this GeoApp on the website of [Fraunhofer ITWM](#) and on the corresponding [module page](#) on our website.

1.11 Adding Custom GeoApps

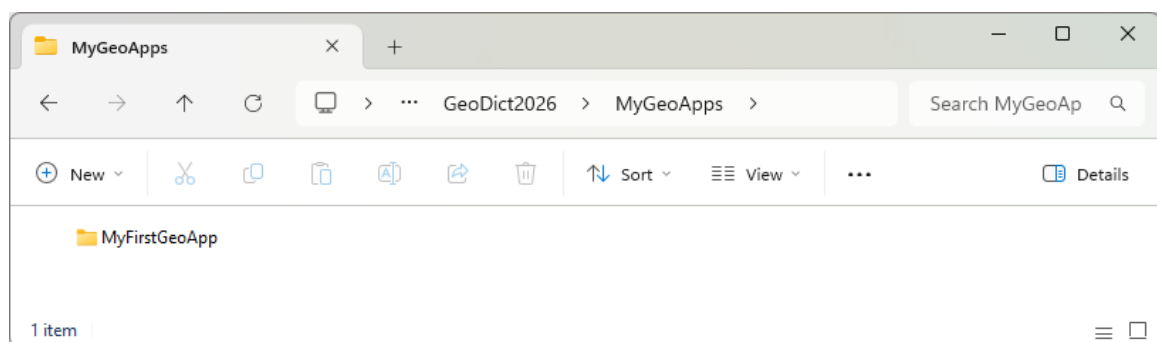
There are two possibilities to add custom GeoApps. They can either be added locally without administrator rights or for all users by the system administrator.

✓ Locally adding custom GeoApps

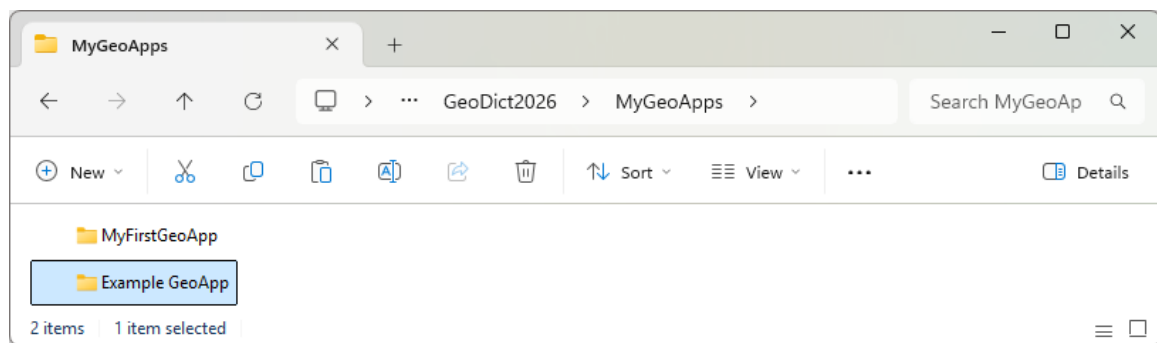
To only locally add your custom GeoApps, browse for the **MyGeoApps** folder in the GeoDict settings folder. For Windows this is located under **C:**

\Users\Username\GeoDict2026\MyGeoApps.

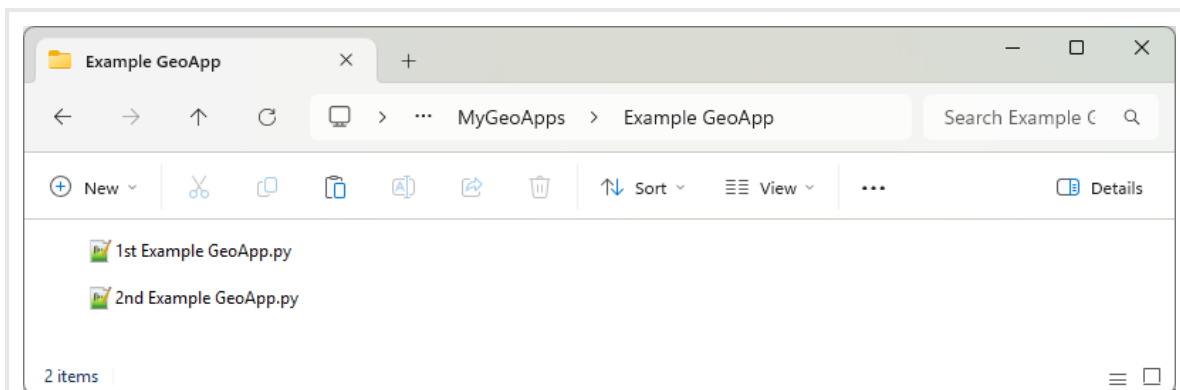
By default, this folder only contains the example MyFirstGeoApp, but you may place additional apps, which then are available for you only.



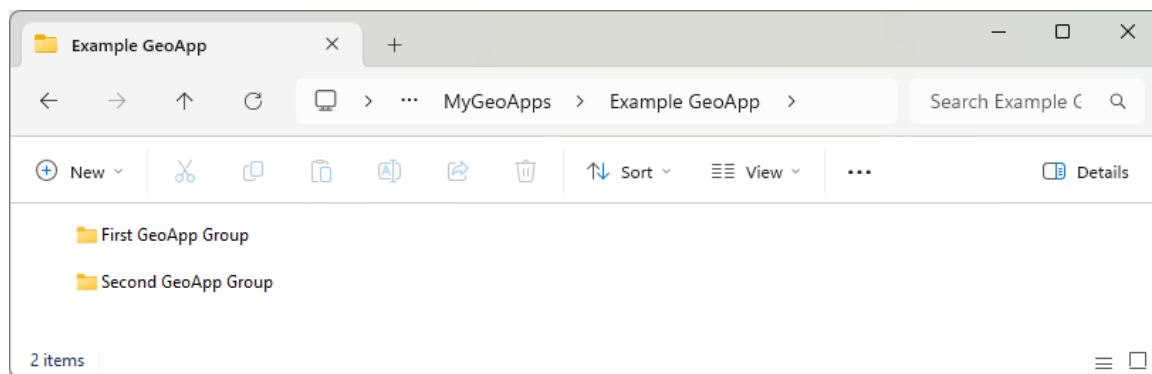
For this, create a new folder inside the MyGeoApps folder. In the example below, the **Example GeoApp** folder is added. The name of this folder will be displayed later under the **GeoApp** menu in the GeoDict Graphical User Interface (GUI).



In the new folder, place the GeoPy files that will be selectable from the pull-down menu in the new GeoApp. Here, for example, the two scripts: **1st Example GeoApp.py** and **2nd Example GeoApp.py**.

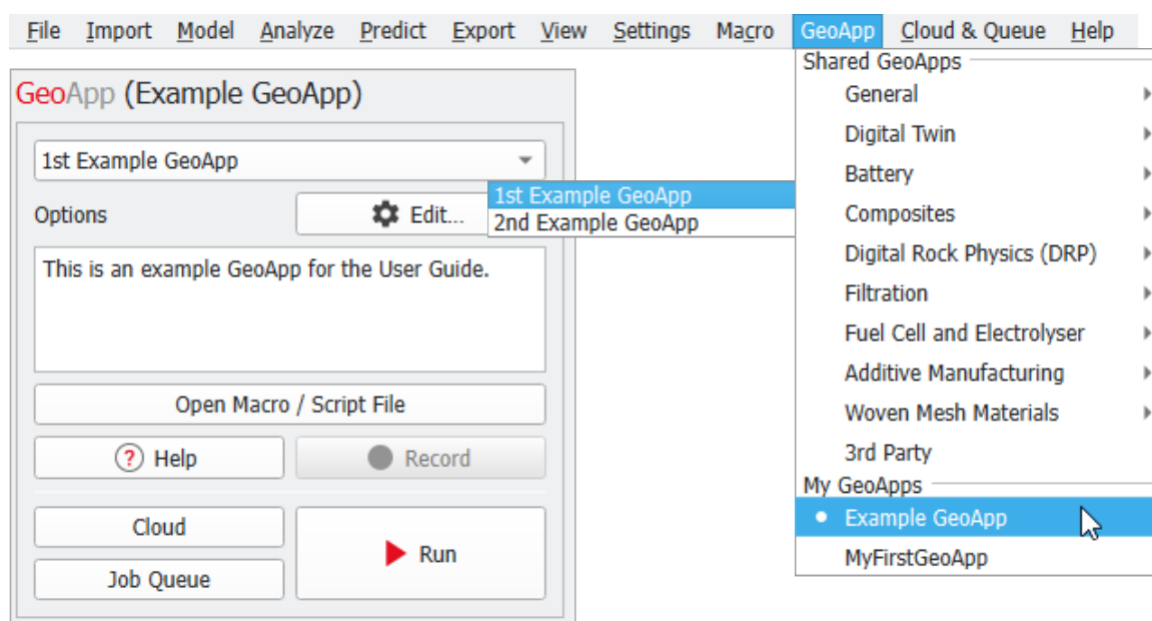


Alternatively, the GeoApps scripts can be grouped into subfolders.

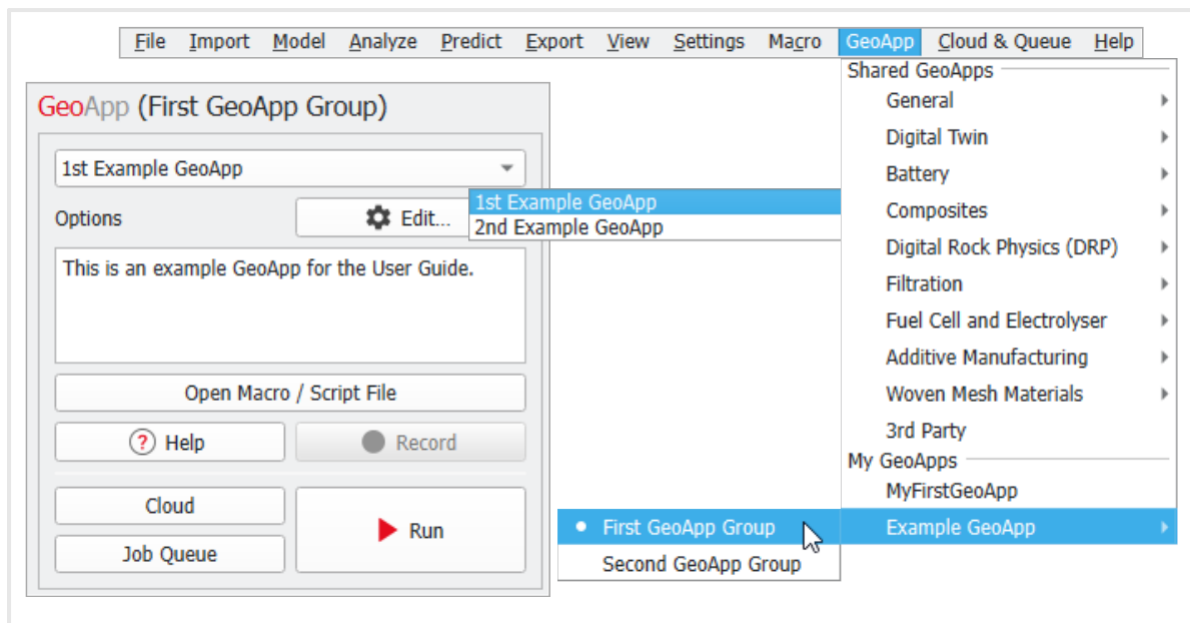


How to create a GeoPy file containing parameters accessible from the GeoDict GUI is described in the GeoPy scripting section.

After restarting GeoDict, the new app will be available from the GeoApp menu. If selected, in the GeoApp section the new apps are displayed in the My GeoApps section and can be opened in a text editor and run as described [here](#).



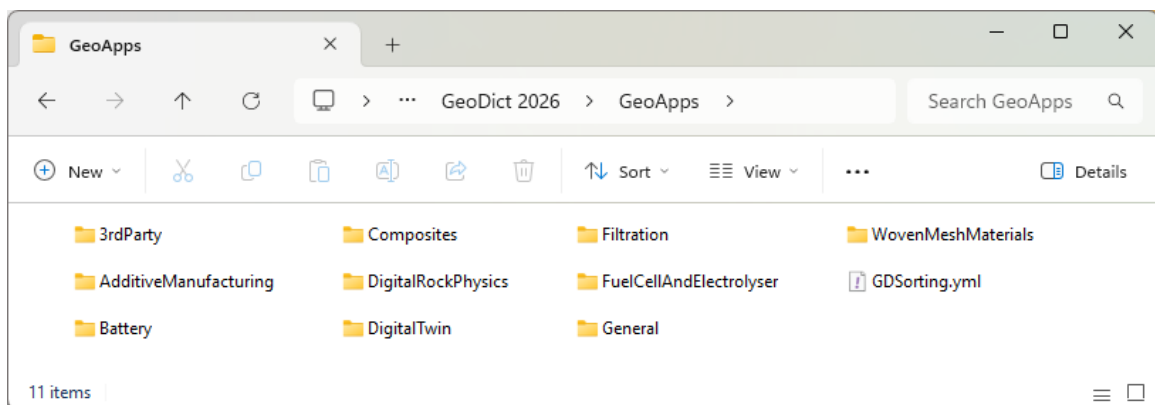
If organizing the GeoPy files in groups the GeoApp menu looks as follows:



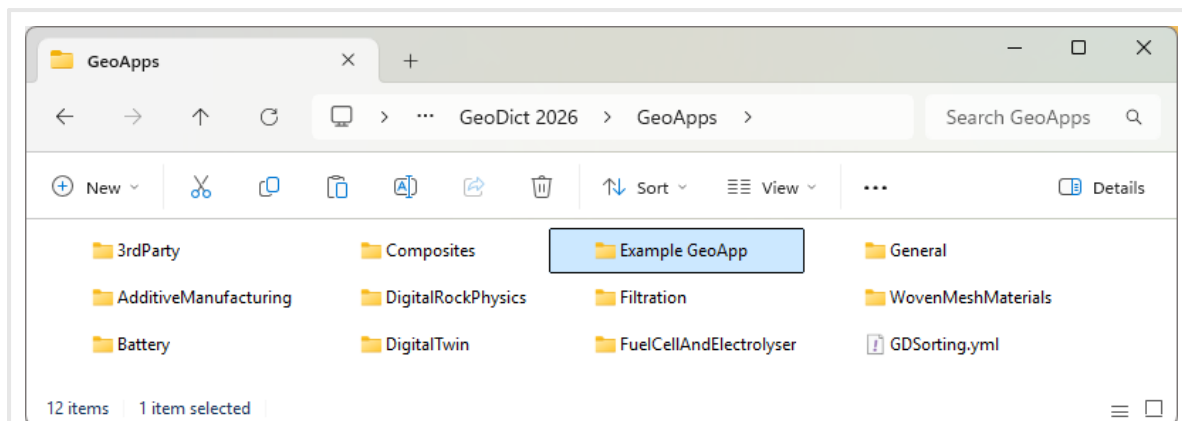
✓ Globally adding custom GeoApps

All GeoApps are stored in the **GeoApps** folder included in the GeoDict installation folder.

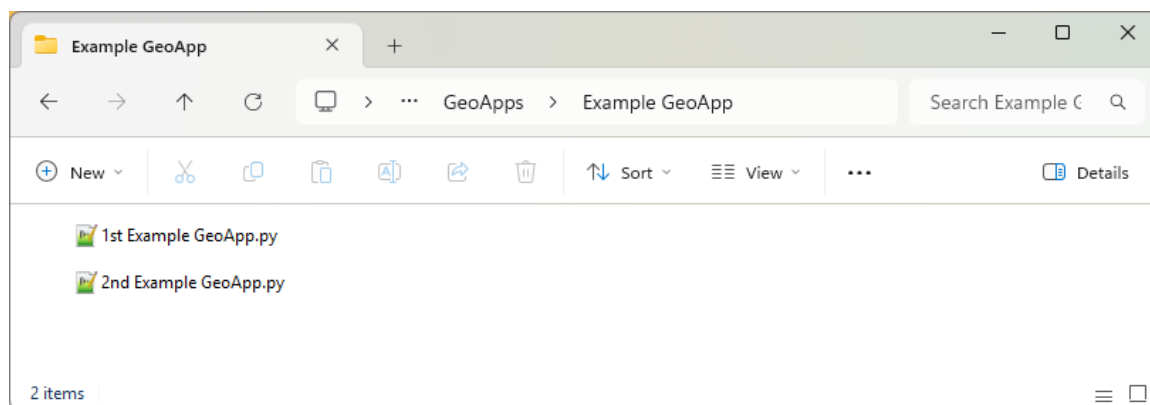
Below, the apps in the installation folder **C:\Program Files\Math2Market GmbH\GeoDict 2026\GeoApps** are shown. Several GeoApp groups are included in the standard installation package, but additional apps may be placed there by your system administrator making them available for all users.



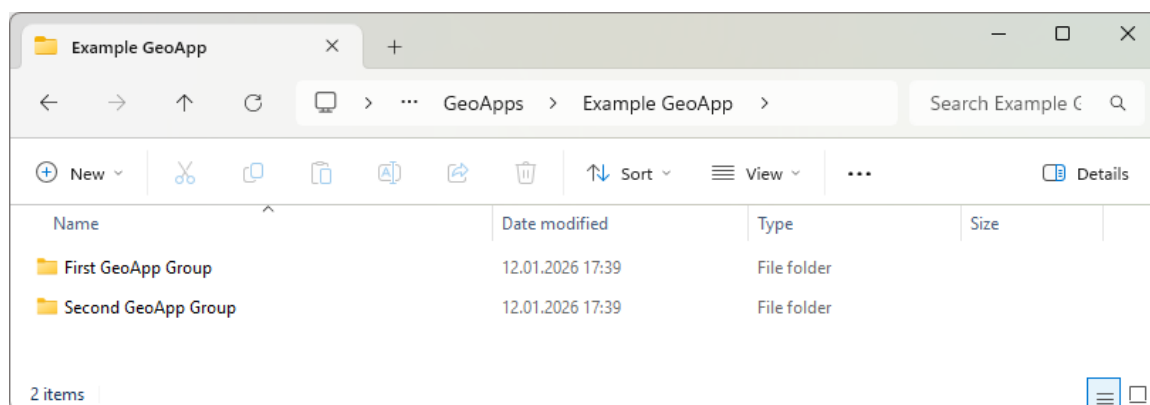
For this, create a new folder inside the GeoApp folder. In the example below, the **Example GeoApp** folder is added. The name of this folder will be displayed later under the **GeoApp** menu in the GeoDict Graphical User Interface (GUI).



In the new folder, place the GeoPy files that will be selectable from the pull-down menu in the new GeoApp. Here, for example, the two scripts: **1st Example GeoApp.py** and **2nd Example GeoApp.py**. How to create a GeoPy file containing parameters accessible from the GeoDict GUI is described in the GeoPy scripting User Guide.

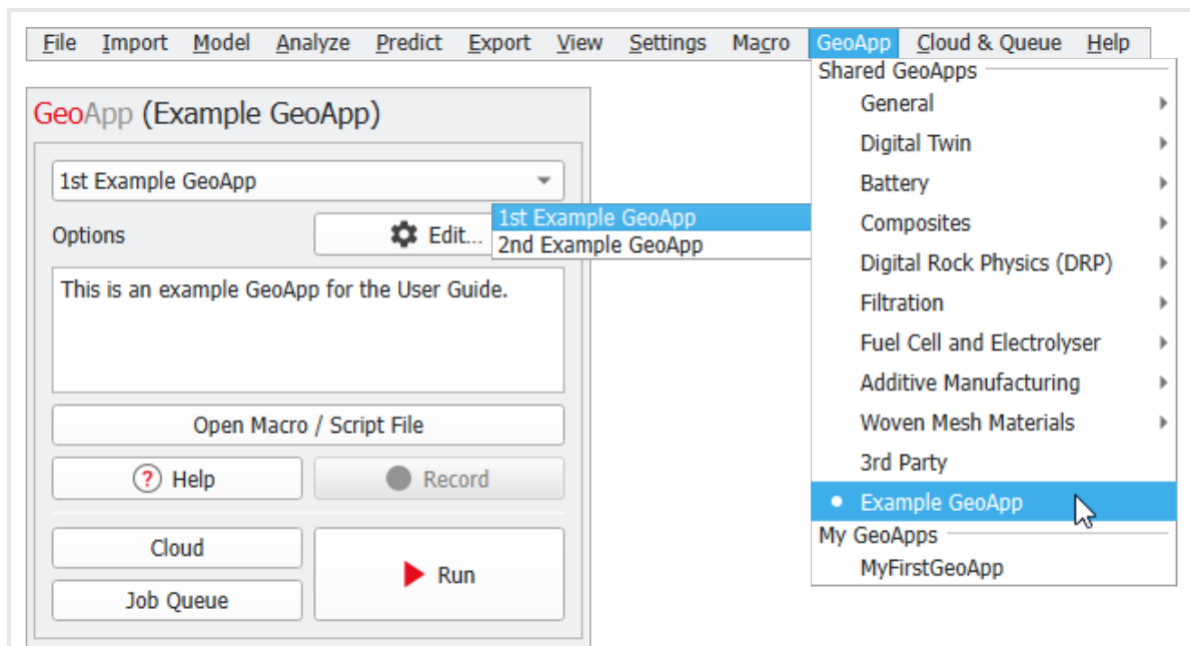


Alternatively, the GeoApps scripts can be grouped into subfolders.

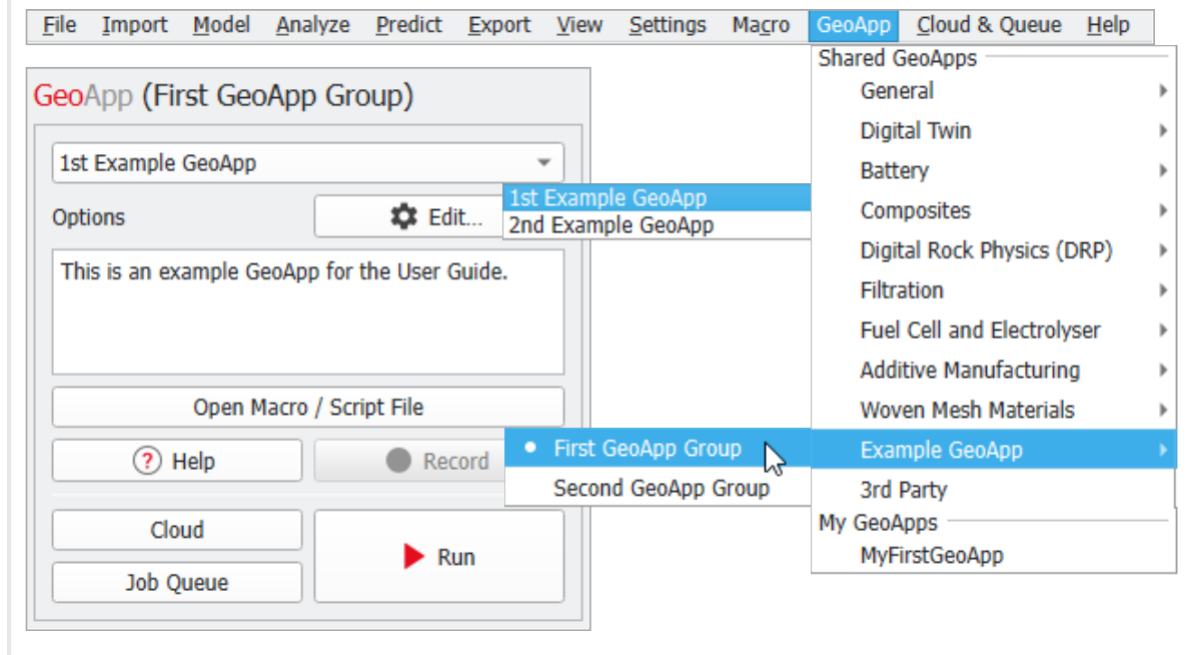


If thematical fitting to one of the existing GeoApp categories, the custom app can of course also be placed there.

After restarting GeoDict, the new app will be available from the GeoApp menu. If selected, in the GeoApp section the new apps are displayed in the Shared GeoApps section and can be edited and run as described [here](#)⁴.



If organizing the GeoPy files in groups the GeoApp menu looks as follows:



1.12 References

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