GeoDict®

Material Database Reference

User Guide

GeoDict release 2022

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GeoDict

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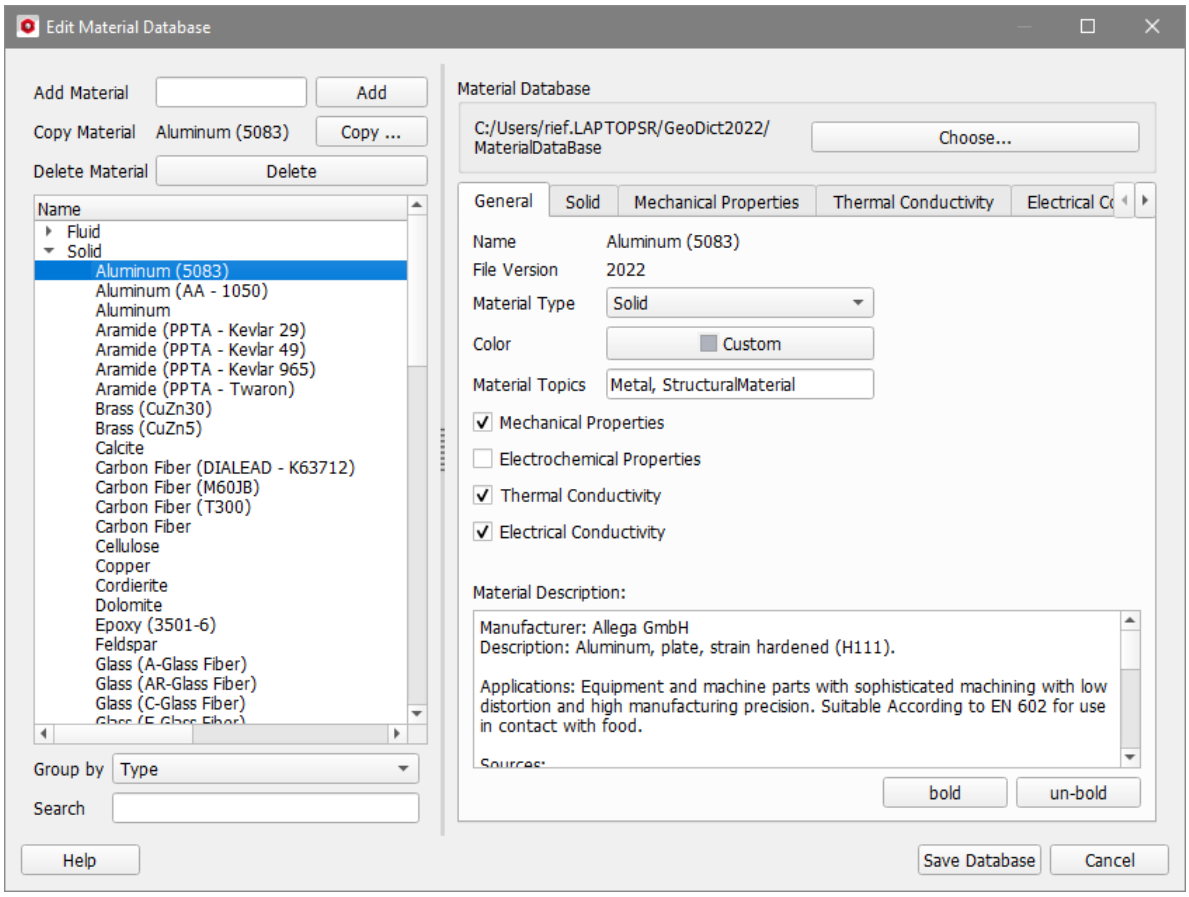
THE GEODICT MATERIAL DATABASE

Structures in GeoDict are 3D voxel images where each voxel has one of 16 possible material IDs. To each of these material IDs, a material can be assigned. This means that a structure in GeoDict can contain up to 16 different materials. Materials in GeoDict can contain all material properties that are needed for simulations in GeoDict.

The GeoDict material database is the place to store material data. A selection of standard materials is already predefined, but the true strength of the database is that it allows the user to define additional materials to be used in GeoDict simulations.

The information for each material in the GeoDict material database is saved as a *.txt file in the material database folder. Therefore, materials can either be edited in the material database editor or by editing the corresponding *.txt file. Materials can be exchanged by copying these *.txt files.



Materials can be assigned to GeoDict structures during the creation with GeoDict structure generation modules (e.g., FiberGeo, GrainGeo, WeaveGeo…) or during the import from e.g., µCT-scans. Additionally, they can be set for the structure currently in memory. When saving a structure in a GeoDict format (as *.gdt or *.gad file), its constituent materials and their properties are saved in that file, too.

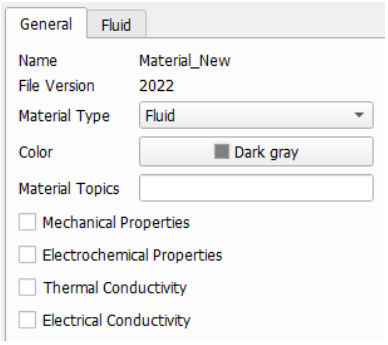
This allows for directly simulating on a structure loaded from its file, there is no necessity to select the materials for the simulation run. However, it is always possible to change the materials and their properties prior to simulation.

MATERIALS IN GEODICT

Three material types are available in GeoDict: **Fluid**, **Porous** and **Solid**. Depending on the material type, different material properties can be assigned.

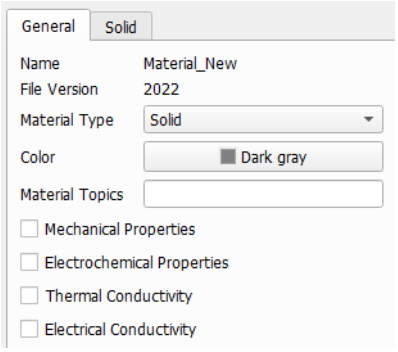
- For a **Fluid**, the density and the dynamic and kinematic viscosity must be defined. Additionally, **Mechanical Properties**, **Electrochemical Properties**, **Thermal Conductivity**, and **Electrical Conductivity** can be selected as optional parameters.

  Thermal Conductivity and **Electrical Conductivity** can be temperature dependent, and the mechanical properties contain the option to add a thermal expansion coefficient.



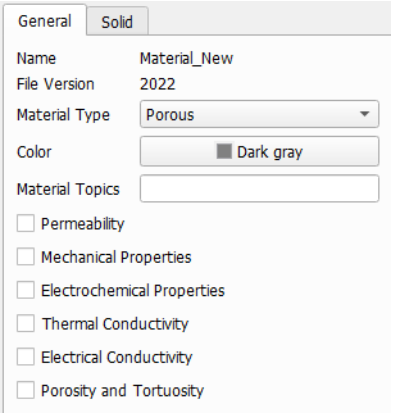
- For **Solid** materials, only the density must be defined. Additionally, **Mechanical Properties**, **Electrochemical Properties**, **Thermal Conductivity**, and **Electrical Conductivity** can be selected as optional parameters.

  Thermal Conductivity and **Electrical Conductivity** can be temperature dependent, and the mechanical properties contain the option to add a thermal expansion coefficient.



- **Porous** materials have the same options as **Solid** materials, but they additionally allow to define the **Permeability** and **Porosity and Tortuosity**.

  The **Porosity** and **Tortuosity** cannot be set to be temperature dependent.

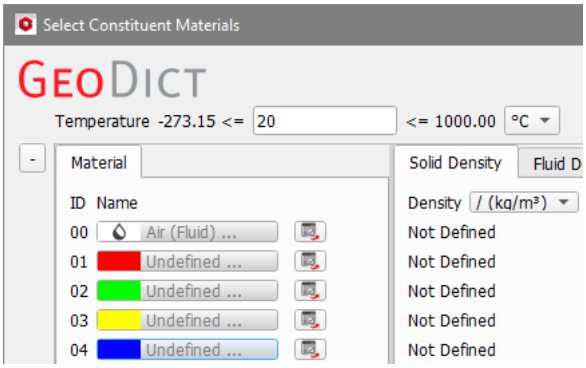


Materials can either be selected from the GeoDict material database or **Manual** materials can be defined during the creation of a microstructure using the GeoDict structure generation modules or prior to simulation with one of the GeoDict predictor modules.

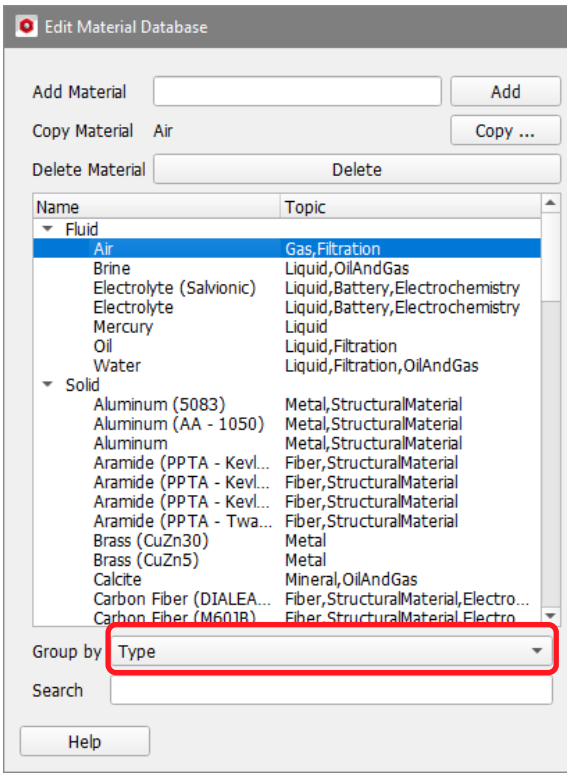
Manual materials allow to quickly set the needed parameters, whereas using materials from the material database allows to reuse them for further simulations. Furthermore, materials defined in the GeoDict material database may have more complex properties than **Manual** materials. For example, when defining a manual material in the ElastoDict settings, it is not possible to select nonlinear material laws.

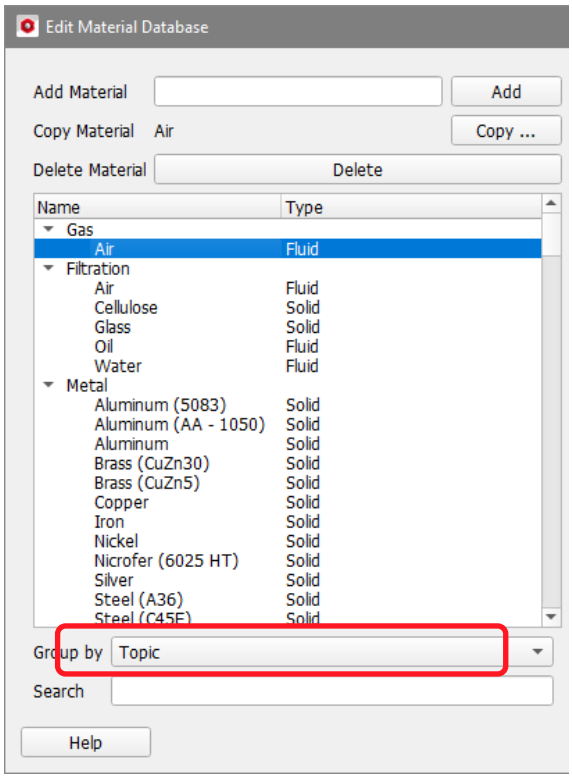
In some cases, the material for a given material ID might be unclear. Then, the material is **Undefined**.

Please choose a material for these IDs before running simulations on the structure.

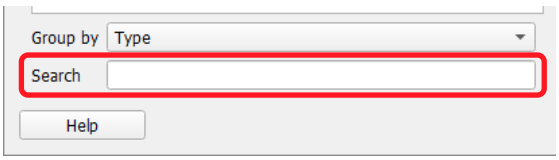


The materials in the material database can be grouped by **Type** or by **Topic**. The types are GeoDicts material categories (**Fluid**, **Solid** and **Porous**), while the topics can be user-defined (See p. 16).





Additionally, the material database can be searched with the search box at the bottom of the material database dialog.

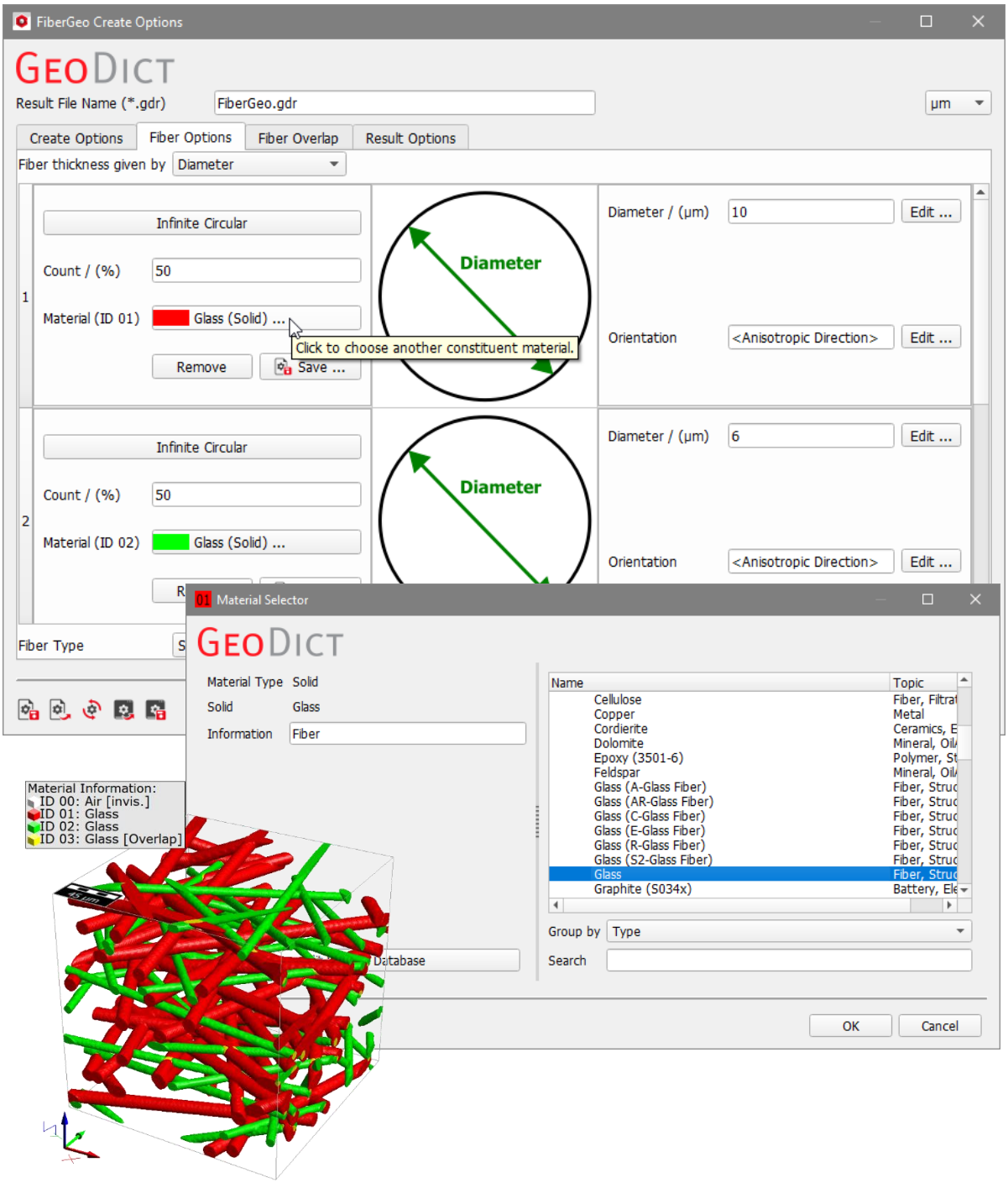


Setting the constituent materials in GeoDict

The constituent materials are selected during the generation of a structure or during the import from 3D image data. Afterwards, the constituent materials can be changed if needed.

Setting materials for structure generation

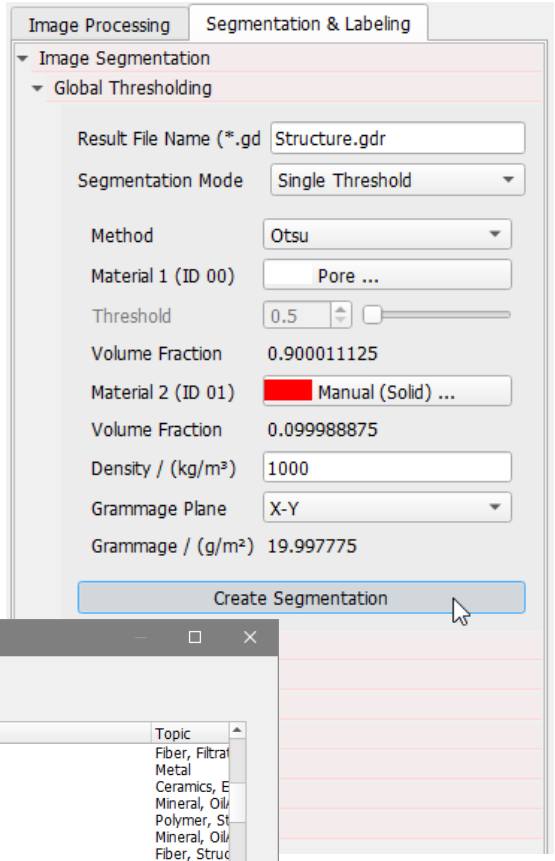
An example for the selection of the constituent materials in FiberGeo is shown below. For each fiber type, the material can be selected by clicking the corresponding button. The **Material Selector** dialog opens, and all materials stored in the current material database are available.

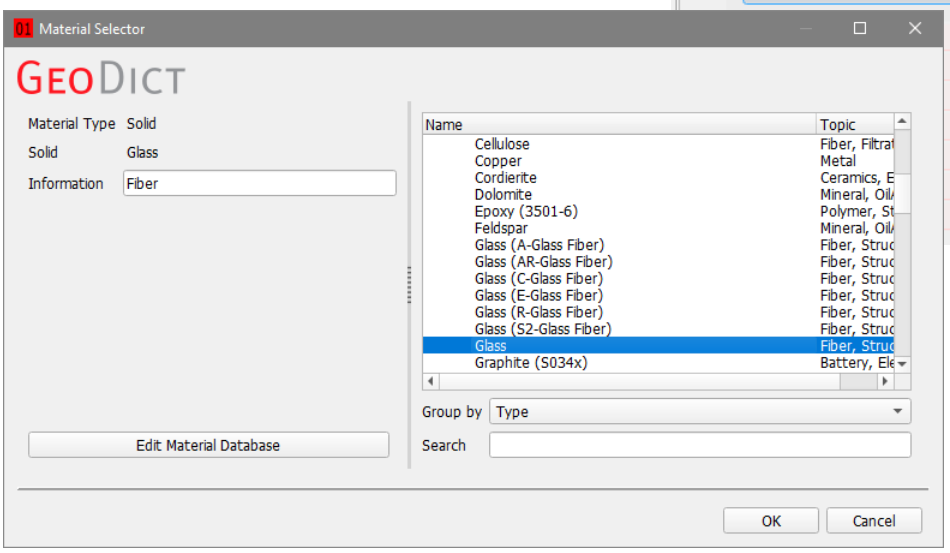


Setting materials during import

When a structure is imported in GeoDict (e.g., from a µCT-scan), its constituent materials can be set during the import.

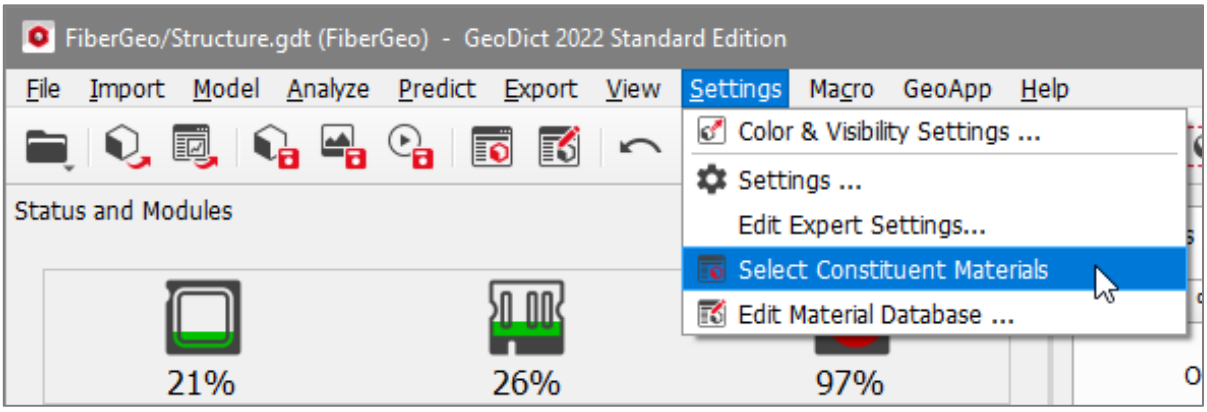
By default, the material with material ID 00 is set to **Pore (Fluid)**, whereas all other material IDs are set to **Manual (Solid)**.

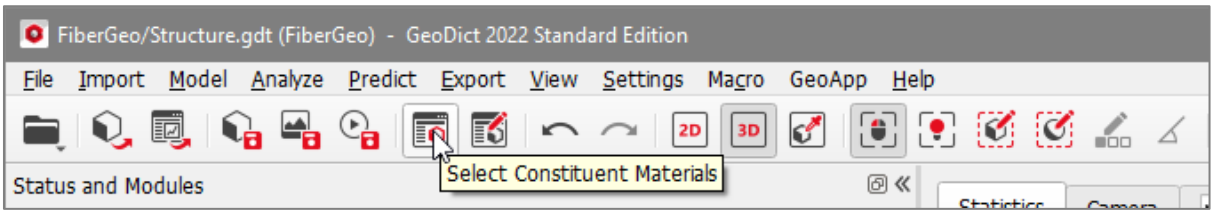




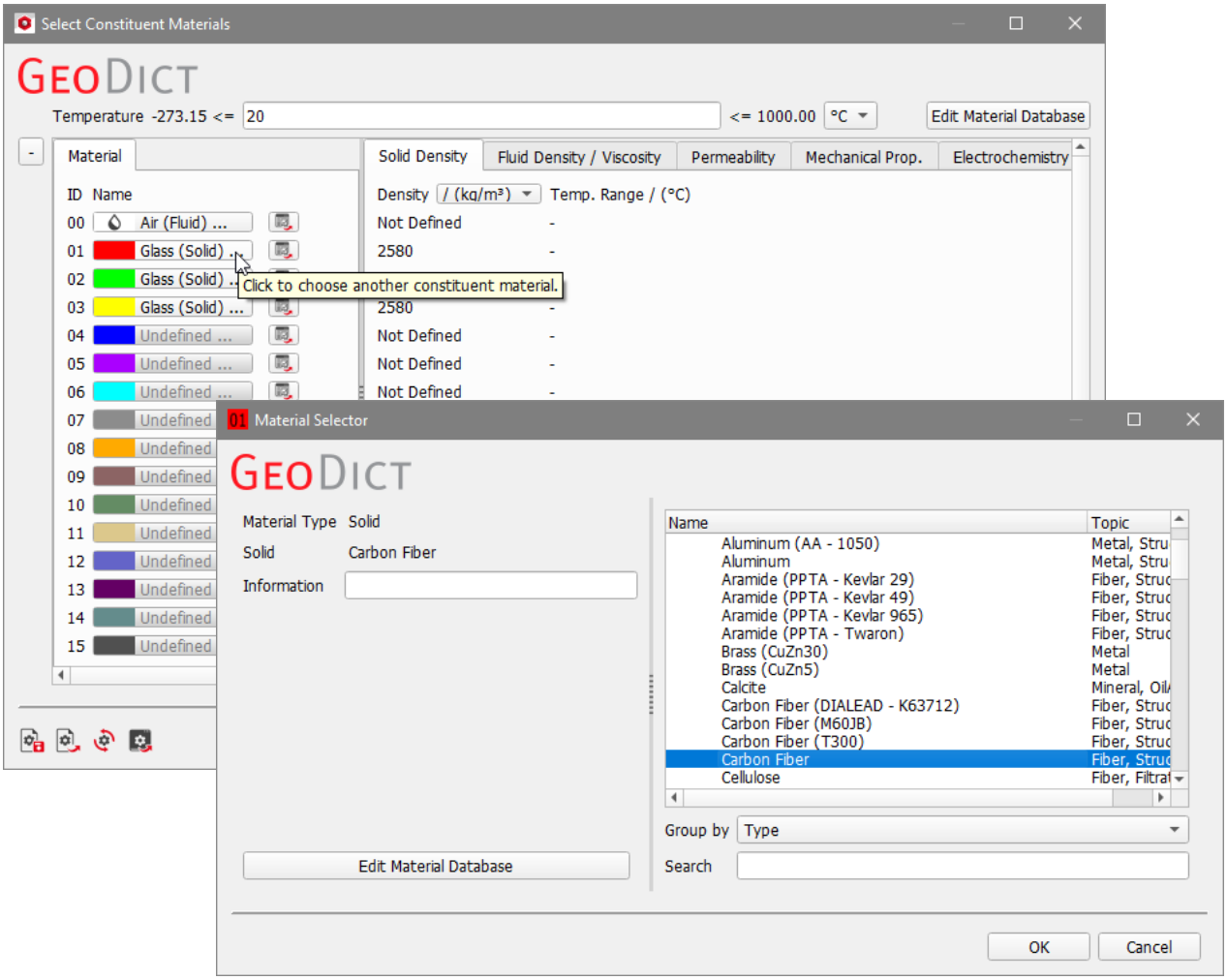
Setting materials for the current structure

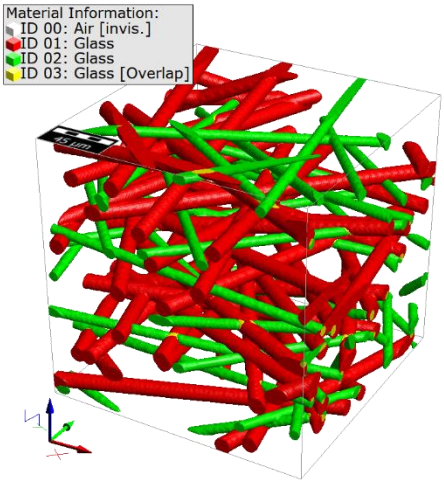
The constituent materials for the structure currently in memory can be changed by selecting **Settings** → **Select Constituent Materials** in the menu bar, or by clicking the corresponding icon in the toolbar.

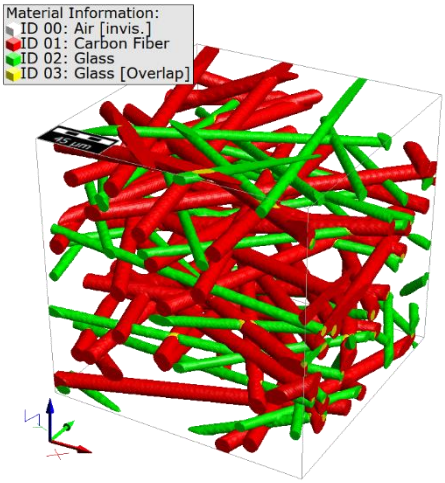




The concept is shown on the structure below: The material assigned to material ID 01 is changed from **Glass** to **Carbon Fiber**.





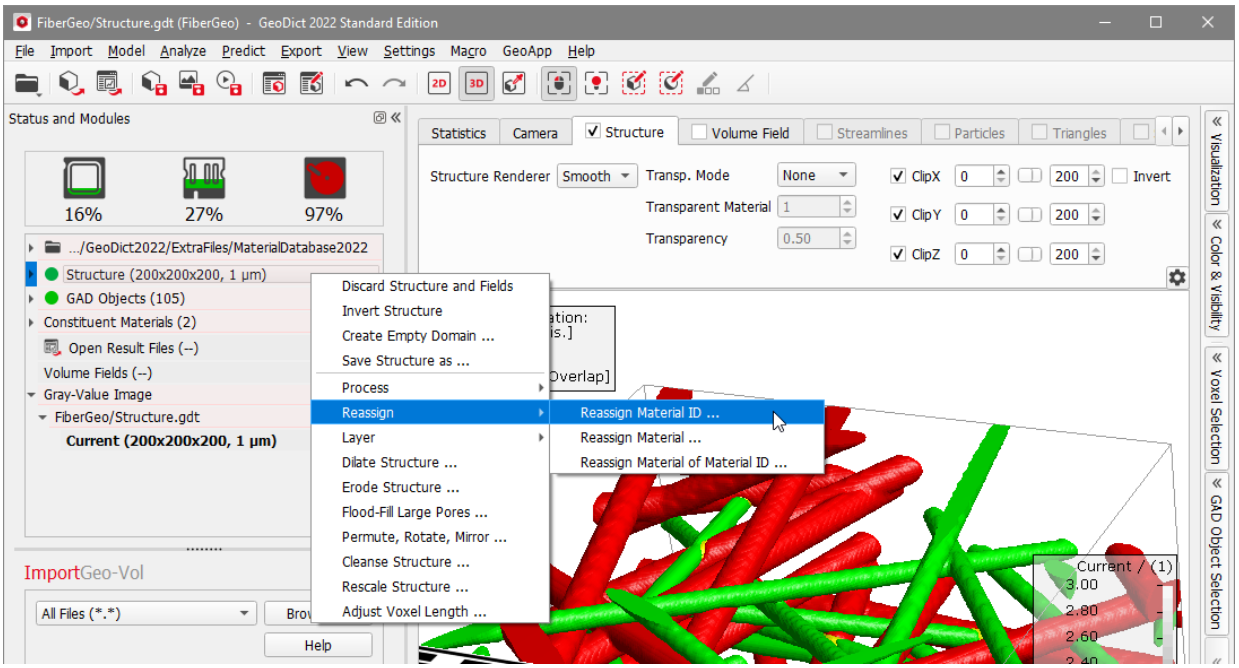


Reassigning Materials and Materials IDs

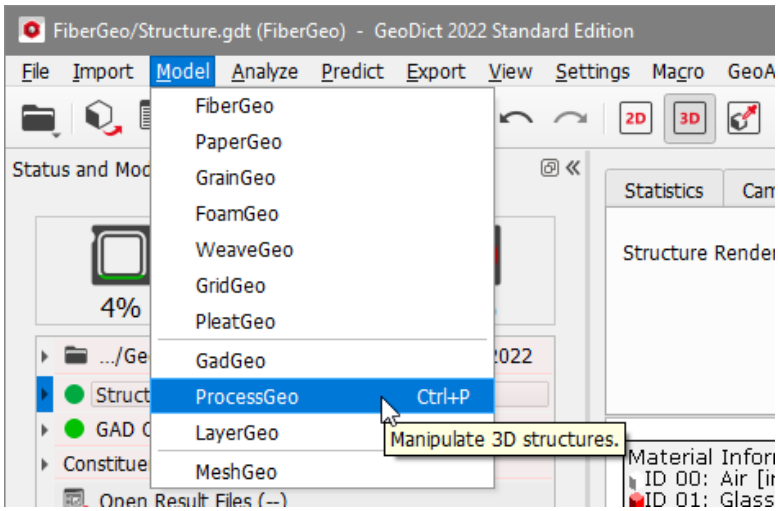
One option to change materials in the structure is the **Select Constituent Materials** dialog, as described above. Depending on the use case, there are other options available through the ProcessGeo module.

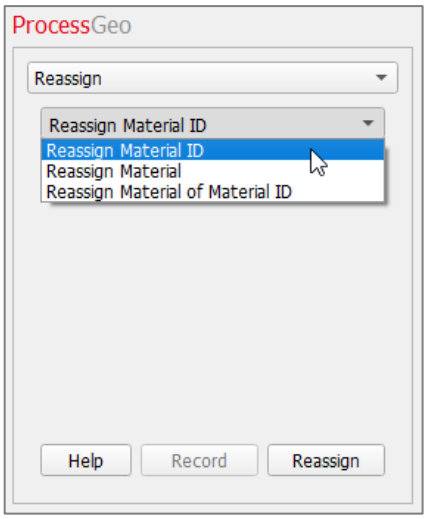
It is possible to **reassign material IDs**, to **reassign materials** and to **reassign the material of a Material ID** (this corresponds to the option in the **Select Constituent Materials** dialog). These options are shortly described here but more information is available in the ProcessGeo handbook of this User Guide.

To access the options for reassigning quickly through a shortcut, right-click on **Structure** in the **Project Status** section on the left side of the GeoDict GUI.



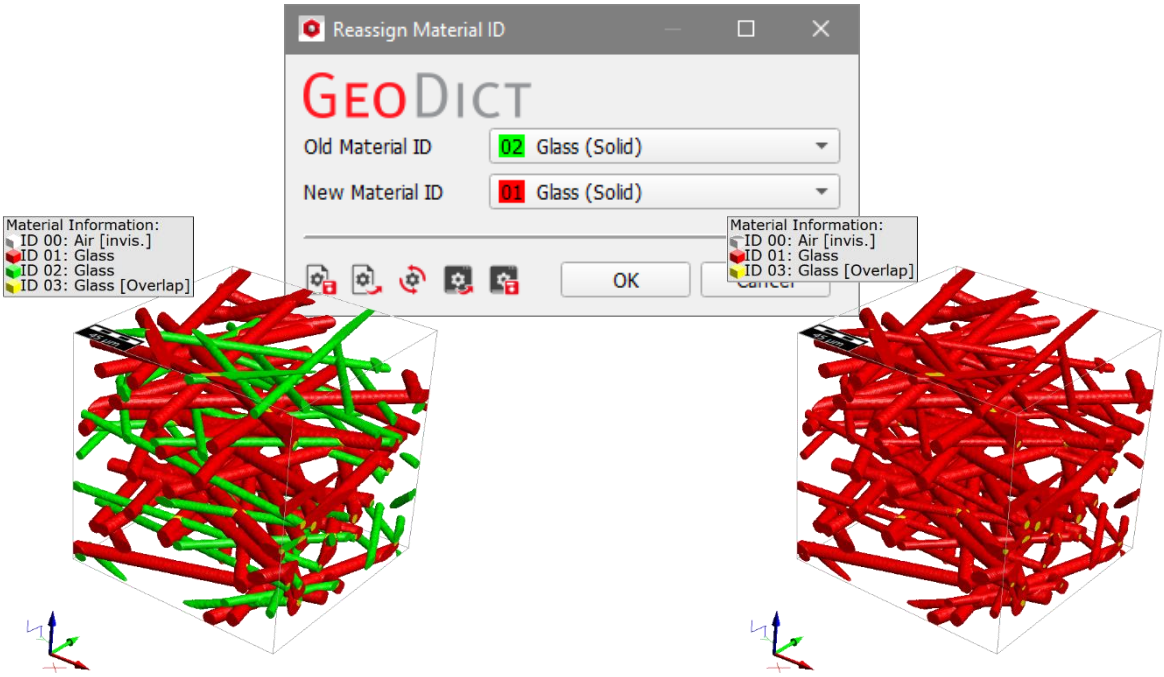
Alternatively, these options are also available from the menu bar by selecting **Model** → **ProcessGeo** → **Reassign.**





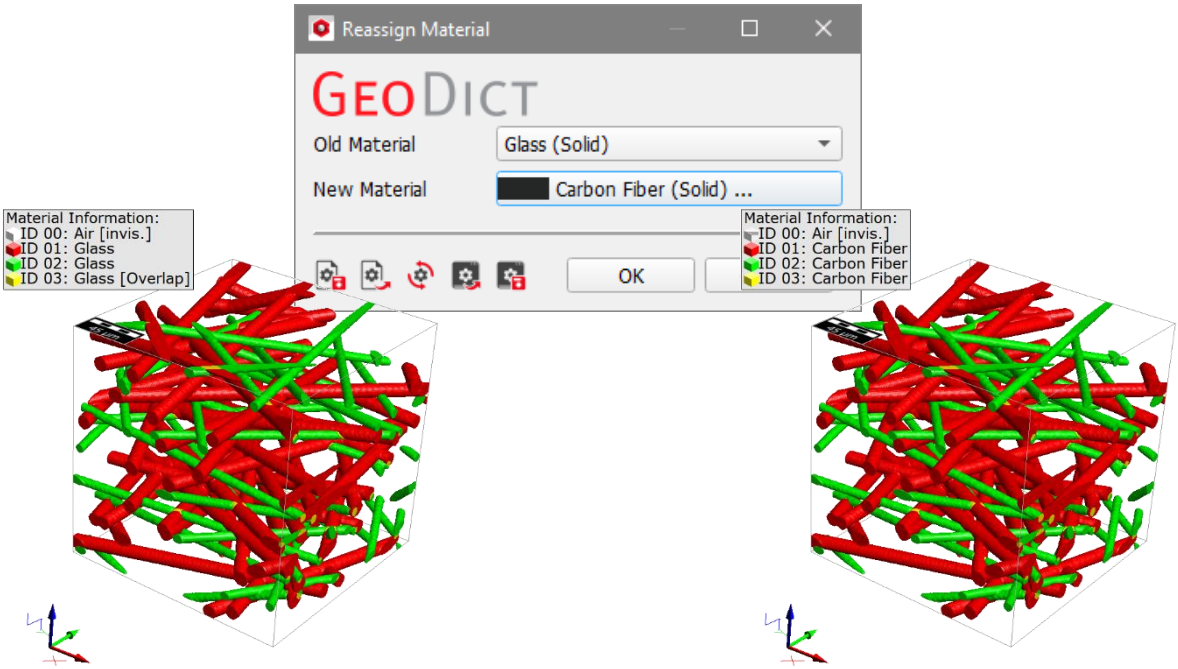
Reassign Material ID

With **Reassign Material ID**, the material ID of the corresponding voxels in the structure is changed. In the example shown below, the material ID 02 is reassigned to the material ID 01. No voxels with material ID 02 remain in the structure, and it is not possible to distinguish which fibers belonged to which ID (01 or 02) after the reassignment.



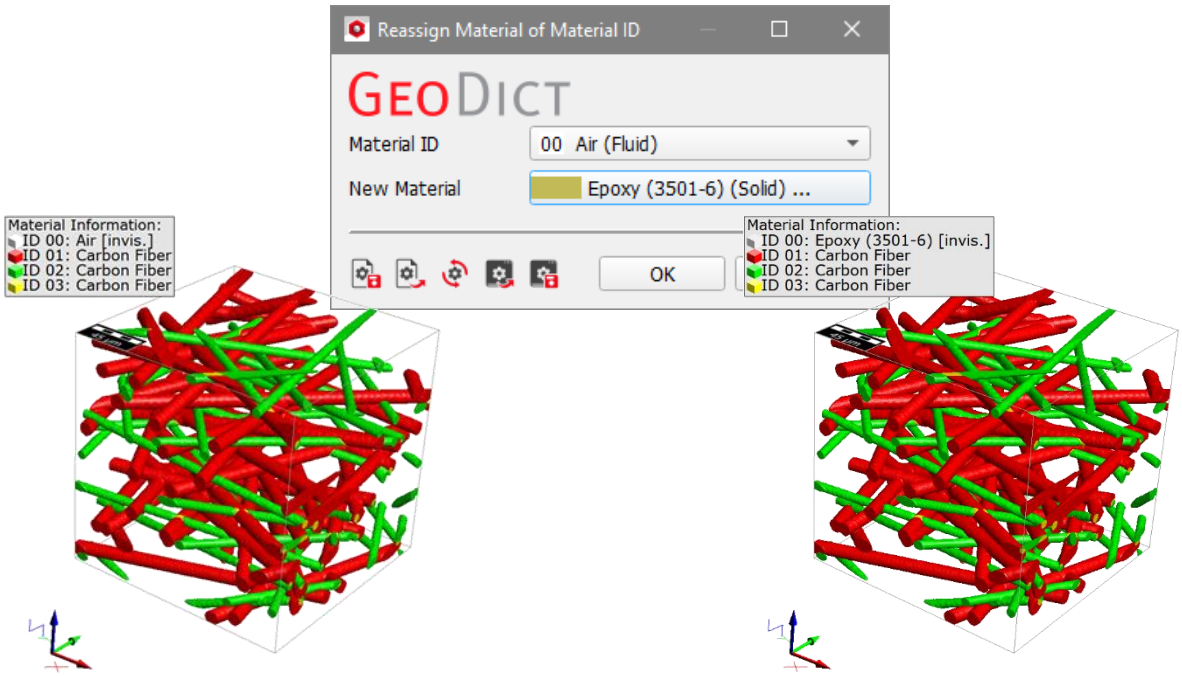
Reassign Material

With **Reassign Material**, a material in the structure is replaced by another material. This means that the material is changed for all material IDs which are set to this material. In the example below, **Glass** is changed to **Carbon Fiber**.



Reassign Material of Material ID

Reassign Material of Material ID corresponds to the option available in the **Select Constituent Materials** dialog. As shown in this example, the material is changed for one selected material ID (here: *Air* to *Epoxy* for Material ID 00).



Material Colors in GeoDict

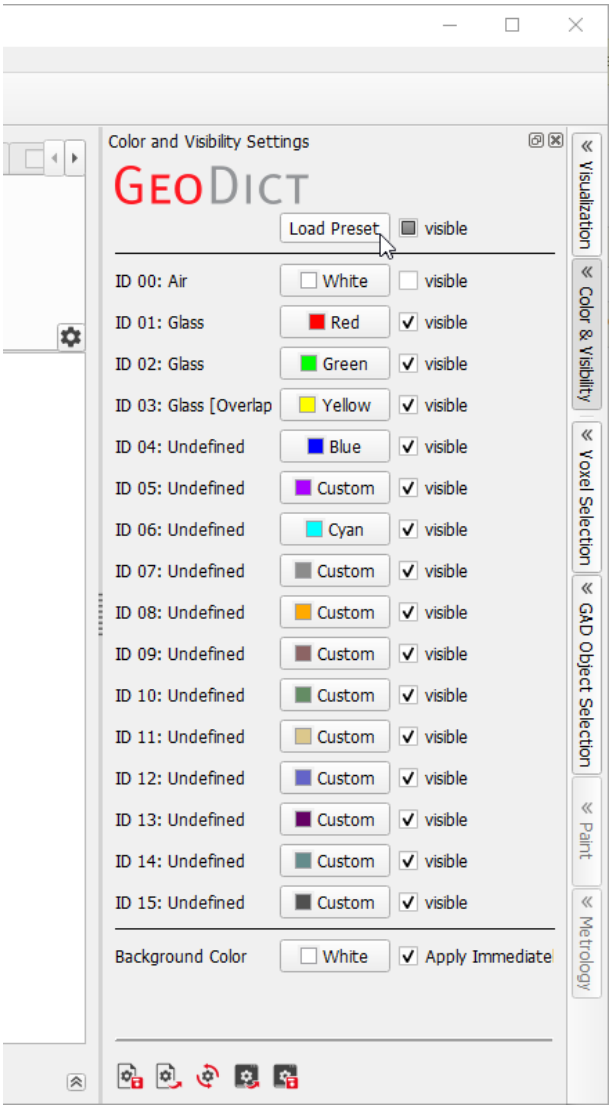
For each material ID in GeoDict, a color can be selected for visualization. These colors are set globally in GeoDict and are not saved in the structure file. For each material in the material database, also a corresponding color is stored (see page 16). In the following, it is described how to use these stored material colors for display.

Color selection

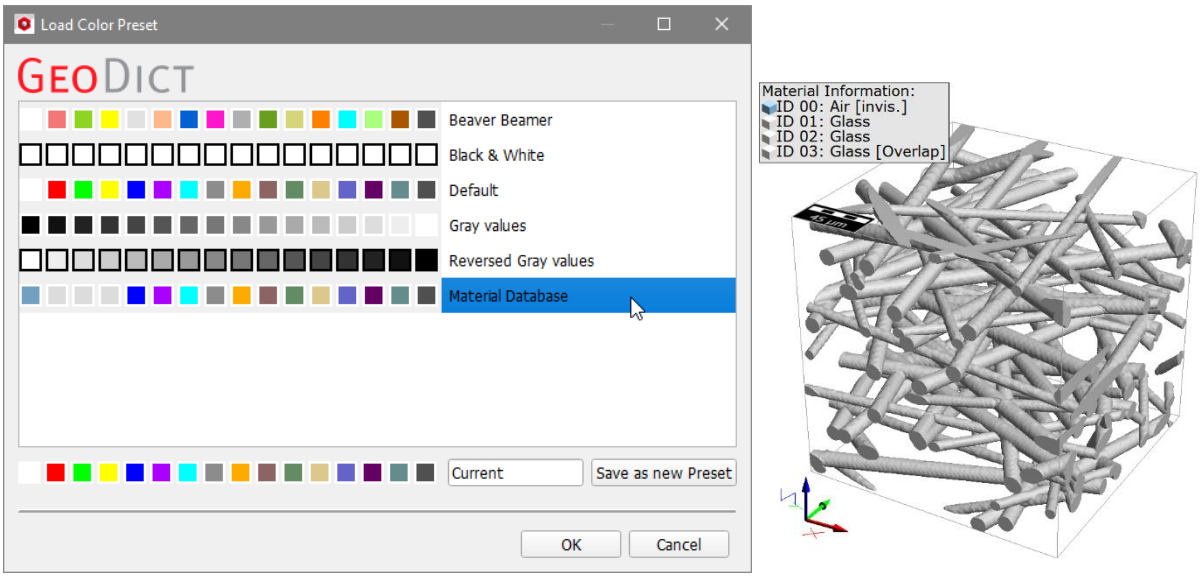
The color of a material in GeoDict can be changed through the **Color and Visibility Settings** dialog by selecting **Settings** → **Color and Visibility Settings** in the menu bar, or by clicking the corresponding icon in the toolbar.

The **Color and Visibility Settings** dialog shows the colors currently assigned to the Material IDs and the Constituent Materials.

To use the colors defined in the GeoDict Material Database, click **Load Preset** and then, choose **Material Database** in the **Load Color Preset** dialog. Confirm the choice with **OK** and close the **Color & Visibility Settings** with **Close**.



For example, the preset color for *Glass* in the material database is a light grey as shown here.



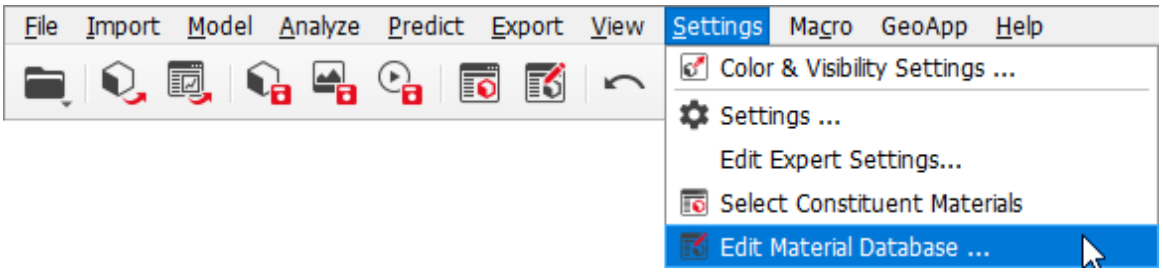
EDIT AND EXPAND THE GEODICT MATERIAL DATABASE

The GeoDict Material Database installed with GeoDict 2022 can be edited and expanded. The following explains how to create new constituent materials and how to edit the properties of materials already included in the GeoDict Material Database.

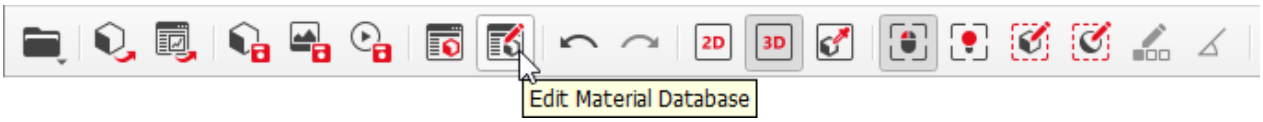
ACCESS THE MATERIAL DATABASE

There are several options to access the Material Database in GeoDict:

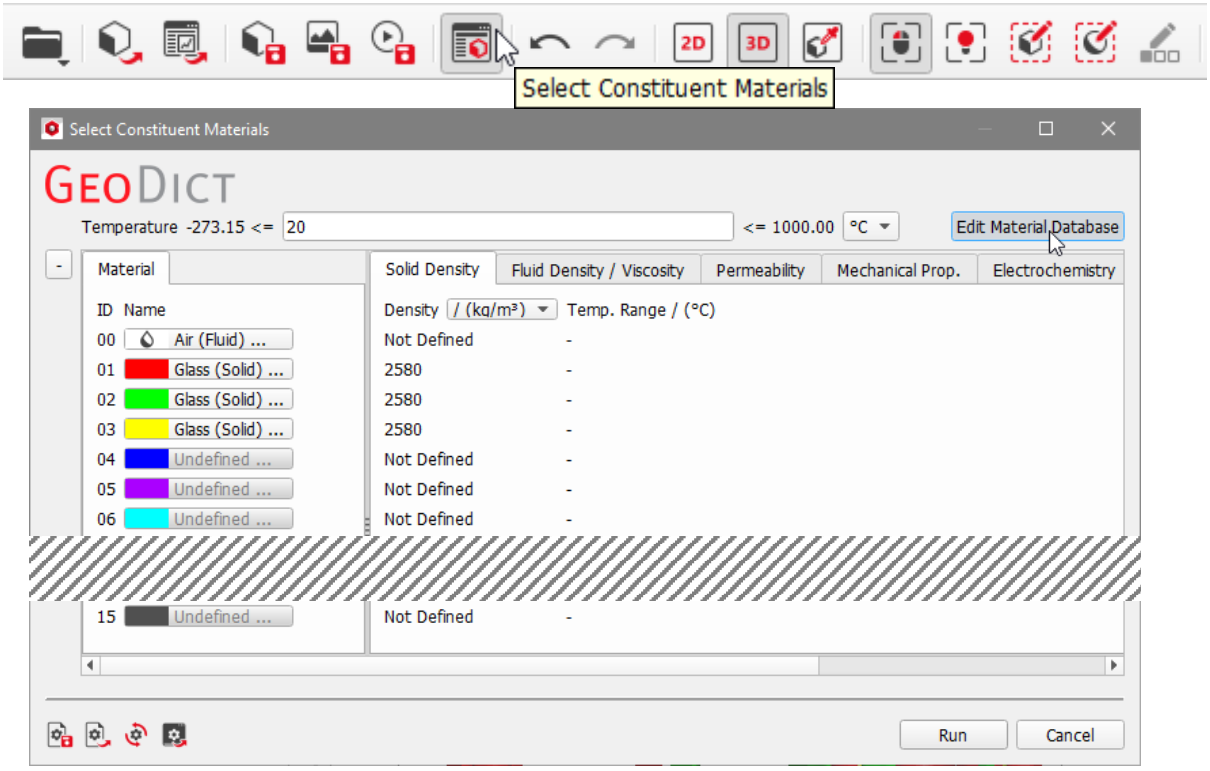
1. Select **Settings → Edit Material Data Base...** in the menu bar



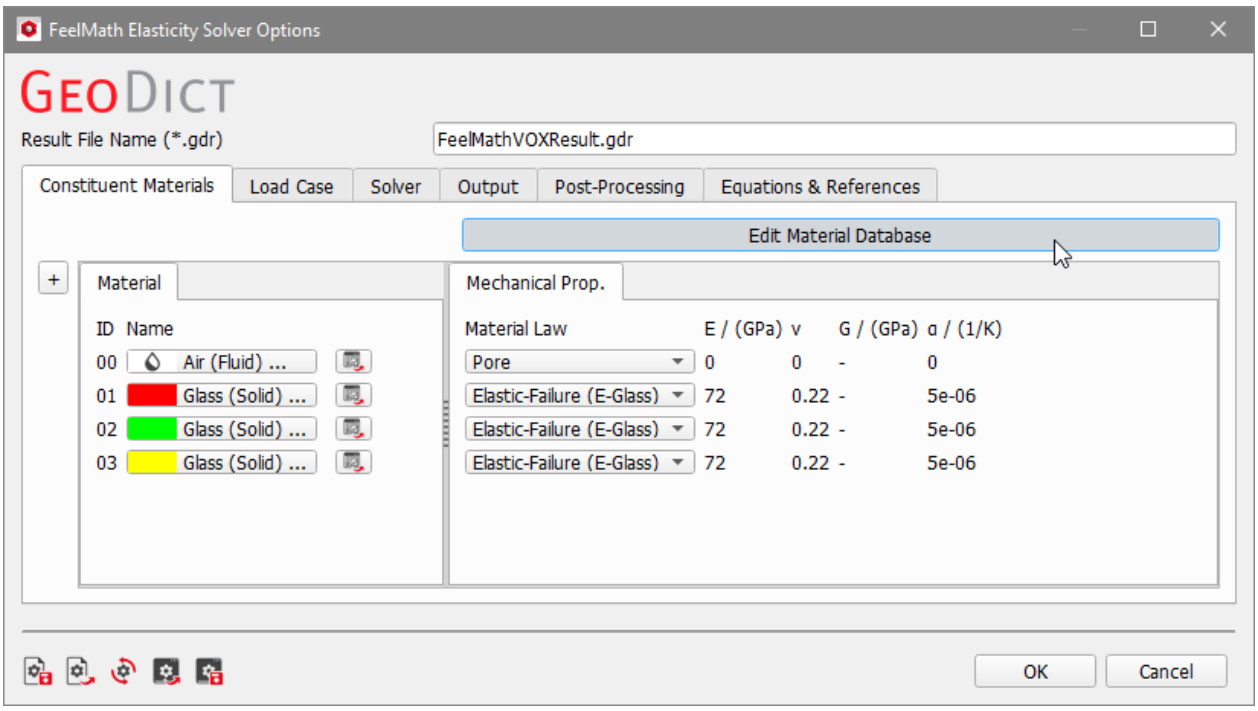
2. Click the **Edit Material Database** icon in the toolbar



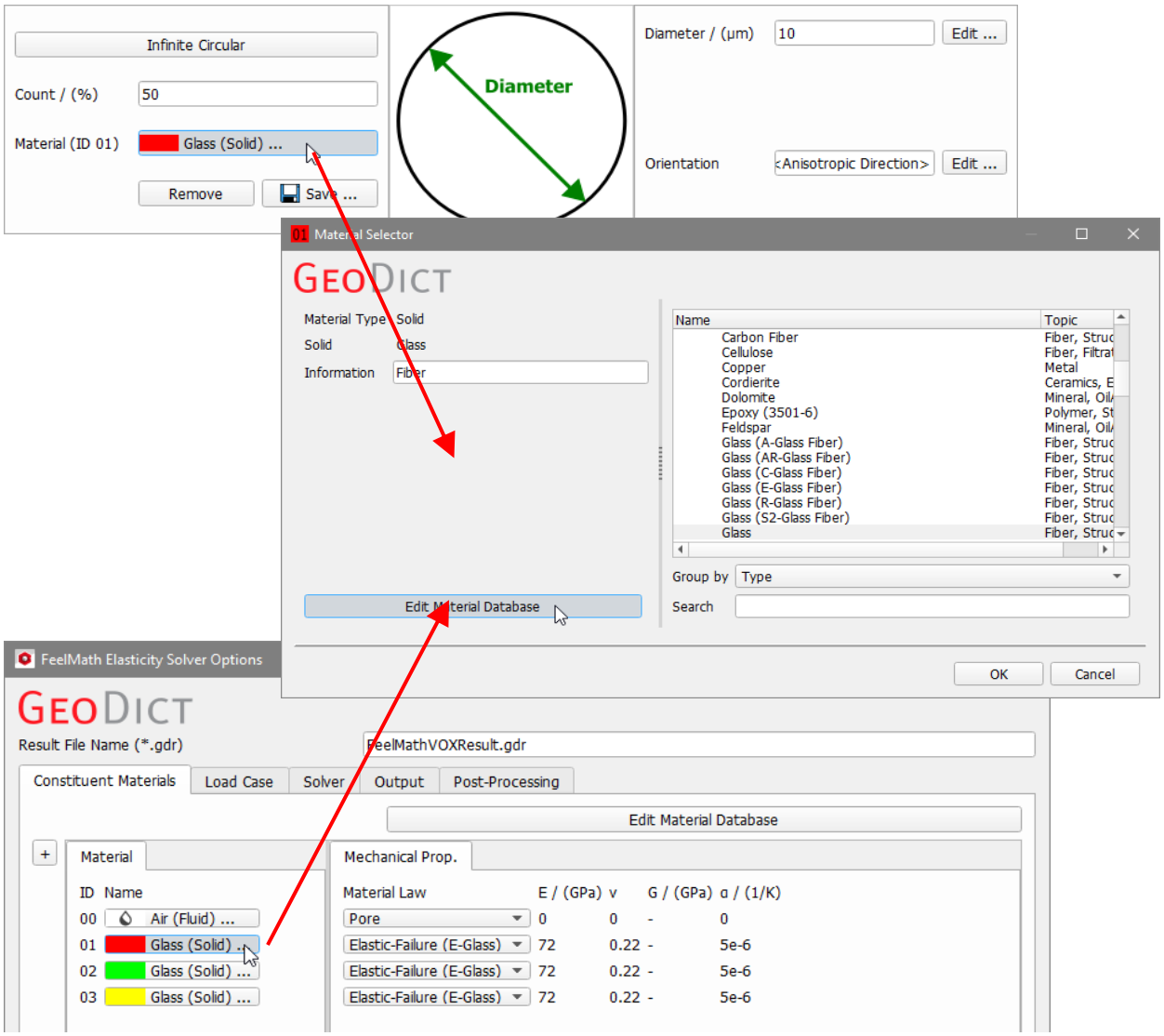
3. Click the **Select Constituent Materials** icon in the toolbar and click **Edit Material Data Base** in the Select Constituent Materials dialog



4. Click the **Edit Material Database** button located in the **Constituent Materials** tab of the **Solver Options** for the predictor modules (ElastoDict, ConductoDict, FlowDict, DiffuDict, FilterDict, etc.):

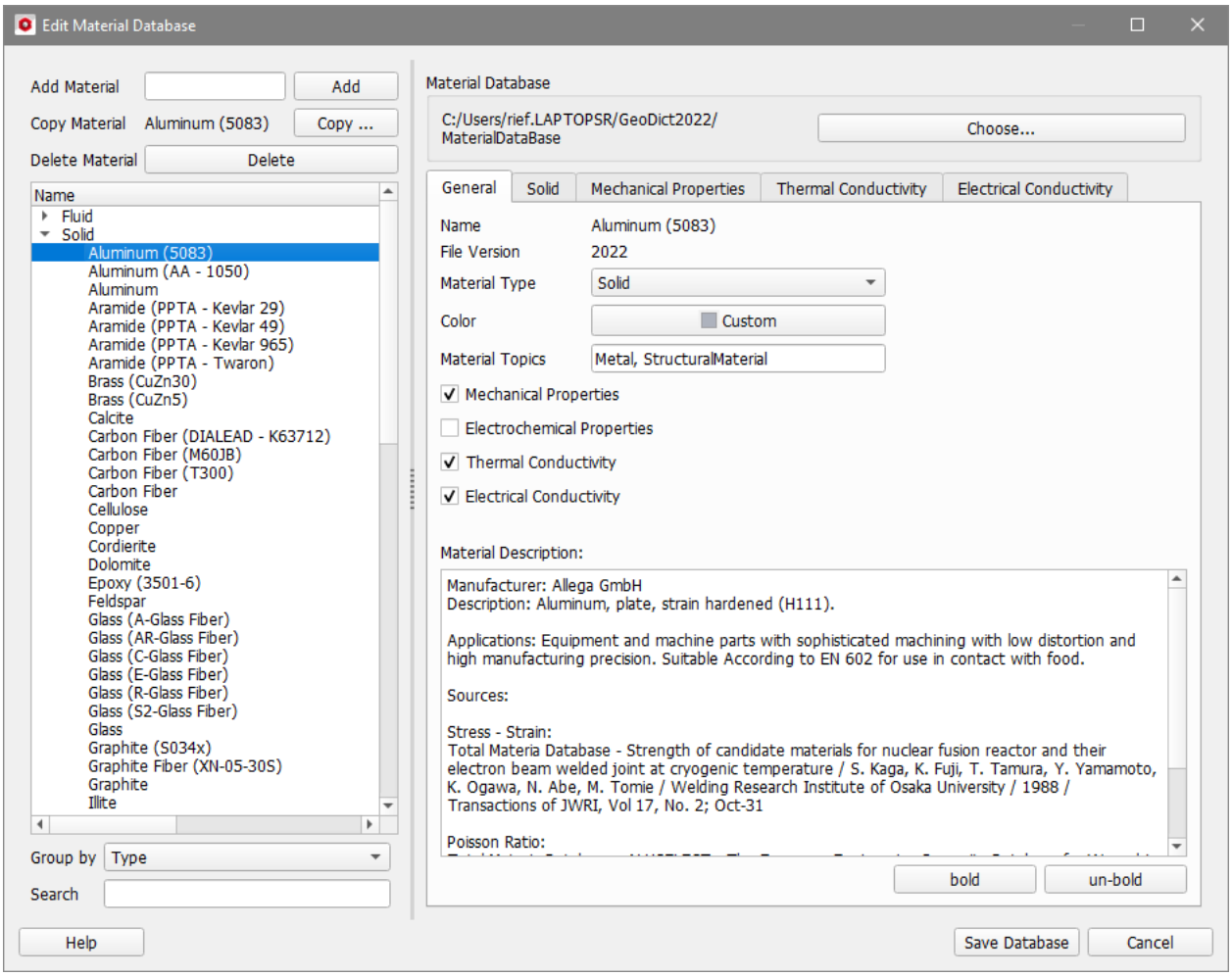


5. Click any material button in generator or predictor modules, and then click **Edit Material Database** in the **Material Selector** dialog box.



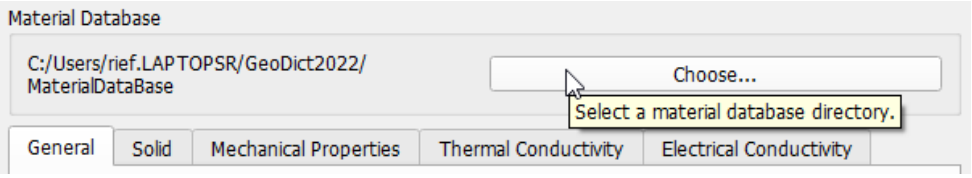
For the predictor modules (ElastoDict, ConductoDict, FlowDict, DiffuDict, FilterDict, etc.), the material buttons are located in the **Constituent Materials** tab of the **Solver Options**.

After clicking **Edit Material Database**, the **Edit Material Database** dialog opens:



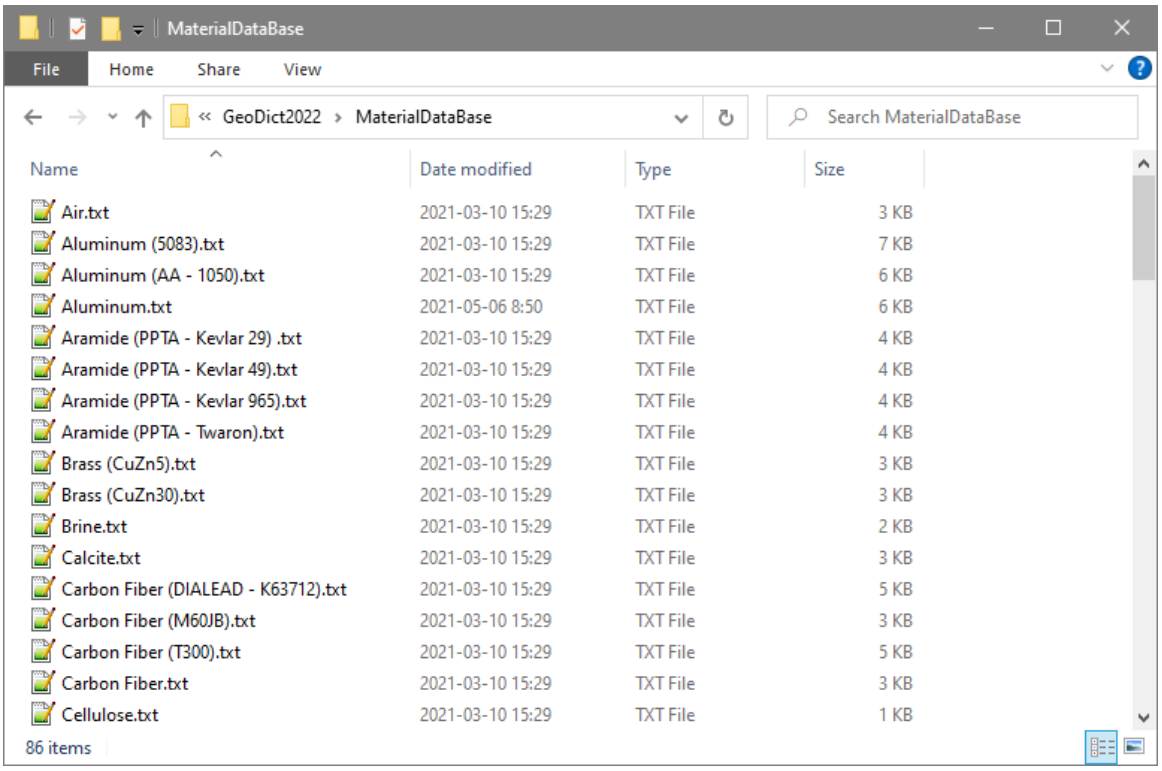
CHOOSE A MATERIAL DATABASE

On the upper right corner of the **Edit Material Database** dialog, click **Choose...** to set the path to a material database directory.



The default path for the GeoDict Material Database is

- `C:\Users\username\GeoDict20XX\MaterialDataBase` for Windows
- `/home/username/.geodict20XX/MaterialDataBase` for Linux



If the default material database needs to be recovered, it can be copied from the GeoDict installation directory, e.g., from:

An arbitrary folder can be chosen as Material Database. For example, a shared network folder could be chosen as material database folder. This way, the same database can be accessed by multiple GeoDict users.

If the current material database folder is deleted, it is automatically recovered from the installation folder at the next start of GeoDict.

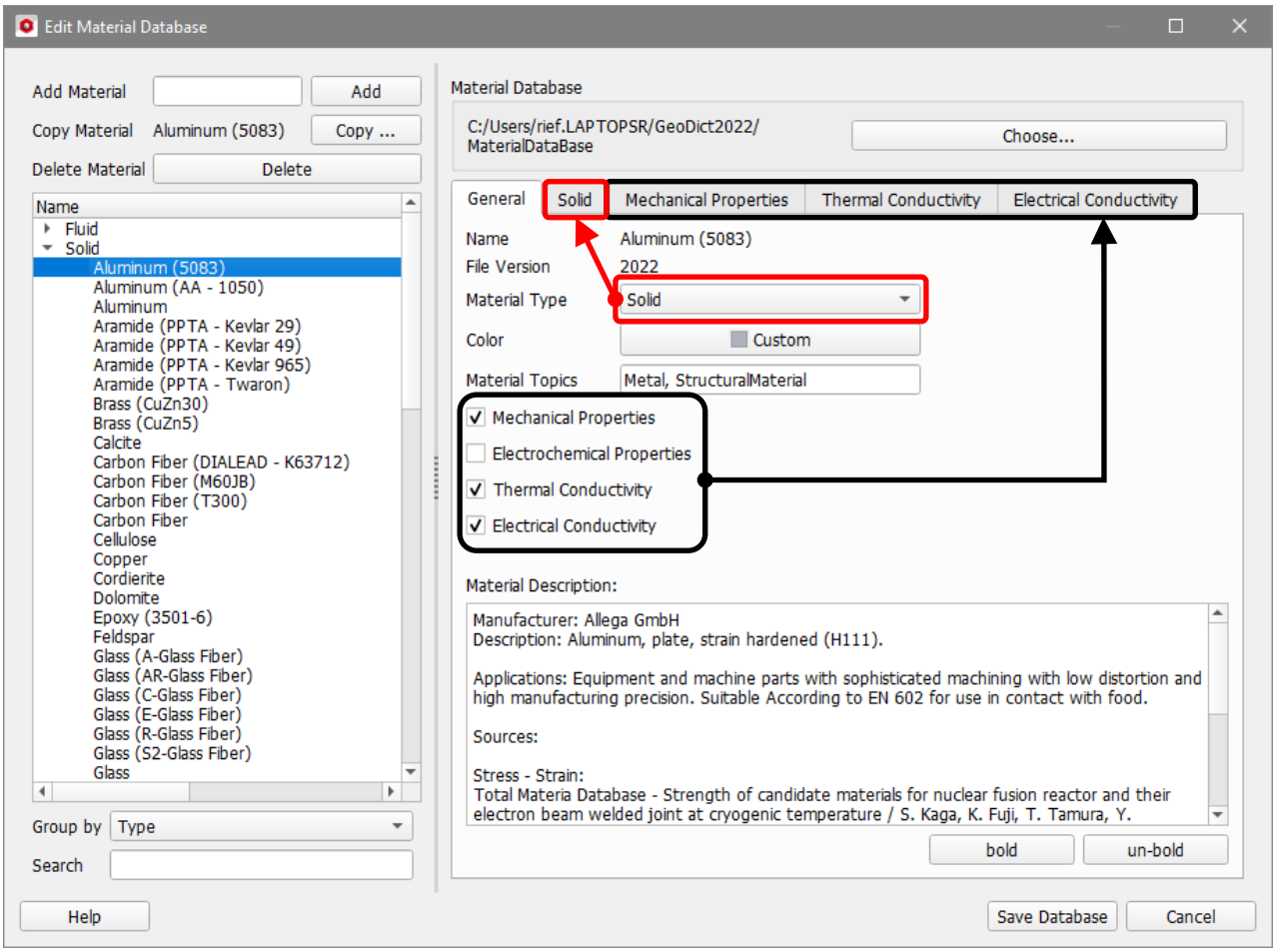
Materials can be added to the Material Database in two ways:

1. Add or copy materials in the material database dialog (see page 18)
2. Copy the corresponding *.txt files from another material database into the MaterialDataBase folder.

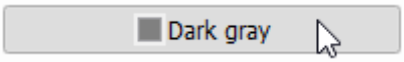
EDIT EXISTING MATERIAL DATABASE ENTRIES

The material database can be edited by modifying or adding properties of constituent materials through the **Edit Material Database** dialog as follows:

1. In the left panel, click to highlight and choose one of the materials in the current GeoDict material database.
2. In the right panel, under the **General** tab, the **Material Type** (Solid, Fluid, Porous), its assigned **Color**, the **Material Topics** (e.g., Battery, Electrochemistry), the material **Properties**, and the **Material Description** can be edited.



Depending on the selection of material type, the next tab after the **General** tab is titled **Solid**, **Fluid**, or **Porous**, and the parameters that apply in each case can be edited. For Solid Materials, a fixed density or a temperature dependent density can be entered. For Fluid materials, a density and the dynamic and kinematic viscosity can be set, which might be also temperature dependent. Porous materials work analogously to solid materials. Additionally, the Permeability, the Porosity and Tortuosity can be defined. The Permeability can be temperature dependent.

The material color can be changed by clicking on the corresponding button, e.g., 

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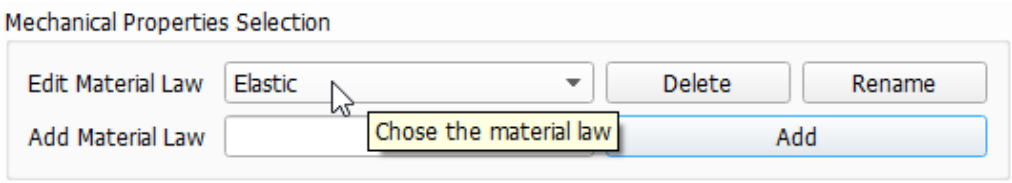
The other tabs depend on the material properties that are selected under the **General** tab.

MECHANICAL PROPERTIES: MULTIPLE MATERIAL LAWS

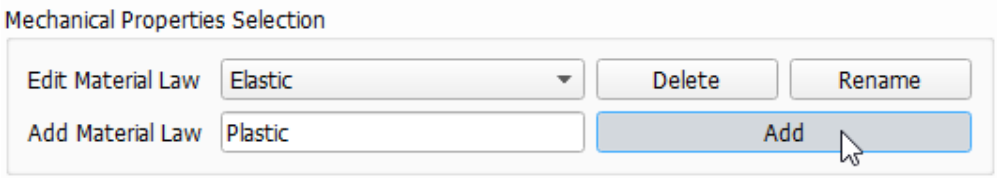
Under **Mechanical Properties**, multiple material laws can be defined and, later, one of them can be selected to run the simulation. For further information about how to define the Mechanical Properties of materials, refer to the ElastoDict 2022 handbook of this User Guide.

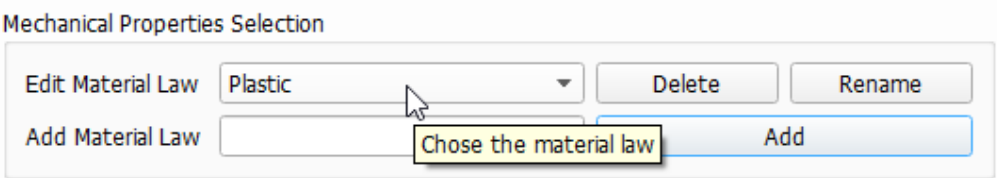
In the material database, it is possible to:

- Edit an existing material law by choosing it under **Edit Material Law** and editing the corresponding parameters below:



- Add a new material law by entering its name in the box **Add Material Law** and clicking **Add**. Afterwards, a material law with the entered name is listed under **Edit Material Law** and can be edited as described above.





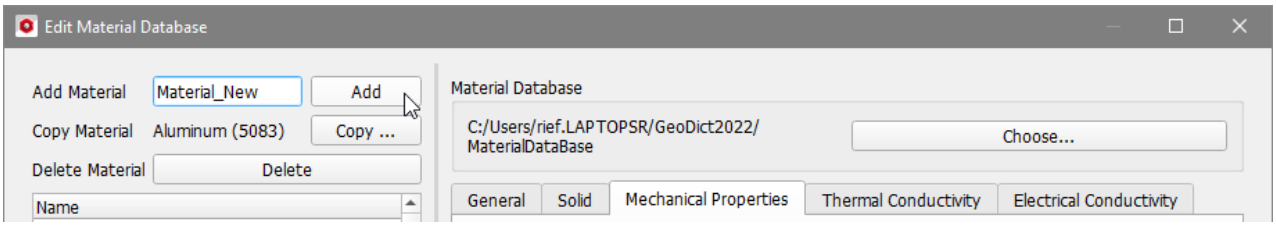
Adding new materials to the database

The material database can be expanded by adding new constituent materials or by copying (and editing) existing materials in the **Edit Material Database** dialog.

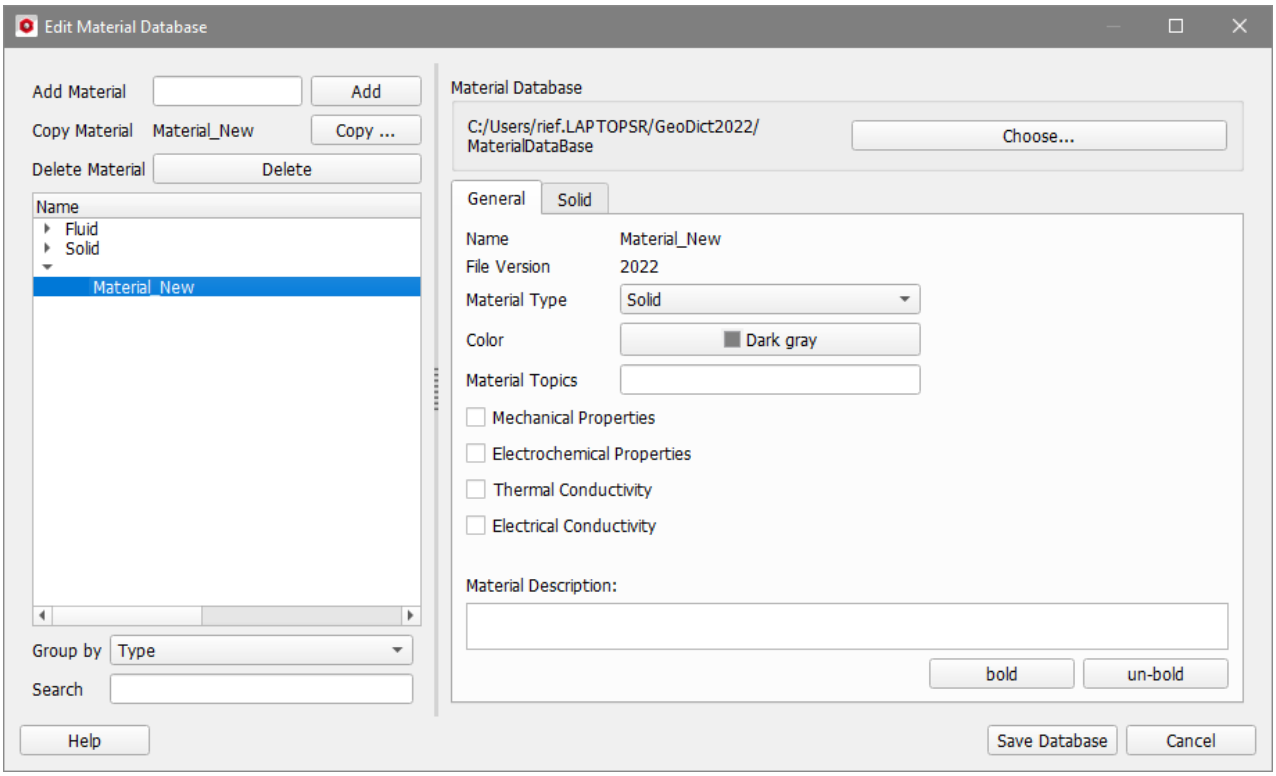
Creating new materials

To add a new material to the database, enter a name for the new material in the corresponding box in the upper left corner of the dialog (e.g., **Material_New** in the example below). Click **Add**.

Material_New appears listed in the left panel and default values appear in the right panel under the General and the Solid tabs.



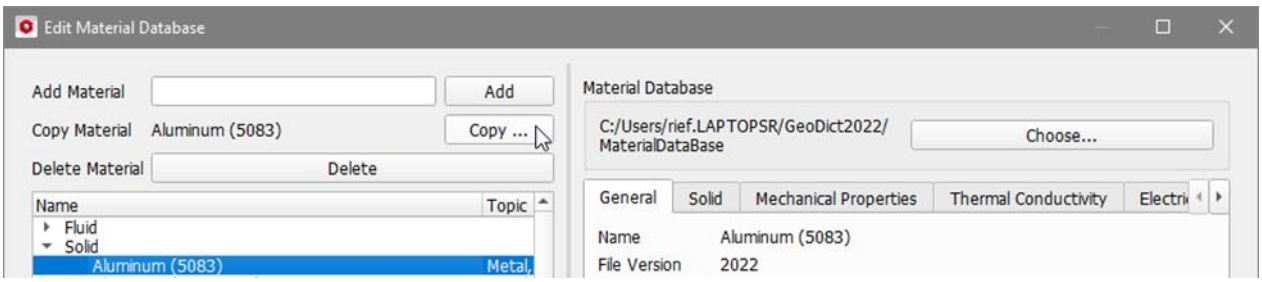
When a material is newly created, its **Material Type** is not yet set and therefore it does not appear under the **Fluid** or **Solid** tree, but separately below.



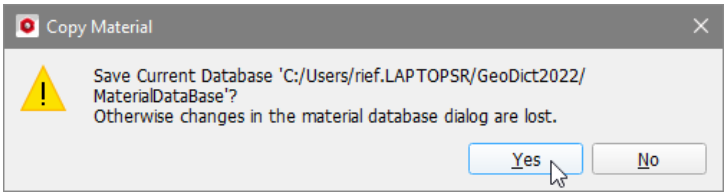
In the next step, the **Material Type** and its properties are set under the corresponding tabs (see the corresponding paragraph on page 16).

Copying existing materials

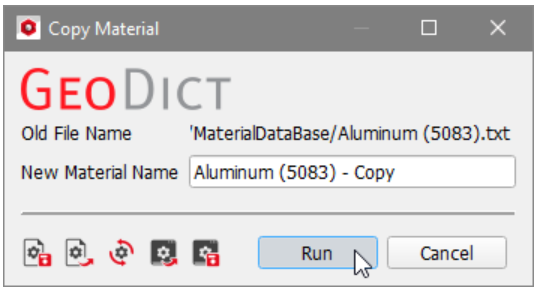
Alternatively, an existing material can be copied by selecting the material and clicking **Copy ...**.



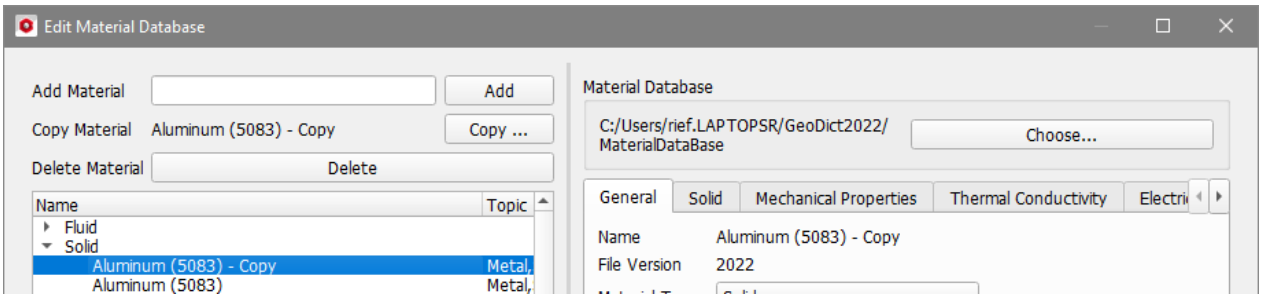
A dialog is shown, which asks if the material database should be saved before adding the copied material. It is recommended to choose yes to proceed.



In the next step, the name for the new copy of the material can be selected. In this example, the default name is kept. Click **Run** to create the material.

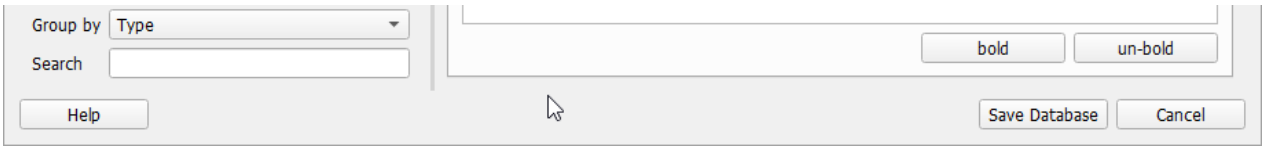


Then, the new material is shown in the material database:



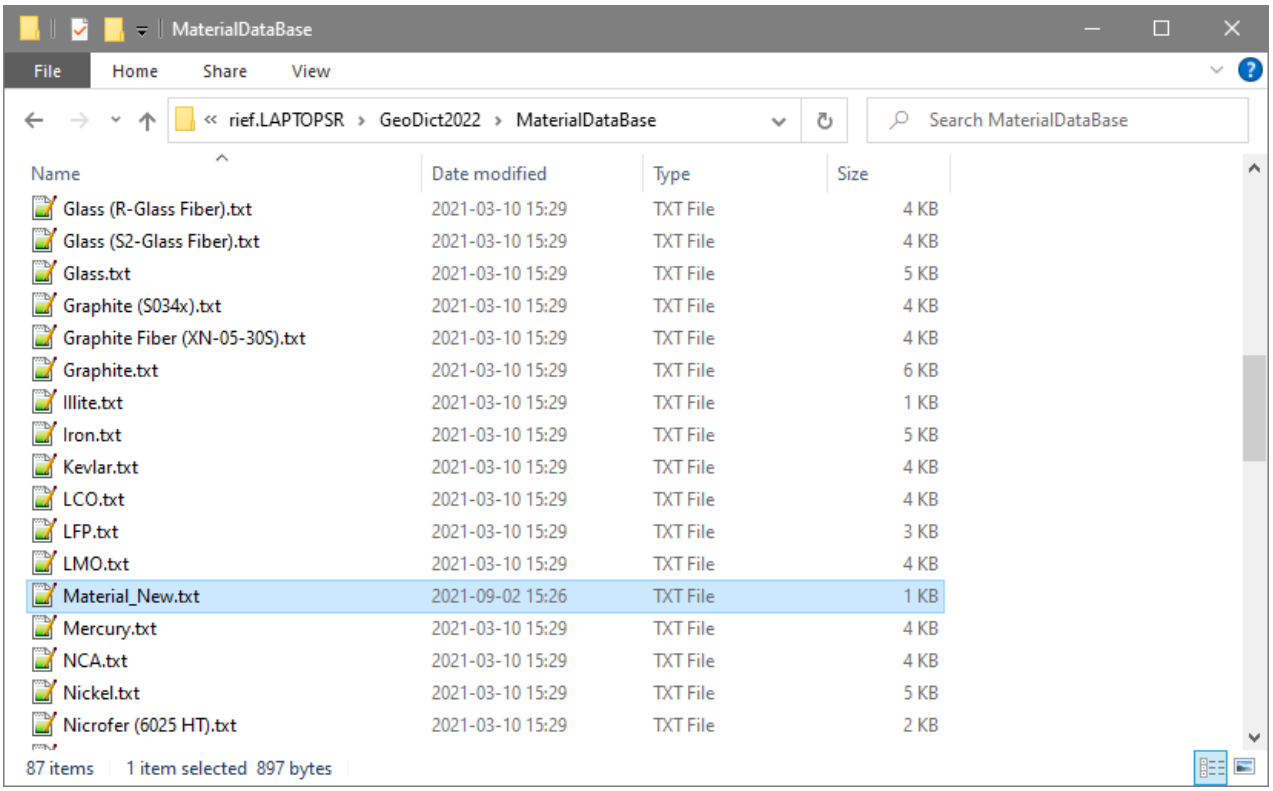
SAVING THE MATERIAL DATABASE

When all parameters are set as desired, either continue with the next material or click **Save Database** at the bottom of the **Edit Material Database** dialog to save all changes to the database.



The material database entries are stored as *.txt files in the current material database folder (either the default GeoDict material database or a user-selected database).

The filename of the *.txt file is the name of the material in the database (here: Material_New.txt). This text file contains all information about the material database entry. It can be shared to other users and copied to other GeoDict material databases.



These text files can be opened and edited with any text editor, such as Notepad++. All parameters can also be changed directly in the *.txt file. As an example, the file for **Aluminum (5083)** is shown on the next page.

C:\Users\rief.LAPTOPSR\GeoDict2022\MaterialDataBase\Aluminum (5083).txt - Notepad++

File Edit Search View Encoding Language Settings Tools Macro Run Plugins Window ?

Aluminum (5083).txt

```
33  <Material>
34    Type                        Solid
35    <Color>
36      RGB                       173,178,189
37    </Color>
38    Topics                      Metal,StructuralMaterial
39    <Solid>
40      Parameter                 None
41      Density                   2660 [kg/m^3]
42    </Solid>
43    <Thermal>
44      <MaterialLaw1>
45        Name                    Iso. Law
46        Parameter               Temperature
47        Type                    Isotropic
48        Temperature             20 [Celsius]
49        Conductivity            112.5 [W/(mK)]
50      </MaterialLaw1>
51    </Thermal>
52    <Electrical>
53      <MaterialLaw1>
54        Name                    Iso. Law
55        Parameter               None
56        Type                    Isotropic
57        Conductivity            16998640 [S/m]
58      </MaterialLaw1>
59    </Electrical>
60    <Elasticity>
61      <MaterialLaw1>
62        <Measurement>
63          Strain                0,3.9,11.52,13.46,15.27,17.94,19.4,21.5,23.32,24.79,25.89,27.25,28.93,30.04,
64          Stress                0,0.171,0.232,0.245,0.267,0.278,0.285,0.279,0.288,0.287,0.29,0.286,0.304,0.3
65        </Measurement>
66        Type                    Isotropic
67        Name                    Elasto-Plastic (20 °C)
68        YoungsModulus           71 [GPa]
69        PoissonsRatio           0.33 [1]
70        AllowThermalExpansion   true
71        ThermalExpansion        2.38e-05 [1/K]
72        PlasticityType          Exponential // Possible values: None, Constant, AffineLinear, Exponential
73        ViscosityType           None // Possible values: None, PerzynaLinear, PerzynaNonlinear, MichelSuquet
74        DamageType              None // Possible values: None, Exponential, Mazar
75        LargeDefoModel          StVenantKirchhoff // Possible values: StVenantKirchhoff, NeoHook, MooneyRivl
76        InitialYieldStress      0.115241 [GPa]
77        HardeningType           Isotropic
78        FirstIsotropicHardening 0.19948 [GPa]
79        SecondIsotropicHardening 8.68635 [1]
80        FailureType             None // Possible values: None, FailStress
81        HasMeasurement          true
82      </MaterialLaw1>
83      <MaterialLaw2>
84        Type                    Isotropic
85        Name                    Elasto-Plastic (-196 °C)
86        YoungsModulus           78 [GPa]
87        PoissonsRatio           0.33 [1]
88        AllowThermalExpansion   false
89        PlasticityType          Exponential // Possible values: None, Constant, AffineLinear, Exponential
90        ViscosityType           None // Possible values: None, PerzynaLinear, PerzynaNonlinear, MichelSuquet
91        DamageType              None // Possible values: None, Exponential, Mazar
92        LargeDefoModel          StVenantKirchhoff // Possible values: StVenantKirchhoff, NeoHook, MooneyRivl
93        InitialYieldStress      0.134927 [GPa]
94        HardeningType           Isotropic
95        FirstIsotropicHardening 0.340126 [GPa]
96        SecondIsotropicHardening 6.81943 [1]
97        FailureType             None // Possible values: None, FailStress
98        HasMeasurement          true
99        <Measurement>
100         Strain                0,0.42,0.86,1.56,2.75,4.31,5.75,7.43,9.35,11.15,13.08,14.89,17.07,19.25,21.6
101         Stress                0,0.122,0.156,0.174,0.198,0.221,0.238,0.26,0.288,0.311,0.329,0.347,0.363,0.3
102       </Measurement>
103     </MaterialLaw2>
104   </Elasticity>
105 </Material>
106
```

Python file | length : 6,824 lines : 106 | Ln : 1 Col : 1 Sel : 0 | 0 | Windows (CR LF) | UTF-8-BOM | INS

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