ElastoDict

User Guide

GeoDict release 2022

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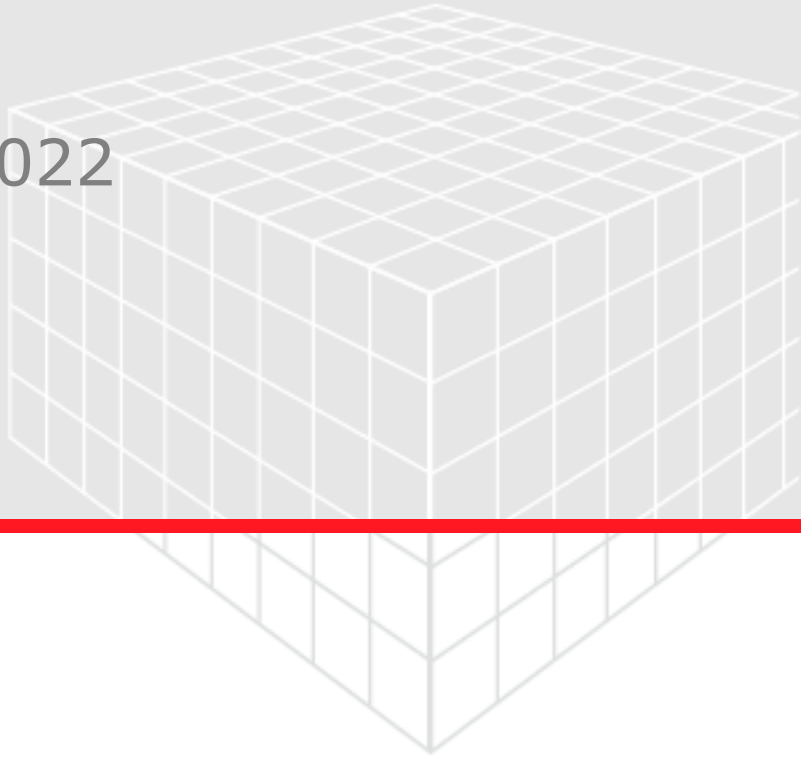

GeoDict

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

ElastoDict: Effective elastic properties and large deformation simulations

The ElastoDict module helps in the development of new materials by providing better understanding of their properties. The key to optimizing your materials are accurate simulations on the 3D micro-structure. ElastoDict is mainly suited for structural materials, these might be e.g., composite materials, ceramics, metals or foams.

As an example, composite materials play a crucial role for light weight applications, but the analysis of their behavior is challenging due to the highly anisotropic behavior and the complex damage mechanisms they exhibit. The expensive, time consuming and often impracticable experimental tests for the study of composites can be supplemented or replaced by simulation.

Using simulation to find answers to mechanical properties and deformation questions is key in many application areas, where the target variables do not necessarily need to be mechanical properties of the materials. For example, the ElastoDict module can be used to simulate how the clamping pressure changes the structure of a gas diffusion layer (GDL) in a PEM fuel cell, or how the properties of rock samples change under in-situ conditions.

All these ElastoDict simulations run at high-speed and are extremely memory-efficient thanks to the integrated FeelMath solver developed at the Fraunhofer ITWM.

ElastoDict contains three sub-modules:

- **FeelMath-AF**
  AF computes analytic approximations and bounds for the linear elastic properties of complex micro-structures. The computation is very fast, as no partial differential equation is solved, and gives a first approximation of the material behavior.
- **FeelMath-VOX**
  VOX accurately computes the linear elastic properties of complex micro-structures by solving the corresponding partial differential equation on the 3D image or model. The results include the local strains and stresses (revealing possible points of material failure), the complete stiffness tensor, and the information on the orthotropic, transversal isotropic or isotropic character of the material, indicative of directionally dependent properties. Additionally, many post-processing steps can be carried out on the VOX results.
- **FeelMath-LD**
  LD simulates nonlinear large deformations. For example, a standard tensile experiment in an arbitrary direction of the 3D micro-structure can be set up. The models of the constituent materials might contain damage, failure, plastic deformation, viscous effects, and many more. For linear elastic materials, new material contacts in the structure can be detected during the simulation. To model the constituent materials, Abaqus UMAT's can be used to include all kinds of possible effects in the nonlinear simulation. Results of the simulation are e.g., a strain-stress curve and local information on the regions where damage sets in and the material ends up failing

REFERENCES

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ELASTODICT WORKFLOW

The computation of mechanical properties in ElastoDict usually follows these steps:

1. Import 3D image data in the form of a stack of (µ)CT scan or FIB-SEM images of an existing material or generate a new structure model in GeoDict.
2. Start ElastoDict and
   - choose the adequate solver,
   - set material parameters using the GeoDict material database,
   - run the mechanical properties computations
   - analyze the results

Solid and porous structures can be used as input for computations with ElastoDict. The mechanical properties of all constituent materials must be given. Including the pore/matrix material, GeoDict handles structures with up to 16 different constituent materials.

As useful convention, for solid materials, the background (Material ID 0) contributes to the computation and is referred to as matrix material. For porous media, Material ID 0 is used for the pore space (void space).

SOLID MATERIALS

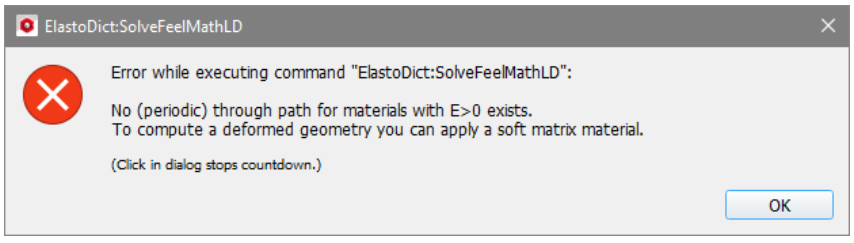
In the solid material case, all constituent materials have non-zero physical material parameters (e.g., Poisson's ratio and Young's modulus for linear elastic materials; see the **Constituent Materials** tab in page 9). In structures consisting of multiple solid materials, like e.g., composite materials, ElastoDict applies perfect contact at the interfaces between different materials.

Many different material models (Plasticity, viscoelasticity, damage, …) are available in GeoDict and you can implement your own Abaqus UMATs.

POROUS MATERIALS

Porous materials in GeoDict are materials where at least one constituent material is selected as Pore (Fluid) material, this means its Youngs's Modulus and Poisson's ratio are both set to zero. No stresses can occur in the pore space.

It is a requirement of all ElastoDict simulations that the solid materials (or more precisely the materials with E>0) are connected. Free-floating objects cannot be handled in a compression or tensile experiment - the movement of those objects would be arbitrary. If no continuous load path exists through the structure, an error message below is shown, and the simulation cannot be started.

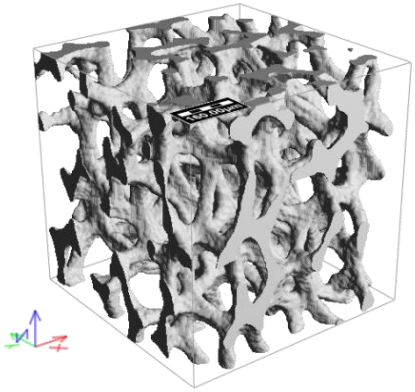


For materials in the pore space, a pore pressure can be set which leads to stresses in the surrounding solid materials. This pore pressure is applied in the first step of the simulation.

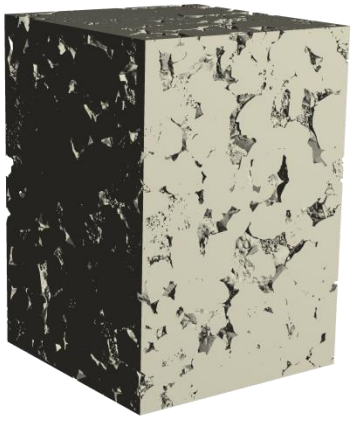
Some structures whose mechanical properties can be calculated with ElastoDict are:

Isotropic fibrous microstructure model generated using FiberGeo

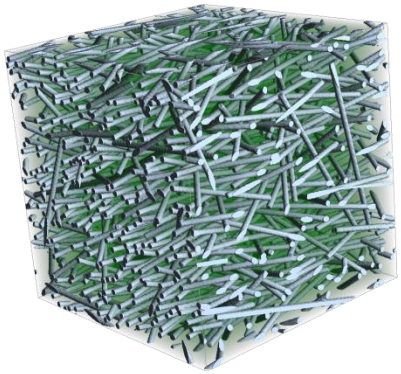
Nickel Foam microstructure model generated using FoamGeo



Berea Sandstone
modeled from imported 3D data using ImportGeo

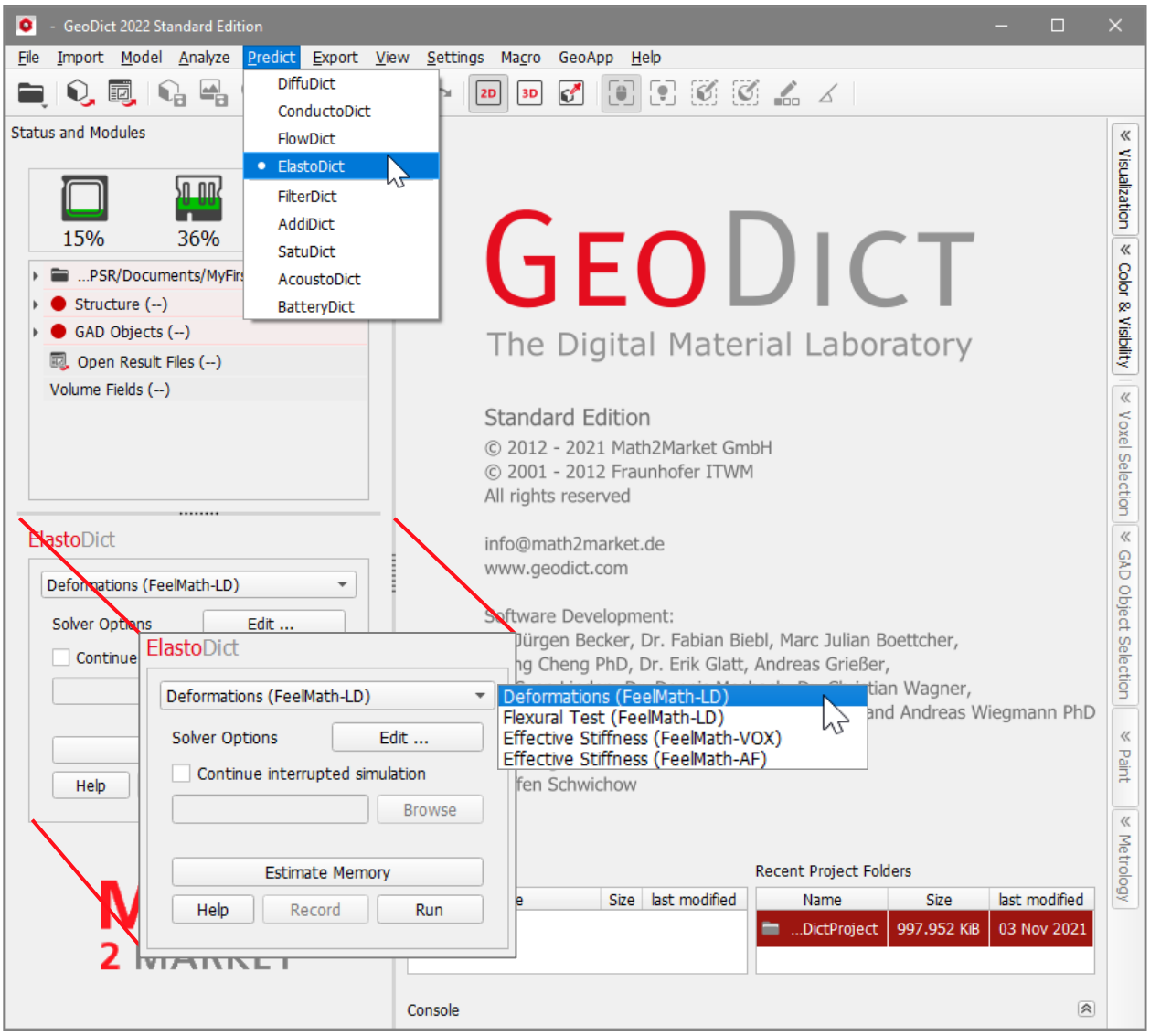


Glass fiber reinforced polymer model generated using FiberGeo



STARTING ELASTODICT

Start ElastoDict by selecting **Predict → ElastoDict** in the menu bar.



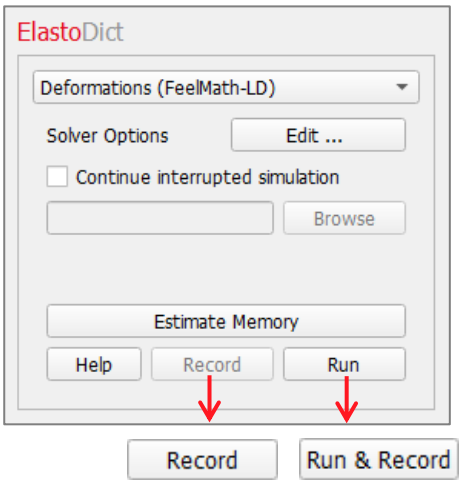
In the **ElastoDict** section located on the left side of the GUI, the solvers are selectable from the pull-down menu:

1. **Deformations (FeelMath-LD)** for the computation of large deformations.
2. **Effective Stiffness (FeelMath-VOX)** for the computation of effective stiffness based on numeric computations.
3. **Effective Stiffness (FeelMath-AF)** for the computation of effective stiffness based on analytic formulas.

The settings for **Solver Options** can be modified through the **Edit...** button. The default parameters can be changed to user-defined parameters for the computation of interest.

For **FeelMath-VOX** and **FeelMath-LD**, the **Estimate Memory** button is present in the **ElastoDict** section. When the structure model of interest is shown in the Visualization area, clicking **Estimate Memory** calculates the memory needed for the computations based on the size of the structure and the parameters entered in the solver options.

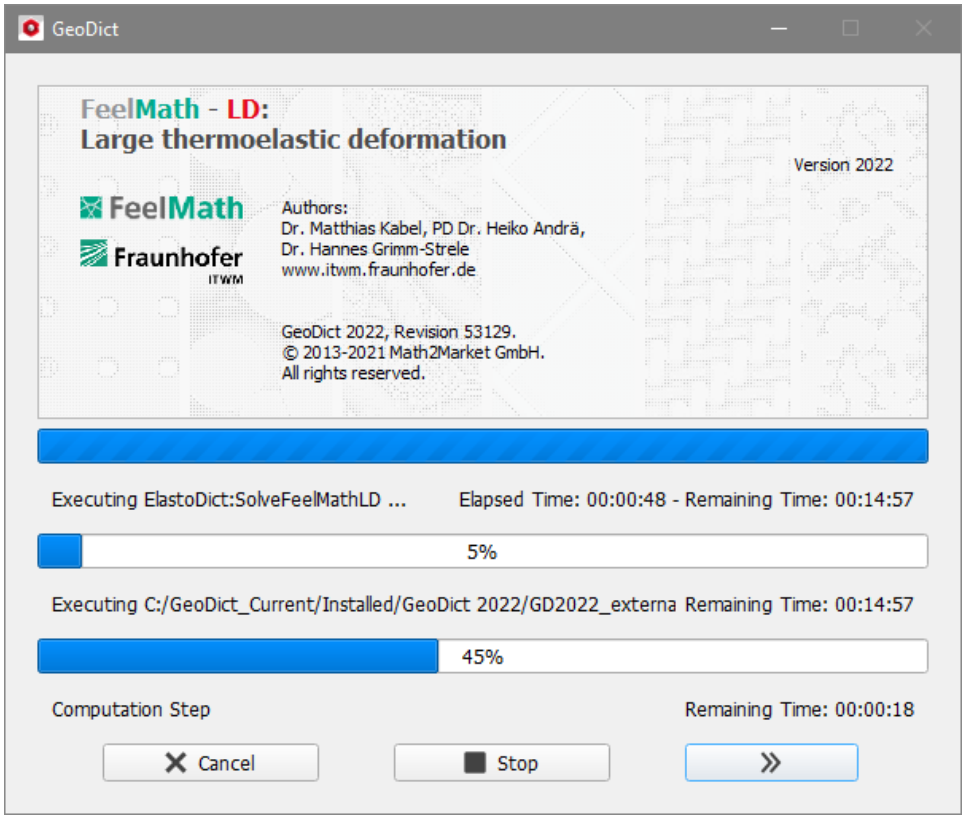
After entering the **Solver Options**, click the **Run** button in the **ElastoDict** section to start the computations. A progress dialog opens to follow the computations.



When recording a macro, the **Record** button becomes active and the **Run** button changes to **Run & Record**.

Clicking **Help** gives direct access to this **ElastoDict2022 handbook** through our web page (https://www.geodict.com).

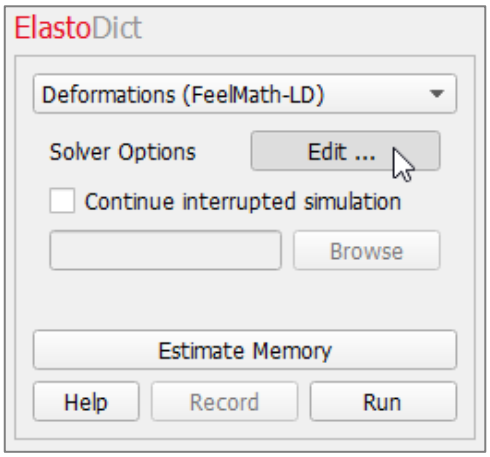
During the computation, the ElastoDict solver process can be cancelled or stopped by clicking **Cancel** or **Stop** button in the progress dialog. With **Cancel**, the computation is terminated, and no further action is taken. With **Stop**, the computation is terminated, and the results file is updated to the current state of the computation. Then, the result file is loaded and shown in the Result Viewer. With the » button, the console is opened which shows additional information about the solver run.

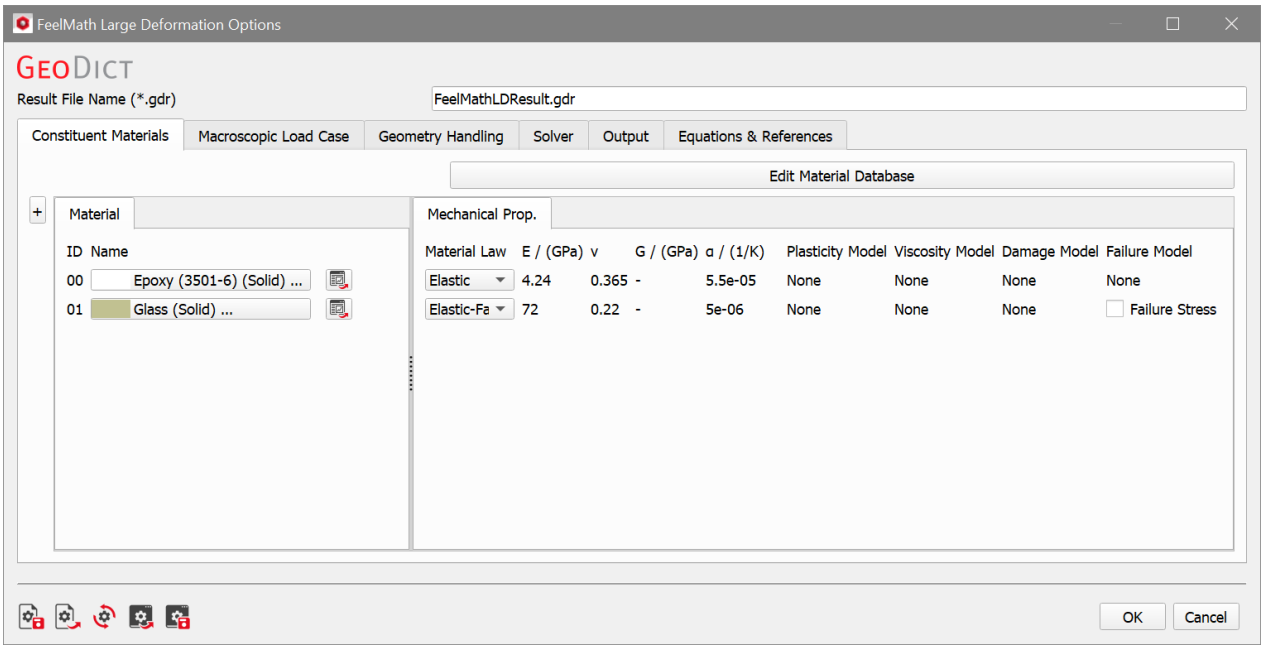


Depending on the solver's internal processes and actual memory usage, terminating the computation may not be instantaneous.

LARGE DEFORMATIONS (FEELMATH-LD)

Click the Solver Options **Edit** button to set the simulations settings for large deformation simulations. In the **FeelMath Large Deformation Options** dialog, choose a **Result File Name (*.gdr)** according to your current project.





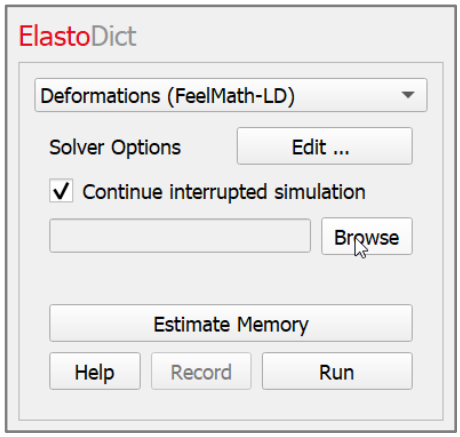
If a GeoDict results file (*.gdr) with the given name already exists in the project folder, a warning message is shown at the start of the creation process. You can either decide to back up the old file, to overwrite it, or to choose a new file name. If no action is taken, the default option **Back-Up** is automatically chosen after a waiting time. Then, the old results files are copied to the folder *00GeoDictBackUp* in the current project folder.

Additional to the results file with the given name, also a corresponding results folder with the same name is written into the current GeoDict project folder. The results file in combination with the results folder contains all information about the current run and allows to reproduce the simulation.

Restarting a simulation

Large deformation simulations can contain many steps, and therefore it may be necessary to interrupt a simulation. Such simulations can be restarted with the option **Continue interrupted simulation**. Click **Browse** to select the corresponding result file and then **Run** to restart the simulation.

For more information about the requirements for restarting simulations, see page 28. If a simulation cannot be restarted, a corresponding error message is shown.

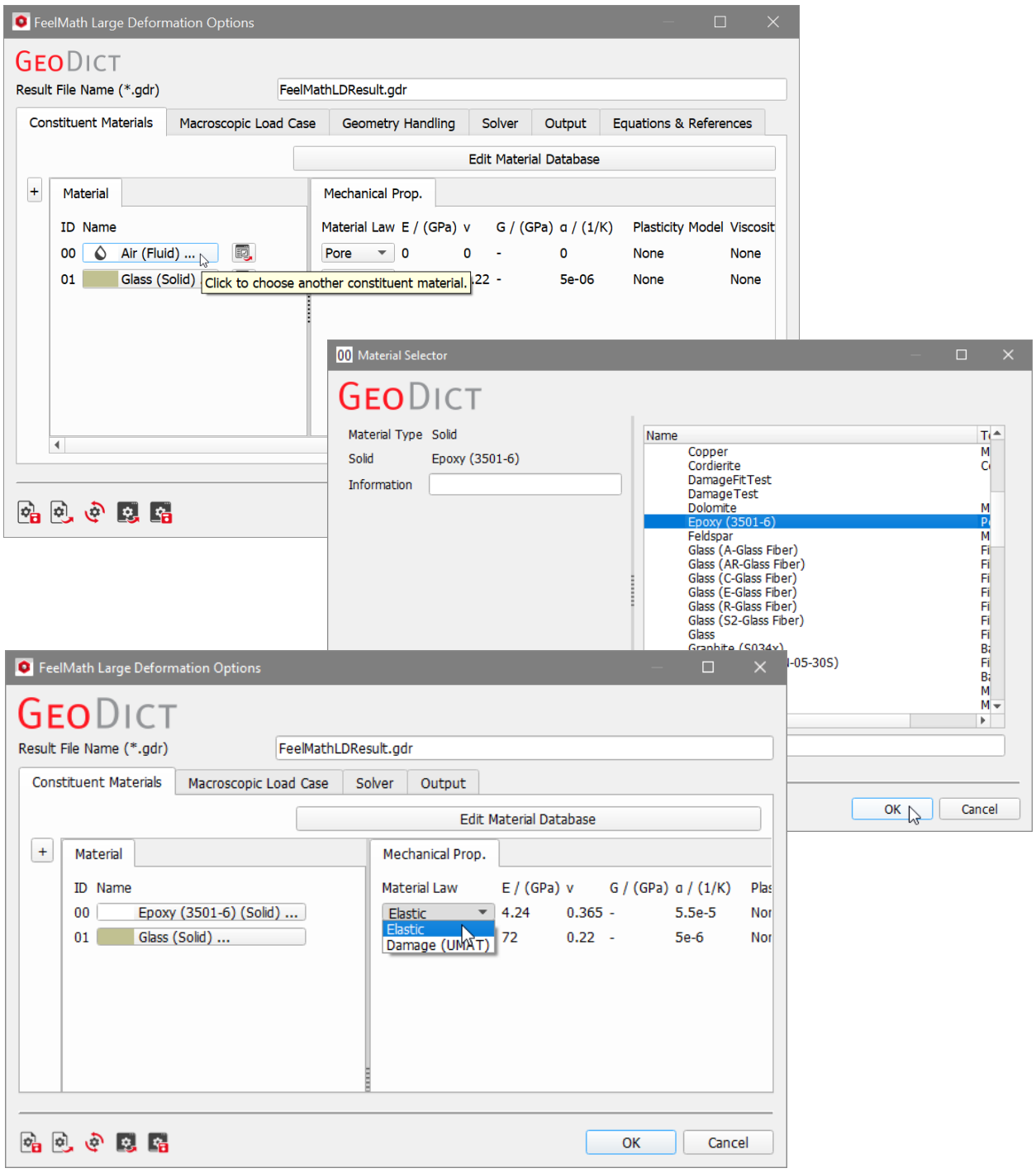


Constituent Materials

For the solver's computations, the materials in the structure model need to be defined under the **Constituent Materials** tab, so that their mechanical parameters, such as the Young's modulus (E) and the Poisson's ratio (ν), are taken into account.

For example, to model a porous material, the constituent material of the empty space can be chosen as pore. To model a composite, it can be chosen to be Epoxy. Simply click on the material name to open the **Material Selector** dialog.

The mechanical properties of the structure's constituent materials are taken directly from the GeoDict Material Database. To enter the material parameters for a linear elastic material manually, choose **Manual (Solid)** as material. If you work with a different set of material constants, transform them to (E, ν) using the formulas given for example, by the Wikipedia page on Hooke's Law.

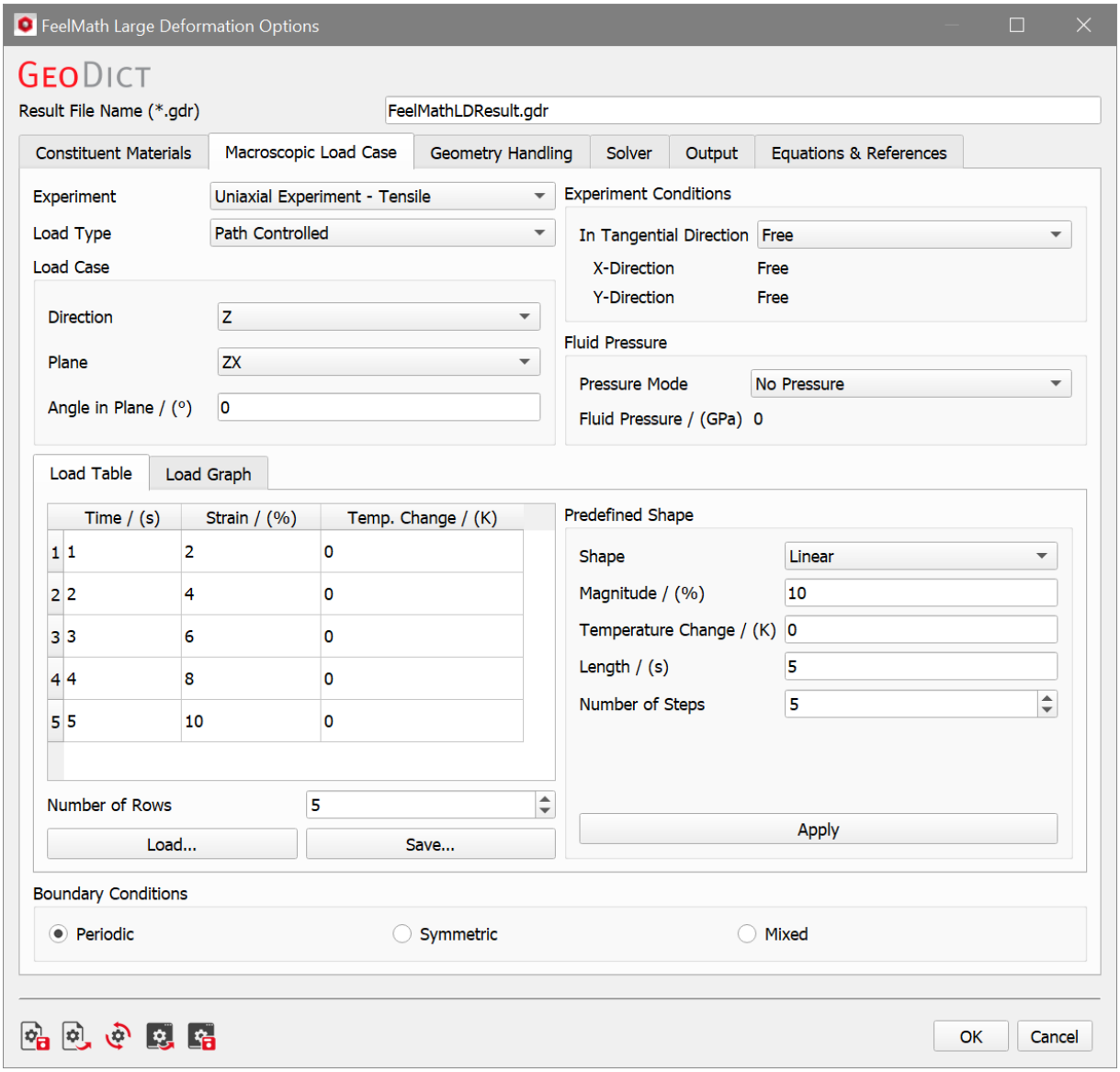


Any values entered manually e.g., those for a user-defined constituent material, can also be added to the material database through the **Edit Material Database...** button. Nonlinear materials can be also created in the **GeoDict Material Database**.

More information on editing, expanding, and using the GeoDict Material Database is available in the Material Database handbook of this User Guide.

Macroscopic Load Case

The parameters which define the general conditions of the **Macroscopic Load Case** are **Experiment** and **Load Type**. Their choice defines which other parameters are available for the experiment.



Experiment

- **Uniaxial Experiment** allows to set up experiments with one load direction (Tensile, Compression or Shear Experiments). The load can be time-dependent, e.g., cyclic. See more on Uniaxial Experiment starting on page 12.
- **Complex Load Experiment** allows to define more elaborate load scenarios, e.g., a tensile experiment followed by a shear load or multiple load directions at the

same time. The load directions can be defined freely as a combination of normal and shear loads. See more on Complex Load Experiment starting on page 14.

Load Type

- **Path Controlled**:

  specify the *mean strain* in the geometry (for geometric linear experiments) or the *mean displacement gradient* in the geometry (for geometric nonlinear experiments) in the load direction.

- **Force Controlled:**

  Specify the *mean stress* in the geometry (for geometric linear experiments) or the *mean nominal stress* in the geometry (for geometric linear experiments) in the load direction. It is important to note, that the mean stress is computed with respect to the complete geometry. If a structure consists of solids and pore space, this means that the average load on the solids is larger than the given mean stress, since the load in the pore space is zero.

  Generally, **Path controlled** should be preferred over **Force Controlled** if possible. One of the challenges with **Force Controlled** is the fact that the Strain-Stress curves for plastic materials are often very flat: This means that a small change in stress can lead to a very large change in strain. On the other hand, a small change in strain leads to an even smaller change in stress. Therefore, the **Path Controlled** simulation is much easier to compute. For simulations with damage, **Force controlled** may be even impossible to solve (because the given stress might be higher than the maximal stress allowed by the material), while **Path Controlled** can always be solved (see also page 81).

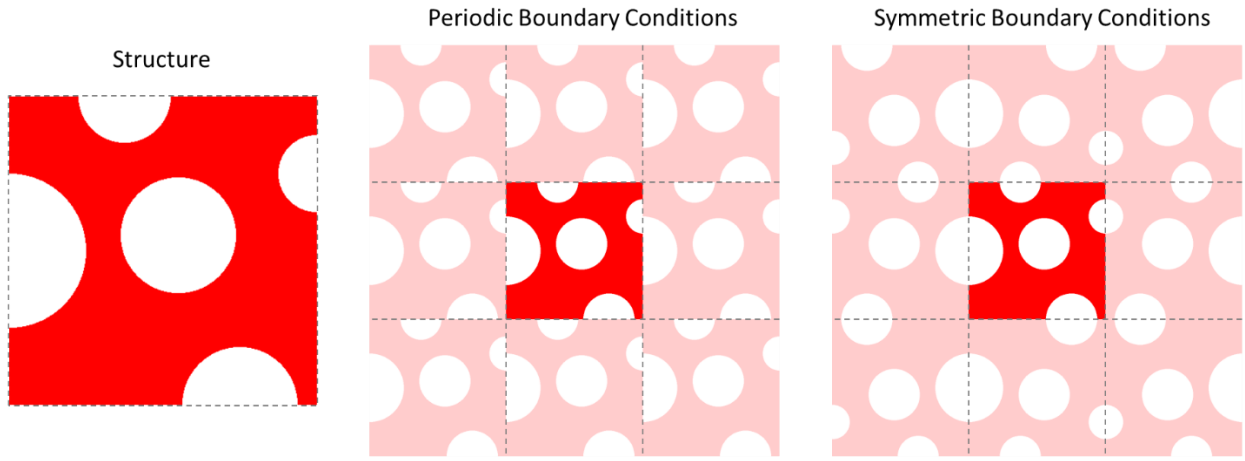
Boundary Conditions

Here, the domain boundary conditions can be set to **Periodic**, **Symmetric**, or **Mixed**.

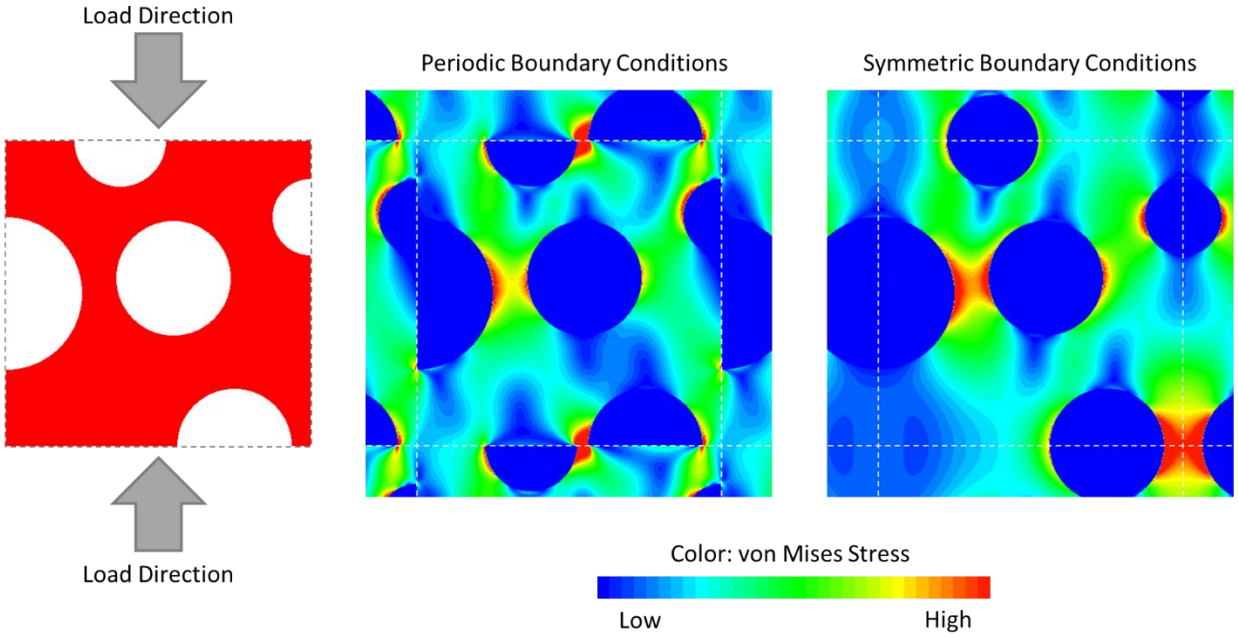
In general, periodic boundary conditions should be used for periodic structures, whereas otherwise symmetric or mixed boundary conditions should be applied.

Mixed boundary conditions mean that symmetric boundary conditions apply in the load direction, whereas periodic boundary conditions apply in the tangential directions. Mixed boundary conditions can only be used for tensile or compression loads along the coordinate directions. In the figure below, periodic and symmetric boundary conditions are illustrated for a non-periodic structure.

The structure below is created only for illustration and does not have a real counterpart.



When periodic boundary conditions are applied to non-periodic structures, it might lead to stress peaks at the boundaries as illustrated below for a uniaxial load.



However, simulations with periodic boundary conditions are much faster and need less memory than simulations with symmetric boundary conditions.

In many cases, for example for composite structures with low fiber percentage, the results for periodic boundary conditions are comparable with the results for symmetric boundary conditions even if the analyzed structure is not periodic.

Therefore, it is recommended to work with periodic boundary conditions until the best simulation settings are found and use symmetric boundary conditions only for the final simulation.

Uniaxial Experiment and Complex Load Experiment

Uniaxial Experiment

In a **Uniaxial Experiment**, the load is applied in one given direction. This direction can be either given by one of the coordinate directions (X, Y, Z), a given angle to one of the coordinate directions in a given coordinate plane (e.g., XZ or YZ), or a shear experiment can be defined.

The available load types are **Tensile**, **Compression** or **Shear**. The choice of **Tensile** or **Compression** only affects the sign of the loads, for example negative tension equals compression.

Load Case

The choices available for the **Load Case** vary depending on whether **Tensile**, **Compression** or **Shear** is selected. For **Tensile** and **Compression** experiments, a direction, a Plane and an **Angle in Plane** must be defined. For **Shear**, the **Shear Load** must be selected. If **Without Geometric Nonlinearity** is chosen, three different shear loads are available: Here, the theory of small deformations applies, therefore the Shear in XY direction corresponds the shear in YX direction. Thus, three different shear options are available in this case: XY, XZ and YZ.

When the theory of small deformations does not apply (**With Geometric Nonlinearity**), there are three different cases for shear in X and Y directions: Shear in XY direction, shear in YX direction (the deformation gradient is asymmetric in those cases) and symmetric shear in X and Y directions (this is a superposition of the two other cases, the deformation gradient is symmetric in this case). Thus, nine different shear options are available for the geometric nonlinear case.

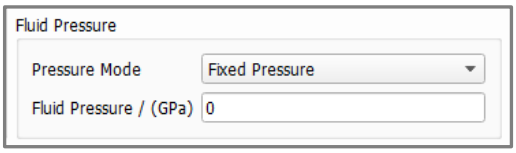
Experiment Conditions

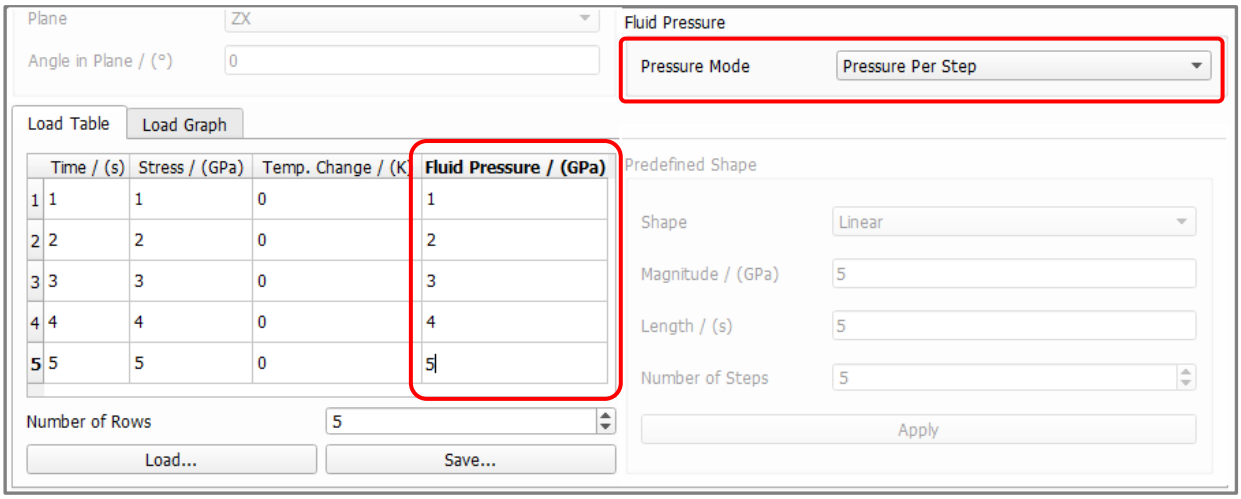
The load conditions in the directions tangential to the load direction can be **Free** (zero mean stress/nominal stress in the geometry), **Confined** (zero mean strain/displacement gradient in the geometry) or **Mixed**. Free means that the structure can expand or contract freely to the load direction, whereas there is no expansion/contraction for confined boundary conditions. With Mixed tangential boundary conditions, two different conditions (**Free** or **Confined**) can be selected for the two tangential directions.

Fluid Pressure

When the structure for the simulation contains pores, a fluid pressure model can be selected. With **No Pressure**, no pressure is applied (this is the default case). With **Fixed Pressure**, a fixed pressure can be given. This fixed pressure is applied at the start of the ElastoDict computations. With the third option, **Pressure Per Step**, the applied pressure can be defined for each simulation step. These pressure steps must be entered in the **Load Table** (see further explanation below).

The pressure is always applied to all fluids in the structure. This means that it is not only applied to pores in the material, but also to the fluid which surrounds the structure.





Load definition (Load Table and Predefined Shape)

The load steps to be computed need to be specified in the **Load Table**, where a plot of the load curve can be seen under the **Load Graph** subtab. It is also possible to use a load curve of Predefined Shape like **Linear**, **Saw-Tooth**, or **Sine**, by selecting it from the pull-down menu on the right and clicking **Apply**, to set it in the **Load Table**. The load table can be loaded from and saved to a *.txt file with the **Load...** and **Save...** buttons.

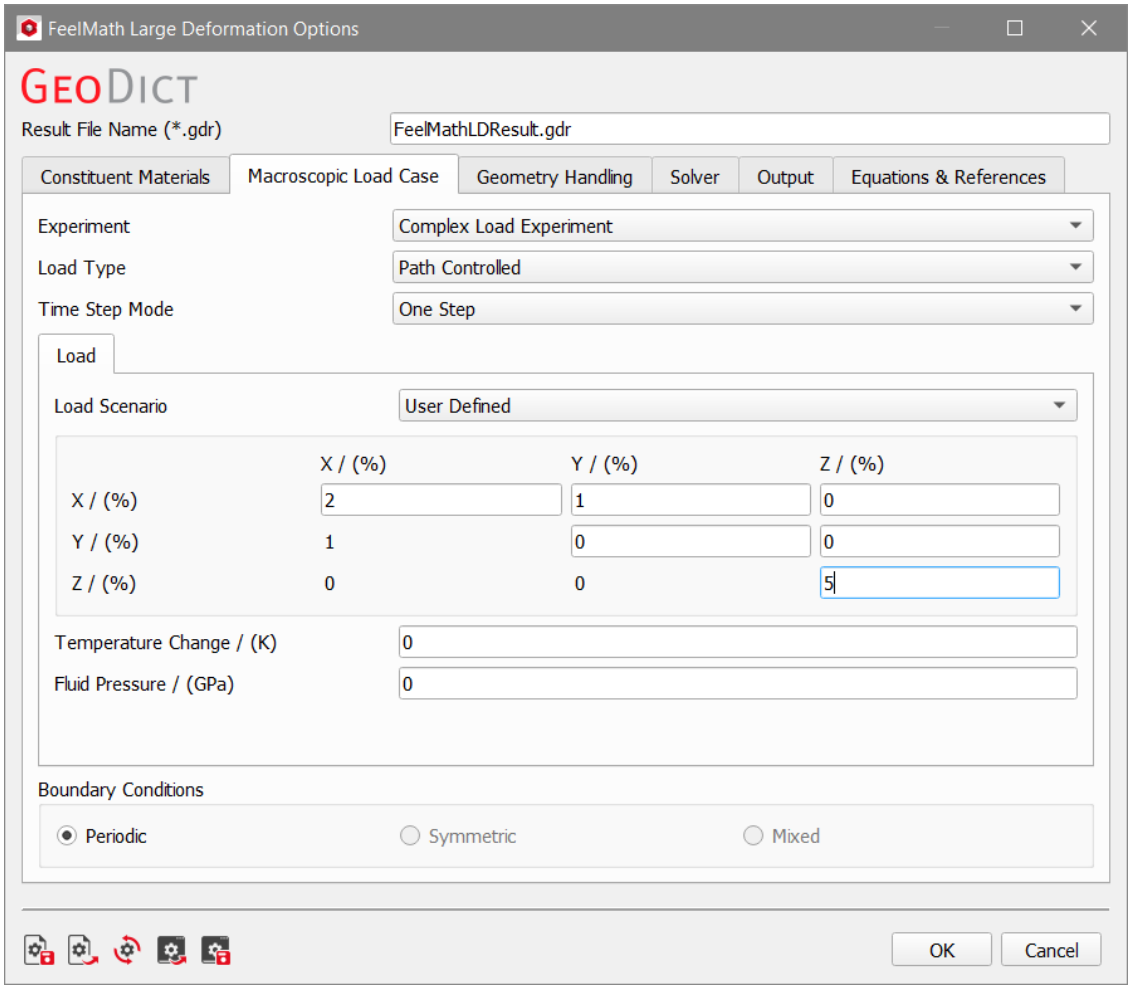
Alternatively, the data from the load table can be entered from other software like Microsoft Excel® via copy and paste.

The time information from the load table is only used if the materials in the structure have a time-dependent behavior. When working with UMATs, this time information is passed to the UMAT.

Complex Load Experiment

For a **Complex Load Experiment**, the complete mean stress (nominal stress) or strain (displacement gradient) tensor for the geometry can be defined.

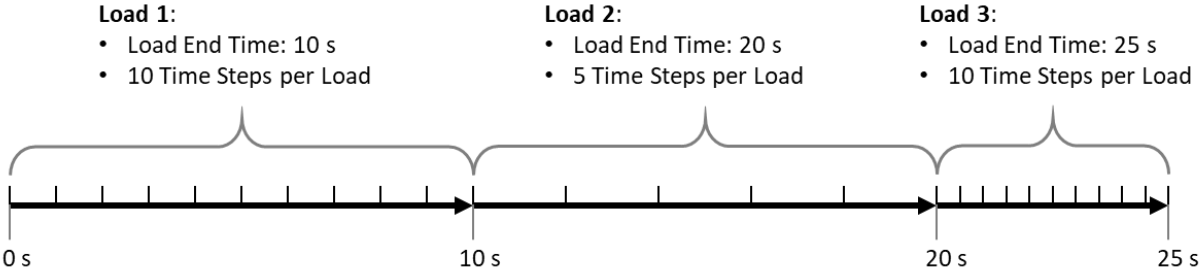
In this way, combinations of multiple loads directions are possible (e.g., biaxial load, triaxial load…). The load directions can be defined freely as a combination of normal and shear loads. In the screenshot below, a tensile strain of 2 % in X-direction, a shear load of 1 % in XY-direction and a tensile strain of 5 % in Z-direction is set.



By selecting **One Step** or **Time Series** from the pull-down menu, time steps and several load cases are specified in terms of a load sequence. With **One Step**, the load is applied in one step.

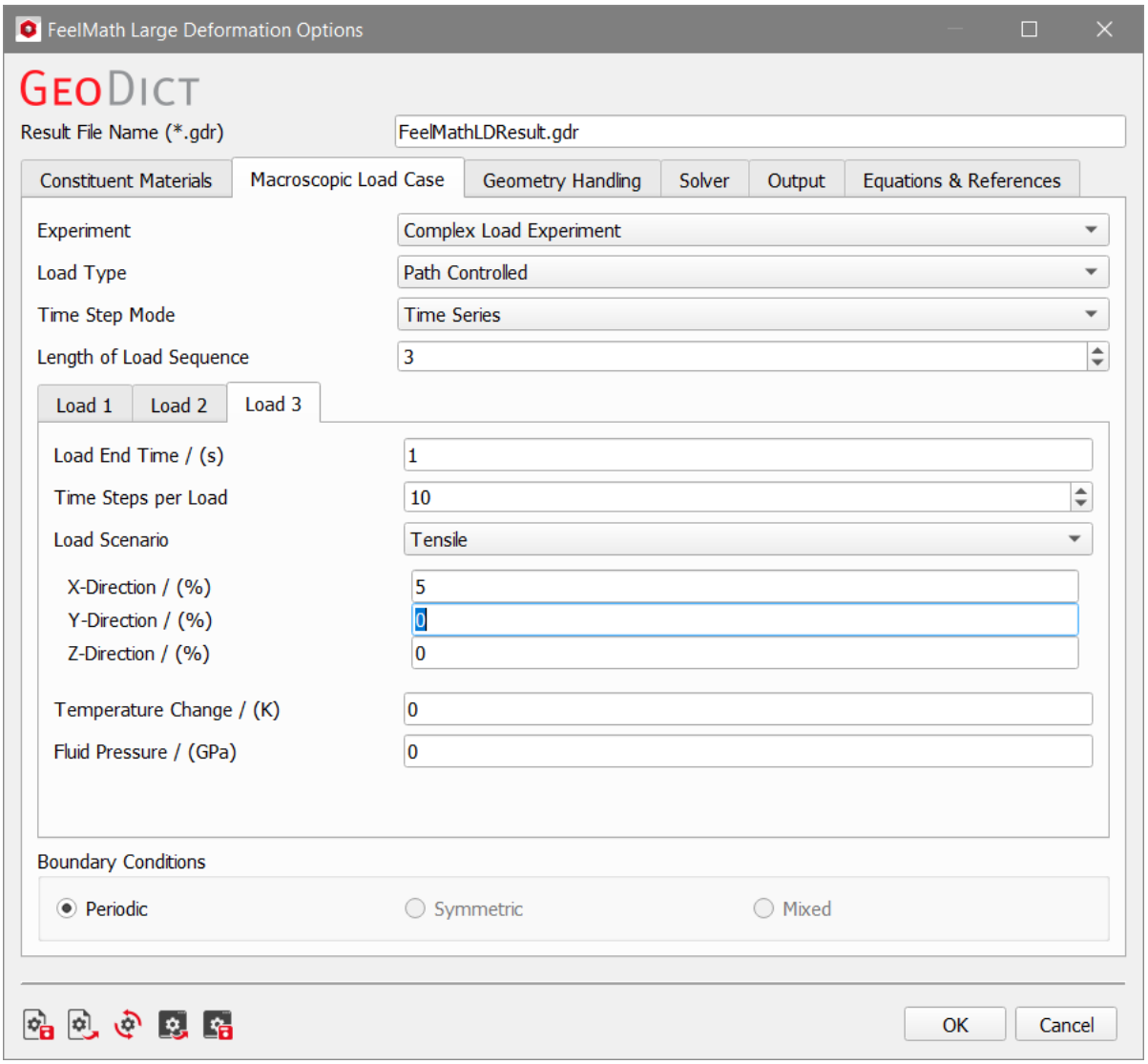
Whereas **One Step** consists of a single load step, a **Time Series** may consist of several load steps (Length of Load Sequence: 1, 2, 3…), where each load step (Load 1, Load 2, Load 3… tabs) is defined by a **Load End Time**, number of **Time Steps per Load** and a **Load Scenario**. The **Load Scenario** can be **Tensile**, **Compression**, **Shear** or **User Defined**.

The total time of the load is the difference of the current **Load End Time** and the previous **Load End Time**; therefore, the load end time must be strictly increasing. Each load is divided in a given number of **Time Steps per Load**. The concept is illustrated in the following figure:



The load sequences can be combined as desired. The user can e.g., do a compression in X-direction followed by a compression in Y-direction and a shear load.

In the example below, for the Load 3 tab, the load is subdivided into 10 timesteps (**Time Steps per Load**) and the load scenario is **Tensile**.

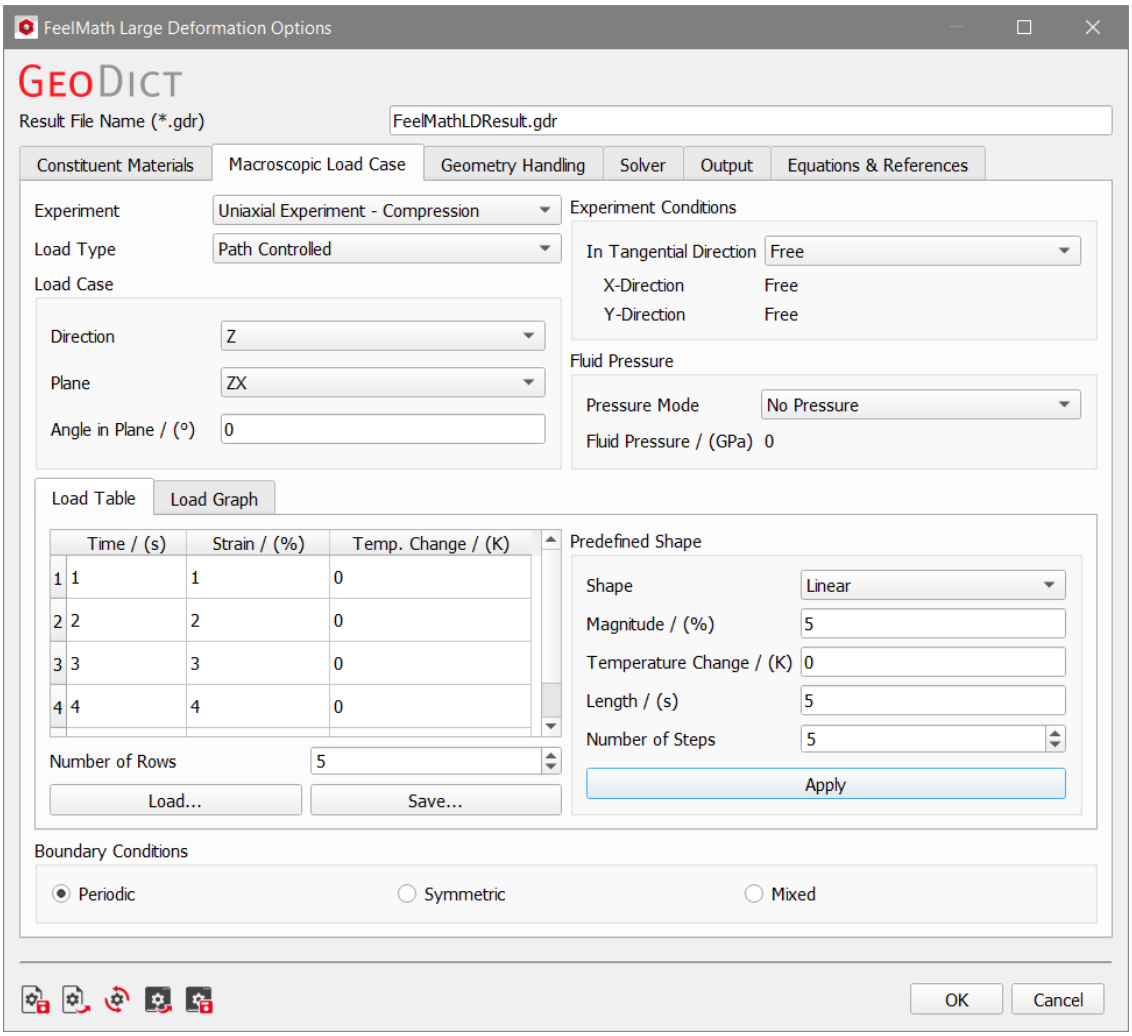

FeelMath Large Deformation Options
GEODICT
Result File Name (*.gdr)
FeelMathLDResult.gdr
Constituent Materials
Macroscopic Load Case
Geometry Handling
Solver
Output
Equations & References
Experiment
Complex Load Experiment
Load Type
Path Controlled
Time Step Mode
Time Series
Length of Load Sequence
3
Load 1
Load 2
Load 3
Load End Time / (s)
1
Time Steps per Load
10
Load Scenario
Tensile
X-Direction / (%)
5
Y-Direction / (%)
0
Z-Direction / (%)
0
Temperature Change / (K)
0
Fluid Pressure / (GPa)
0
Boundary Conditions
Periodic
Symmetric
Mixed
OK
Cancel

EXAMPLE: SETTINGS FOR UNIAXIAL COMPRESSION

In this example, we set a compression by 5% along the z-axis. Choose **Uniaxial Experiment - Compression** as Experiment and **Path Controlled** as the Load Type (to prescribe the compression ratio).

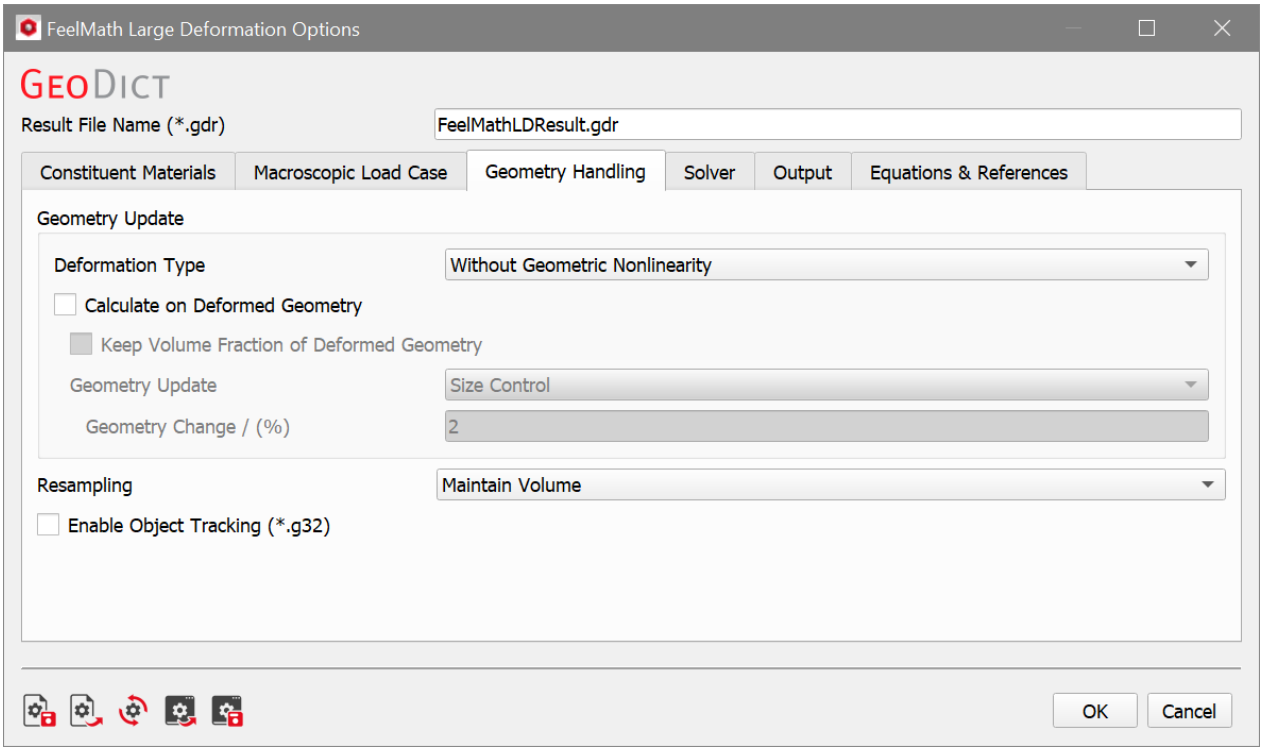
Keep the default settings for **Load Case** to compress along the Z-axis. The tangential boundary condition should be chosen depending on the needs, here we set it to **Free** to allow expansion in tangential direction.

Under **Predefined Shape**, choose **Linear**, set a **Magnitude** of 5%, a **Length** of 5 s, and a **Number of Steps** of 5. Generally, the time and number of steps should be chosen depending on the user needs. More steps always mean more computing time. After the settings for the **Predefined Shape** are made, click **Apply** to update the **Load Table** to these values.



Geometry Handling

The Geometry Handling tab contains all options relating to the geometry handling during the simulation.



Deformation Type

Under **Deformation Type**, the theory which is used for the structural mechanics is selected:

- **Without Geometric Nonlinearity**: This approach is faster and more reliable than the geometric nonlinear case. More material models are available in GeoDict for this case (e.g., Plasticity and Damage models). The boundary conditions for this experiment type are given as mean strains or mean stresses in the analyzed volume.
  - Here, the **infinitesimal strain theory** applies (see more information on Wikipedia). This is the linearized form of the *finite strain theory* (which applies to **With Geometric Nonlinearity**).
  - It is assumed that only small deformations occur, for example it is assumed that no rotations occur.
  - This is the simpler theory, but it is much more robust and easier to solve and is therefore preferable in most use cases. This means, one should always try **Without Geometric Nonlinearity** first.
  - The usual strain and stress definitions apply only here.
- **With Geometric Nonlinearity**: Should be used when the theory of small deformations does not hold anymore. A nonlinear problem must be solved; therefore, the computation might be considerably slower and less reliable than for the geometric linear case. The boundary conditions for this experiment type are given as mean displacement gradient or mean nominal stresses in the analyzed volume.

- Here, the **finite strain theory** applies (see more information on Wikipedia)
- Here, large deformations are considered, this means that also the effect of rotations is considered correctly.
- This theory is more complete, but also *much more complicated to solve* (Finite Strain Theory).
- Here, many different definitions for the stresses and strain are possible. The usual strain and stress definitions do not apply here. Nevertheless, as long as the deformations are small, the strains in the nonlinear definitions do not deviate largely from the strains in the linear definition (e.g., for small strains, the Green Lagrange Strain is close to the Strain for **Without Geometric Nonlinearity**).

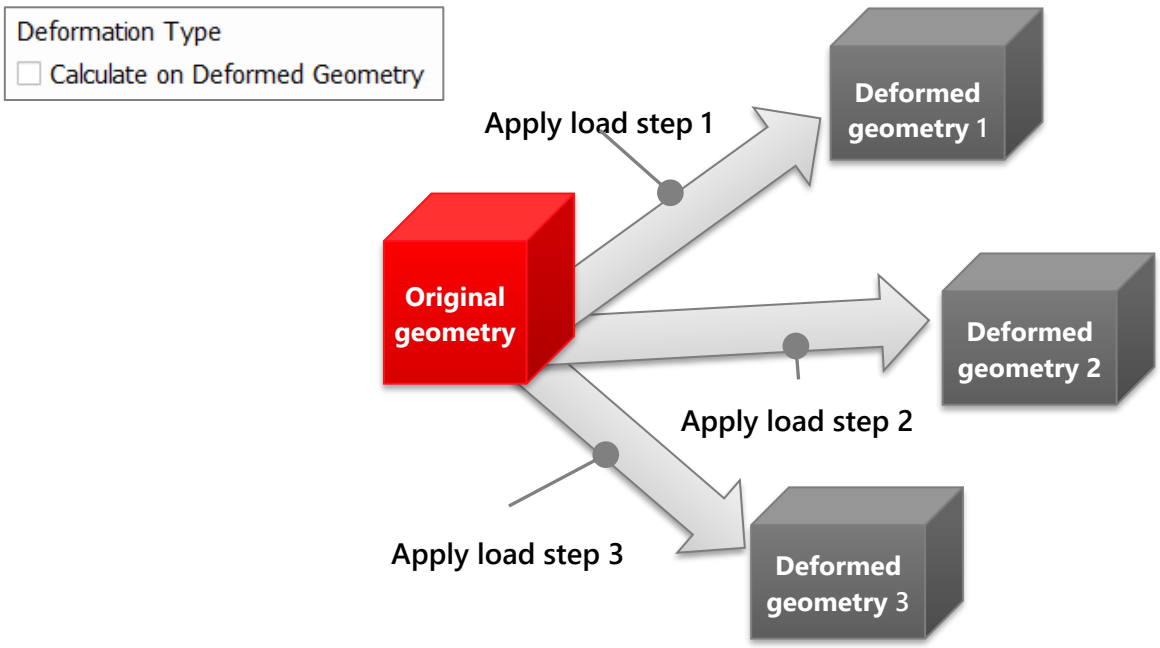
The difference between the geometric linear and nonlinear case is not special to GeoDict. This concerns all structural mechanics simulations – one always needs to choose between the simpler, but robust theory (**Without Geometric Nonlinearity**) and the more general theory (**With Geometric Nonlinearity**), which is much more complicated to solve and understand, but necessary in some cases. The two options ("With/Without Geometric Nonlinearity") might have slightly different names in other software, but the theory behind them is the same.

CALCULATE ON DEFORMED GEOMETRY

With **Calculate on Deformed Geometry** checked, the deformed geometry is re-sampled, and this geometry is used for the calculations in the next step. With this method, it is possible to detect new object contacts during deformation and e.g., to observe the effect of stiffening during compression. **Calculate on Deformed Geometry** can only be used without geometric nonlinearity.

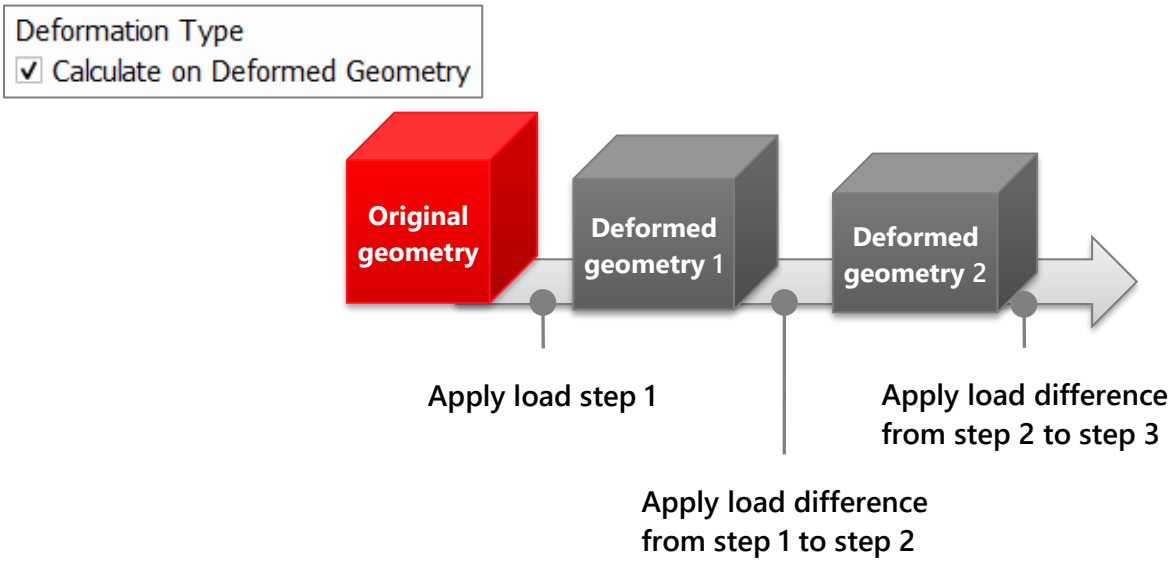
A resampling step is done if the conditions defined under Geometry Update are met. It is important to choose these settings appropriately for the current geometry and deformation steps: With each resampling step, discretization errors occur, and these errors accumulate if too many resampling steps are done. Therefore, the resampling should only be done after a significant change in the geometry size. This can be achieved by choosing the mode **Size Control** for **Geometry Update** (see page 20).

- **Off:** The deformation is always calculated relatively to the original geometry



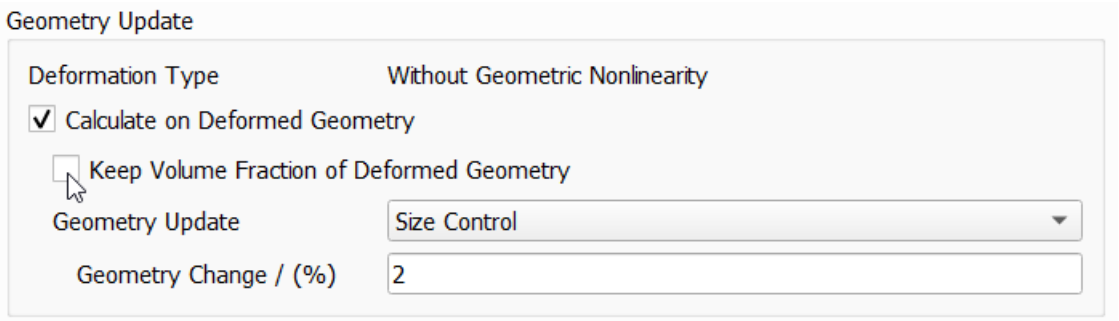
- **On**:

  If the conditions defined under **Geometry Update** are met, the deformed geometry is calculated, and the deformation is calculated relative to the previous geometry. In the figure below, the behavior of the setting **All** for **Geometry Update** is shown.



Keep Volume Fraction of Deformed Geometry

If **Keep Volume Fraction of Deformed Geometry** is checked, the accurate volume fraction information for each material ID after the deformation is kept and updated in memory (Please refer to page 21 for further information about the volume fractions). This needs more memory but leads to a more accurate geometry deformation if many (small steps) are computed. Without this information, the volume fractions are converted into a structure in each deformation step and the volume fraction is lost.

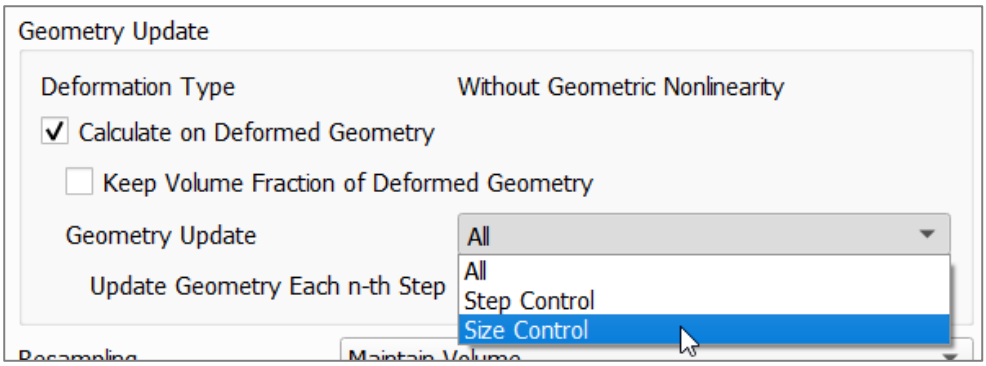


Geometry Update

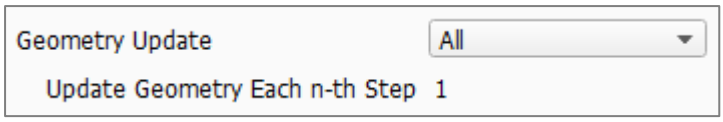
Under **Geometry Update**, it can be selected when the next simulation step is computed on the newly deformed geometry, or if it is computed based on the existing geometry.

Use the mode **Size Control** for the Geometry Update when using **Calculate on Deformed Geometry**. With this mode, the size of the deformation is checked after each step.

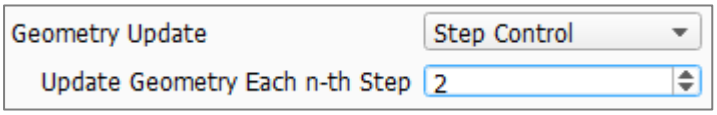
Only if the deformation is larger than the given threshold, **Calculate on Deformed Geometry** is used for this step. Otherwise, the step is done without **Calculate on Deformed Geometry**. We strongly recommend using this mode for simulations of this type.



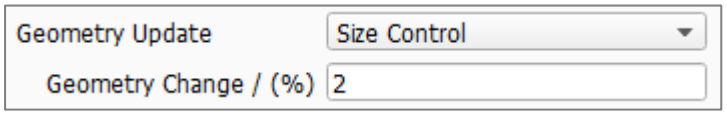
- **All** – The geometry is updated in every step



- **Step Control** – Choose how often the geometry is updated with **Update Geometry Each n-th Step**.



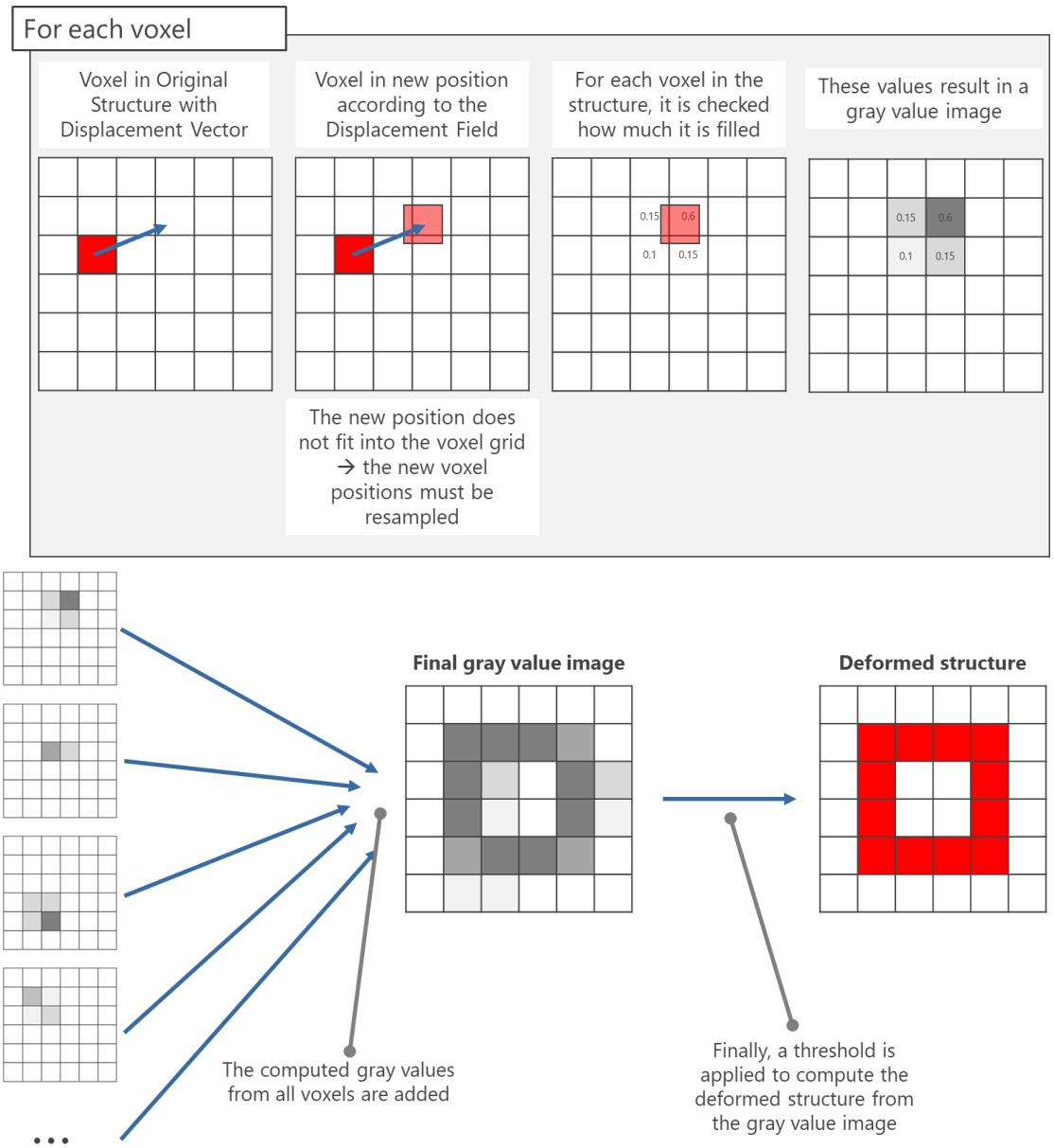
- **Size Control** – If the geometry is updated or does not depend on the change of the domain size. If the size change for one domain side is larger than the value defined for **Geometry Change / %**, the geometry is updated.



RESAMPLING

For **Resampling**, two options can be chosen: **Maintain Volume** or **Maintain Mass**. Deformation in ElastoDict is computed and stored as a displacement field. For each voxel, this displacement field contains the information on how far it is displaced in the current deformation step.

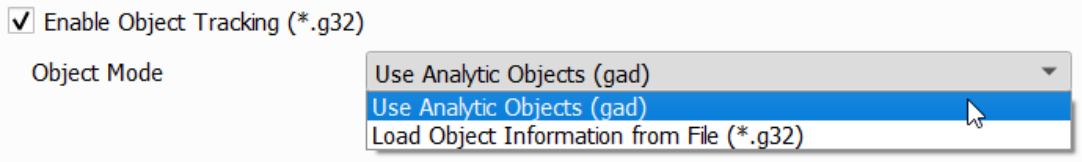
Internally, the new material positions are calculated based on this displacement information. Since the new positions do not necessarily lie on the voxel grid, a gray value image with material **Volume Fractions** is computed for each material ID. These volume fractions contain the information "how much" of a given material is contained in a voxel after the deformation. These volume fractions must be resampled to the voxel geometry. In the figures below, this resampling is shown in a simplified example for one material ID. The deformed geometry is generated by thresholding the resulting gray value image containing the volume fractions.



With **Maintain Volume**, the resampling threshold is chosen in such a way that the volume of each solid material in the structure stays roughly the same. With **Maintain Mass**, the threshold for each voxel is set to 0.5. This means, **Maintain Volume** is a good choice when it is expected that the volume of a material doesn't change during the deformation. When deformations occur where the volume of the material changes significantly during the computations, e.g., thermal expansion or expansion due to a negative Poisson's' ratio, **Maintain Mass** should be used.

Enable Object Tracking (*.g32)

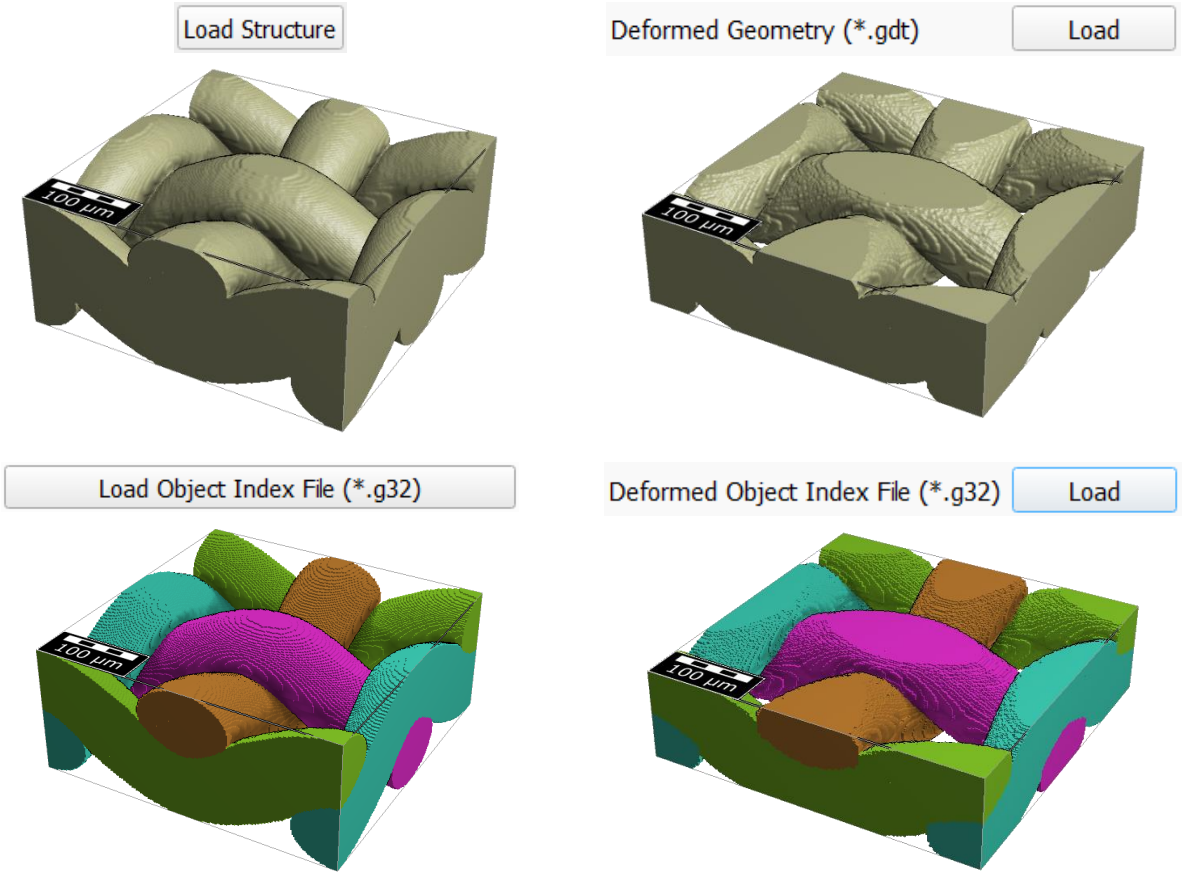
With the object tracking option, a *.g32 file with the object indices for all objects in the structure is created for each deformed geometry. This way, the deformation of each object in the structure can be tracked during the deformation.



OBJECT MODE

The choice for **Object Mode** depends on the available information: If a structure with analytic object information (e.g. from GeoDict's structure generator modules FiberGeo, GrainGeo, FoamGeo, …) is used, this information can be used with **Use Analytic Objects (gad)**. In this case, a *.g32 file with object indices is automatically created and saved in the results folder. If no analytic object information is available, **Load Object Information from File (*.g32)** must be selected and a *.g32 file must be loaded. A *.g32 file can be created e.g. with GrainFind for all grains in the structure.

In the example below, a weave structure from WeaveGeo with the corresponding object indices is shown before and after deformation in ElastoDict. These structures can be loaded directly from the result viewer with the corresponding buttons (shown below).



SOLVER

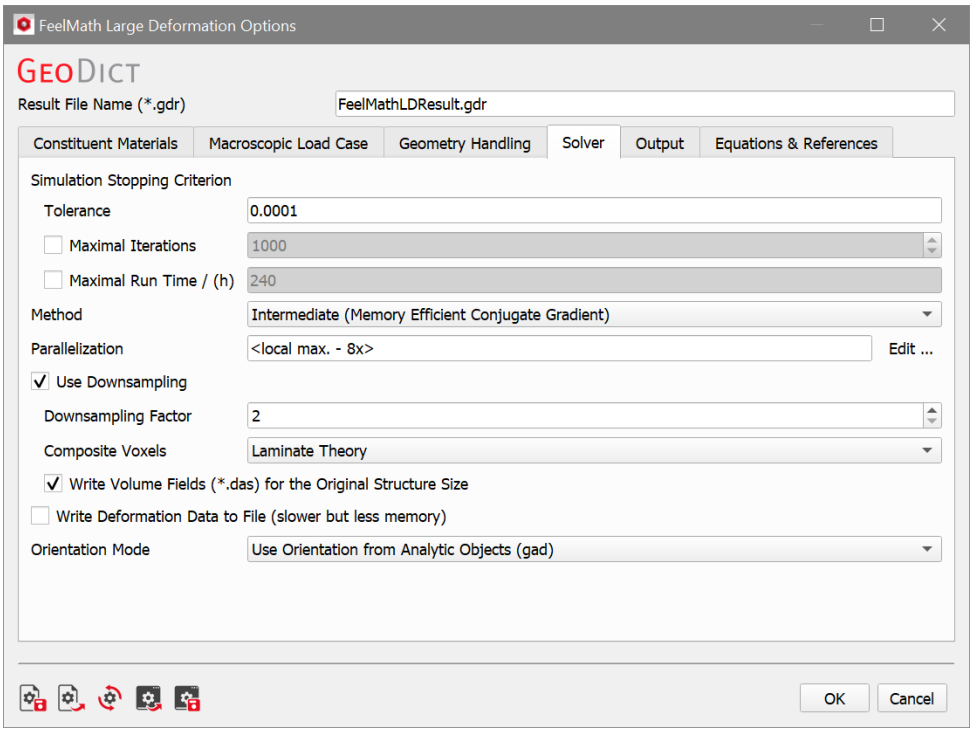
Internally ElastoDict uses an iterative solver to solve the equations that describe the mechanical problem at each voxel. The basic idea of an iterative method is:

1. Start with an initial guess for the unknown values.
2. Improve the current values in each iterative step. The speed of the improvement depends on the problem parameters.
3. Repeat the iterative process until one of the stopping criteria occurs.

Simulation Stopping Criterion

The iterative process of the solver is controlled by setting the values for **Tolerance**, **Maximal Iterations**, and **Maximal Run Time (h)**. Only the tolerance must be set, the two other parameters are optional.

For each iteration step, the relative error of the current solution is computed. If this relative error is smaller than the given tolerance, the computation is finished. When there is doubt about the quality of the solution, decrease the tolerance value by a factor of ten for that solver. In general, it is recommended to keep the default setting for tolerance.



When the solver stops because the **Maximal Iterations** or the **Maximal Run Time (h)** are reached, the quality of solution might be doubtful since the requested accuracy is not achieved. Therefore, those two options are disabled by default and should only be selected if there are strong constraints on the allowed runtime.

Method

For the **FeelMath-LD** solver, three different iterative methods are available: **Fast (Conjugate Gradient)**, **Intermediate (Memory Efficient Conjugate Gradient)** and **Memory Efficient (Neumann Series)**.

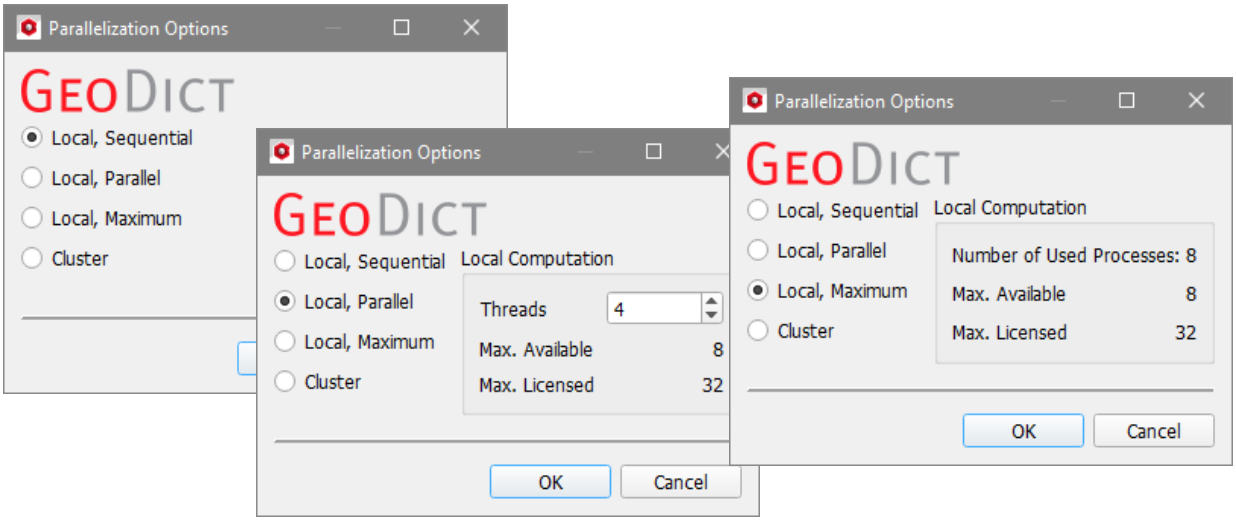
The **Fast** method converges faster, especially for strongly varying material parameters and nonlinear material laws (as e.g. plasticity or damage), but needs about four times as much memory as the **Memory Efficient** method.

The **Intermediate Method** needs approximately 40 % less memory than the **Fast** method but is 20-30 % slower. The **Estimate memory** button, in the **ElastoDict** section (see page 5), can be used to decide which method is applicable for the current structure on the available computer.

In general, it is recommended to use the default (**Memory Efficient Conjugate Gradient**) or the **Conjugate Gradient** method. The **Neumann Series** method should only be used if the memory is not enough for the other methods.

PARALLELIZATION

The ElastoDict run can be accelerated by using multiple CPU cores. The **Parallelization Options** dialog opens when clicking the **Edit...** button, to choose between **Local, Sequential**, **Local, Parallel**, **Local, Maximum** and **Cluster**.



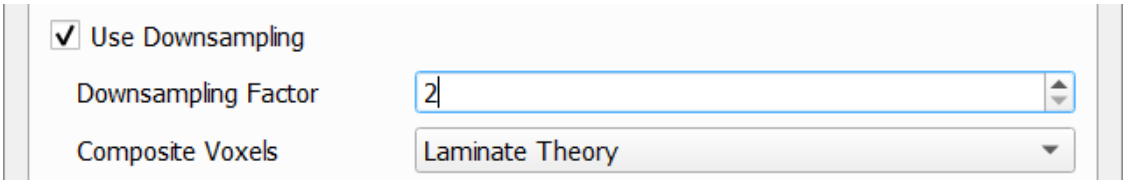
The number of **Threads** to run can be entered after choosing **Local Parallel**. **Local, Maximum** is the default and provides the fastest possible computation based on the available and licensed processes. With **Local, Sequential**, only one thread is used and no parallel computation is done.

For information on how to set up and use ElastoDict in a **Cluster** configuration, contact support@math2market.de

USE DOWNSAMPLING

Downsampling reduces the structure size by combining multiple voxels. By default, the **Downsampling Factor** is set to two – this means that 2x2x2 voxels are combined to one voxel. The material model used for each voxel in the downsampled structure is a combination of the material model (e.g., a **Composite Voxel**) of the original voxels. Since the simulated structure size is much smaller than the original structure, **Downsampling** allows to speed up the simulation and to quickly obtain results even on computers with little memory. This option should not be used if highest accuracy is required.

In most cases, a **Downsampling Factor** of 2 is the best choice, but it can also be set to 4 if needed. Then, the computation will be faster, but the results will be more inaccurate.



To be able to use downsampling, the features (e.g., fibers or grains) in each material ID must have a diameter of at least the Downsampling factor in voxels (e.g., 2 voxels for a **Downsampling Factor** of 2). Otherwise, the computation of the material properties might not work properly. Since GeoDict 2021, an error message is shown

if all features in the structure are smaller than this diameter, and the simulation cannot be started.

Composite Voxels

Two different methods to compute the **Composite Voxels**: **Laminate Theory** (the default), and **Arithmetic Mean**. When using **Laminate Theory**, the composite material properties are computed based on the laminate theory of composite materials. With this option, also direction dependent properties are represented correctly. With **Arithmetic Mean**, the material properties of the composite voxel are the average of the material properties of the original voxels. This method is less accurate, but the simulation might be more stable, especially if the structure contains many pores (as e.g., in foams). Nevertheless, it is recommended to keep the default **Laminate Theory** in most use cases for the higher accuracy.

Write Volume Fields (*.das) for the Original Structure Size

The result fields can be written in the downsampled resolution (by disabling **Write Volume Fields (*.das) for the Original Structure Size**, which is the default). Writing the fields in the downsampled resolution is much faster and saves disk space, since the files are 8 times smaller for a **Downsampling Factor** of 2, or even 64 times smaller for a **Downsampling Factor** of 4 (2x2x2 or 4x4x4 voxels in the original structure correspond to 1 voxel in the downsampled structure). Therefore, it is recommended to keep this default for most use cases. Nevertheless, if **Laminate Theory** is selected as mode for the **Composite Voxels**, the fields in the original resolution contain more information. In this case, the composite material also contains directional information, which can lead to a gradual change of the strains and stresses inside a single composite voxel. This change is only resolved by writing the fields in the original resolution.

Write Deformation Data to File

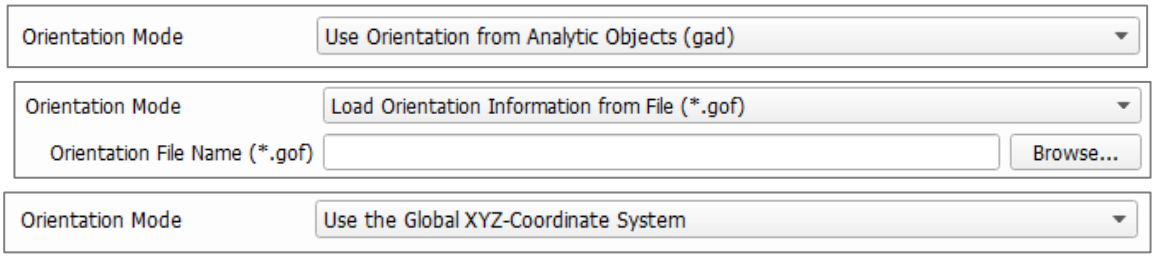
For the computation of the deformed structures, intermediate data is computed which describes the displacement for each voxel. Before this computation, it is not clear how large this data will be, since a voxel in the original structure might be partially moved in multiple voxels in the deformed structure. Therefore, this data might not fit in the main memory of the computer. Due to this, the deformation data was always written to the hard drive in GeoDict 2020 and before. Nevertheless, there is an issue with this approach: Writing and loading data form the hard drive is many times slower that writing and loading data in the main memory (even if the drive is an SSD). This causes a bottleneck, which can slow the simulation down.

Therefore, GeoDict 2021 and later allows to keep the deformation data in memory. This is the new default, since the data fits in the main memory in most cases, and this option is many times faster (See benchmark results on page 40). To get the old behavior from GeoDict 2020 and before, check the option **Write Deformation Data to File**. We recommend keeping this option disabled, and to select it only if the simulation fails because the data doesn’t fit in the RAM.

Orientation Mode

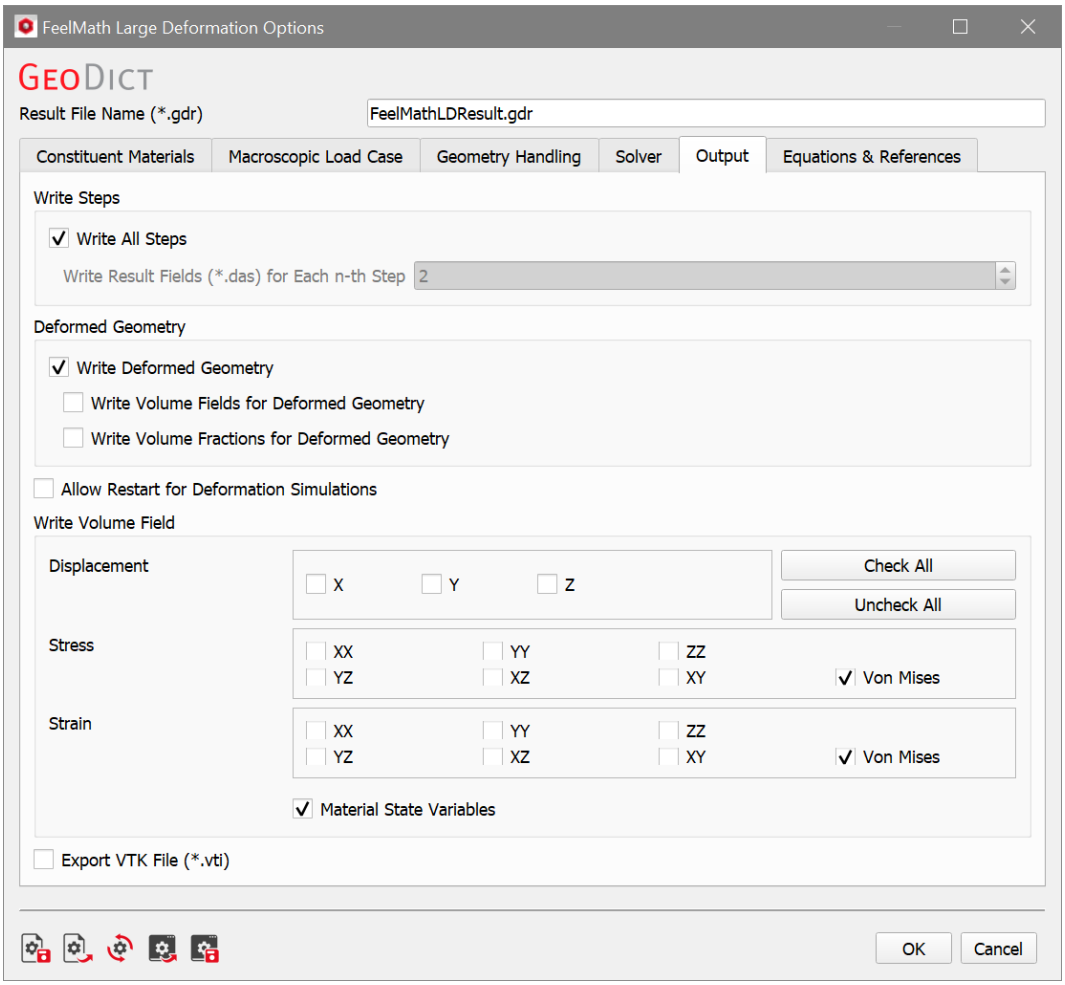
ElastoDict can handle non-isotropic constituent materials. For these materials, an orientation has to be additionally specified. If the analyzed structure consists of analytical objects (gad data), the orientation of these objects is used when **Use Orientation from Analytic Objects (gad)** is selected.

Alternatively, with **Load Orientation Information from File (*.gof)**, orientation information can be loaded from a file. Such a file can be generated for example with GrainFind for granular structures. The third option, **Use the Global XYZ-Coordinate System**, allows to use anisotropic materials even if no orientation information for the structure is available.



OUTPUT

The options available in the Output tab control which information is saved to the hard disk during the computation. Choosing only the necessary variables might help to save computation time.



WRITE ALL STEPS

When **Write all Steps** is chosen, the results fields selected under **Write Volume Field** are written after each computation step. Otherwise, the number of steps after which the results fields are saved can be selected. When computing with many steps, disabling **Write all Steps** saves considerable computation time.

Deformed Geometry

When **Write Deformed Geometry** is chosen, a geometry with the current displacements is resampled and saved after each step. Deformed geometries are written at each step, even if **Write all Steps** is disabled. Writing the deformed geometries is mainly interesting for visualization purposes and to check possible problems in the simulation setup when **Compute on Deformed Geometry** is chosen in the **Macroscopic Load Case** tab.

With **Write Volume Fields on Deformed Geometry**, also the result fields are resampled with the current displacements so that they match the deformed geometries.

With **Write Volume Fractions for Deformed Geometry**, the volume fractions for each material ID in each voxel after the deformation are written to the *.das files. This information is necessary for the computation of the deformed geometries (For further understanding, check out the explanations on page 21). In general, it is not necessary to select this option.

Allow Restart for Deformation Simulations

If you want to be able to restart a simulation after an interruption, the complete stress and strain information must be saved for each step. With the option Allow Restart for Deformation Simulations, the necessary volume fields are automatically saved.

Since GeoDict 2022, restarting is also available for simulations with **On Deformed Geometry**.

Write Volume Field

Checking or un-checking the boxes for **Displacement**, **Stress**, and **Strain** determines whether these results outputs are available for visualization and post-processing after the run of the FeelMath-LD solver. Additionally, it is possible to save the deformed geometry and to save the solution fields (for stress and strain) for the deformed geometry. Depending on the structures size, the result files can become large (up to several GB), so it is recommended to deselect all options which are not needed for the current task.

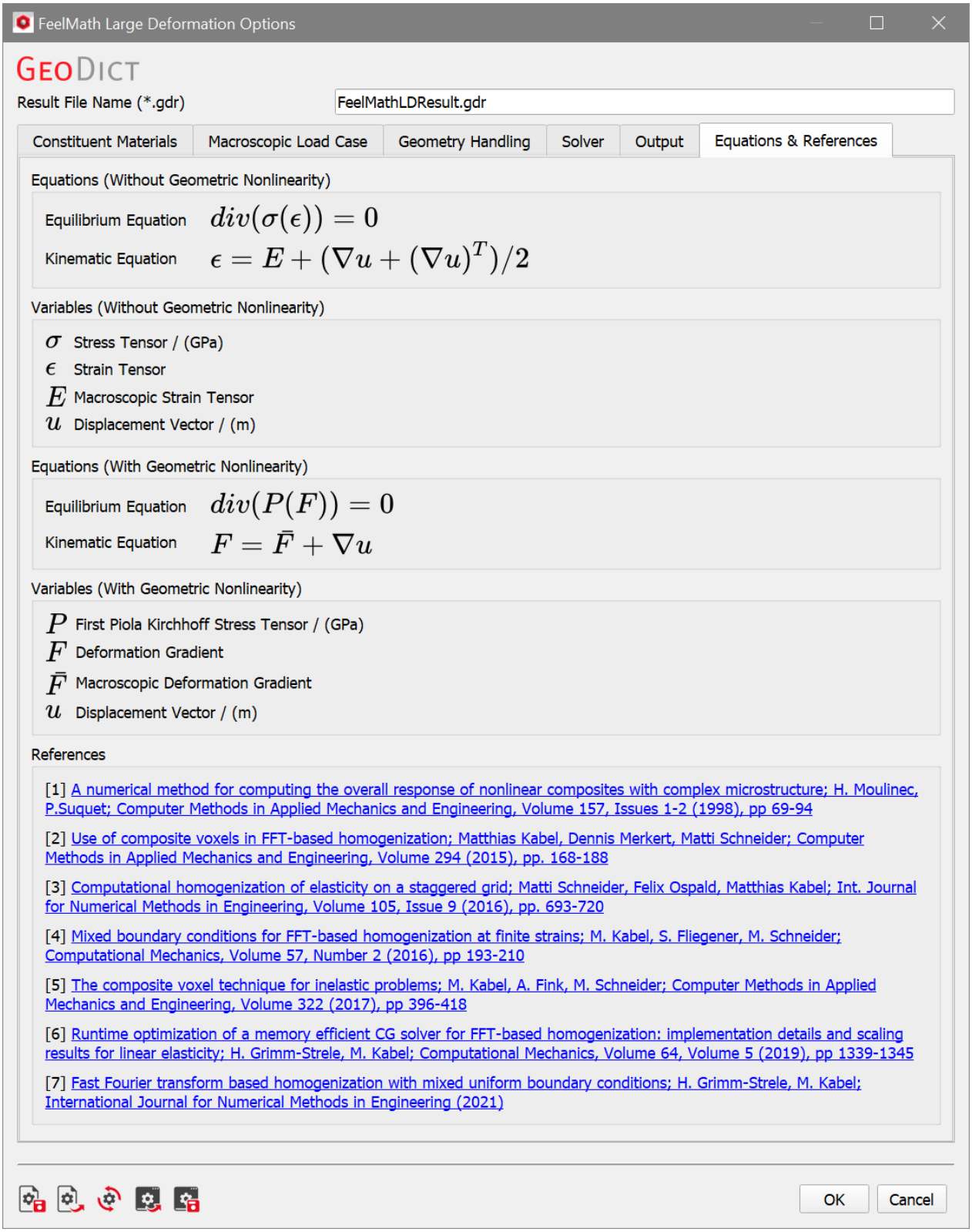
For nonlinear materials, additional state variables might be defined. For example, for plastic deformation, these are the elastic and plastic strains. For materials with damage behavior, this is the damage variable. When **Material State Variables** is checked, these variables are saved as Volume Fields.

Export VTK File

Besides using GeoDict's own visualization tools, it is possible to export the solution in the commonly used VTK (Visualization Toolkit) format (see: https://vtk.org/ and, https://www.paraview.org/).

Equations & References

The differential equations solved in the simulation are listed under the **Equations & References**. Additionally, the tab contains the references for the methods used by the FeelMath solver in ElastoDict (see page 2 for links).



RESULT FILE (.GDR)

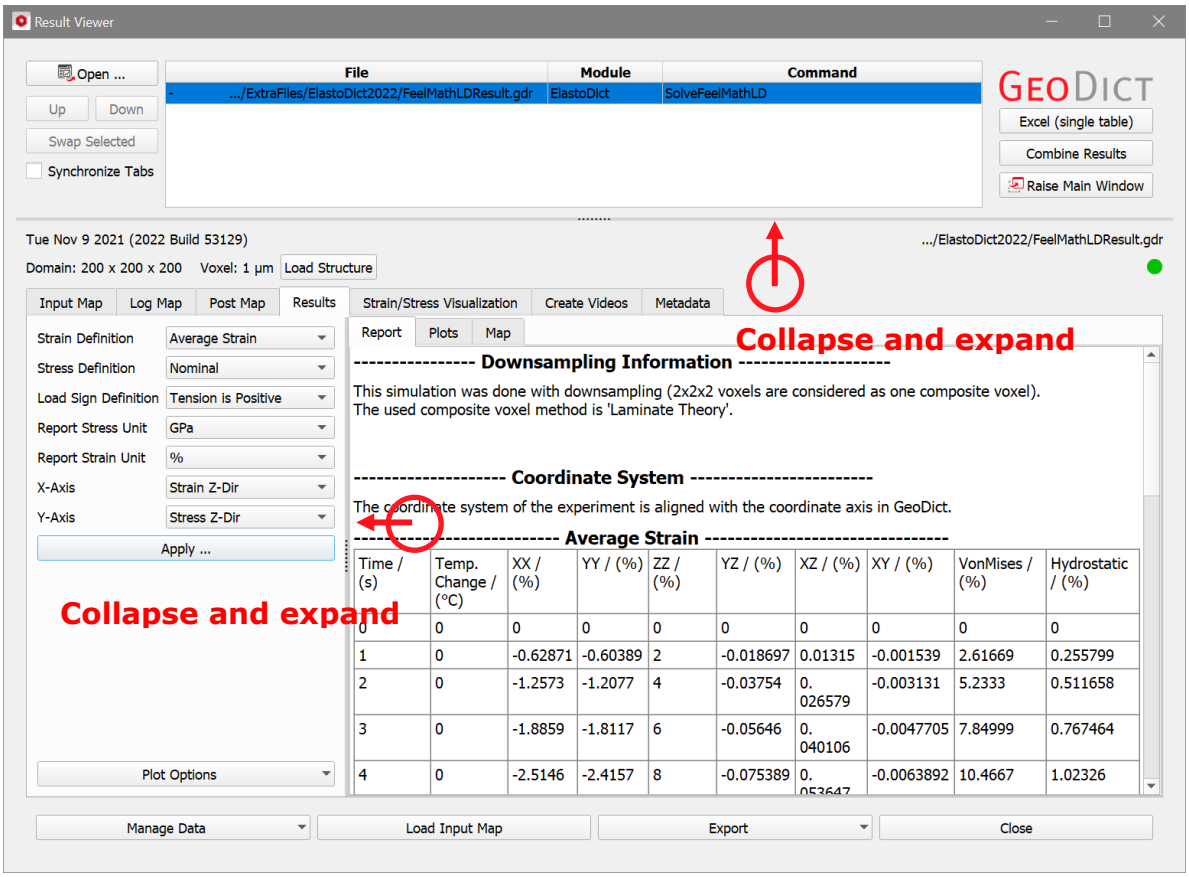
After the solver has finished, the result file (.gdr) is saved in the project folder and the Result Viewer opens automatically.

In the **Result Viewer**, the list of all open result files and the path to them is shown in the header section. Results from older runs are accessible by opening their *.gdr files (**File → Open *.gdr File...** in the menu bar). The name of the result file currently displayed is highlighted in blue in the header section. Multiple results files can be opened at the same time. To compare their results, use **CTRL+right-click** to select multiple results files in the Result Viewer. The selected result files are shown side-by-side.

The header section and the post-processing section (left panel of the **Results** tab) can be collapsed (and expanded) by pulling up/down or left/right on the dotted line.

The green dot in the right side of the Result Viewer indicates that the results shown are computed for the structure displayed in the visualization area (in memory) at this time. The dot is red when the structure in memory is not the one for which the values in the opened result file were calculated. The corresponding structure can be loaded by clicking **Load Structure** in the Result Viewer.

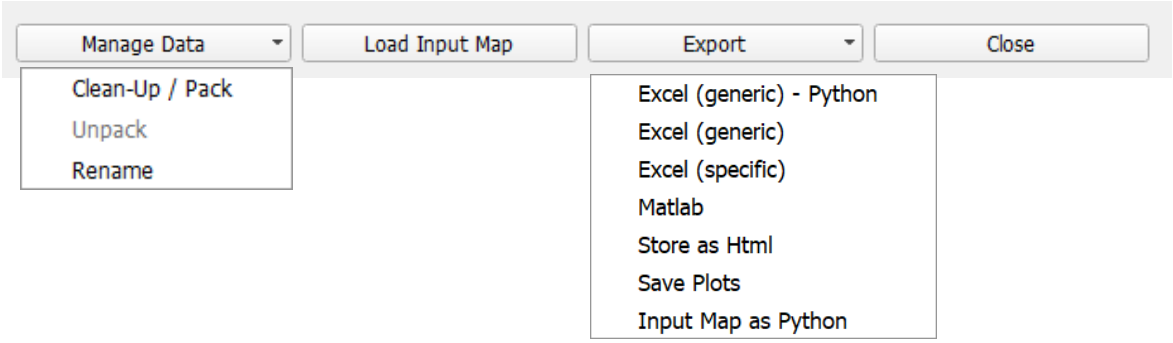
When two result files have green dots, it indicates that both result files correspond to the structure shown in the **Visualization area** and might be the results from two simulations with different ElastoDict settings. Since GeoDict 2020, it is possible to **Combine Results** files, for further information please refer to the Result Viewer handbook of this User Guide.



The Result Viewer contains seven main tabs and subtabs:

- **Input Map** - all input parameters
- **Log Map** - solver specific values
- **Post Map** - parameters of the current plot
- **Results** - numerical results and plots
  - **Report**
  - **Plots**
  - **Map**
- **Strain/Stress Visualization** - 3D data which can be loaded in GeoDict for visual inspection
- **Create Videos**
- **Metadata** - description and user defined parameters

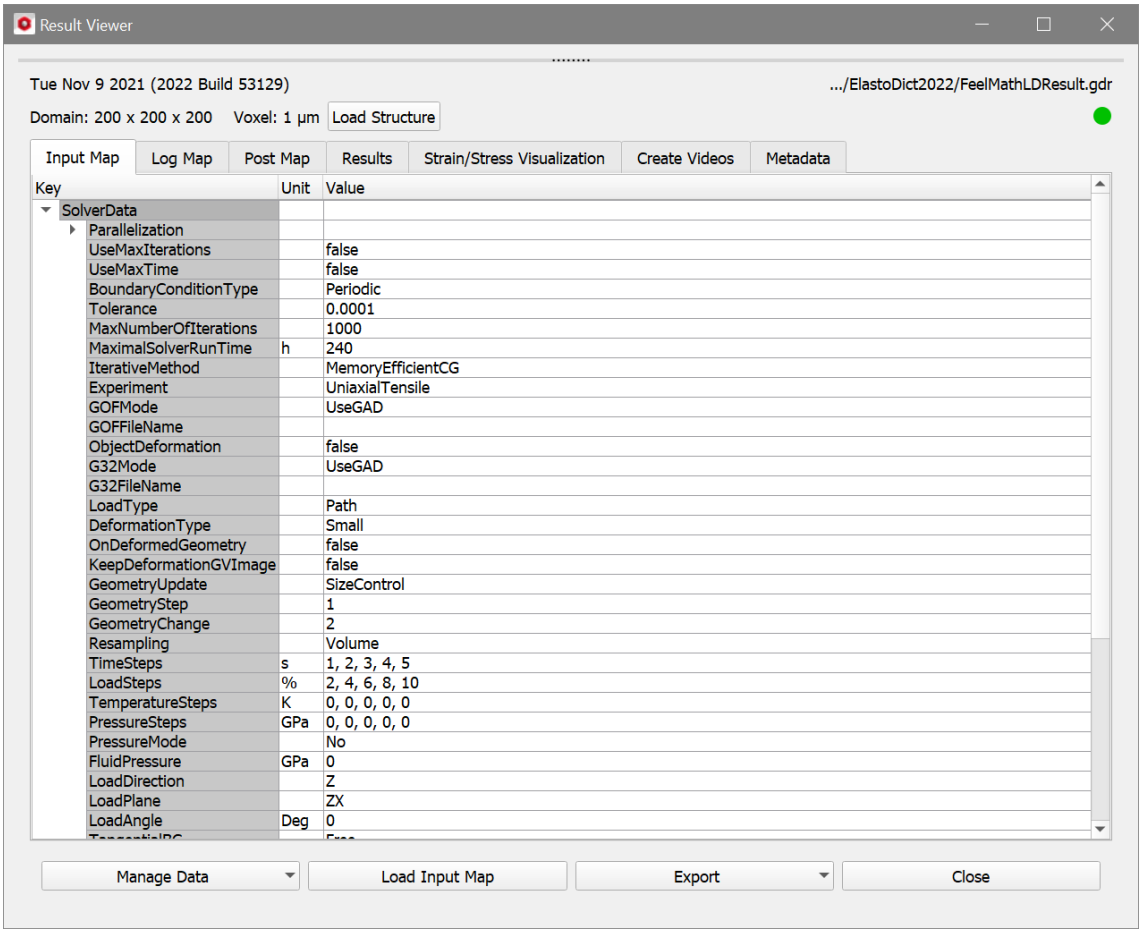
At the bottom of the Result Viewer, several buttons are available:



- Use the Manage Data option to **Clean-Up**, **Pack**, **Unpack** or **Rename** the result files. For the packing and unpacking operations, the additional software 7-zip is needed which can be installed with the GeoDict Required Tools installer.
- Load the solver options that were used for the calculations into the ElastoDict GUI by clicking **Load Input Map**.
- **Export** data:
  - Analyze and plot computation results in Microsoft Excel® using GeoDexcel provided with GeoDict by clicking **Excel (specific)**, **Excel (generic)**. The specific import loads the results report (see page 33) as a formatted excel table, whereas the generic import loads all information from the *.gdr file. GeoDexcel is only available for Windows®. See the GeoDexcel handbook of this User Guide for more information. **Excel (generic) – Python** provides the same functionality as **Excel (generic)** using Python and works on Windows and Linux.
  - Analyze computation results in MATLAB® using GeoDict's MATLAB® interface GeoLab by clicking **Matlab**. All information included in the results file is loaded into MATLAB® automatically.
  - Save the information in the result file in *.html format by clicking **Store As HTML**.
  - **Save Plots** to save images for all plots in the current results file
- Close the results file by clicking **Close**.

Input Map

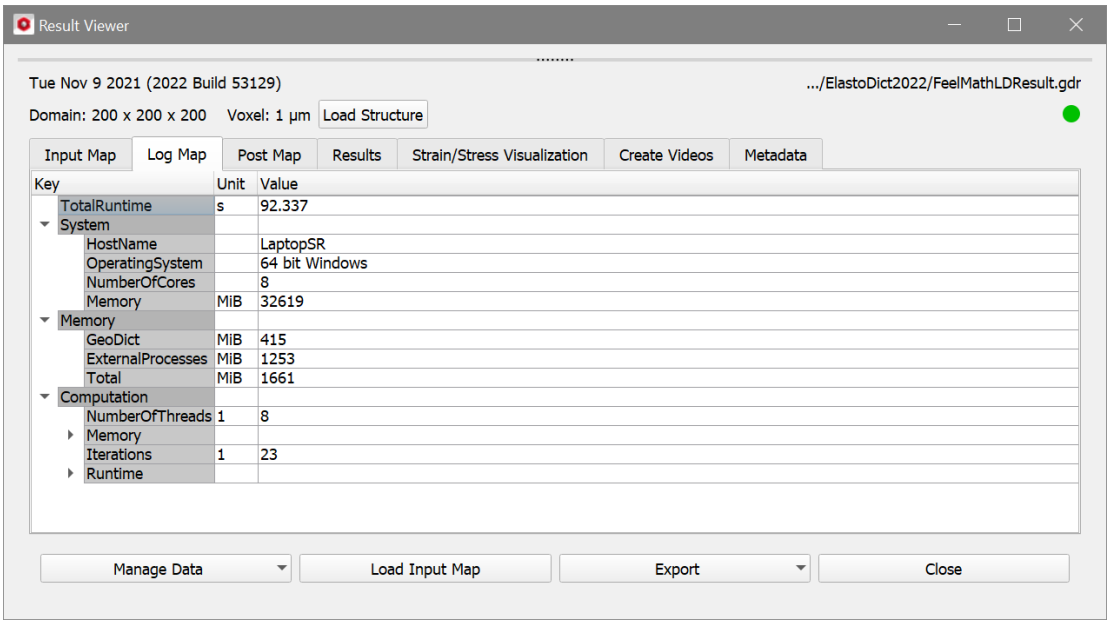
The **Input Map** contains all parameters which were used for the simulation. With the option **Load Input Map** at the bottom of the Result Viewer, all parameters are loaded into the GeoDict GUI and a new simulation with the same parameters can be started.



Key	Unit	Value
SolverData		
Parallelization		
UseMaxIterations		false
UseMaxTime		false
BoundaryConditionType		Periodic
Tolerance		0.0001
MaxNumberOfIterations		1000
MaximalSolverRunTime	h	240
IterativeMethod		MemoryEfficientCG
Experiment		UniaxialTensile
GOFMode		UseGAD
GOFFileName		
ObjectDeformation		false
G32Mode		UseGAD
G32FileName		
LoadType		Path
DeformationType		Small
OnDeformedGeometry		false
KeepDeformationGVImage		false
GeometryUpdate		SizeControl
GeometryStep		1
GeometryChange		2
Resampling		Volume
TimeSteps	s	1, 2, 3, 4, 5
LoadSteps	%	2, 4, 6, 8, 10
TemperatureSteps	K	0, 0, 0, 0, 0
PressureSteps	GPa	0, 0, 0, 0, 0
PressureMode		No
FluidPressure	GPa	0
LoadDirection		Z
LoadPlane		ZX
LoadAngle	Deg	0

Log Map

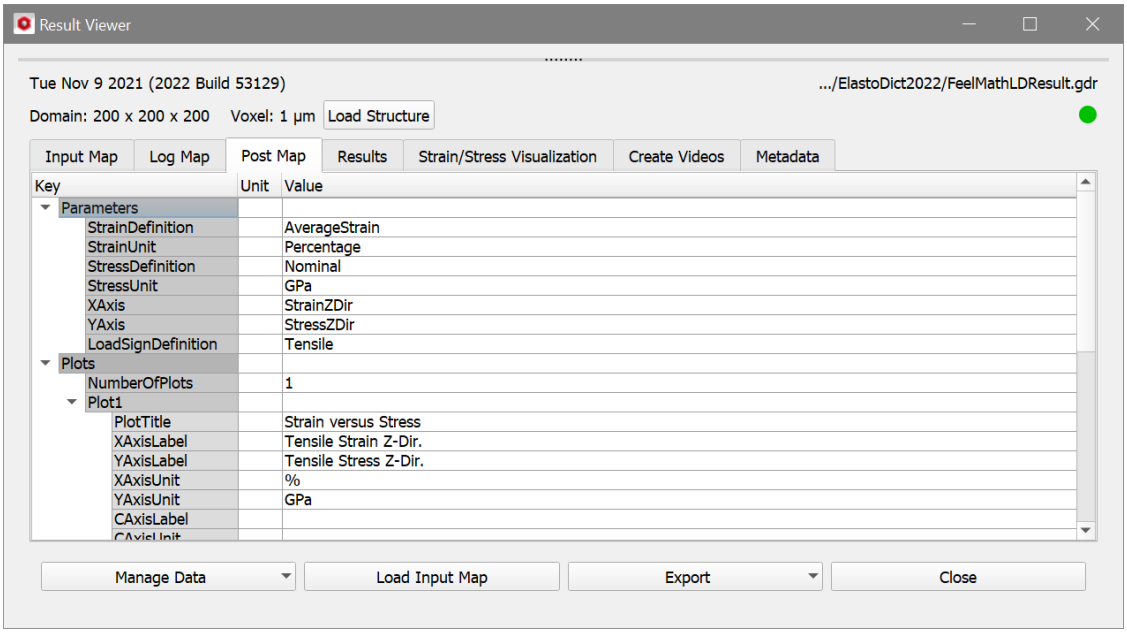
The **Log Map** contains detailed information about the runtime and memory consumption during the simulation.



Key	Unit	Value
TotalRuntime	s	92.337
System		
HostName		LaptopSR
OperatingSystem		64 bit Windows
NumberOfCores		8
Memory	MiB	32619
Memory		
GeoDict	MiB	415
ExternalProcesses	MiB	1253
Total	MiB	1661
Computation		
NumberOfThreads	1	8
Memory		
Iterations	1	23
Runtime		

Post Map

The **Post Map** tab contains all information about the current plot under the Results tab.

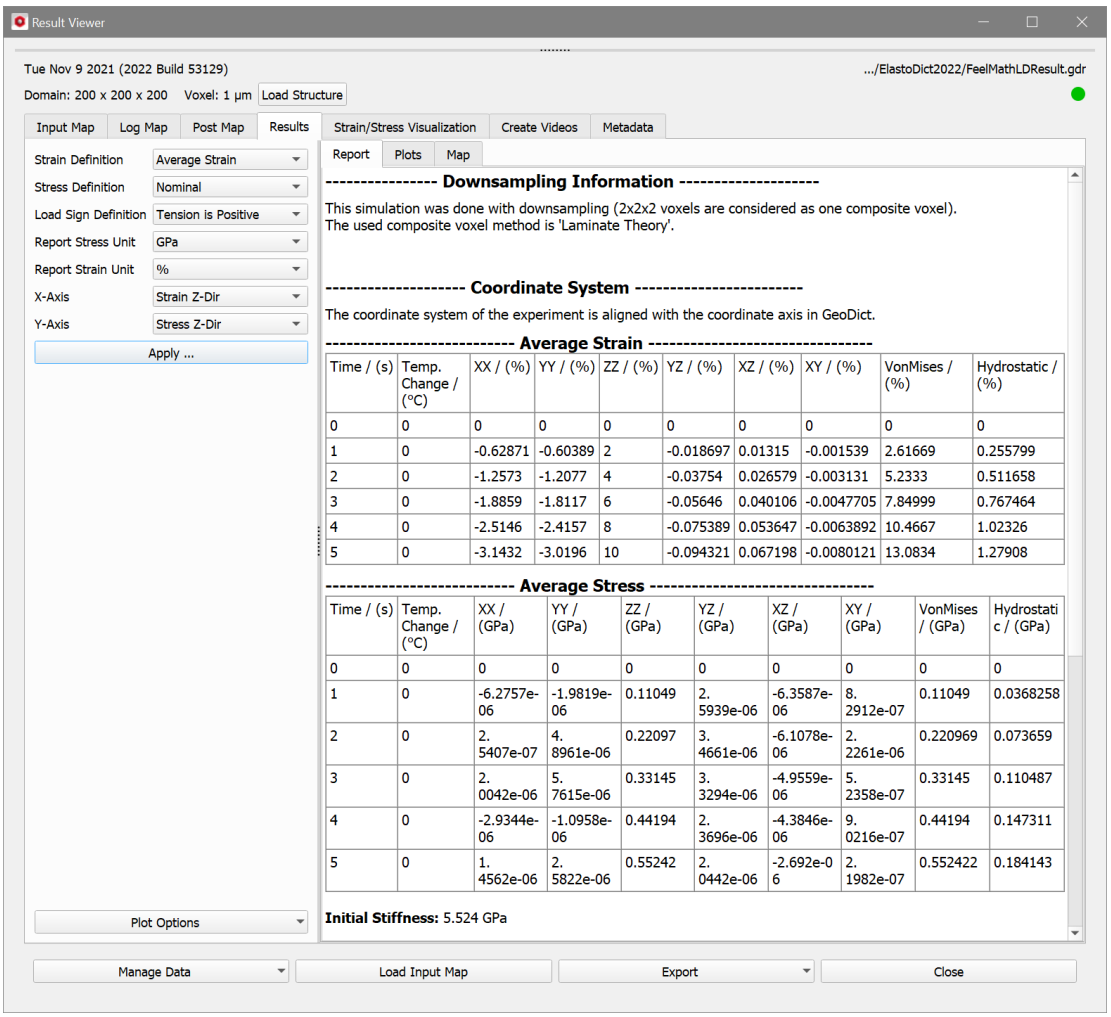


Results

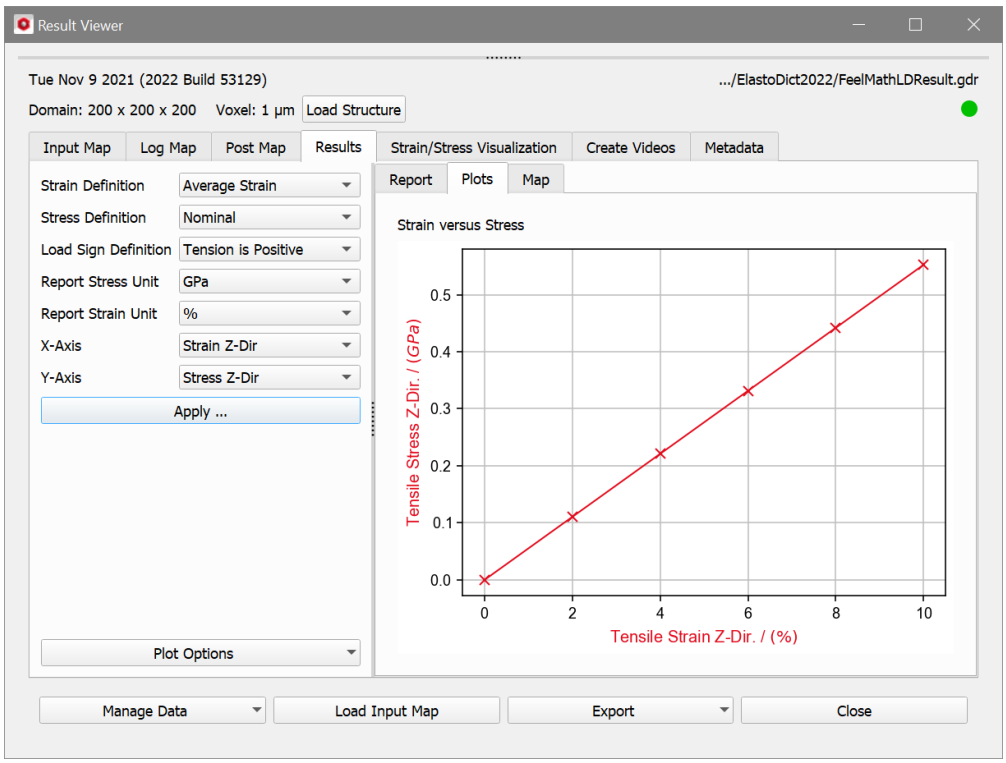
The **Results** tab gives access to the computed values for the parameters calculated by the selected ElastoDict process.

The **Results** tab is divided into two or into three subtabs:

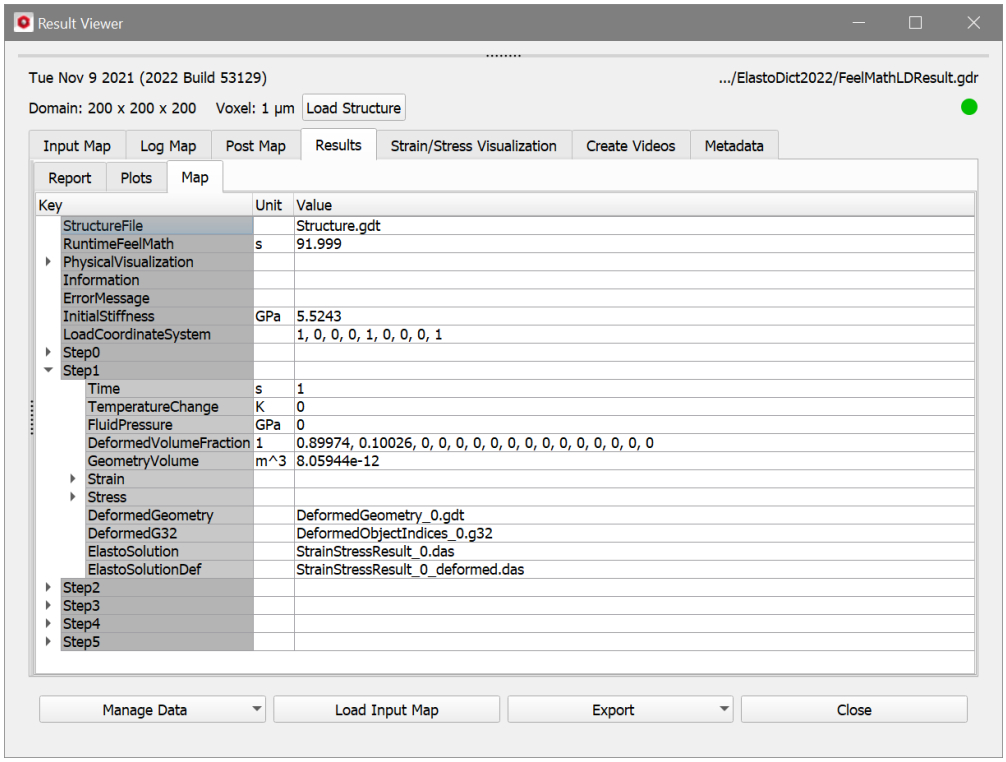
- The **Report** subtab shows the average strain (displacement gradient when using geometric nonlinearity) and stress values in the experiment.



- The **Plots** subtab shows the strain-stress diagram by default. The parameters on the X/Y-Axis and the corresponding units can be specified to the left of the plot. The new plot is created by clicking **Apply**. By right-clicking on the plot, it is possible to adjust the plot settings, for example, the font sizes, data range etc. Additionally, the plot can be saved as an image and the data can be saved as a *.txt file.

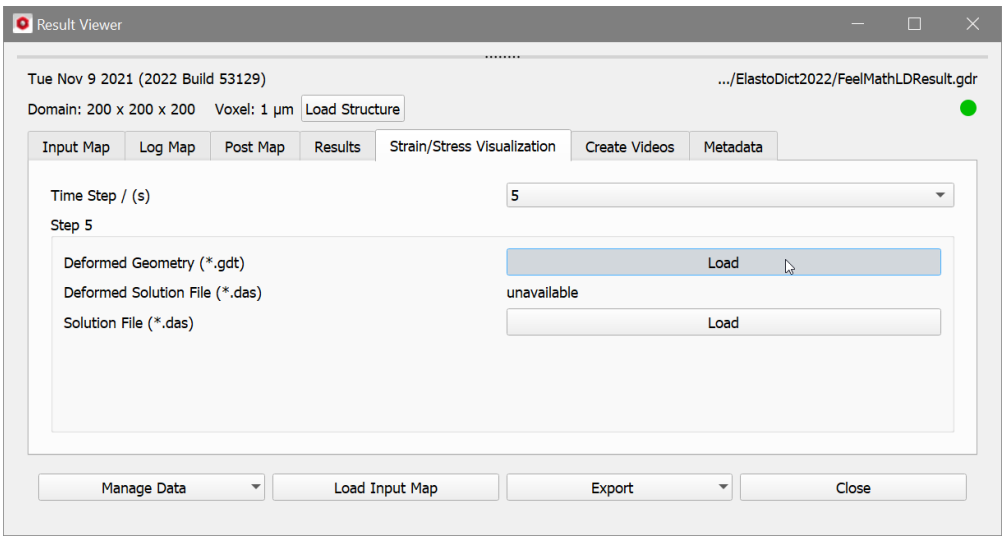


- The **Map** subtab contains all result values.



Strain/Stress Visualization

In the **Strain/Stress Visualization** tab, the computed result fields (*.das) and deformed geometries (*.gdt) can be loaded into GeoDict for visualization.

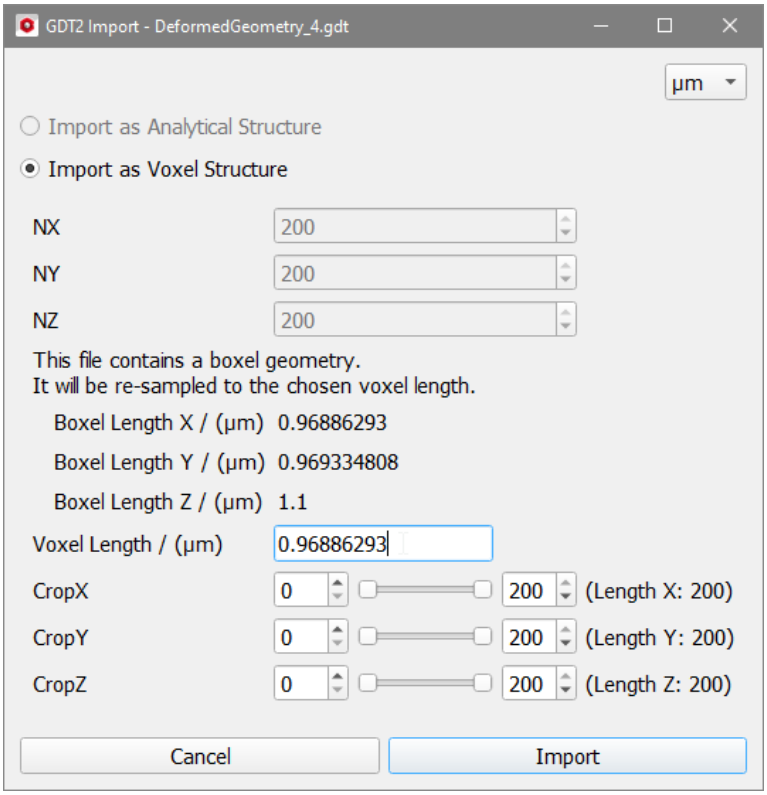


Since GeoDict 2022, the deformed geometries and volume fields are saved in boxels (instead of voxels as before).

Internally, ElastoDict works on boxels (cuboids with different side lengths), while GeoDict works on voxels (cubes). Until GeoDict 2021, ElastoDict automatically resampled the structure to a voxel structure with the original voxel length (therefore, the voxel length did not change). In GeoDict 2022, ElastoDict saves the boxel structure directly. This change was necessary to enable the restart for simulations with **On Deformed Geometry**: The solver in ElastoDict needs the boxel structure for restarting the computations. With boxels, the number of elements does not change during the simulation.

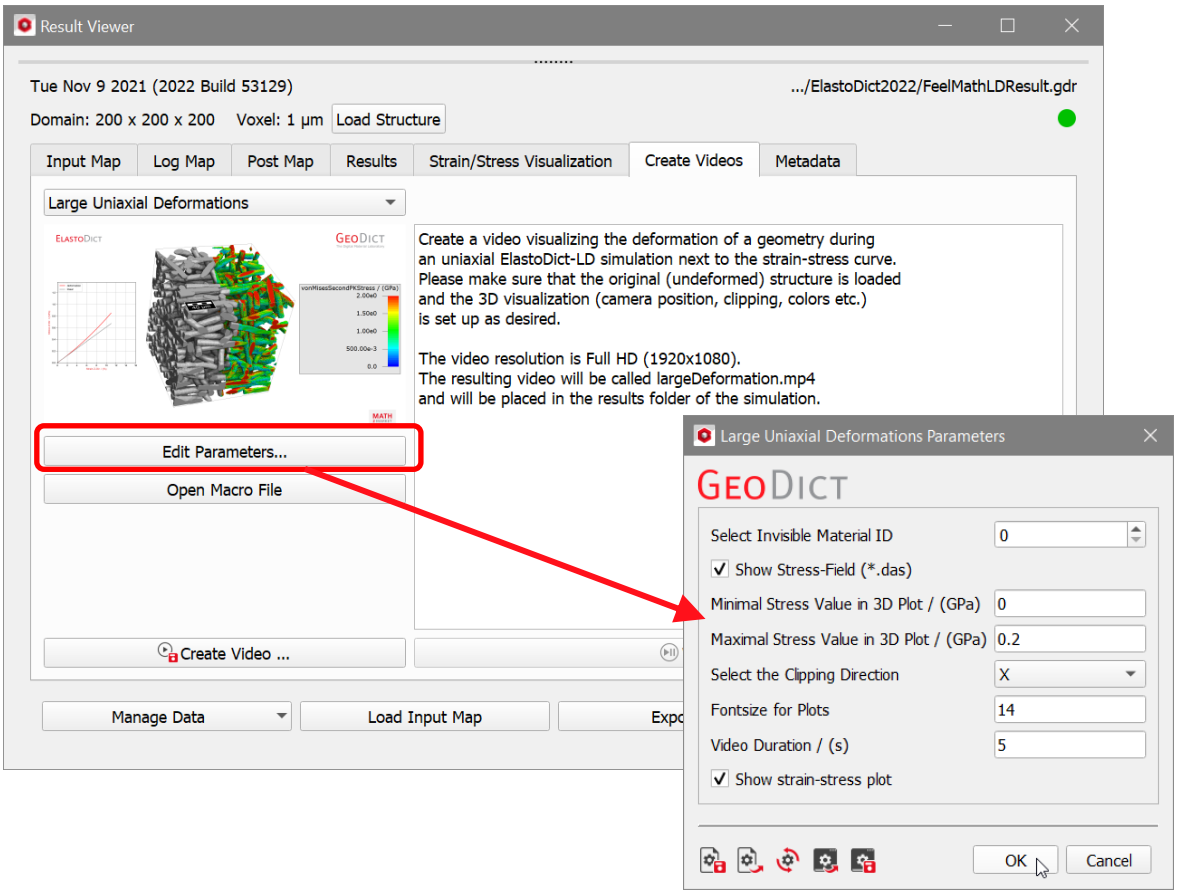
Now, the resampling to a voxel structure is done when the structure is loaded in GeoDict. The smallest boxel side length is selected as the new voxel length (instead of the original voxel length as before). With this choice, more detail can be preserved especially for compression simulations and the structure is shown with more details.

It is also possible to load the structure with the original voxel length (as before in GeoDict 2021). For this, the structure must be imported with ImportGeo-Base instead of loading it directly. Then, the voxel length for the structure can be selected:

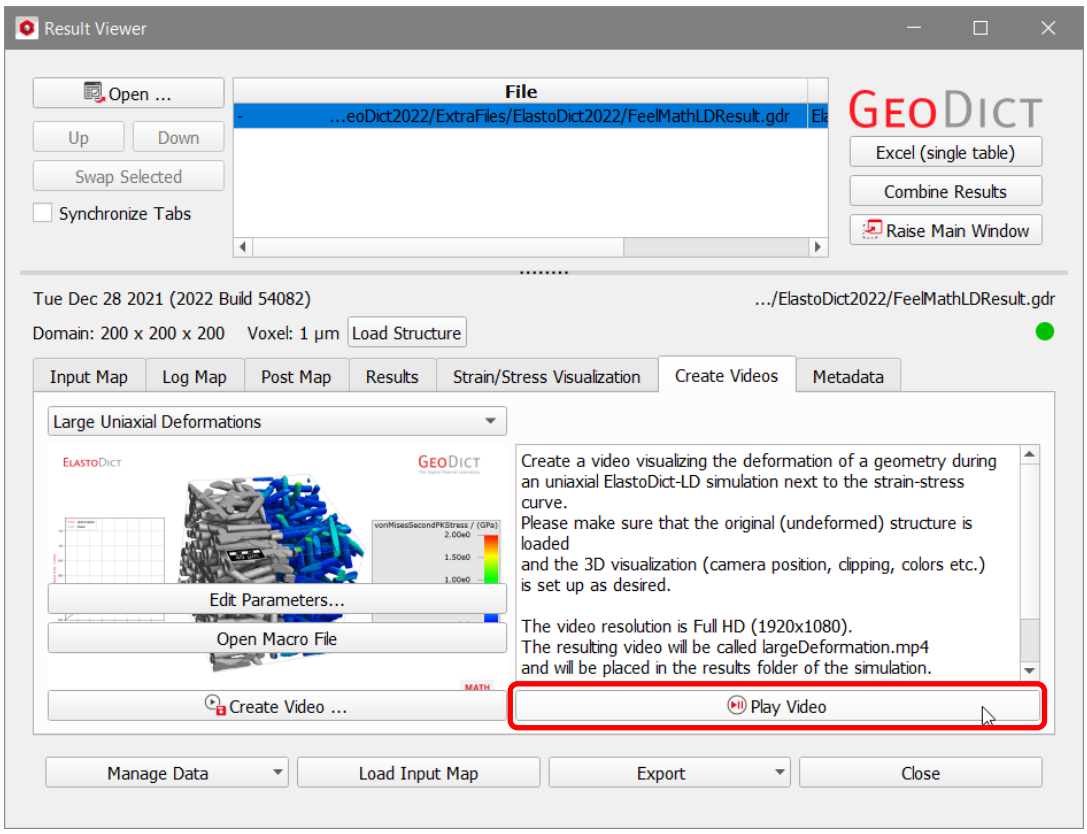


Create Videos

The **Create Videos** tab allows to create a video of the current large deformation simulation directly from the results viewer. **Click Create Video...** to use the default settings or **Edit Parameters...** to set them to your needs. The video creation is performed with an underlying python macro which can be opened and edited with the **Open Macro File** button.



After the parameters are set, click **Create Video ...** to create the video. After the generation is finished, the video file is saved in the result folder and can be opened with the **Play Video** button (see screenshot below).

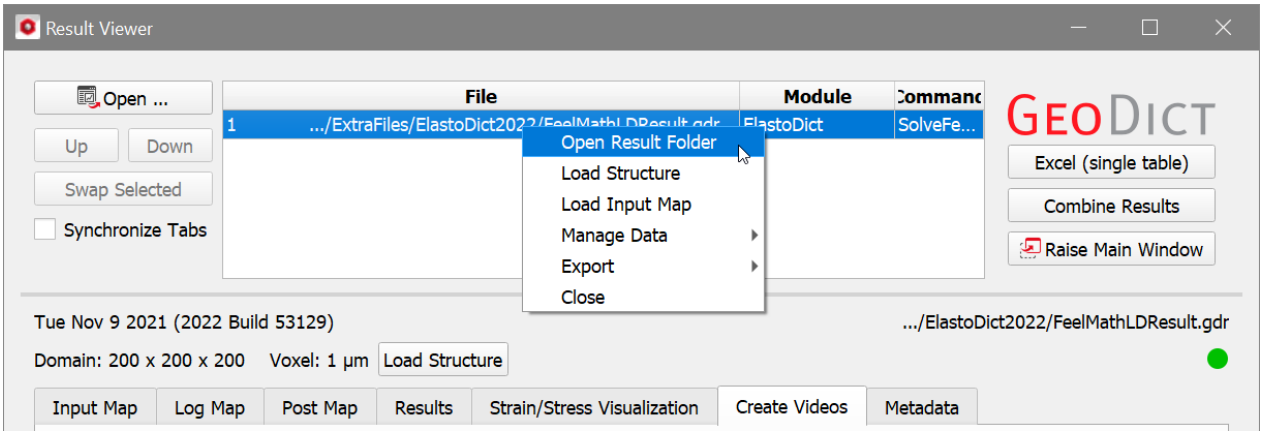


Metadata

The **Metadata**-tab contains a free text field for additional input.

Also contains the macro parameters when the simulation was started through a macro.

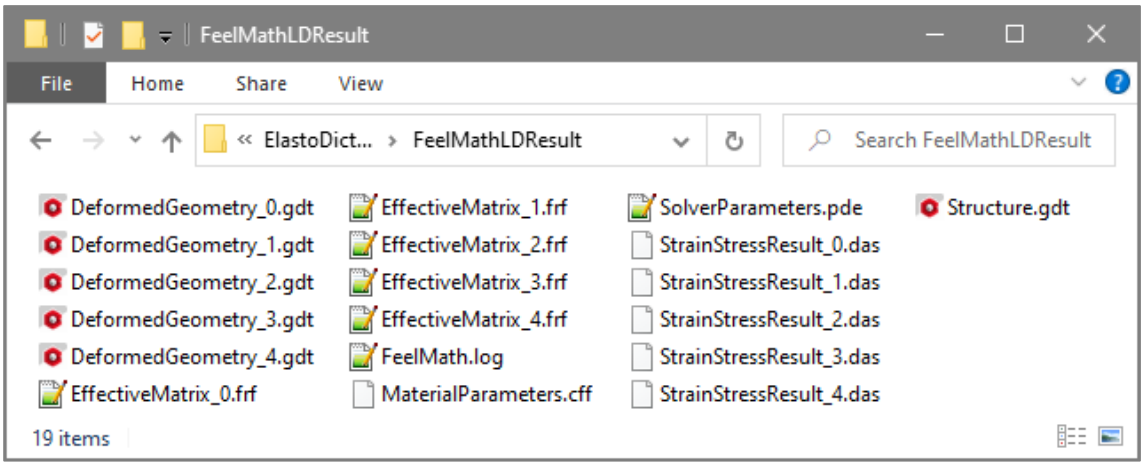
Result folder



The result folder has the same name as the result file and is saved in the current project folder. It can be opened directly from the result viewer by right-clicking on the result file name and selecting **Open Result Folder**. The result folder contains the following file formats:

- ***.gdt**: geometry data, e.g., the original structure and files with the deformed geometry (e.g., `DeformedGeometry_1.gdt`)

- ***.frf**: Free Report Form file (e.g., `EffectiveMatrix_2.frf`). It contains the results of each solution step. This information can also be found in the Results tab in the Results viewer.
- ***.cff**: coefficient file format (e.g., `MaterialParameters.cff`). This file contains the material properties of the materials in the structure as input data for the solver.
- ***.das**: e.g., `StrainStressResult_0.das`. These files contain the result fields and can be visualized in GeoDict. They can be loaded directly from the results viewer.
- ***.log**: e.g., `FeelMath.log`. A log file of the current solver run.
- ***.pde**: e.g., `SolverParameters.pde`. This file contains the parameters of the current simulations as input data for the FeelMath solver.
- ***.fmr** for `FeelMathRestart.fmr`: If a simulation is aborted, a restart file might be written which contains information to be used for a restart of the simulation. These files can be quite large, therefore they should only be kept if the simulation will be restarted later.

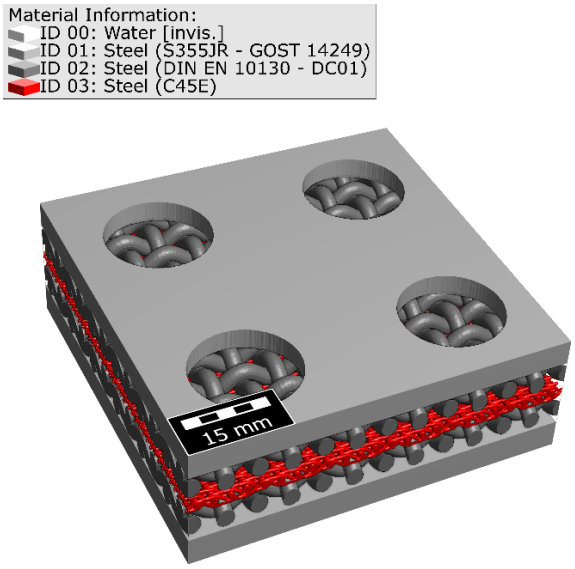


BENCHMARK RESULTS FOR FEELMATH-LD

In GeoDict 2021 and GeoDict 2022, the runtime for FeelMath-LD is reduced significantly if the deformation data is not written to a file.

As an example, the compression of a sand control screen is shown here.

The structure consists of 660 x 660 x 232 voxels (i.e., approximately 100 million voxels). A compression of 25% is computed in 10 steps with plastic deformation of the structure.



The computation was run on our server, with 2 x Intel E5-2697A v4 processors with 16 cores each, running with a maximum of 3.60 GHz, and 128 GB RAM under Linux.

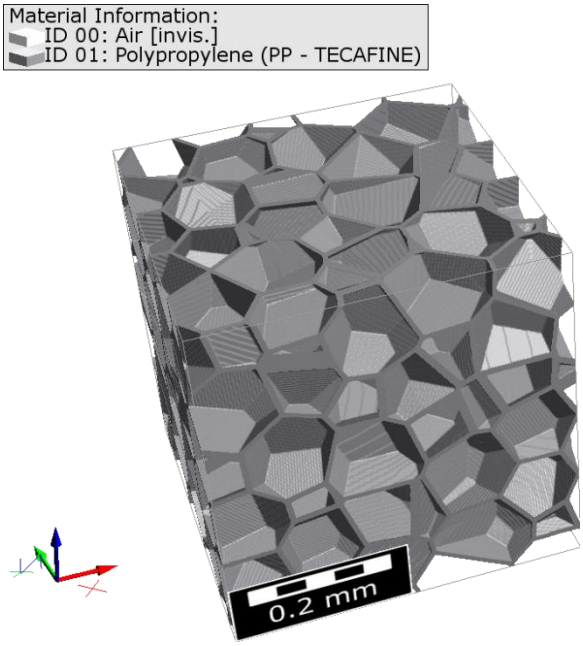
Without writing the deformation data to a file, the computation with 32 processes, needs 50% more memory, but the runtime is reduced by 40% compared to GeoDict 2020. With GeoDict 2022, the runtime is further reduced by 10% compared to GeoDict 2021.

GeoDict release	Runtime /h	Memory / GB
2020 SP3	32.8	82
2021 (r42253)	19.6	123
2022 (r52998)	17.7	133

If keeping the deformed geometry in memory is combined with downsampling, computation time can be reduced even further.

The example shown next is the compression of a foam structure.

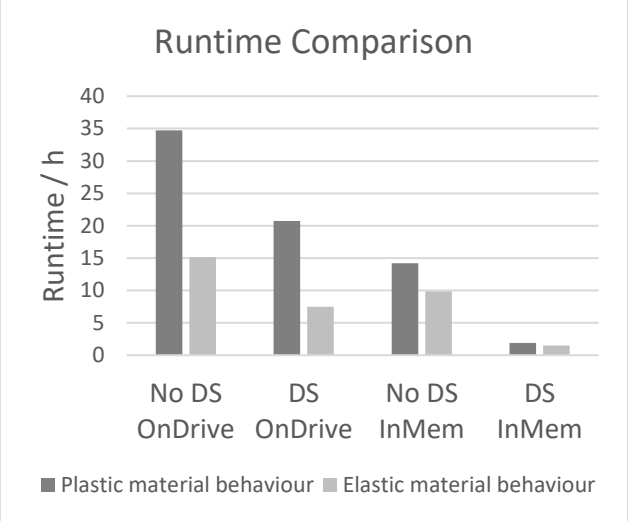
For a structure size of 500 x 500 x 500 voxels, a compression of 80% is computed with FeelMath-LD in 40 steps.

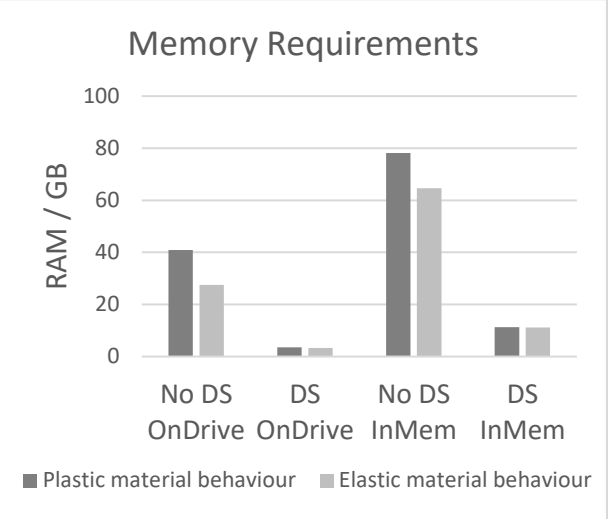


Again, computations were run with 32 processes on our server mentioned above.

Each computation is run twice, once for elastic, and once for plastic material behavior with GeoDict 2022. Runtimes and memory requirements for the computation with and without downsampling (DS), as well as for keeping the deformed geometry in memory (InMem) or writing the deformation data to a file (OnDrive) are compared in the following figures.

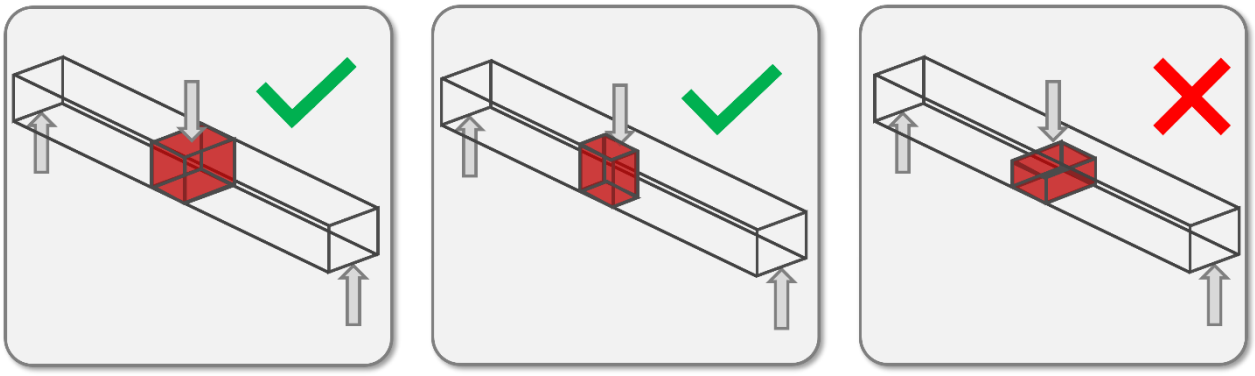
With downsampling and keeping the deformed geometry in memory, runtimes can be reduced for the foam structure by more than 90%, by reducing the required memory to 50% for elastic case, and to 20% for plastic case.



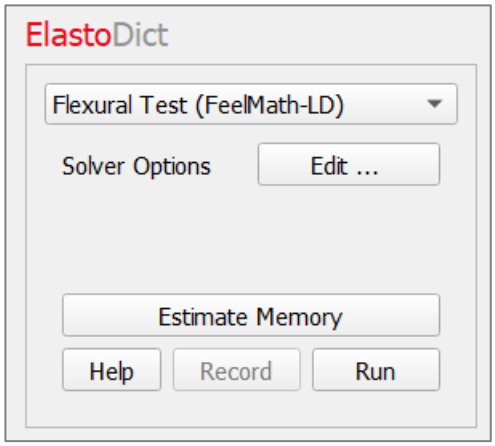


Flexural Test (FeelMath-LD)

With the **Flexural Test** option in ElastoDict, the reaction of a material to bending loads can be analyzed. As in most applications in GeoDict, only a small domain of the structure is needed for the simulation. However, it is necessary that the structure in GeoDict contains the complete height of the real structure.



Click the Solver Options **Edit** button to set the simulations settings for large deformation simulations. In the **FeelMath Flexural Test Options** dialog, choose a **Result File Name (*.gdr)** according to your current project.

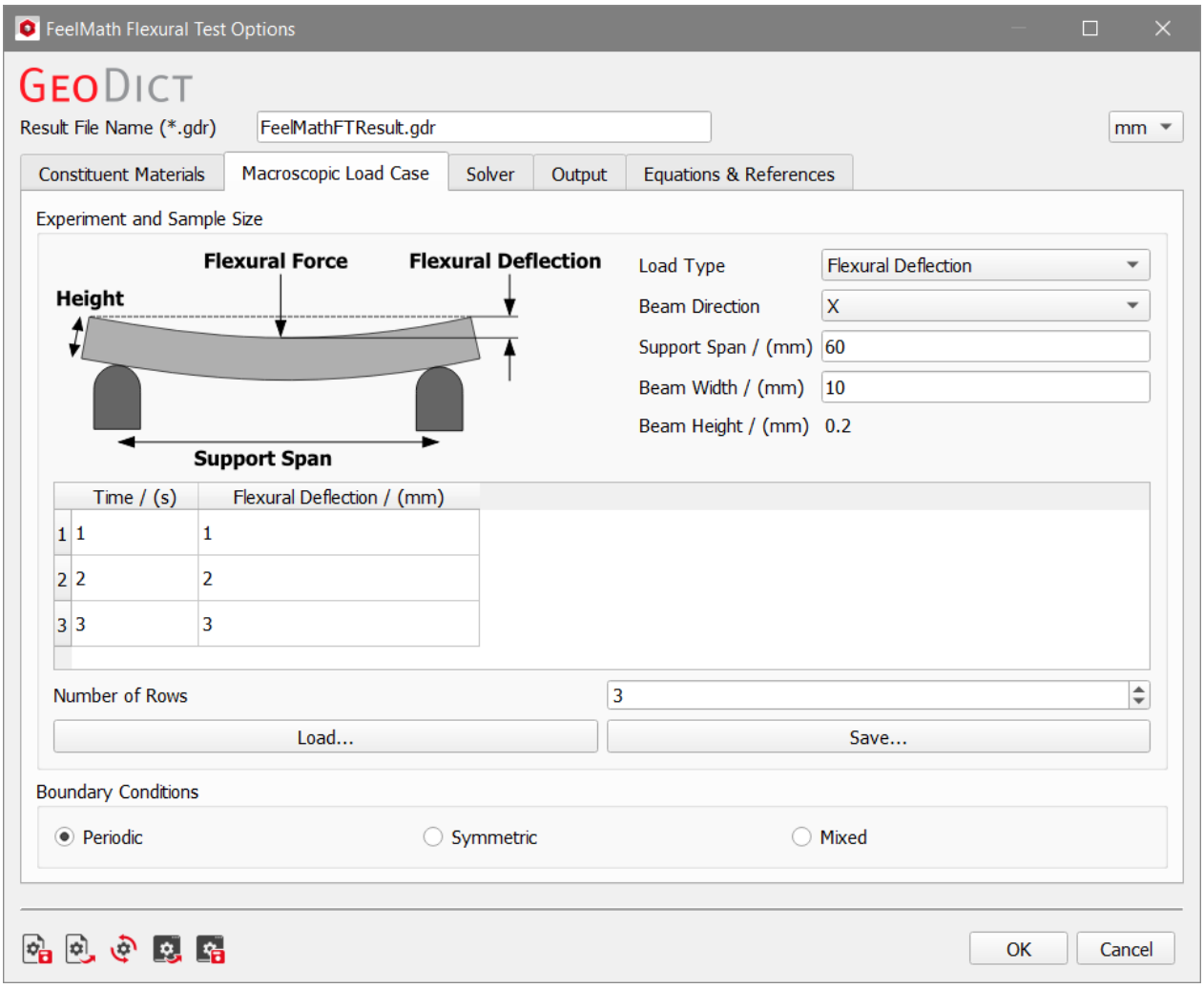


Constituent Materials

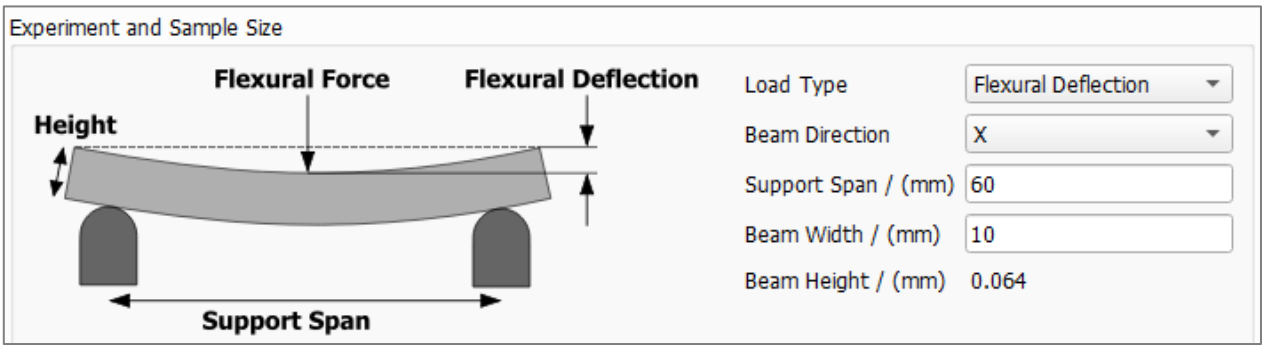
Select the constituent materials of the structure model as indicated above in page 9 for FeelMath-LD. For the flexural test, linear and nonlinear materials can be used.

Macroscopic Load Case

Under the **Macroscopic Load Case** tab, the experiment settings for the flexural test are defined.



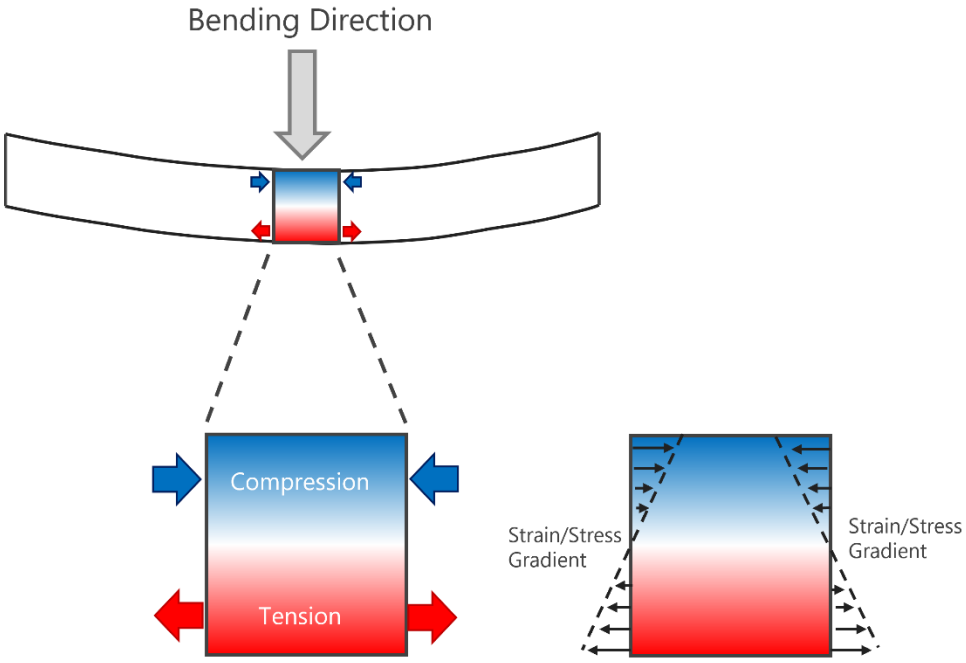
Experiment and Sample Size



Load Type

The bending of the beam leads to compression in the upper part of the beam, and to tension in the lower part. This can also be understood as a **Strain Gradient** and **Stress Gradient** (see also the figure below). In GeoDict, the flexural test is computed

based on these gradients. If **Flexural Deflection** or **Flexural Force** are defined, these gradients are automatically computed by GeoDict.



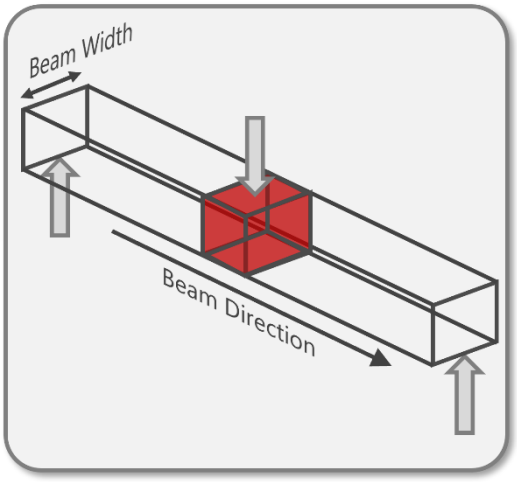
The load type can be defined as **Flexural Deflection** or **Flexural Force**, or alternatively as **Strain Gradient** or **Stress Gradient**. It is recommended to only use **Flexural Deflection** or **Flexural Force** here, the other (gradient) options are expert options. If possible, **Flexural Deflection** should be used, since it usually leads to a better convergence behavior than **Flexural Force** (see page 11 and page 81 for further information).

Support Span

The support span is the distance between the two supporting pins as indicated in the picture under **Experiment and Sample Size**. It must be entered in the user interface, since the structure in GeoDict is usually only a small cutout of the full sample.

Beam Width & Beam Height

The **Beam Width** is perpendicular to the beam and bending directions. It influences the ratio between load and deflection (since the beam can carry higher loads if it is wider), but it has no influence on the effective material parameters like the flexural modulus. The value of the **Beam Height** cannot be changed, since height of the beam is the height of the structure in GeoDict.



Load Table

In the **Load Table**, the load steps and the corresponding times can be defined. For computing the flexural modulus, one step is sufficient. For analyzing more complicated effects like plasticity and damage, more load steps are necessary.

Solver

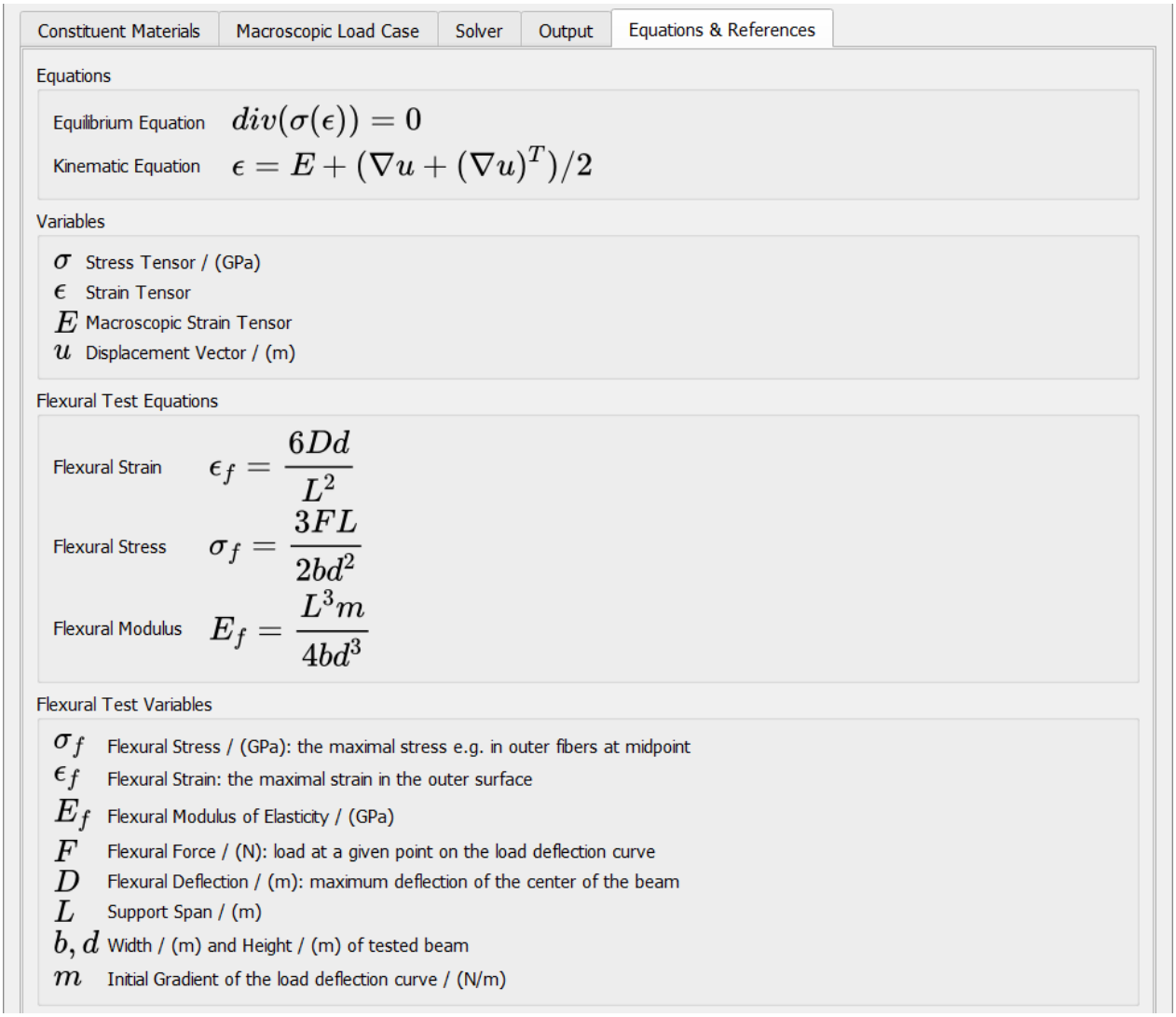
The Solver tab is identical to the solver tab in … (see page 23).

Output

The options under the output tab are identical to those in … (see page 27)

Equations & References

The differential equations solved in the simulation and additional equations relevant for flexural tests are listed under the **Equations & References**. Additionally, the tab contains the references for the methods used by the FeelMath solver in ElastoDict (see page 2 for links).

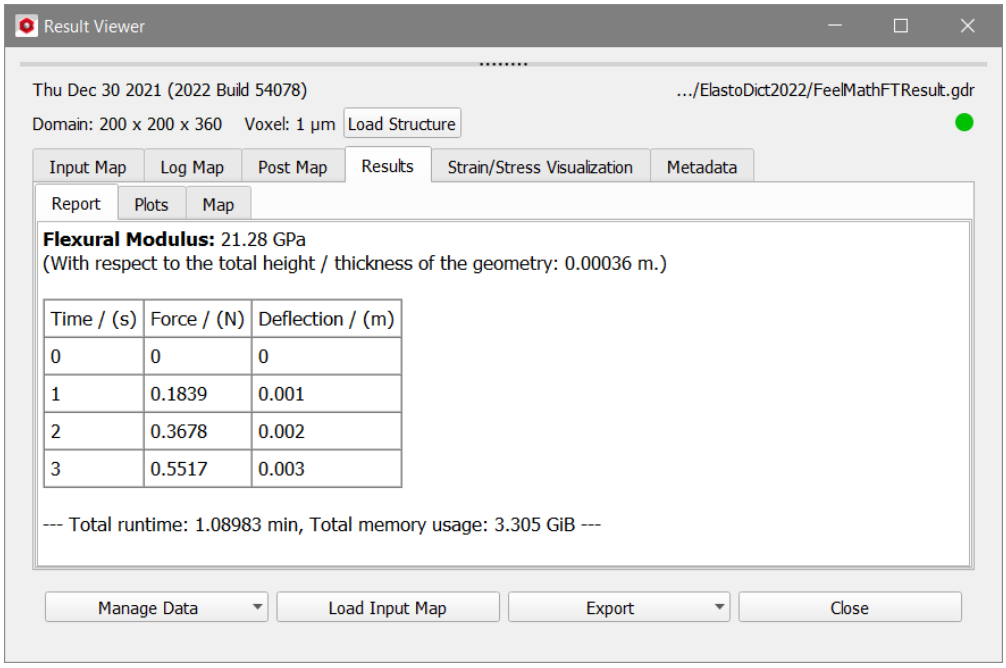


Results File (.GDR)

The handling of the result file works analogous as for FeelMath-LD (see page 30), therefore only the features specific for the flexural test are explained here in detail.

Results

The results tab contains a table with the forces and corresponding deflections in the experiment. Additionally, the flexural modulus is computed based on the first step of the simulation.

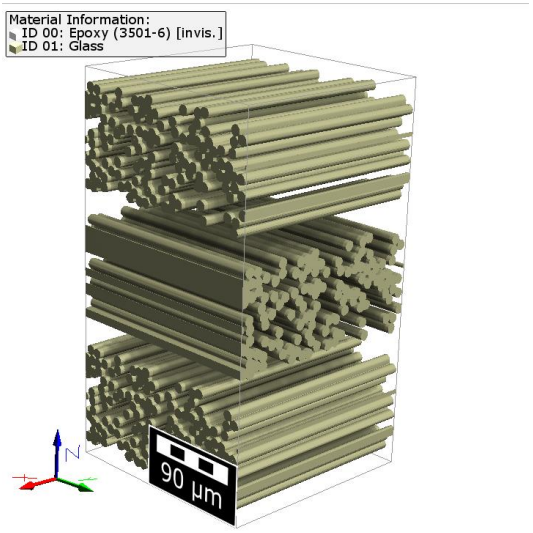


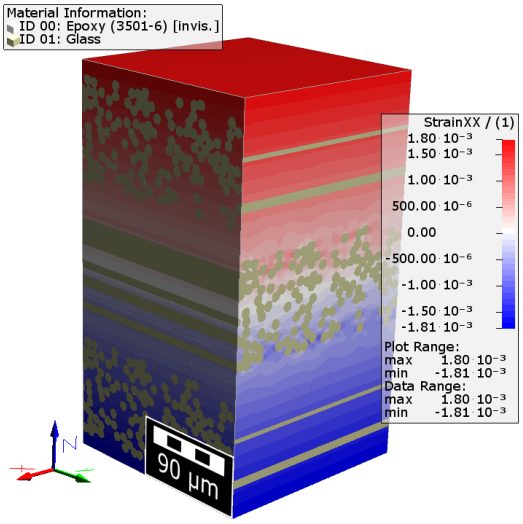
Strain/Stress Visualization

In the **Strain/Stress Visualization** tab, the computed result fields (*.das) and deformed geometries (*.gdt) can be loaded into GeoDict for visualization.

In the example below, a flexural test is done on a beam with a material structure as shown on the left. On the right, the distribution of the strain in X-direction is shown, and it is visible that the compressed on the top (negative strain, colored in blue) and stretched on the bottom (positive strain, colored in red).

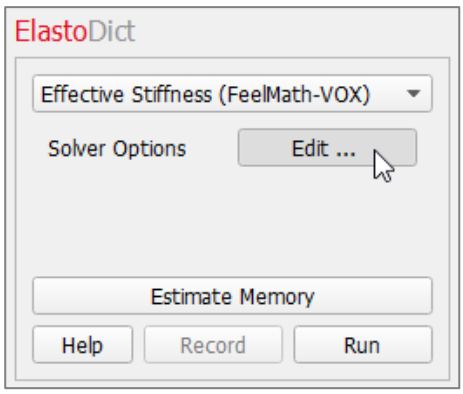
The simulation is based on the strain or stress gradients in the beam in the load direction. Therefore, it is not possible to see the bending in the results. This corresponds to the idea of analyzing a very small part of the beam.


Material Information:
ID 00: Epoxy (3501-6) [invis.]
ID 01: Glass
N
90 µm

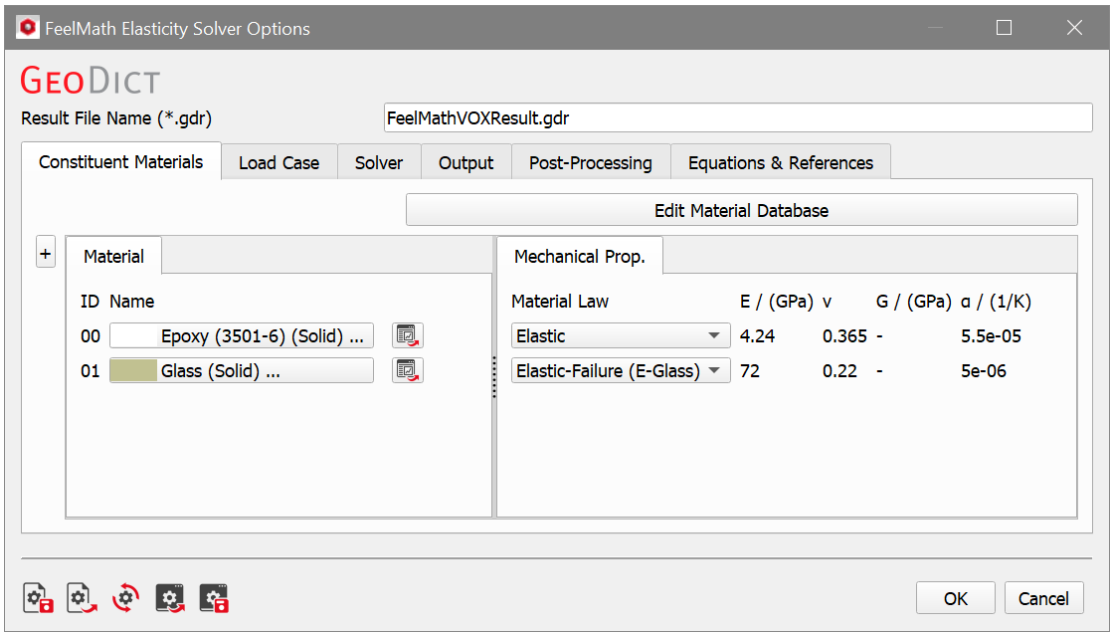

Material Information:
ID 00: Epoxy (3501-6) [invis.]
ID 01: Glass
StrainXX / (1)
1.80 10⁻³
1.50 10⁻³
1.00 10⁻³
500.00 10⁻⁶
0.00
-500.00 10⁻⁶
-1.00 10⁻³
-1.50 10⁻³
-1.81 10⁻³
Plot Range:
max 1.80 10⁻³
min -1.81 10⁻³
Data Range:
max 1.80 10⁻³
min -1.81 10⁻³
N
90 µm

Effective Stiffness (FeelMath-VOX)

FeelMath-VOX is the solver in ElastoDict for computing the effective elastic properties in GeoDict. Effective elastic properties are the mechanical properties of a homogeneous material which shows the same elastic behavior as the given non-homogenous material.



In the **FeelMath Elasticity Solver Options** dialog, choose the **Result File Name (*.gdr)** as you wish.



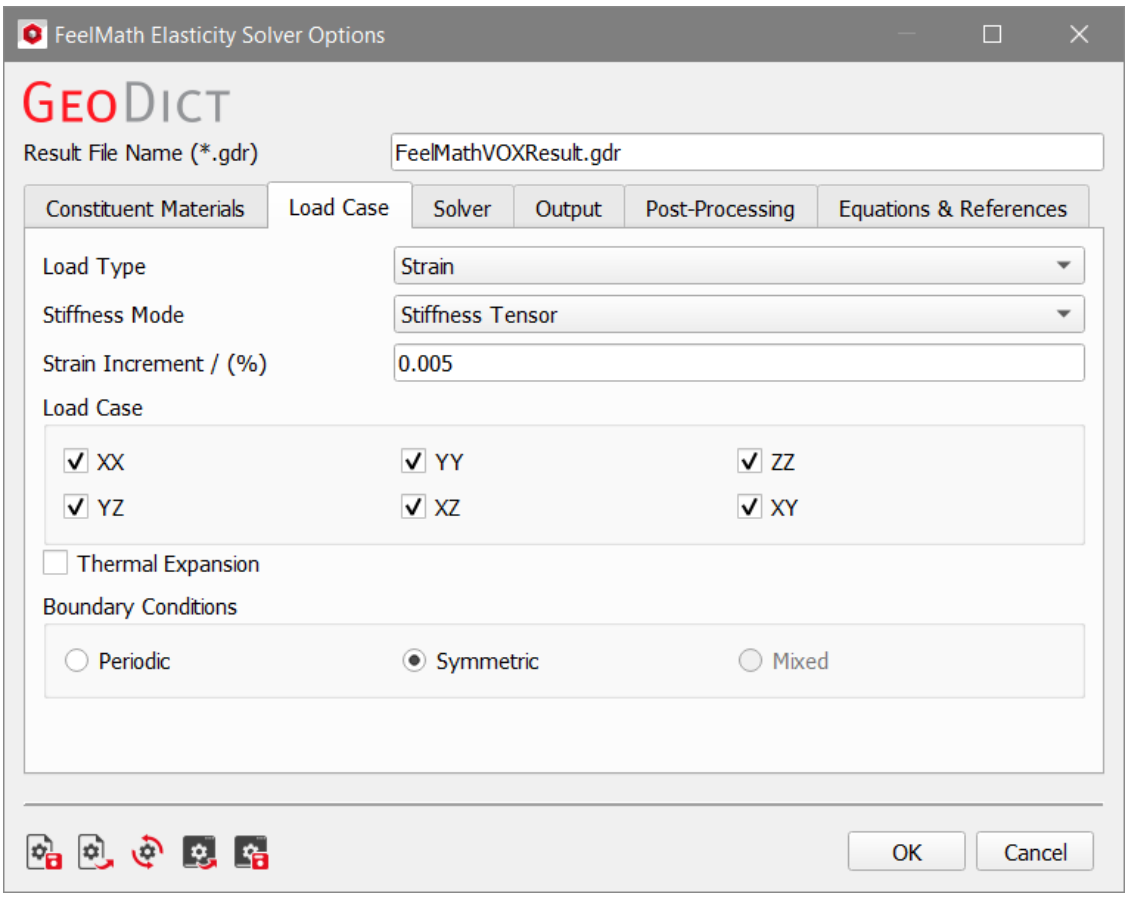
If a GeoDict results file (*.gdr) with the given name already exists in the project folder, a warning message is shown at the start of the creation process. The user can either decide to back up the old file, to overwrite it or cancel and choose a new file name. If no action is taken, the default option back-up is automatically chosen after a waiting time.

Constituent Materials

Select the constituent materials of the structure model as indicated above in page 9 for FeelMath-LD. In FeelMath-VOX, only linear elastic materials can be used.

Load Case

In the **Load Case** tab, the loads applied to the geometry are defined.

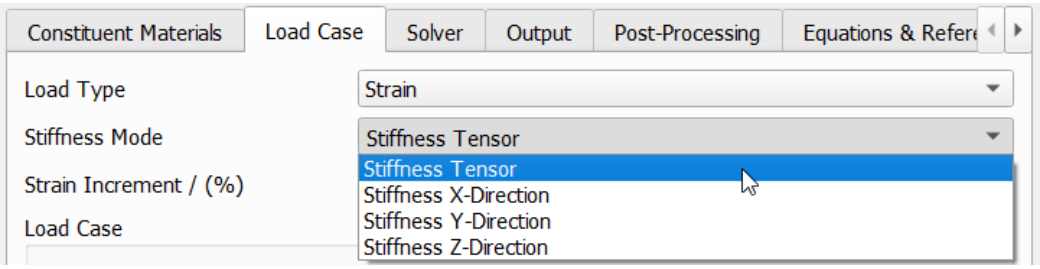


Load Type

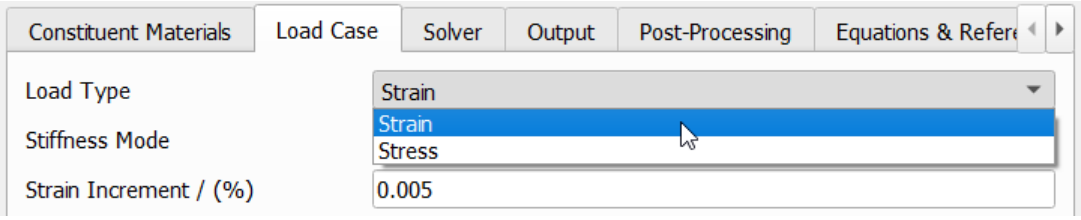
Choose whether the load applied to the material should be **Strain** or **Stress** from the pull-down menu. Choosing **Strain** is favorable for the solver and is often faster, but the choice has no effect on the quality of the solution.

Stiffness Mode

Either the **Stiffness Tensor** for the structure, or the effective stiffness for a selected direction can be computed (**Stiffness X-Direction**, …).



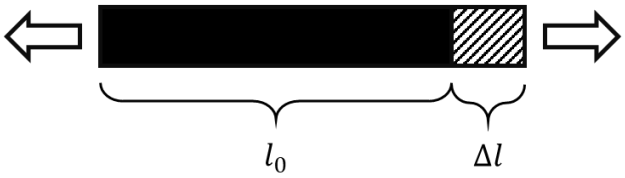
The stiffness tensor contains more information and allows to understand the properties of the structure more thoroughly. Nevertheless, if only the information for one direction is needed, the option to compute only a selected direction is much faster.



Strain/Stress Increment

Depending on the selected **Load Type**, a **Strain** or **Stress Increment** must be set. Generally, it is recommended to keep the default settings. Since the equation solved in FeelMath-VOX is linear, scaling the input increment (**Strain** respectively **Stress**) by a factor also scales the output (**Stress** respectively **Strain**) by the same factor. In conclusion, changing the input increment does not change the computed stiffness tensors.

$$\text{Strain Increment } \varepsilon = \frac{\Delta l}{l_0} \times 100\ \%$$



Load Case

Choose the **Load Directions** in which the effective stiffness should be computed by the FeelMath-VOX solver. The complete stiffness tensor can only be computed if all six load case directions are simulated (See the Appendix about the effective elastic properties on pages 105 ff. for an exemplary analysis of FeelMath-VOX results). Otherwise, only part of the stiffness tensor is calculated. If only parts of the stiffness tensor are computed, the results might be inaccurate, especially if the structure is highly anisotropic. Therefore, we recommend using the option to compute the stiffness in selected directions (see **Stiffness Tensor**, page 49) instead of computing only parts of the stiffness tensor.

For the strain equivalence principle (see the **Solver** tab), each load case adds one column to the stiffness tensor. For the energy equivalence principle, only the entries of the stiffness tensor can be calculated, for which both the load case belonging to the column-number and the load case belonging to the row-number, have been solved.

Thermal Expansion

When thermal expansion is chosen, the tensor with the thermal expansion coefficients is computed for the current structure. Thermal expansion is a separate load case independent from the strain or stress loads. The temperature change is then specified as **Temperature Increment [K]**.

Boundary Conditions

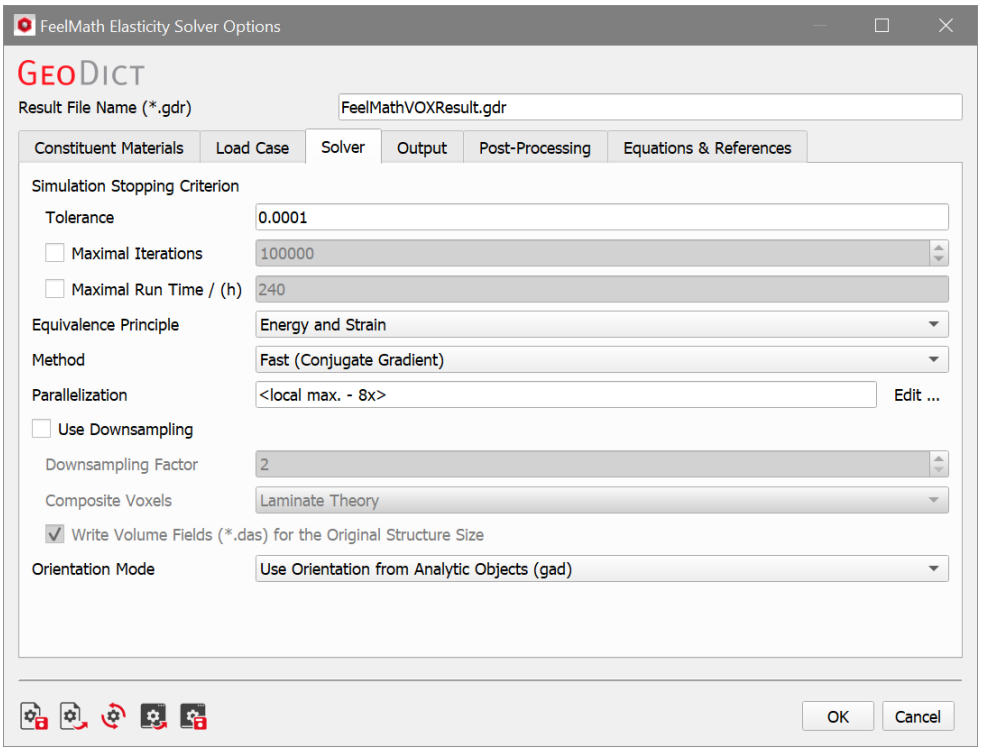
Here, the domain boundary conditions can be set. In general, periodic boundary conditions should be used for periodic structures, whereas otherwise symmetric boundary conditions should be applied. For further explanations, see the corresponding paragraph in the FeelMath-LD section (pages 11 ff.).

However, periodic boundary conditions are much faster and need less memory than symmetric boundary conditions. In many cases, for example for composite structures with low fiber percentage, the results for periodic boundary conditions are comparable with the results for symmetric boundary conditions even if the analyzed structure is not periodic.

If the **Stiffness Mode** is set to **Stiffness Tensor**, only **Periodic** or **Symmetric** boundary conditions are available. For **Stiffness in X,Y or Z-Direction**, also **Mixed** boundary conditions can be set.

Solver

The FeelMath-VOX solver options are mostly the same as for the FeelMath-LD solver (see page 23). Here, the Equivalence Principle can be chosen whereas for FeelMath-LD, resampling options can be set which do not apply for FeelMath-VOX. Additionally, when using Downsampling, the strain and stress fields can be written in the downsampled resolution.



Equivalence Principle

The **Equivalence principle** defines the equations which are solved for the computation of the effective properties of the structure. In principle, the effective properties are the properties of a homogeneous material with the same properties as the given structure. There are two approaches to compute these properties:

- Based on **Strain Equivalence**: the stress caused by a given strain is the same for the homogeneous and non-homogeneous material
- Based on **Energy Equivalence**: the elastic energy stored in the material caused by a given strain is the same in the homogeneous and non-homogeneous material

In FeelMath-VOX, either only **Strain Equivalence** or **Energy and Strain Equivalence** can be chosen. By computing both, also the deviation in the results of

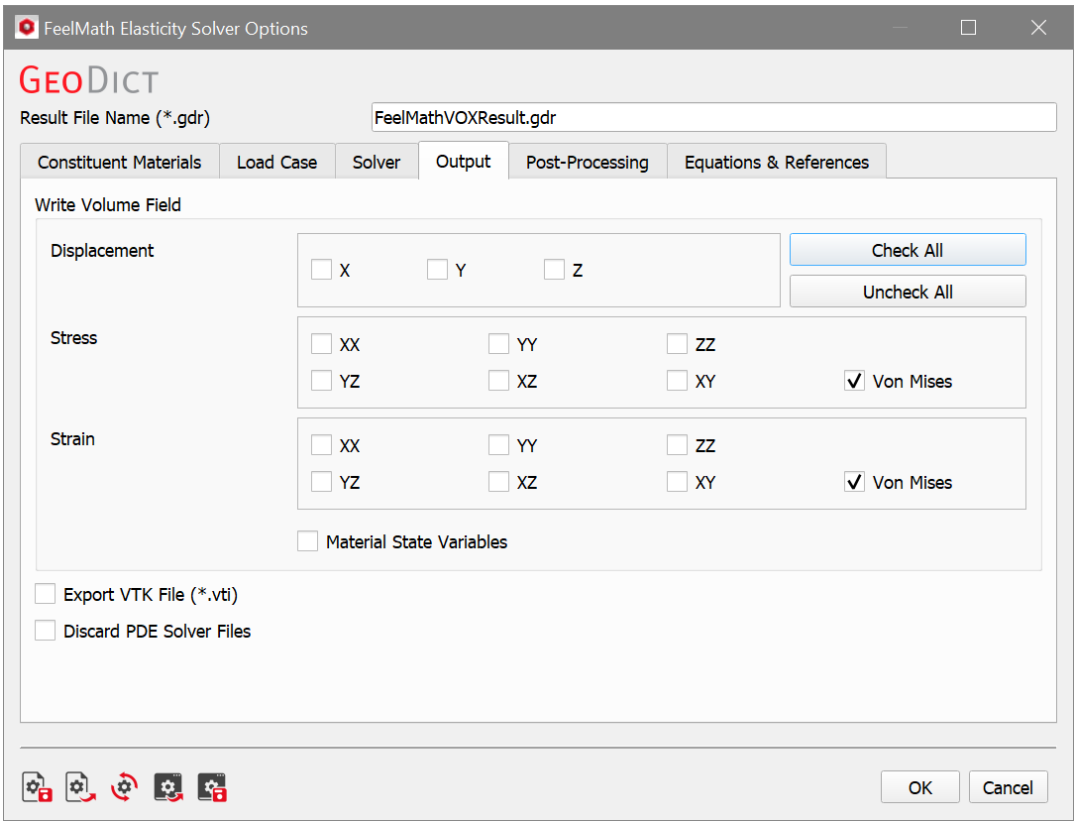
both methods is evaluated in the result file and provides a measure for the quality of the solution. Depending on the structure, both methods might lead to slightly different results.

Downsampling

For **Downsampling**, all options are the same as for large deformation simulations (see page 25).

Output

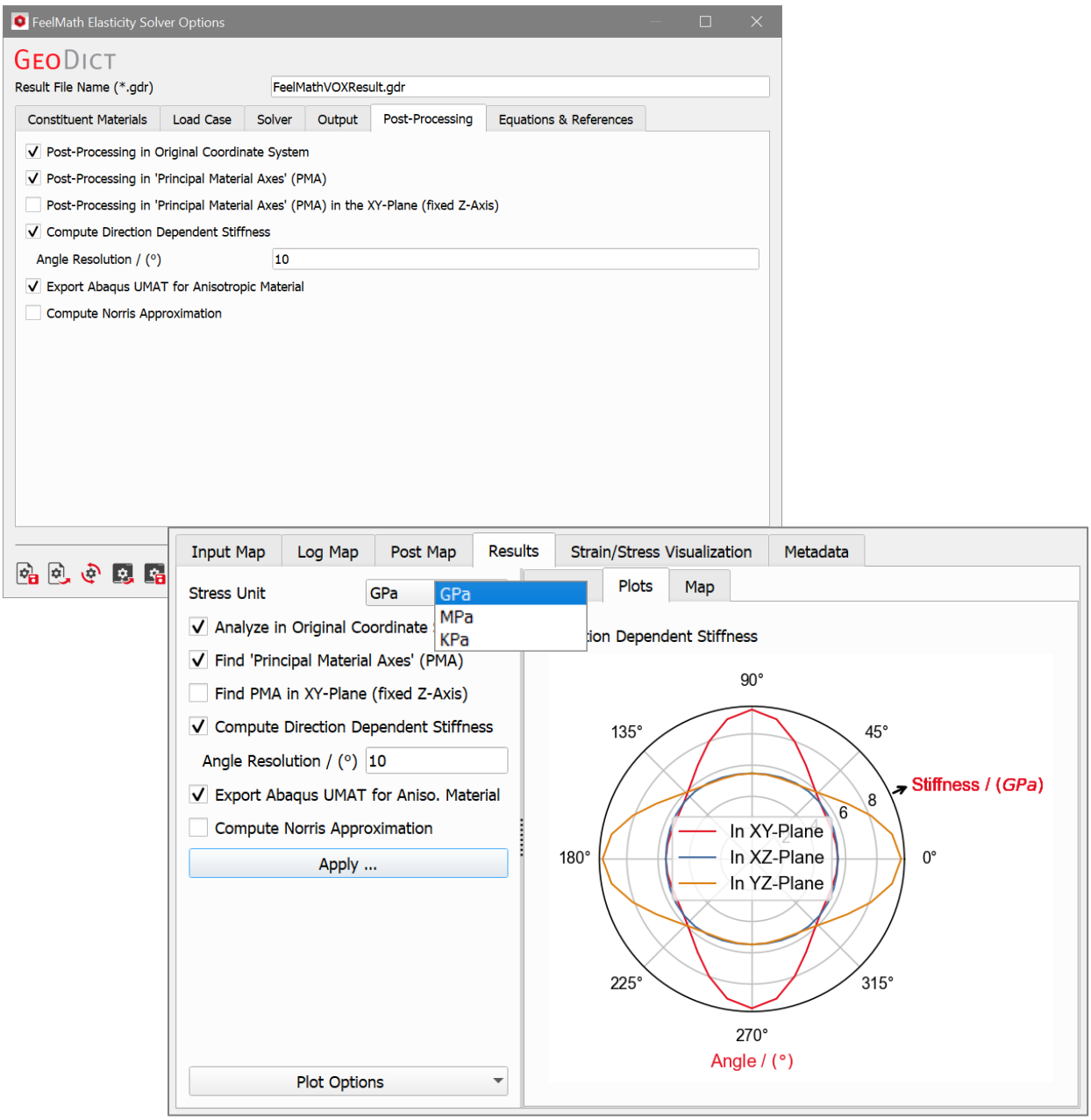
The FeelMath-VOX **Output** options are mostly the same as for FeelMath-LD (see page 27). The option to **Discard PDE Solver Files** is only available in VOX. When this option is chosen, only the .gdr file is kept after the run and the corresponding solver files are deleted (log files, solver input files, result files, …). This option is useful when only the effective properties are of interest and no result fields are needed.



Post-processing

The options available under **Post-Processing** are optional and they can also be set later in the Result Viewer of the result file (*.gdr) after the computations.

In the figure below, the options in the FeelMath-VOX settings are shown in the image below (on the top-left). How they look in the Result Viewer is shown at the bottom right. **Post-Processing in Original Coordinate System** is always available and selected by default. All other post-processing options are only available if all load directions (XX, YY, ZZ, YZ, XZ, and XY) have been previously checked under the **Load Case** tab.



Stress Unit

When post-processing the plots in the Result Viewer, the **Stress Unit** for the results can be selected. This choice has an effect on the values under the Report subtab and on the Plots subtab. The stress unit in the Results – Map subtab is always GPa.

Post-Processing in Original Coordinate System

Check **Post-Processing in Original Coordinate System** to compute the engineering parameters and elasticity-tensor approximations in the original coordinate system (X, Y, Z).

Post-Processing in Principal Material Axes (PMA)

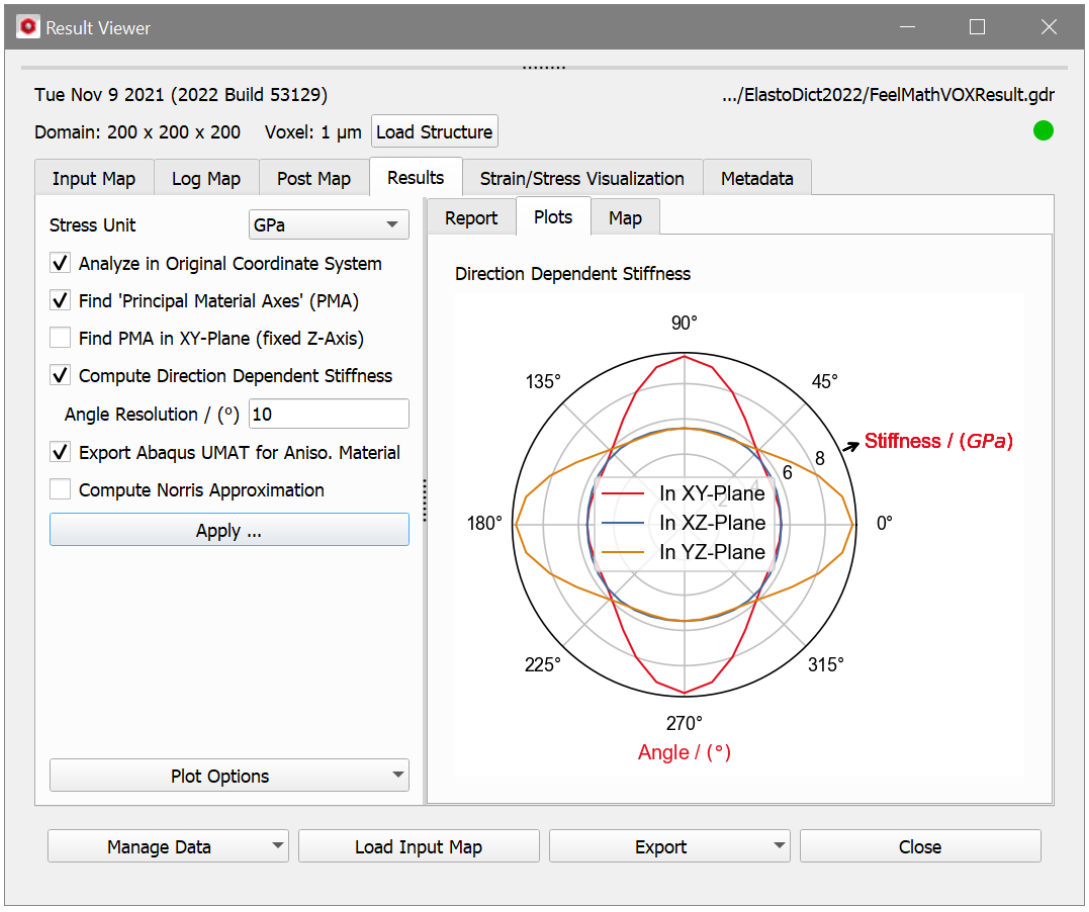
Check **Post-Processing in Principal Material Axes (PMA)** to find the PMA of the material and compute the engineering parameters and elasticity-tensor approximations in the PMA system. This is only possible if all six load cases (under **Load Case** tab) are calculated.

Post-Processing in Principal Material Axes (PMA) in the XY-Plane

Check **Post-Processing in Principal Material Axes (PMA) in the XY-plane** to find the PMA of the material in the XY-plane and to compute the engineering parameters and elasticity-tensor approximations in this PMA system. This is only possible if all six load cases (under **Load Case** tab) are calculated.

Compute Direction-Dependent Stiffness

Check **Compute Direction-Dependent Stiffness** to calculate the material stiffness in the XY, XZ, and YZ plane, in the original coordinate system. Additionally, enter an **Angle Resolution (°)** to analyze the material stiffness for arbitrary angles. The result file obtained after computations includes a table showing the calculated Young's Modulus **E** in the three planes according to the entered angle resolution. Additionally, a plot for the direction dependent stiffness can be found in the results file under the **Plots** tab.



Export Abaqus UMAT for Anisotropic Material

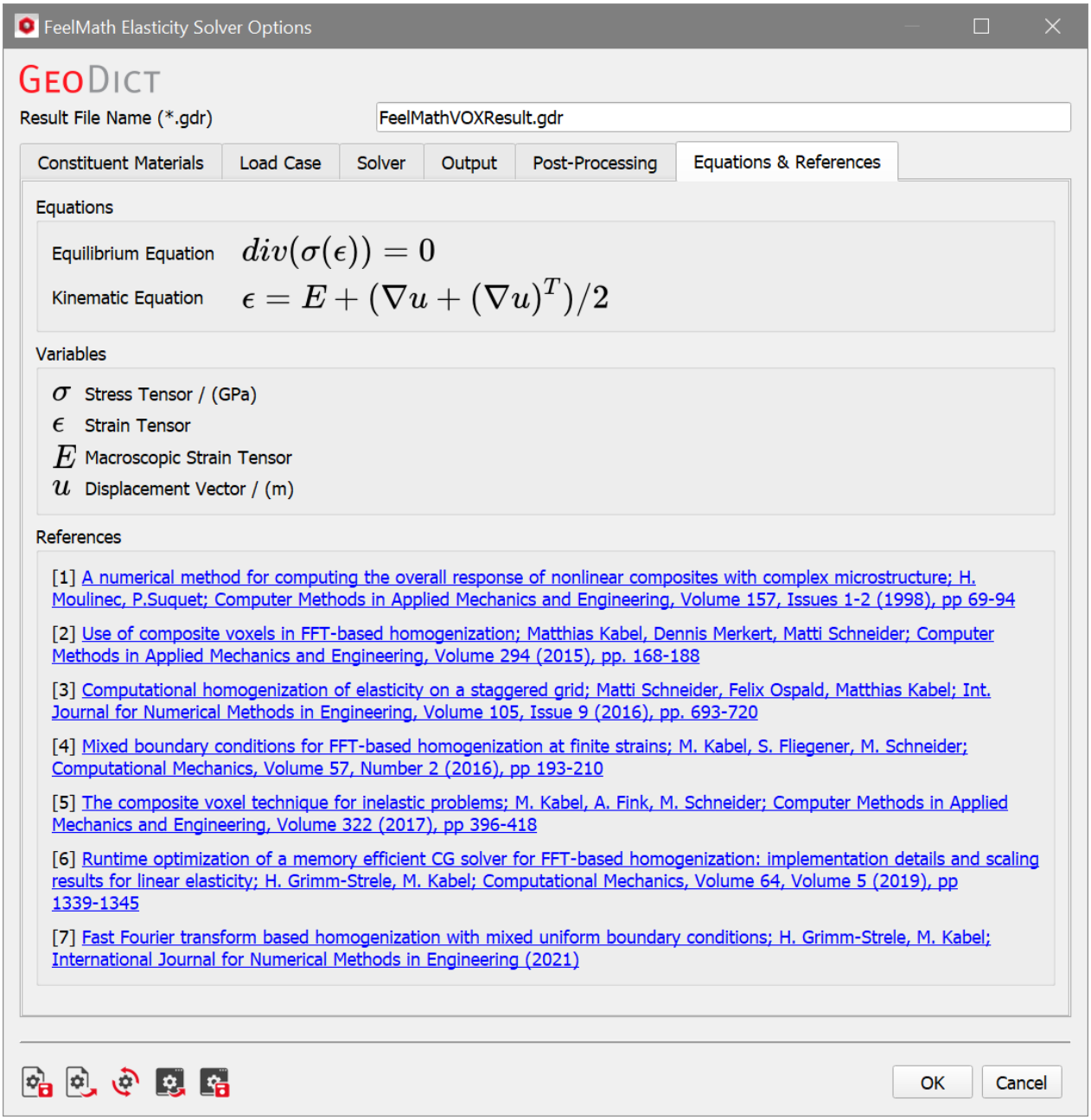
When Export Abaqus UMAT for Anisotropic Material, an UMAT with the computed anisotropic material properties is exported and can be found in the result folder. This UMAT can directly used in Abaqus, or it can also be used as material in GeoDict.

Compute Norris Approximation

Check **Compute Norris Approximation** to compute the cubic elasticity tensor approximation following Norris (A. Norris, Elastic Moduli Approximation, J. Acoust. Soc. Am. Vol 119, No 4, April 2006). See also the section about the effective elastic properties in the Appendix on pages 105 ff. This is only possible if all six load cases (under **Load Case** tab) are calculated.

Equations & References

The differential equations solved in the simulation are listed under the **Equations & References**. Additionally, the tab contains the references for the methods used by the FeelMath solver in ElastoDict (see page 2 for links).



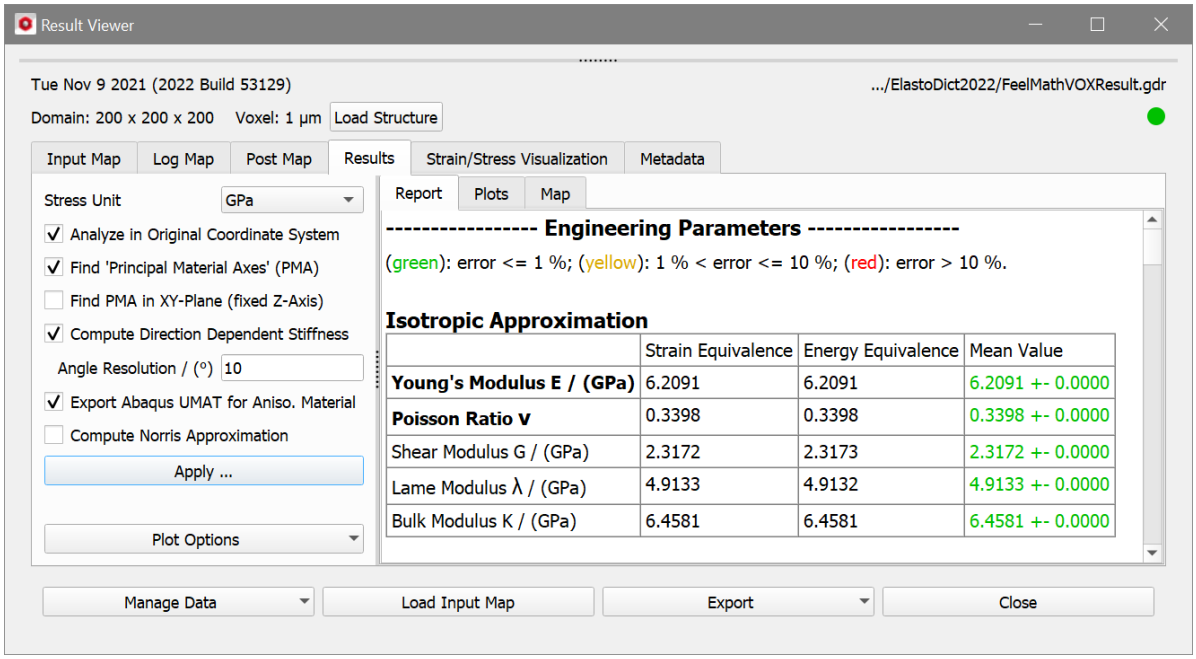
RESULT FILE (.GDR)

The handling of the result file works analogous as for FeelMath-LD (see page 30), therefore only the features specific for FeelMath-VOX are explained here in detail.

RESULTS

The **Results** tab gives access to the computed values for the parameters calculated by the selected ElastoDict process. The **Results** tab is divided into two or three subtabs:

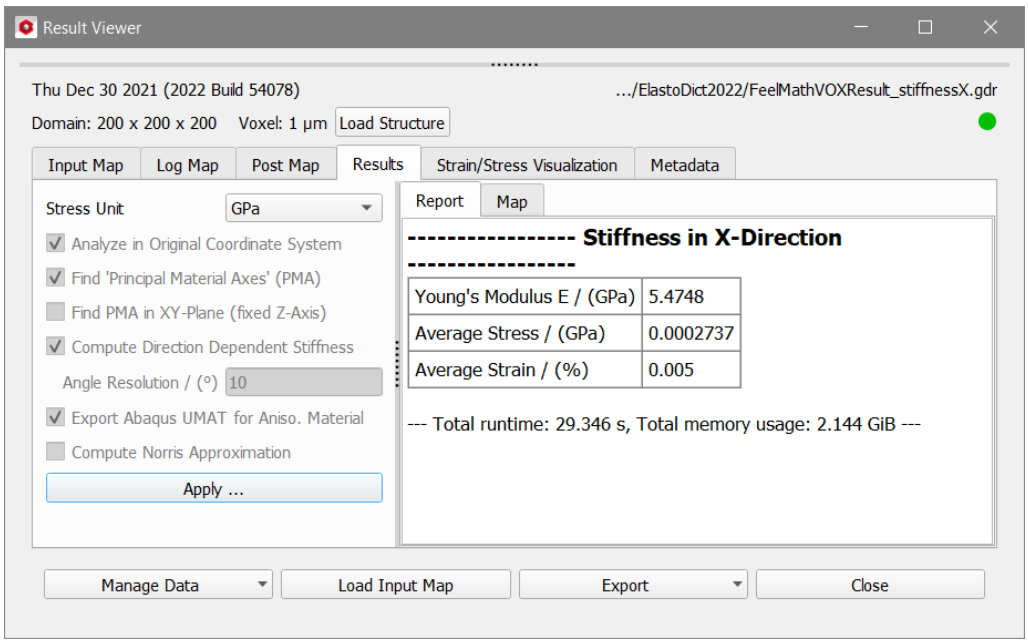
- The **Report** subtab shows the values of the computed mechanical properties. These values can be exported by selecting **Store As Html** from the **Export** pull-down menu at the bottom of the Result Viewer.



  For FeelMath-AF and FeelMath-VOX, if all 6 load cases have been computed, an analysis of the effective stiffness tensors can be carried out on the tables shown in this view. This analysis allows to judge, whether the material exhibits some degree of symmetry, such as transverse isotropy.

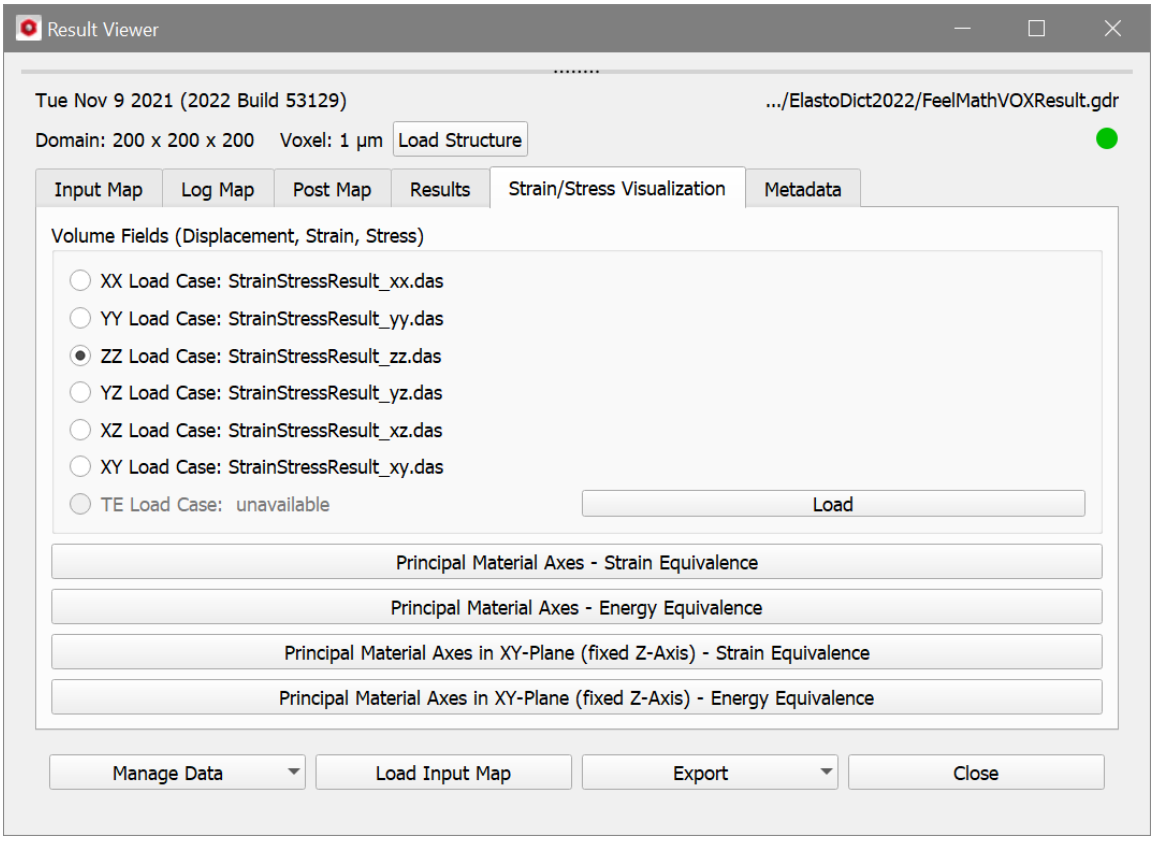
- In the FeelMath-VOX result file, the **Plots** subtab shows a plot of the direction dependent stiffness in the X-, Y- and Z-planes (see page 54 for further explanation). Right-clicking on the plot view allows generating an image or exporting the values as .txt file.
- The **Map** subtab shows a structured list of all result values.

If only the stiffness in one direction is computed instead of the complete stiffness tensor (by selecting e.g. **Stiffness in X-Direction** as **Stiffness Mode** under the **Load Case** tab), the results report is much simpler. It contains only the Young's modulus in the selected direction, and the average strain and the average stress in the structure (see example below).



Strain/Stress Visualization

In the **Visualization** tab, the computed solution volume fields (*.das) and visualizations of the principal material axes (PMA) can be loaded (see pages 69ff. for an example).

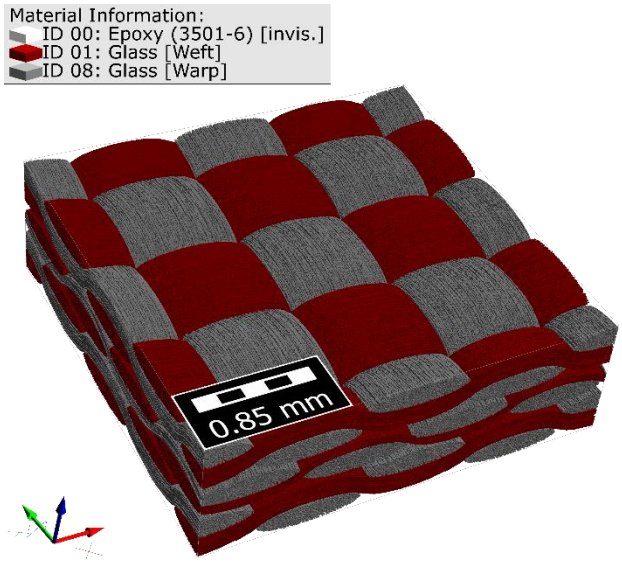


Clicking **Load Structure** in the result file loads the original structure to the visualization area at any time.

See an example of the possibilities of visualizing the results from ElastoDict's FeelMath-VOX, below starting on page 63.

Benchmark Results for FeelMath-VOX

For the weave structure shown here, the effective stiffness is computed with FeelMath-VOX. All fibers are fully resolved in the structure of 2,590 x 2,590 x 821 voxels (i.e., in total ~5.5 billion voxels).



For strain load type and periodic boundary conditions, all six load cases are computed using the conjugate gradient method.

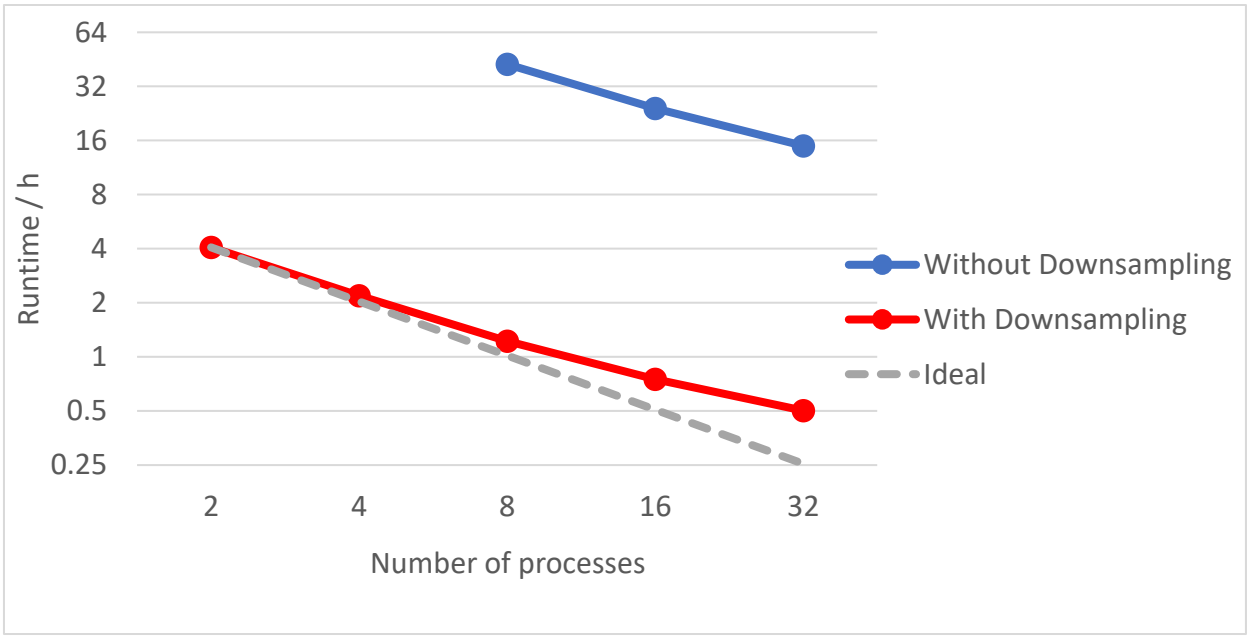
The computation was run on our server, with 2 x Intel E5-2697A v4 processors with 16 cores each, running with a maximum of 3.60 GHz, and 1024 GB RAM.

To show the possible benefit of using downsampling, runtime and memory requirements are compared with and without downsampling, for a different number of processes, using GeoDict 2022 (r52859).

Runtime results are shown in the following figure. The computation, which needs 54 h with 8 processes, can be run in 36 min with 32 processes and downsampling. Even without increasing the number of processes, the runtime is reduced by 97%.

The memory requirement is reduced by 97% as well. The computation that needed 1 TB of RAM without downsampling requires only 30 GB with downsampling and thus can be run on a standard laptop or desktop computer.

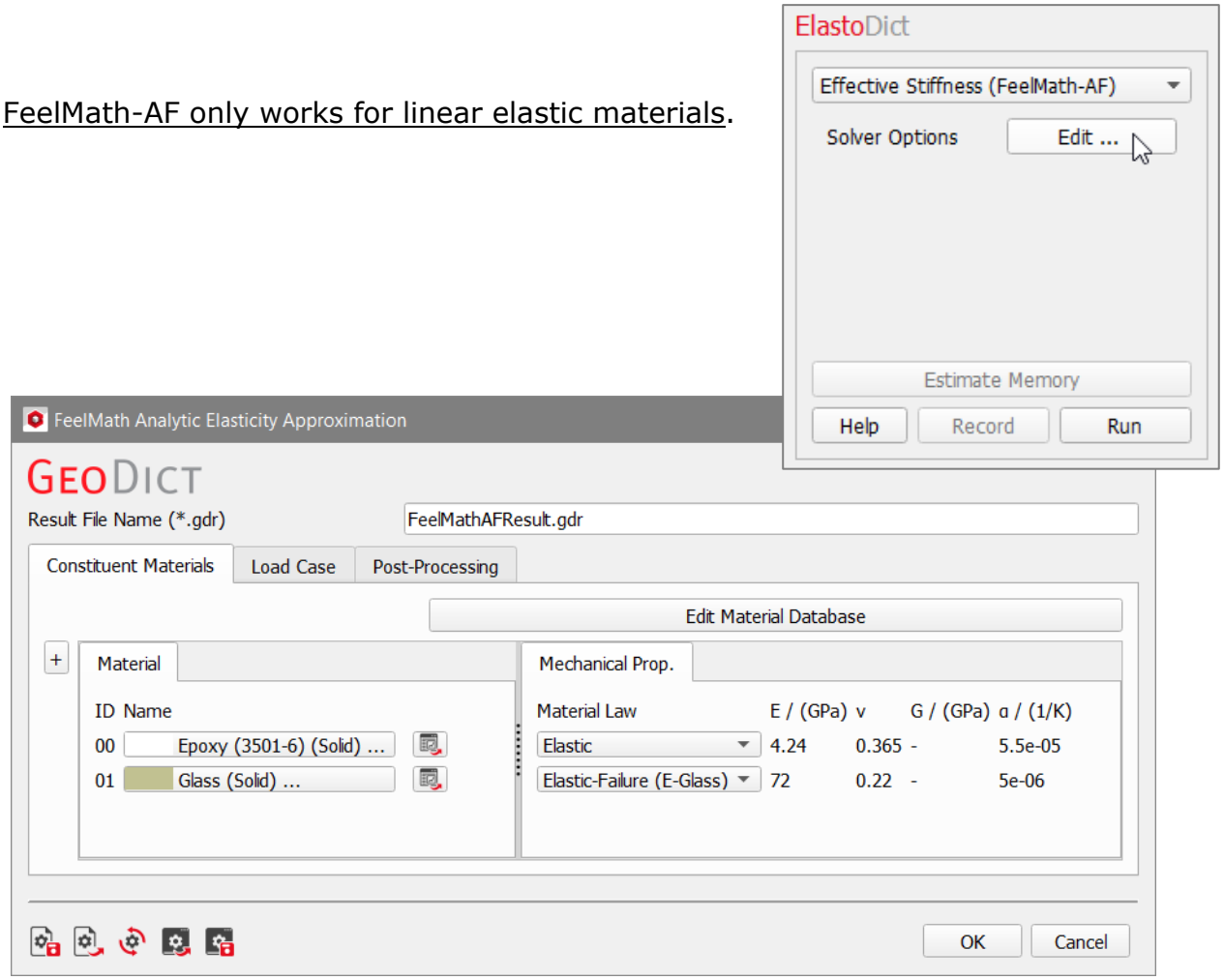
The ideal speedup, i.e., getting half the runtime for twice the number of processes is also shown in the figure for the computation with downsampling. Computations with FeelMath-VOX have a very good speedup compared to the ideal line, which is usually not possible to reach for real life examples.



Effective Stiffness (FeelMath-AF)

The FeelMath-AF solver provides a fast analytic approximation of the effective elastic properties. It computes the **Voigt** (upper bound), the **Reuss** (lower bound) and the **Mori-Tanaka** approximations.

FeelMath-AF only works for linear elastic materials.



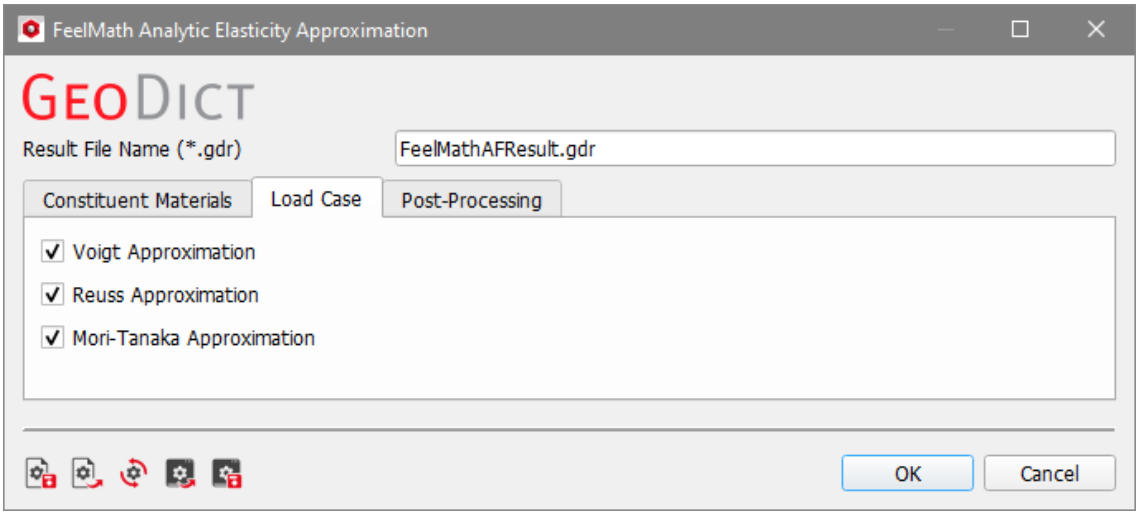
Constituent Materials

Select the constituent materials of the structure model as indicated above on page 9 for FeelMath-LD. As mentioned above, FeelMath-AF only works for linear materials. Choosing nonlinear materials results in an error message when starting the solver.

Load Case

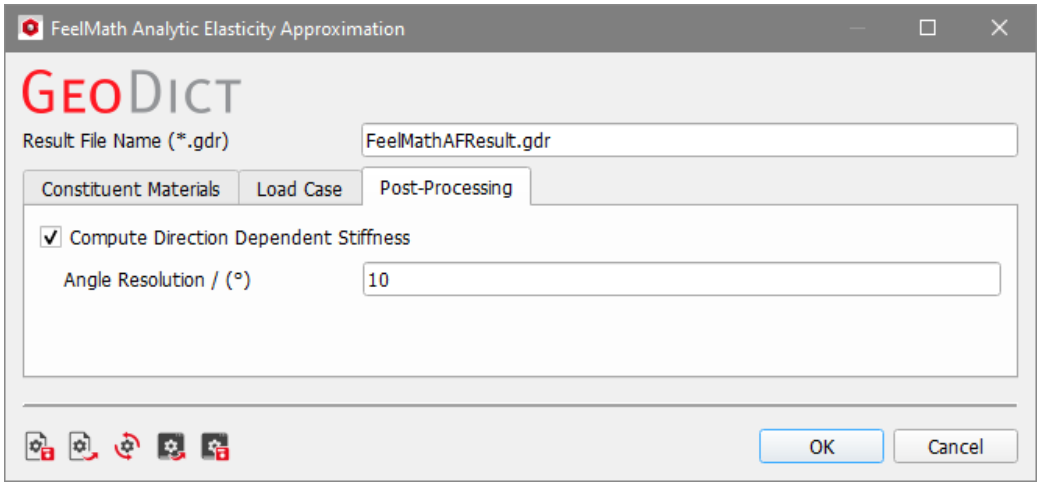
The **Voigt** and **Reuss** approximations can be interpreted as the ratio of average stress and average strain within the microstructure. The stress and strain are generally unknown and expected to be non-uniform.

The upper bound (**Voigt**) assumes that the strain is uniform everywhere. The lower bound (**Reuss**) assumes that the stress is uniform everywhere. The **Mori-Tanaka** approximation works for Ellipsoids and circular fibers and needs the input of analytic data (*.gad files).



Post-processing

Analogous to FeelMath-VOX, the post-processing options can also be chosen after the computation in the Result Viewer. For FeelMath-AF, only the option **Compute Direction Dependent Stiffness**, and the option to set a corresponding **Angle Resolution** is available. Refer to page 54 in the FeelMath-VOX section for further details.



Result file (.gdr)

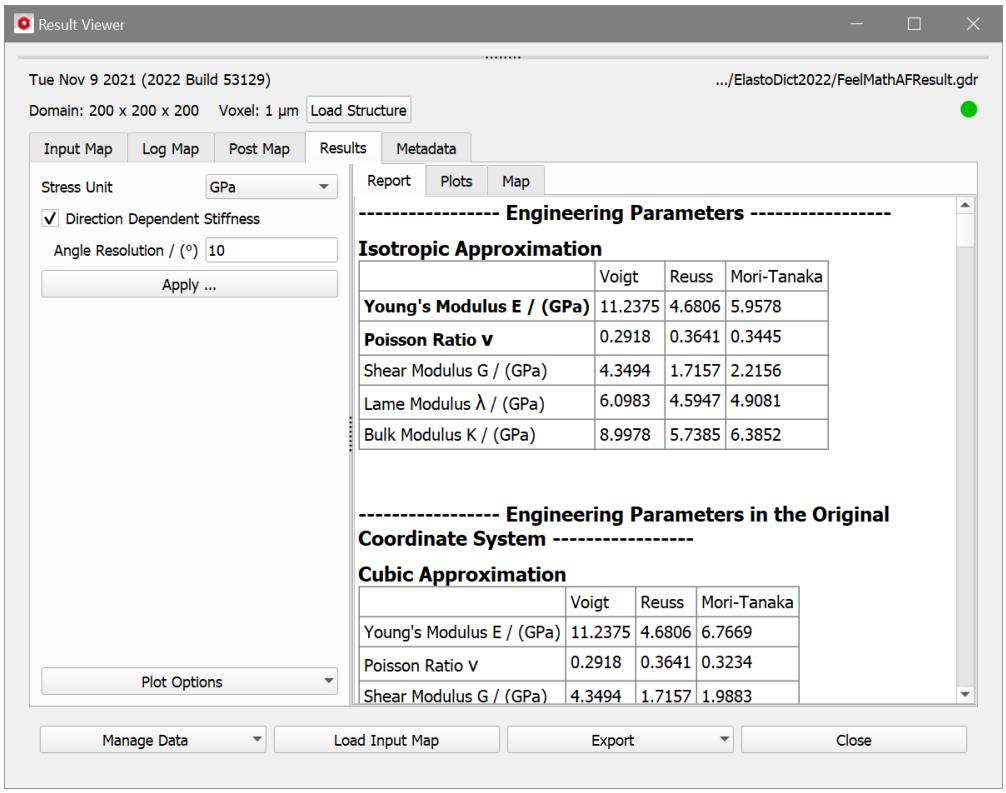
The handling of the result file is analogous to that of the FeelMath-LD (see page 30). Therefore, only the features specific for FeelMath-AF are explained here in detail.

Results

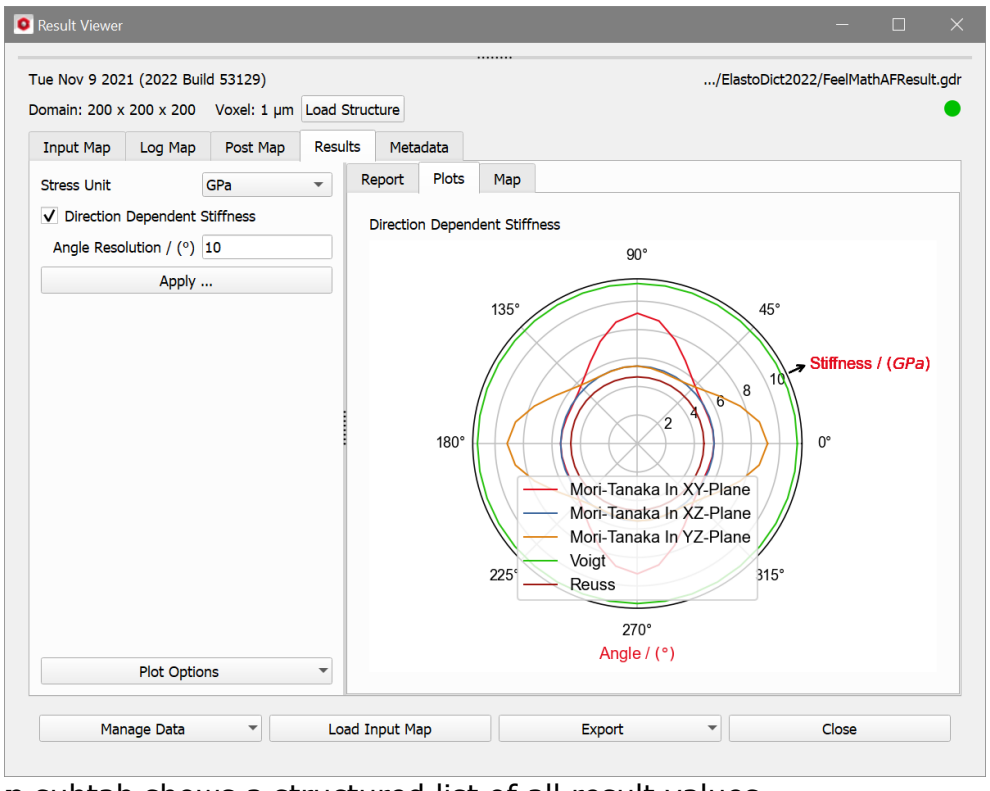
The **Results** tab gives access to the computed values for the parameters calculated by the selected ElastoDict process. The **Results** tab is divided into two or into three subtabs:

- The **Report** subtab shows the values of the computed mechanical properties. These values can be exported by clicking **Store As Html** at the bottom of the Result Viewer.

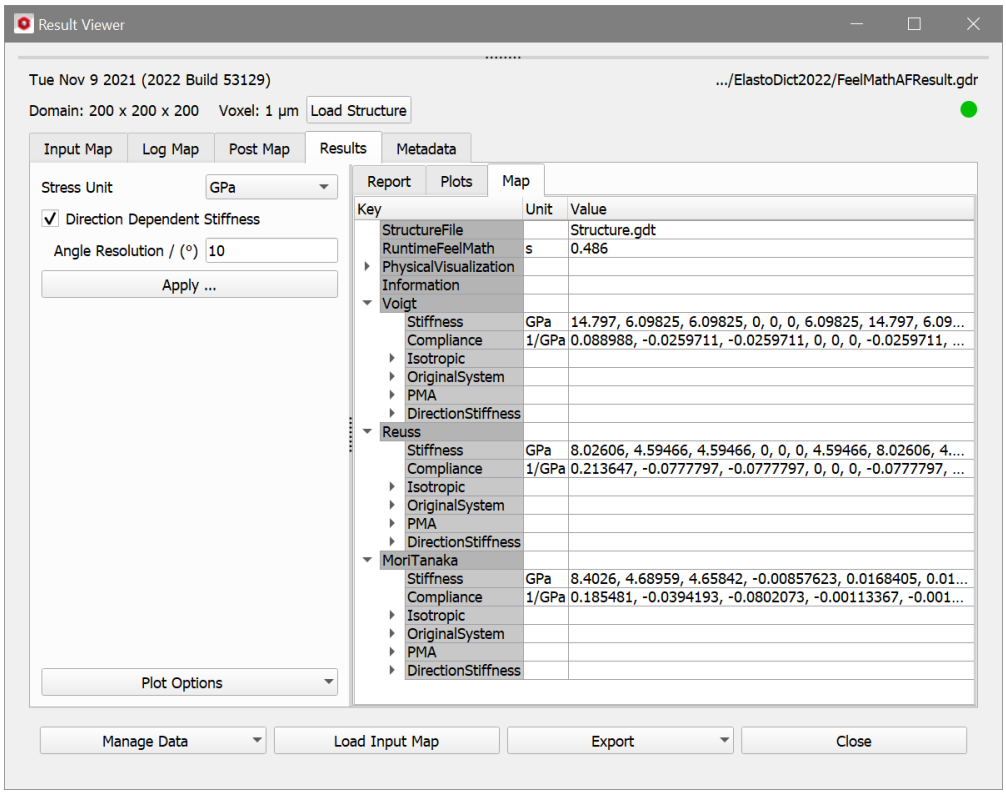
For FeelMath-AF, an analysis of the effective stiffness tensors can be carried out on the tables shown in this view. This analysis allows to judge, whether the material exhibits some degree of symmetry, such as transverse isotropy.



- In Result Viewer of the FeelMath-AF result file, the **Plots** subtab shows a plot of the direction dependent stiffness in the X-, Y- and Z-planes as shown below. Right-clicking on the plot view allows generating an image or exporting the values as .txt file.



- The **Map** subtab shows a structured list of all result values.


Result Viewer
Tue Nov 9 2021 (2022 Build 53129)
.../ElastoDict2022/FeelMathAFResult.gdr
Domain: 200 x 200 x 200 Voxel: 1 µm
Load Structure
Input Map
Log Map
Post Map
Results
Metadata
Stress Unit
GPa
Direction Dependent Stiffness
Angle Resolution / (°)
10
Apply ...
Plot Options
Report
Plots
Map
Key
Unit
Value
StructureFile
Structure.gdt
RuntimeFeelMath
s
0.486
PhysicalVisualization
Information
Voigt
Stiffness
GPa
14.797, 6.09825, 6.09825, 0, 0, 0, 6.09825, 14.797, 6.09...
Compliance
1/GPa
0.088988, -0.0259711, -0.0259711, 0, 0, 0, -0.0259711, ...
Isotropic
OriginalSystem
PMA
DirectionStiffness
Reuss
Stiffness
GPa
8.02606, 4.59466, 4.59466, 0, 0, 0, 4.59466, 8.02606, 4....
Compliance
1/GPa
0.213647, -0.0777797, -0.0777797, 0, 0, 0, -0.0777797, ...
Isotropic
OriginalSystem
PMA
DirectionStiffness
MoriTanaka
Stiffness
GPa
8.4026, 4.68959, 4.65842, -0.00857623, 0.0168405, 0.01...
Compliance
1/GPa
0.185481, -0.0394193, -0.0802073, -0.00113367, -0.001...
Isotropic
OriginalSystem
PMA
DirectionStiffness
Manage Data
Load Input Map
Export
Close

Appendix I: Examples and Visualization

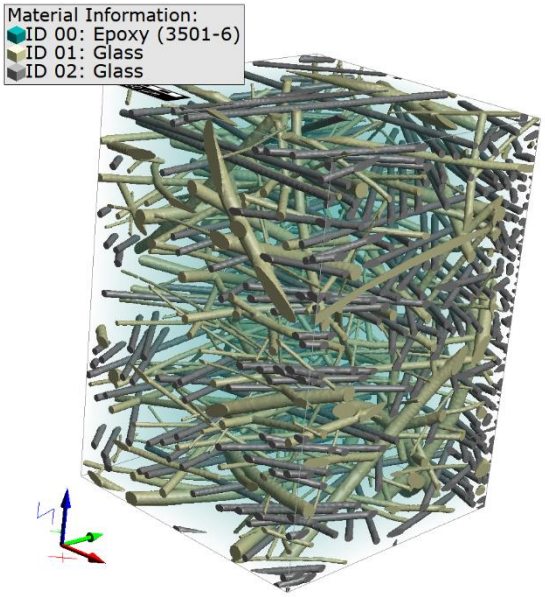
This section contains examples for FeelMath-VOX and for FeelMath-LD. For some of the examples, also suggestions for possible visualizations are made.

FeelMath-VOX

The general visualization options for FeelMath-VOX are presented here. These options apply for arbitrary FeelMath-VOX runs. The simulation settings are not relevant here.

Visualizing the structure

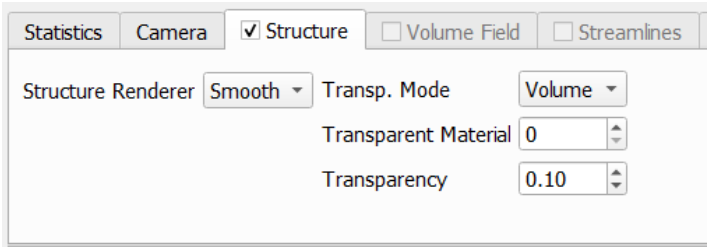
The structure used in this example is shown on the right and the settings for the visualization of this image are shown below.

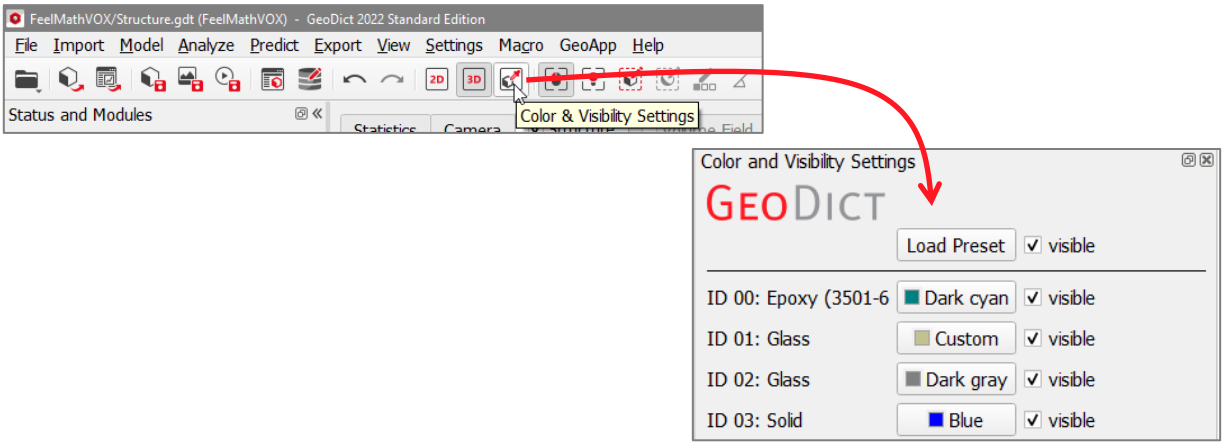


Render the structure in 3D (by clicking ) and go to the **Structure** tab in the visualization panel (above the Visualization area). Set the **Structure Renderer** to **Smooth**. Then, select **Transp. Mode** to **Volume**, set the **Transparent Material** ID to 0, and set the **Transparency** value to 0.10.

Usually, the material with ID 00 is set to invisible, so the transparency setting has no effect.

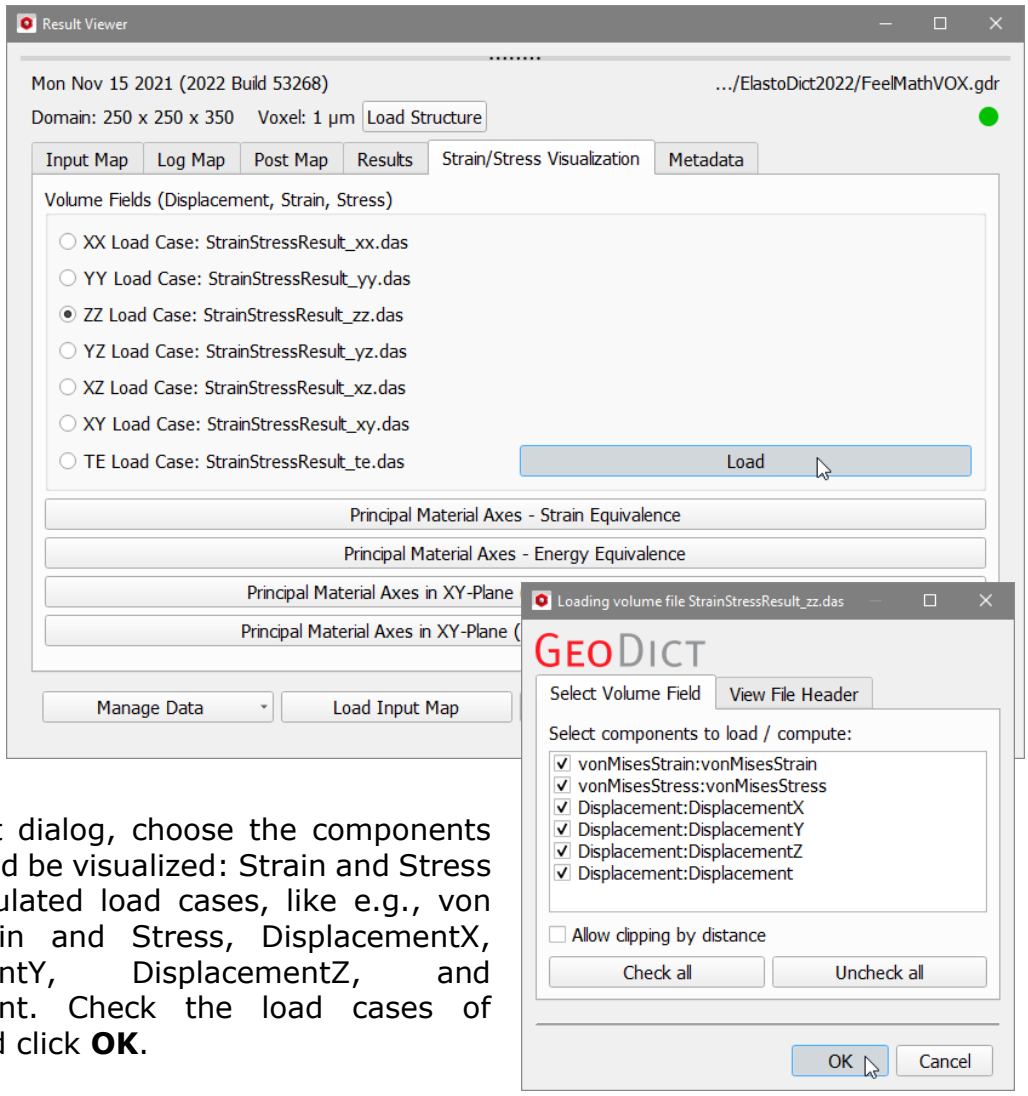
Click  to open the **Color & Visibility Settings** dialog and check **visible** to enable visibility for the material ID 00.





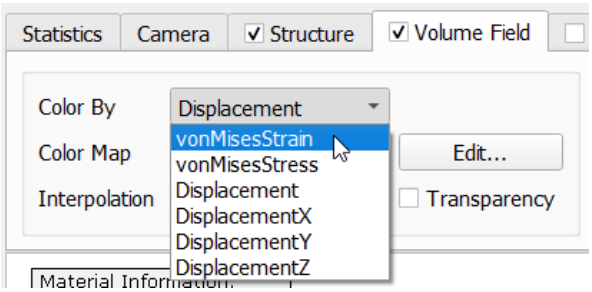
VISUALIZATION OF DISPLACEMENT AND STRESSES

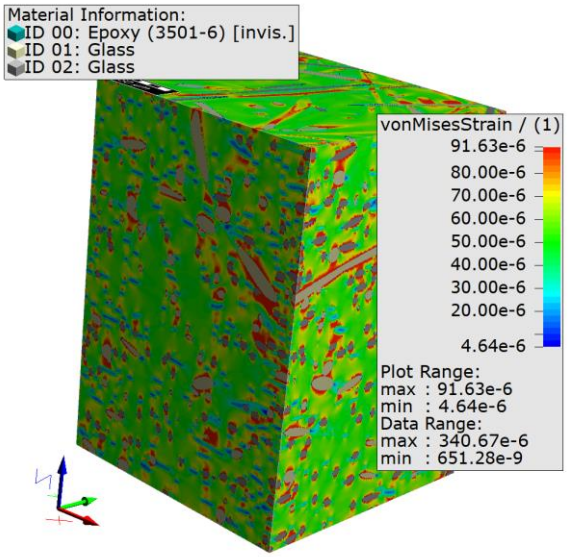
After all selected load cases have been computed, results fields can be loaded by choosing the corresponding *.das file and clicking **Load Results** in the Result Viewer (*.gdr).



In the next dialog, choose the components which should be visualized: Strain and Stress for all calculated load cases, like e.g., von Mises Strain and Stress, DisplacementX, DisplacementY, DisplacementZ, and Displacement. Check the load cases of interest and click **OK**.

Choose the displayed data through the **Color by** pull-down menu, under the **Volume Field** tab, in the Visualization panel above the Visualization Area.

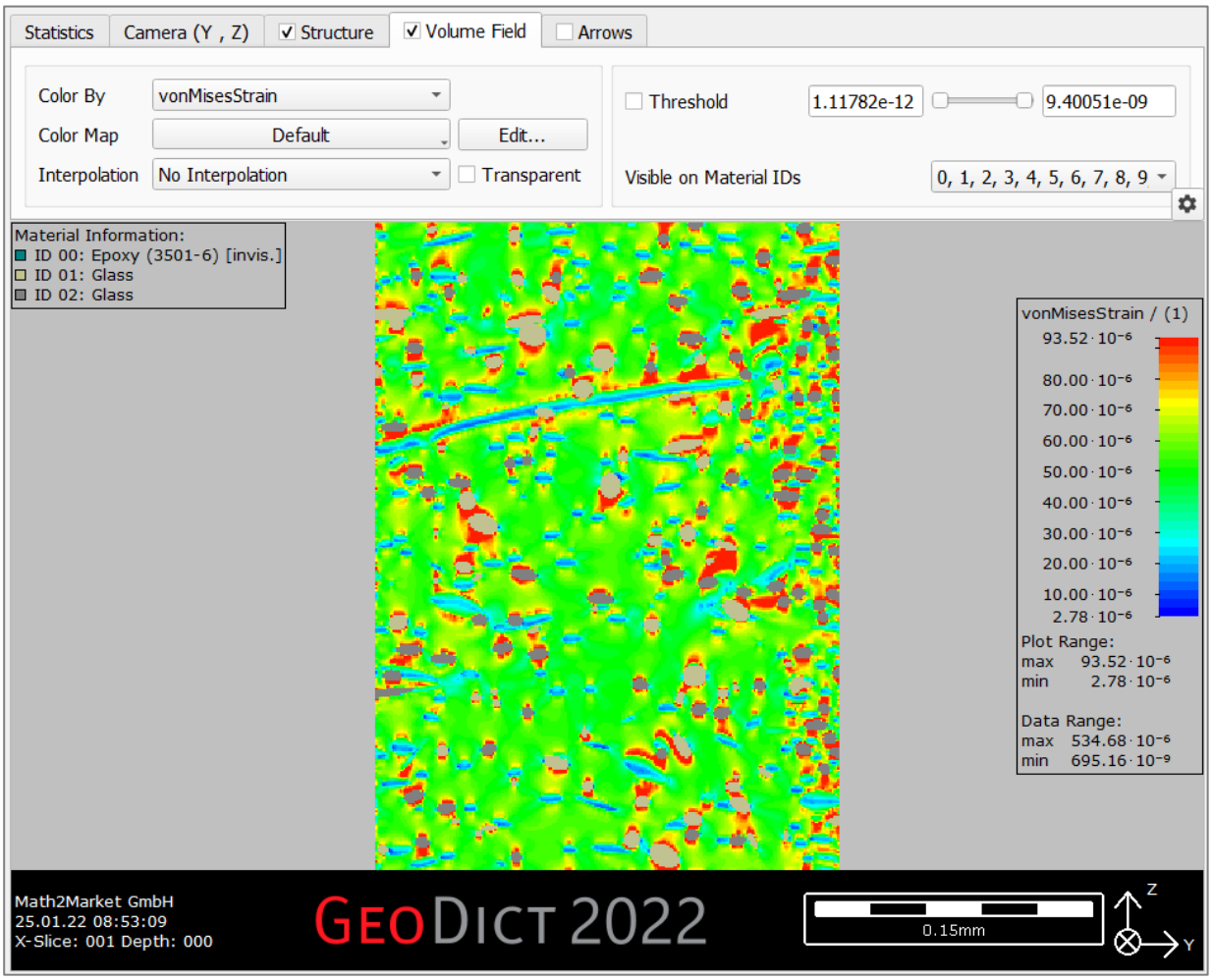




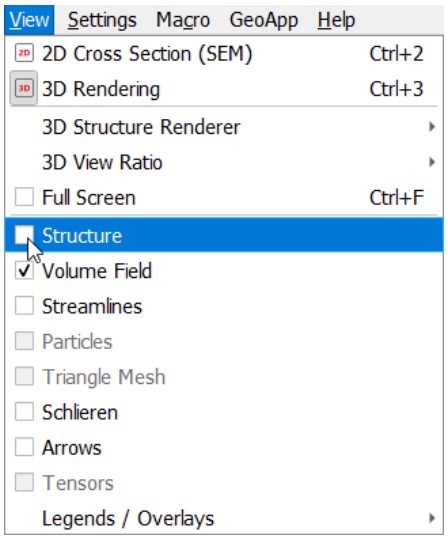
The visualization parameters of the results can also be set under the **Results** tab in the Result Viewer.

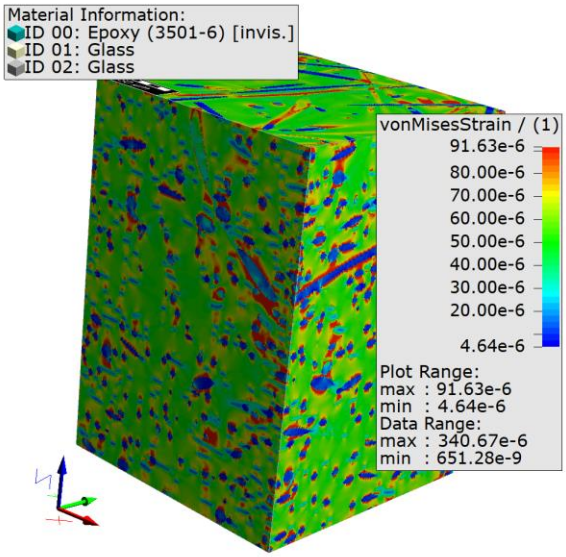
Tools are available for the visualization in 2D Cross Section (SEM) and in 3D Rendering.

For 2D visualization, select **View → 2D Cross Section (SEM)** in the Menu bar. The control of 2D visualization parameters is also done through the Visualization panel above the Visualization Area.



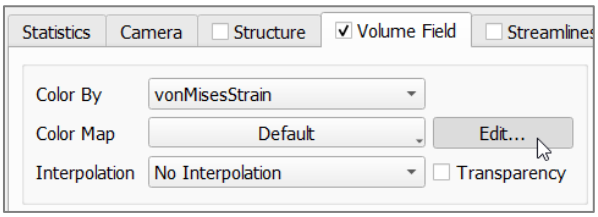
The structure in the model can be set to invisible to observe only the results (Volume Field). For this, select **View** and un-check **Structure** in the menu bar.

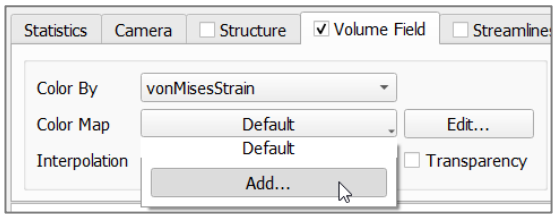




In 2D and 3D Rendering, a color bar appears to the right (if the default position is not changed) during the visualization of the result file, indicating the gradation of the currently selected property.

Click the **Edit...** button to edit the Default Color Map or add a new Colormap by choosing **Add...** in the dropdown menu (and then click the **Edit...** button). Alternatively, new colormaps can also be defined in the **Color Map** dialog.

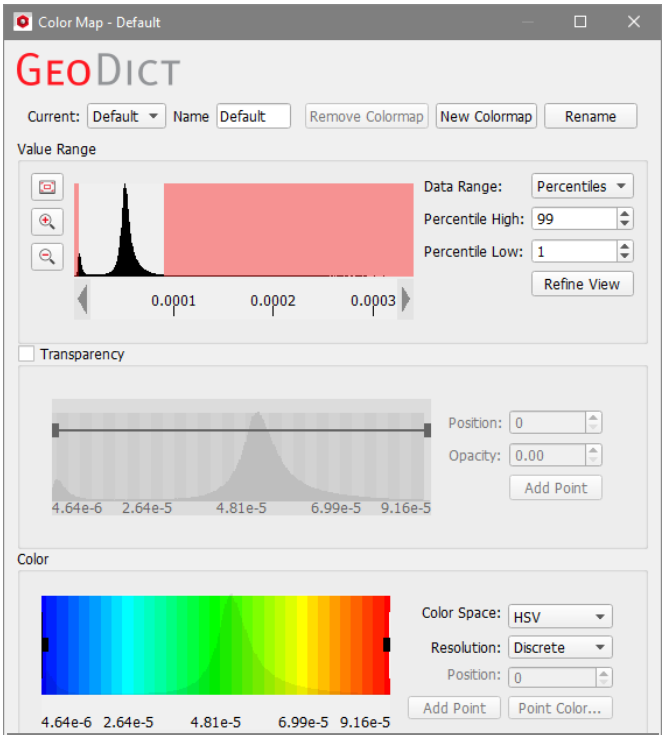


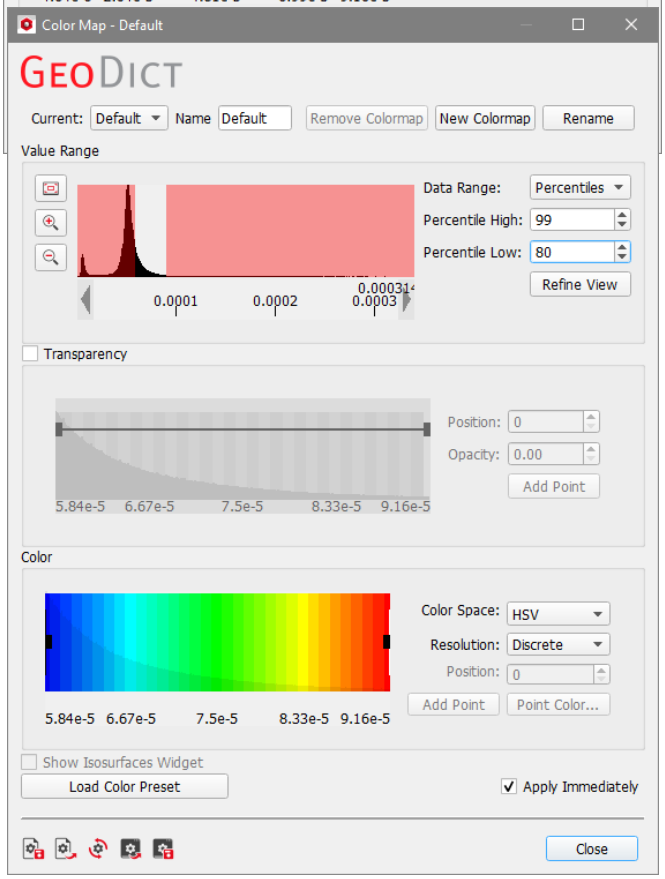


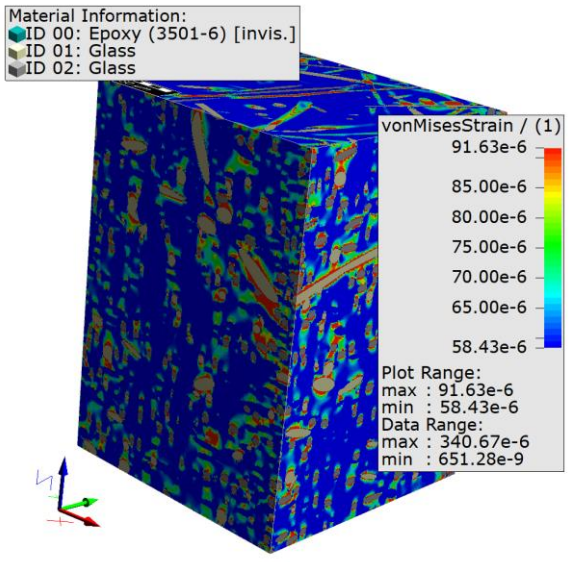
In the **Color Map** dialog, you can define the upper and lower limits of the color scale, add transparency to the visualized result field and assign a particular **Color Space** (RGB, HSV, LAB). The values entered in the **Color Map** dialog can be saved into *.gps (GeoDict Project Settings) files and/or loaded from them.

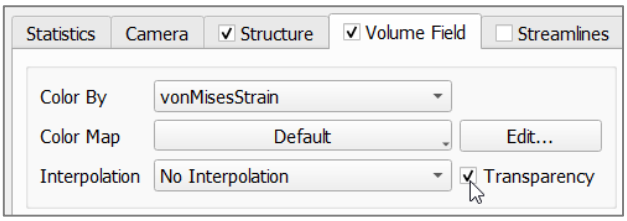
As you can observe in the histogram in the **Value Range** panel, the values concentrate in an area below a value 5.0e-05. To highlight the areas with high strain, we increase the **Percentile Low** to 80.

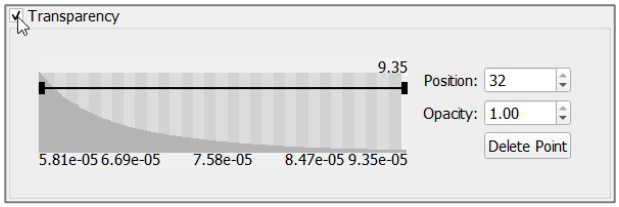
Note how the color of the result field in the Visualization area and the histogram change accordingly.





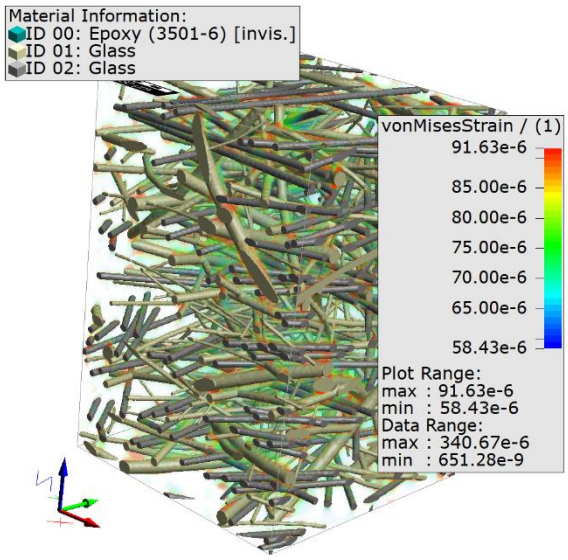


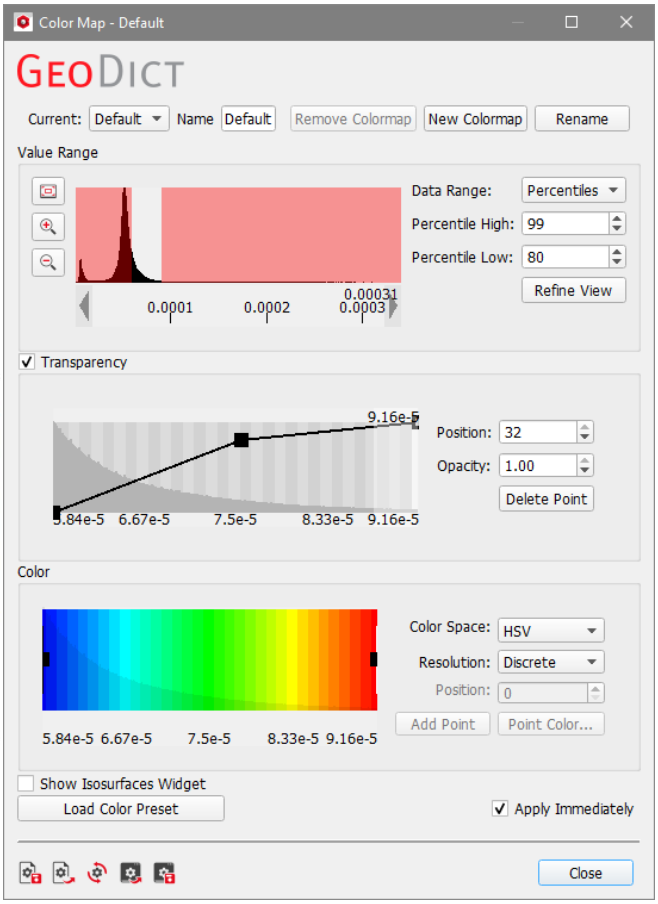




To emphasize the areas where the strain is elevated, you can activate **Transparency** under the Volume Field tab or directly in the **Color Map** dialog. Make sure that **No Interpolation** is selected in the **Interpolation dropdown menu** and then modify the transparency curve in the Color Map dialog, as indicated in the image on the right.

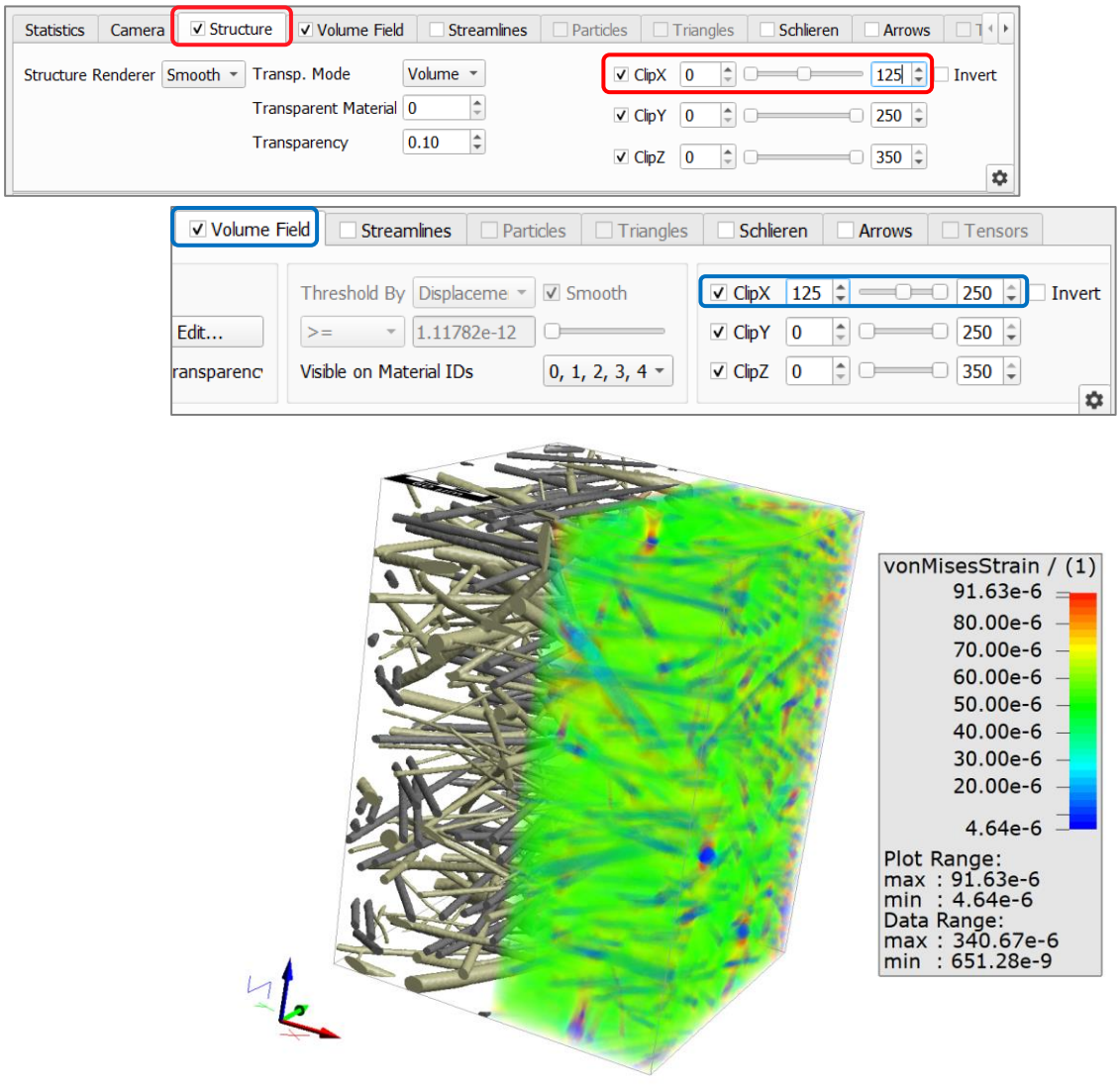
In the figure below, the transparency for low values is increased to see through these areas, and upper values with a high transparency are highlighted.





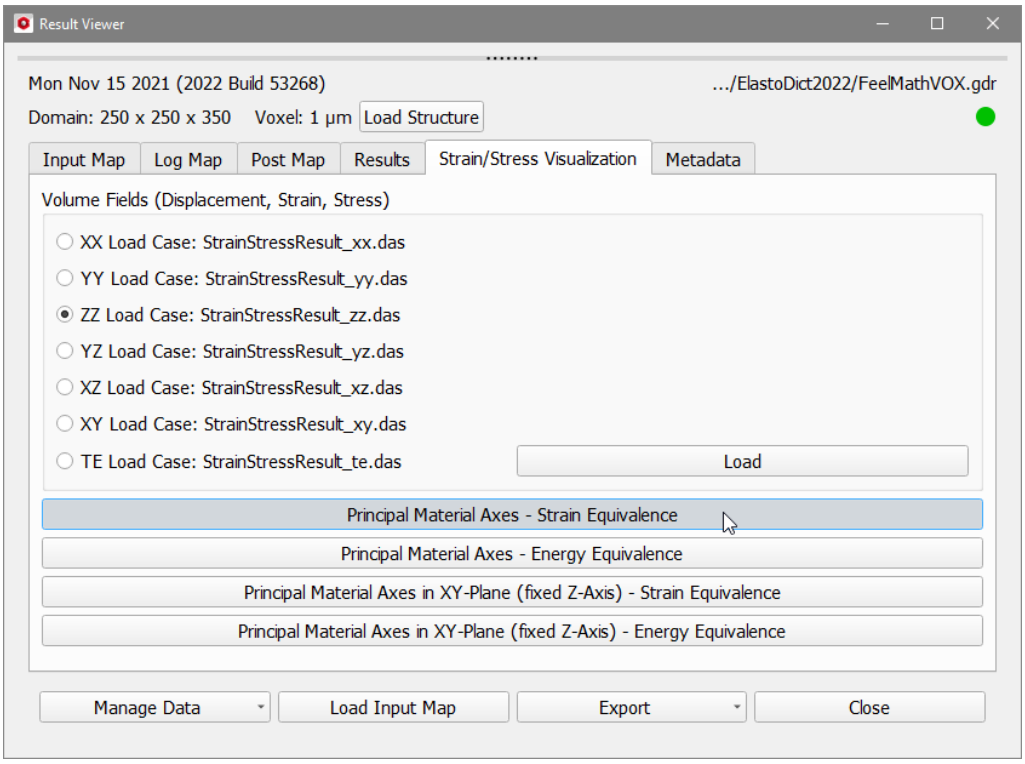
CLIPPING STRUCTURE AND RESULTS

The displayed results can also be clipped spatially in all three directions (**ClipX, ClipY, ClipZ**) with the sliders or by direct input. This enables the simultaneous visualization of the structure and the corresponding results. Make sure that the structure is set to visible (**View** → checked **Structure**).

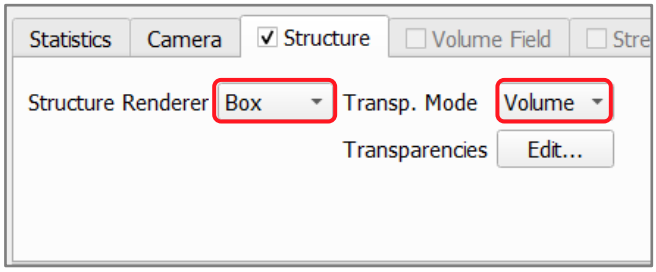


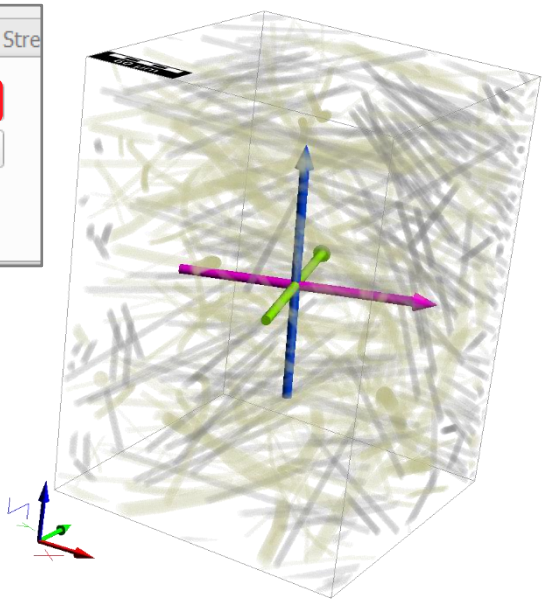
Visualization of Principal Material Axes

When all load cases (XX, YY, ZZ, XY, XZ, YZ) have been computed, the principal material axis can be visualized by clicking **Principal Material Axes – Strain Equivalence** or **Principal Material Axes - Energy Equivalence** under the Strain/Stress Visualization tab of the Result Viewer.



The axes are best to observe when the structure is transparent. For this, switch off the visualization of the results (**View** → uncheck **Volume Fields**), choose the Structure Renderer to **Box** and set the **Transp. Mode** to **Volume** (both options under the **Structure** tab in the Visualization panel).





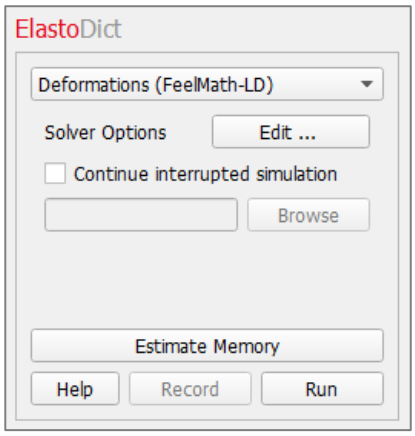
FeelMath-LD

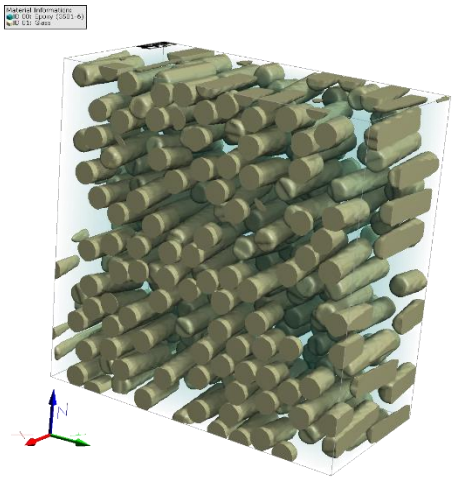
For FeelMath-LD, this section contains an example of how to simulate and visualize matrix damage.

MATRIX DAMAGE

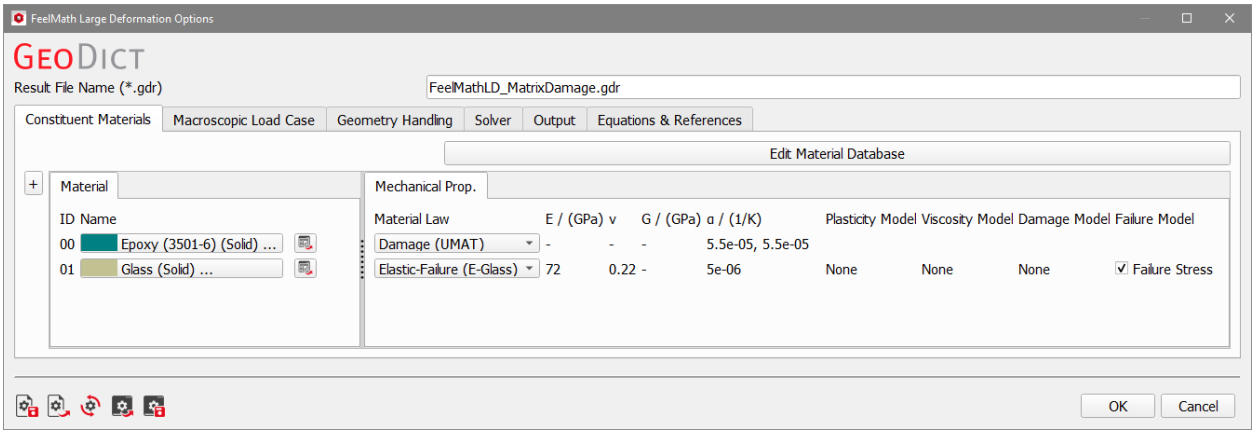
FeelMath-LD can be used to determine matrix damage in a composite model. In this example, E-Glass fibers are combined with an epoxy matrix. The structure used for this example is generated with FiberGeo.

Select the **Deformations (FeelMath-LD)** solver.



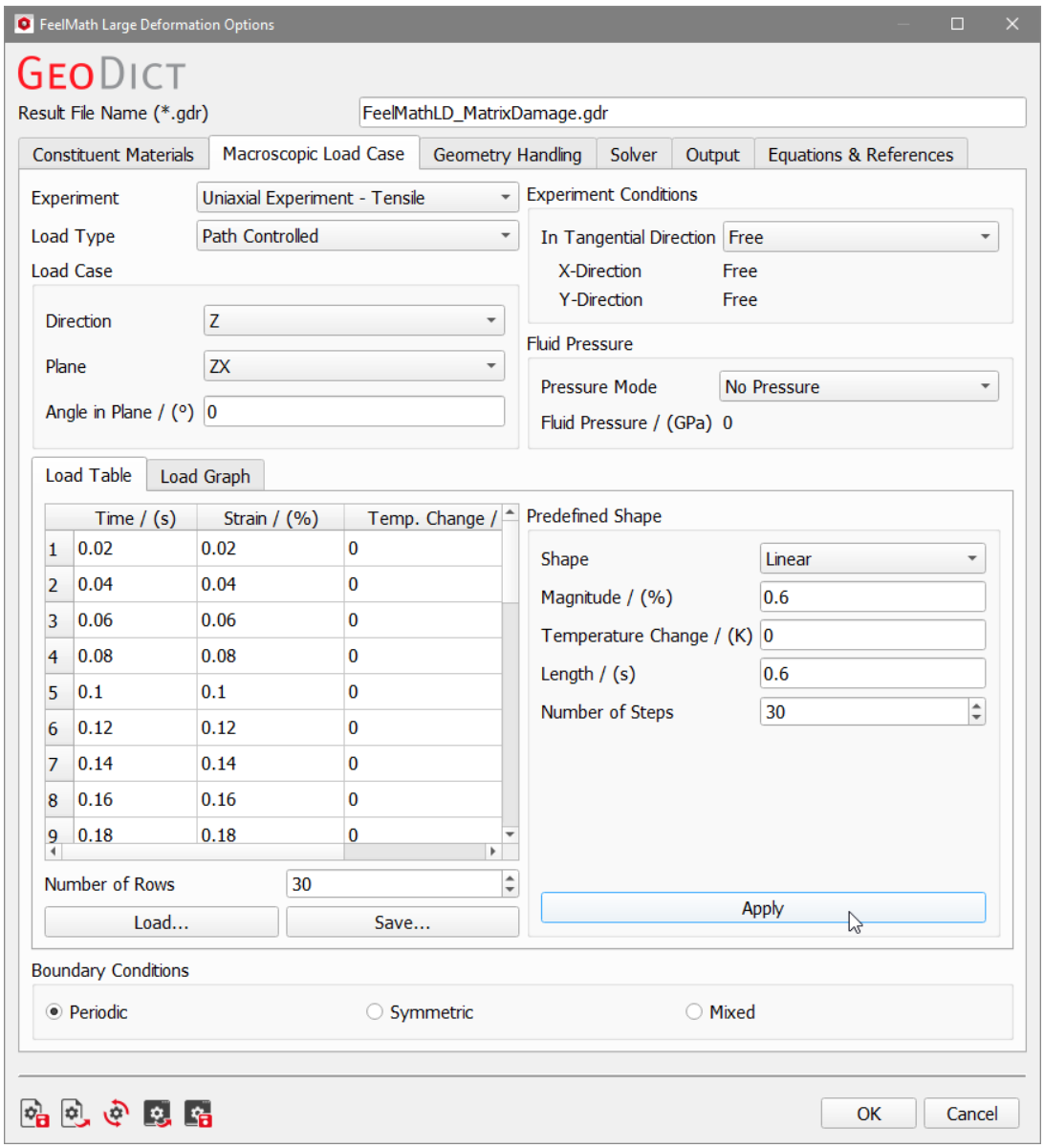


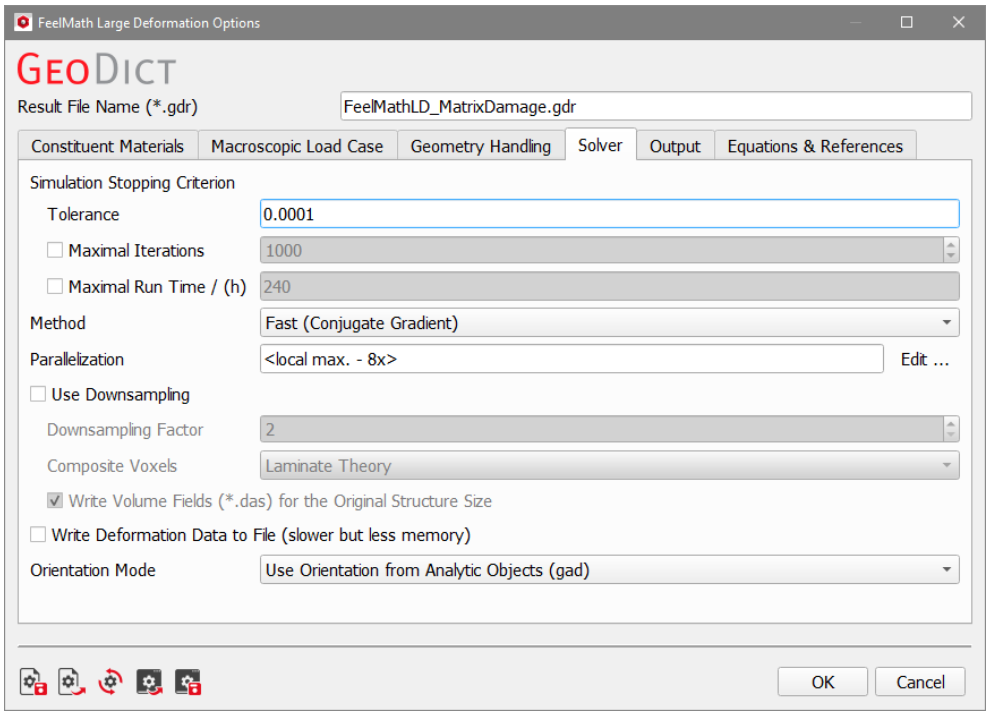
In the **FeelMath Large Deformation Options** dialog, under the **Constituent Materials** tab, set the materials to *Epoxy (3501-6)* with the *Damage (UMAT)* material model and *Glass* with the *E-Glass (Isotropic)* material model. The **Failure Stress** option for *Glass* can additionally be enabled, although it is not necessary for this example.



Under the **Macroscopic Load Case** tab, the experiment is set to **Uniaxial Experiment - Tensile**. A maximal strain of 0.6% is applied in 30 steps (choose **Predefined Shape**, set **Magnitude** to 0.6%, **Length** to 0.6 s and the **Number of Steps** to 30. Click apply to set the load in the **Load Table**). For damage simulations, it is useful to choose small steps (here, 0.2%).

Under the **Solver** tab, keep the default method **Fast (Conjugate Gradient)**.Keep the **Tolerance** at the default of 0.0001 to since a high accuracy is important especially for simulations with damage. Keep the default settings under the **Geometry Handling** tab.

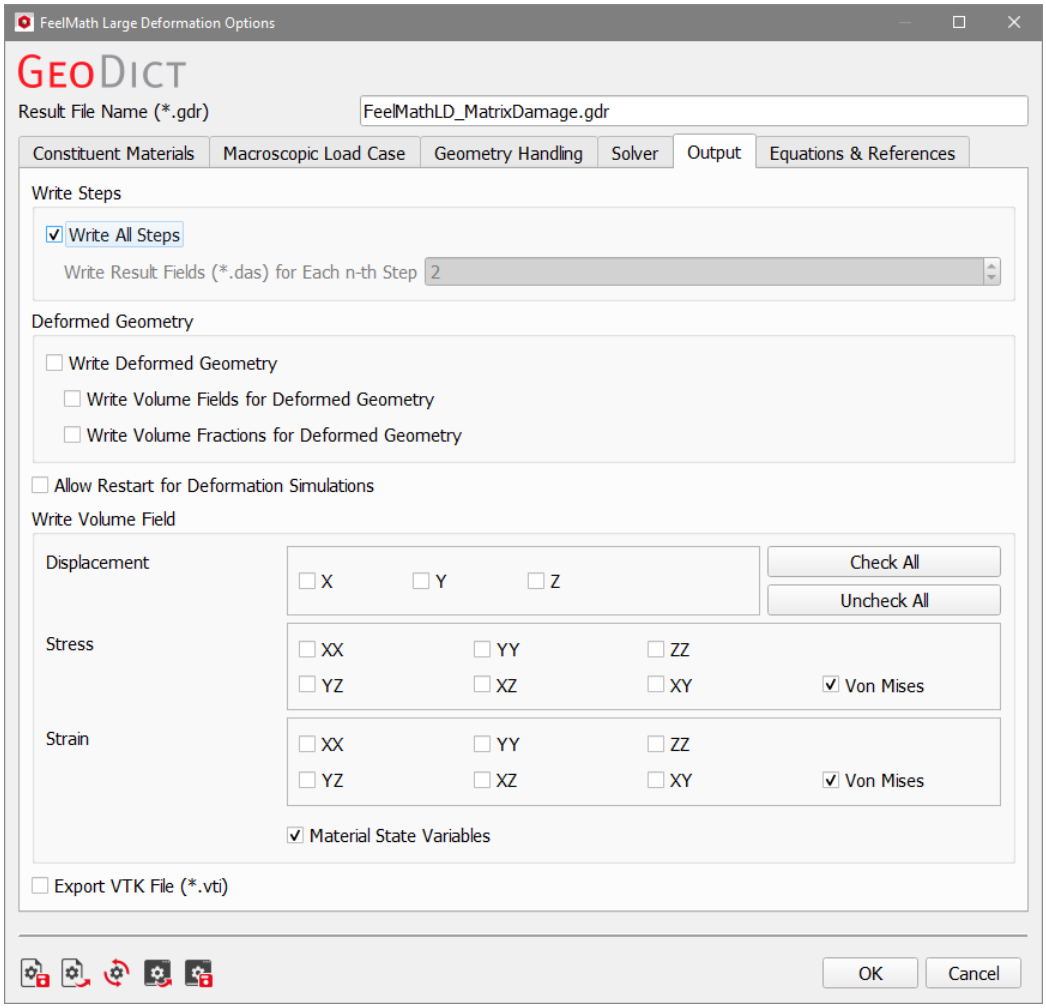

FeelMath Large Deformation Options
GEODICT
Result File Name (*.gdr)
FeelMathLD_MatrixDamage.gdr
Constituent Materials
Macroscopic Load Case
Geometry Handling
Solver
Output
Equations & References
Experiment
Uniaxial Experiment - Tensile
Load Type
Path Controlled
Load Case
Direction
Z
Plane
ZX
Angle in Plane / (°)
0
Experiment Conditions
In Tangential Direction
Free
X-Direction
Free
Y-Direction
Free
Fluid Pressure
Pressure Mode
No Pressure
Fluid Pressure / (GPa)
0
Load Table
Load Graph
Time / (s)
Strain / (%)
Temp. Change /
1 0.02 0.02 0
2 0.04 0.04 0
3 0.06 0.06 0
4 0.08 0.08 0
5 0.1 0.1 0
6 0.12 0.12 0
7 0.14 0.14 0
8 0.16 0.16 0
9 0.18 0.18 0
Number of Rows
30
Load...
Save...
Predefined Shape
Shape
Linear
Magnitude / (%)
0.6
Temperature Change / (K)
0
Length / (s)
0.6
Number of Steps
30
Apply
Boundary Conditions
Periodic
Symmetric
Mixed
OK
Cancel


FeelMath Large Deformation Options
GEODICT
Result File Name (*.gdr)
FeelMathLD_MatrixDamage.gdr
Constituent Materials
Macroscopic Load Case
Geometry Handling
Solver
Output
Equations & References
Simulation Stopping Criterion
Tolerance
0.0001
Maximal Iterations
1000
Maximal Run Time / (h)
240
Method
Fast (Conjugate Gradient)
Parallelization
<local max. - 8x>
Edit ...
Use Downsampling
Downsampling Factor
2
Composite Voxels
Laminate Theory
Write Volume Fields (*.das) for the Original Structure Size
Write Deformation Data to File (slower but less memory)
Orientation Mode
Use Orientation from Analytic Objects (gad)
OK
Cancel

Under the **Output** tab, uncheck **Deformed Geometry** and keep only the volume fields **Von Mises** for **Stress** and **Strain** and the **Material State Variables** (containing the damage and failure variables in this example).

Uncheck **Write Deformed Geometry**, since generating the deformed geometries takes additional computation time and the deformed geometries are not relevant in most damage simulations (since the strain at the point of failure is often very low).

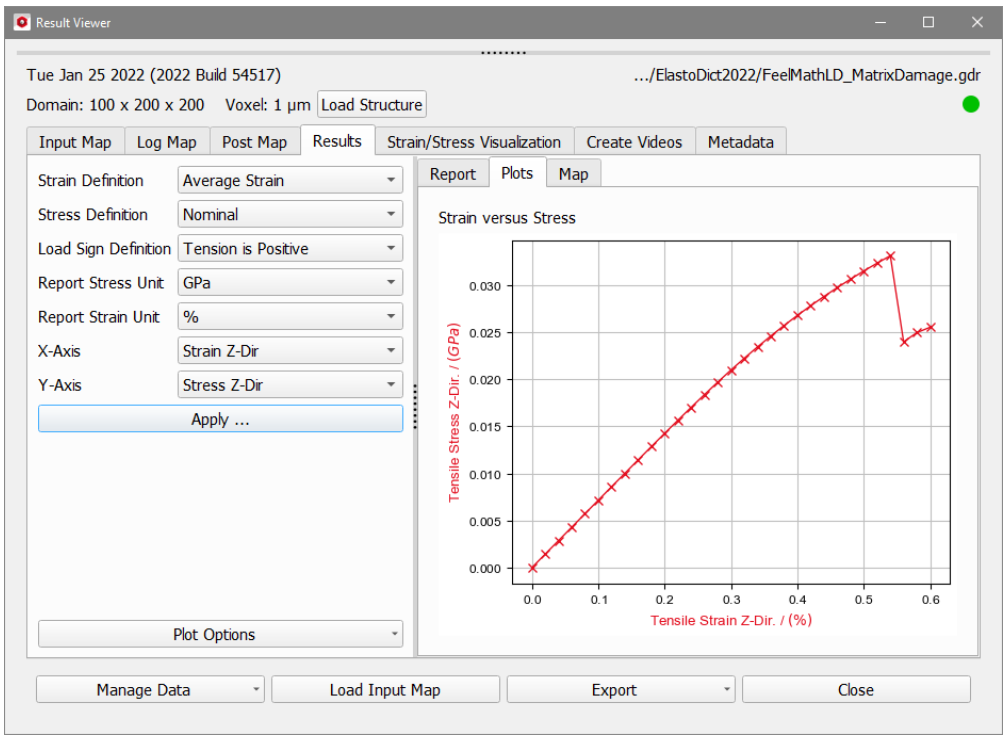
Analogously, writing volume fields might take a significant amount of disk space and time, depending on the size of the structure. Some disk-space and computational time is saved by unchecking stress, strain, and displacement fields which do not need to be visualized.



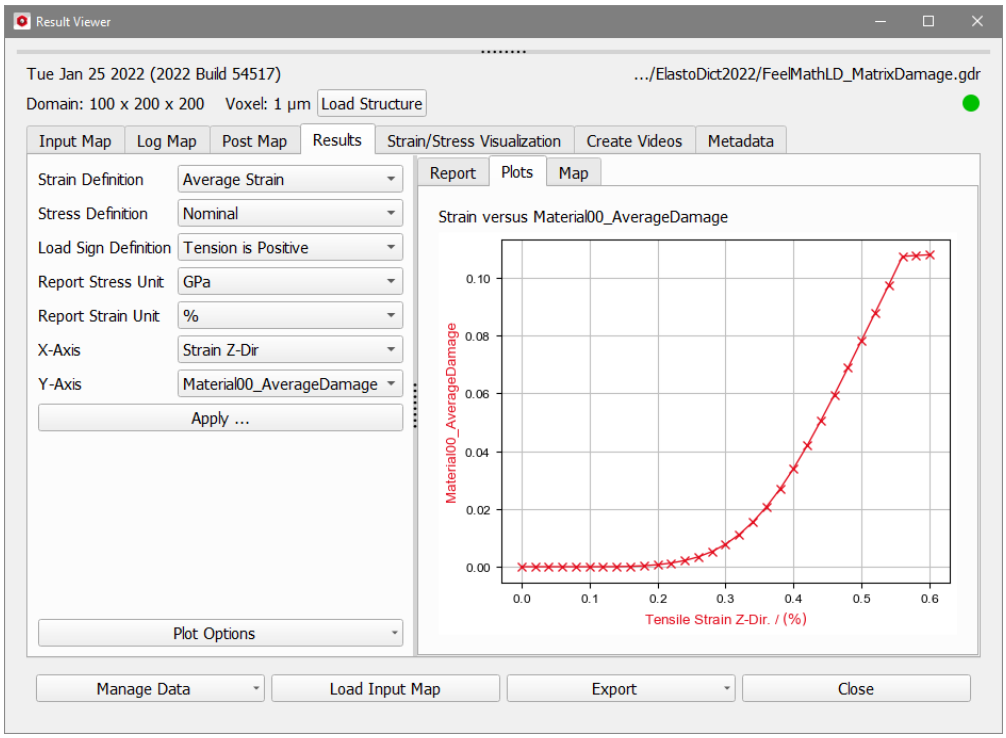
Click **OK** to close the **Options** dialog and start the simulation by clicking **Run** in the GeoDict GUI main screen.

After the simulation is finished, the result file is opened automatically in the Result Viewer at the **Results - Report** subtab.

Under the **Results - Plots** subtab, the results of the deformation during the time series experiment are plotted as **Stress-Strain** chart (X-Axis: Strain Z-Dir; Y-Axis: Stress Z-Dir). Increasing damage leads to decreasing stiffness in the structure.



Choose **Material00_Damage** for the Y-Axis and click **Apply...** to plot the average matrix damage in the the matrix material (0 is no damage, 1 is maximal damage). As it can be observed in the plot, the average damage increases constantly until the point of failure (which can be recognized on the drop in the strain-stress curve at a strain of 0.56% in the plot above), but it reaches a plateau (with a much smaller increase) after failure. Failure in a composite is a local phenomenon: As soon as a crack occurs (with a high local damage), the rest of the structure is unloaded.

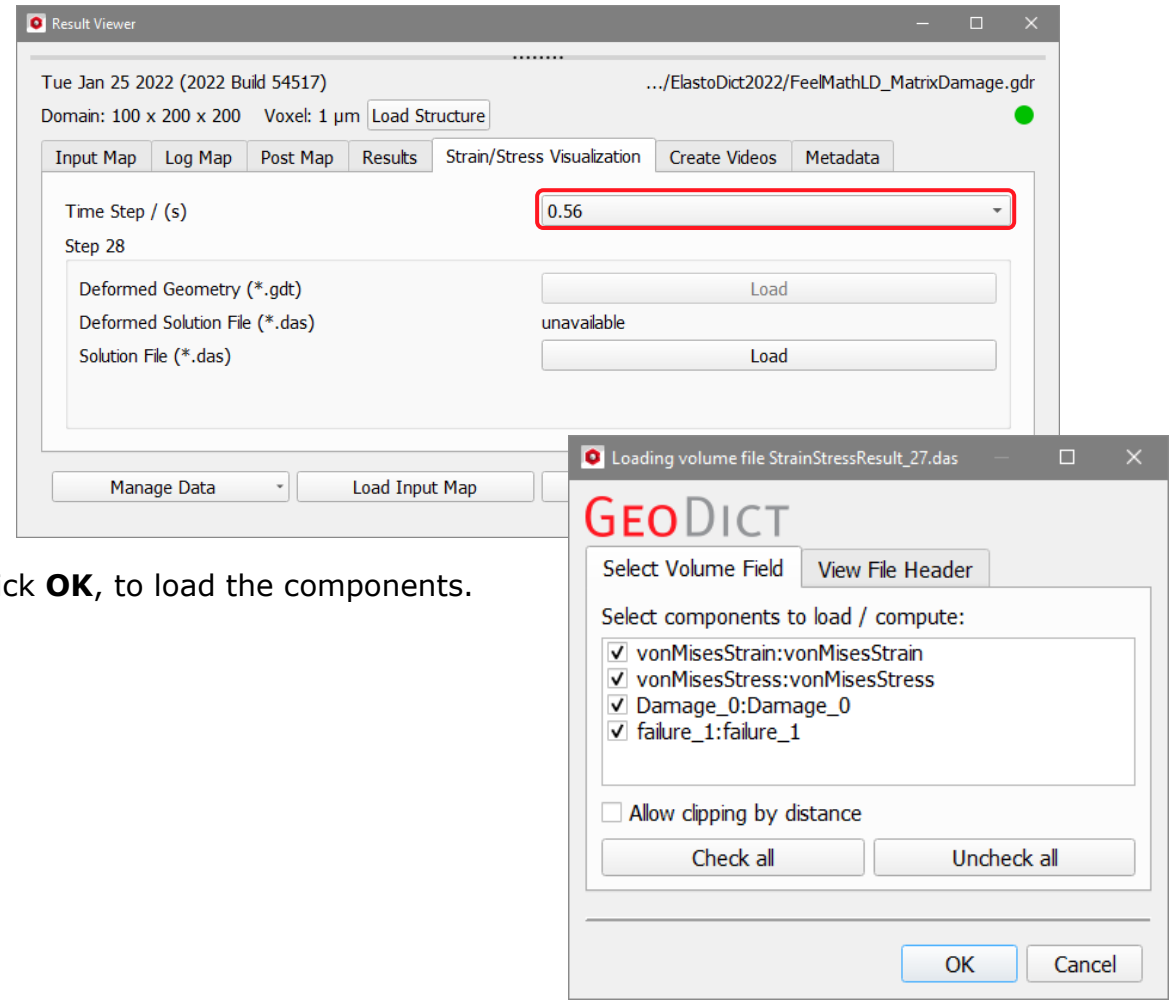


Other graphs of interest can be plotted by changing the selections of the **X-Axis** and the **Y-Axis** pull-down menus.

The original structure can be loaded with the **Load Structure** button.

The **Strain/Stress Visualization** tab contains the volume fields of the **Time Steps**, which can be selected from the pull-down menu (here, the point of failure at 0.56 s is selected) and loaded by clicking **Load**.

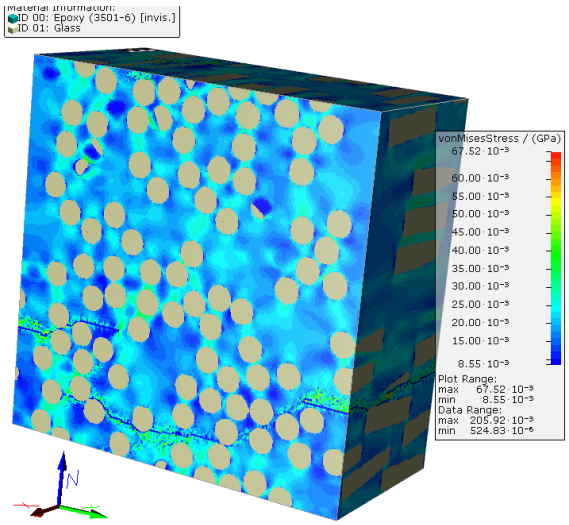
The components whose results can be visualized are checked in the list e.g., here von Mises Strain, von Mises Stress, Damage (Damage_0) and failure (failure_1). The numbers (0 in Damage_0 and 1 in failure_1) stand for the Material IDs to which the volume fields belong.



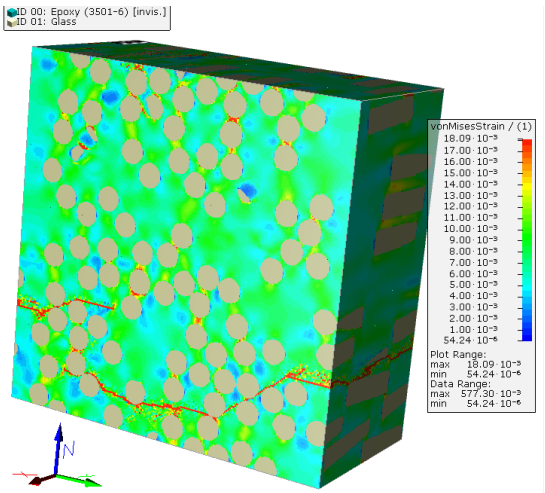
Click **OK**, to load the components.

In 2D and 3D Rendering, a color bar appears to the right (default position) during the visualization of the result file, indicating the gradation of the selected component.

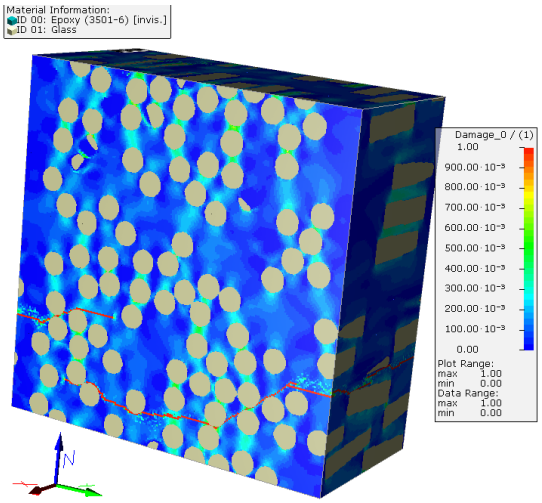
The visualization parameters can be set under the **Results** tab in the Visualization panel, above the Visualization Area. For more information, see the Visualization handbook of this User Guide.



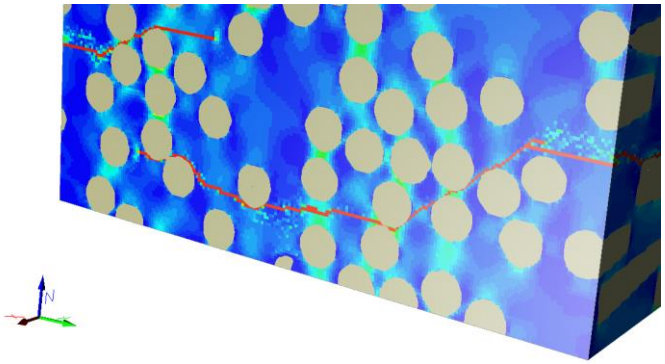
The structure is loaded in Z-direction, therefore the highest stresses in the material occur in the areas between fibers which lie closely together. In the lower area of the structure, the crack can be seen in the matrix where the stresses are close to zero.



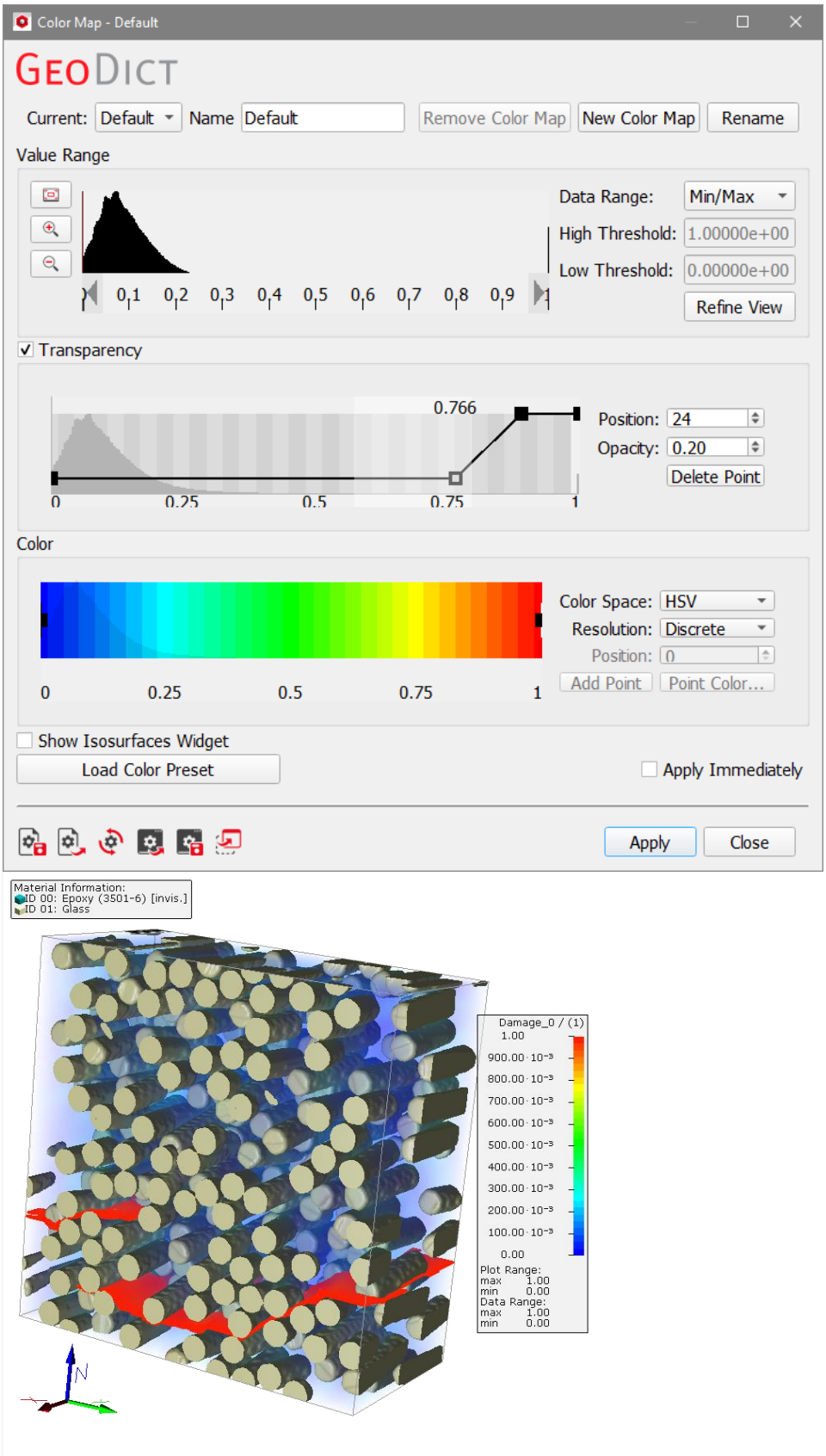
The highest strain can be observed at the crack. There, the stiffness of the matrix material is lowered due to the damage, which leads to high strain values and low stress values.



When damage is visualized, it is recommended to set the **Data Range** in the **Color Map** dialog to **Min/Max** or manually to a minimal value of 0.0 and a maximal value of 1.0 (see also screenshot on the next page). Then, the areas which are fully damaged are clearly visible.



The crack in the material can be best visualized with the **Transparency** option for the volume field. For this, set the transparency as shown in the screenshot below: Choose low values (e.g. 0.2) for low damage values (in this example, for damage values lower than 0.75), and high values (1, which means no transparency) for high damage values (here, for damage values above 0.875).



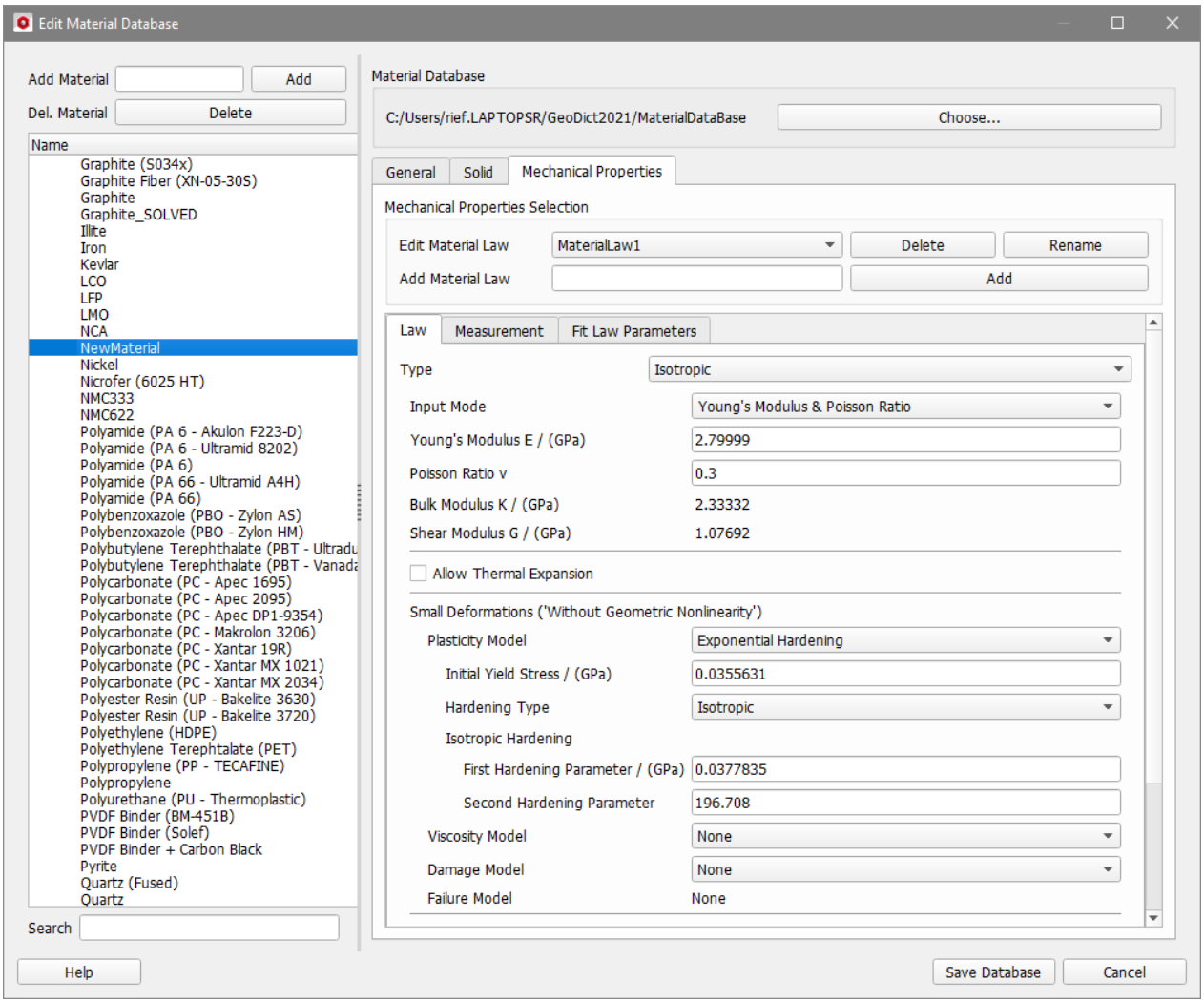
Appendix II: Nonlinear material models in ElastoDict

In ElastoDict, several types of nonlinear material laws are integrated. The next section explains how these material laws can be set up. Additionally, it is also possible to program user-defined material laws through the UMAT interface (see page 89)

Internal nonlinear material laws in FeelMath

Several nonlinear material laws are delivered with GeoDict and can conveniently be set up in the GeoDict Material Database dialog. see the Material Database handbook for more information.

The available material laws are: **Plasticity**, **Damage**, **Viscosity** and **Failure**. All these material models are only available **Without Geometric Nonlinearity**.

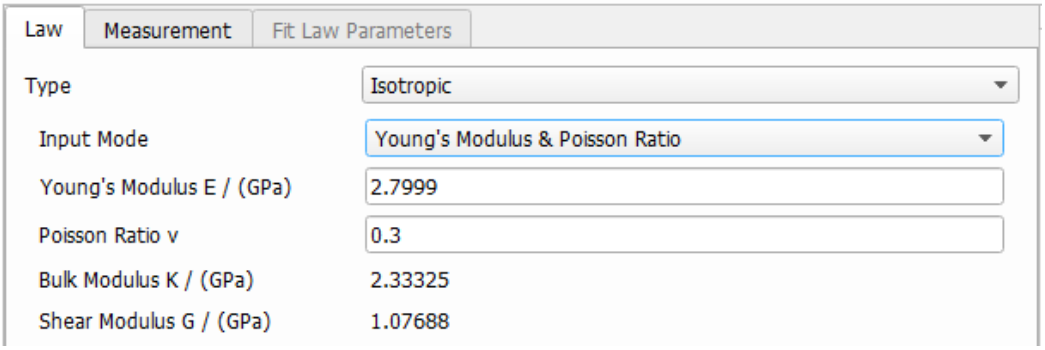


These material laws can be combined in different ways:

- Plasticity, damage and viscosity can be combined. For these combinations, only the exponential damage model is available.
- The Mazars damage model cannot be combined with any other model.
- The Failure model cannot be combined with any other model.

Linear Elasticity

The constants for linear elastic materials need to be defined for each material law in ElastoDict. All nonlinear material laws that can be selected in GeoDict's material Database are based on linear isotropic elastic materials, except of the failure model, which is also available for transverse isotropic materials.

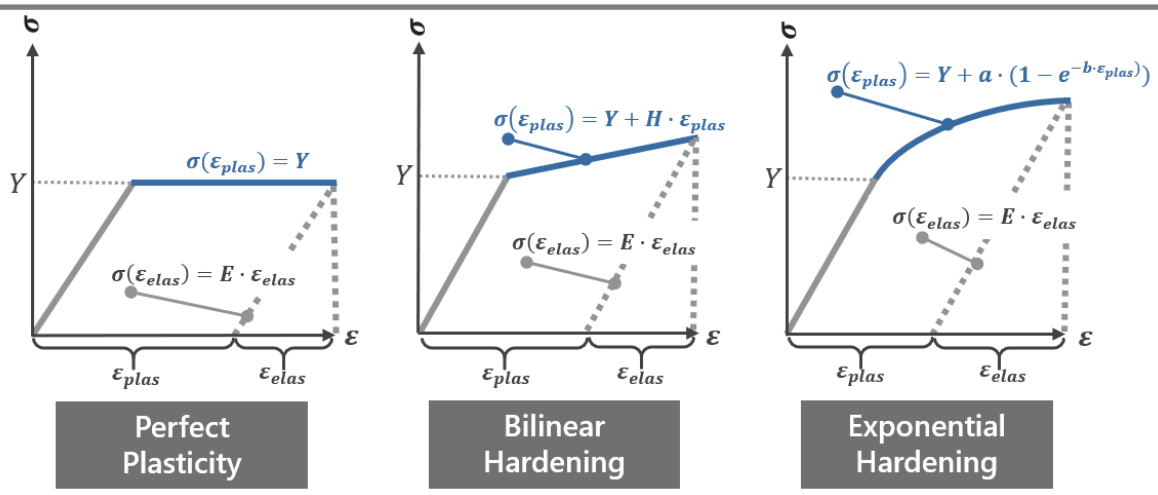


Plasticity

Plasticity in materials describes the effect that a deformation remains when the load is removed. In GeoDict, three different plastic material laws are available: **Perfect Plasticity**, **Bilinear Hardening** (Affine linear Hardening) and **Exponential Hardening**.

For understanding plastic material laws, the two most important parameters are the elastic strain ε_{elas} and the plastic strain ε_{plas} which add up to the strain ε. The elastic strain is recoverable, whereas the plastic strain remains in the material after unloading. The relation of the elastic strain ε_{elas} to the stress σ is described by Hooke's law, and the relation of the plastic strain ε_{plas} to the stress σ is described by the chosen plastic material law.

As long as the stress is lower than the yield stress Y of the material, the deformation is purely elastic. After this point, an increase in stress leads to a combination of elastic and plastic strains. The yield stress increases through the plastic deformation, which means that the material is elastic up to this point under a new load. Nevertheless, the course of the plastic material always depends on the initial yield stress.



The parameters are: ε_{elas}: elastic strain, ε_{plas}: plastic strain, σ: stress, Y: yield stress, H: plastic strain hardening modulus, a: first hardening parameter, b: second hardening parameter

The three available plastic material laws differ in the relation between the plastic strain and the stress:

- **Perfect Plasticity**: As soon as the initial yield stress Y is reached, the stress remains at that level. From this point, the elastic strain stays constant, and all additional strain is purely plastic.
- **Bilinear (Affine linear) Hardening**: The stress is a linear function of the plastic strain

  $$\sigma(\varepsilon_{plas}) = Y + H \cdot \varepsilon_{plas}$$

  where H is the **Plastic Strain Hardening Modulus**.

  The plastic strain hardening modulus is not the slope of the strain-stress curve, since it only takes the plastic strain into account. The slope of the strain-stress curve (after the yield stress is reached) is the **Tangential Modulus** T. The **Plastic Strain Hardening Modulus** and the **Tangential Modulus** are related as

  $$H = \frac{T}{1 - \frac{T}{E}}$$

  with the young's modulus E. In the material definition in GeoDict, either the **Plastic Strain Hardening Modulus** or the **Tangential Modulus** can be set.
- **Exponential Hardening**: The stress is related to the plastic strain via an exponential function

  $$\sigma(\varepsilon_{plas}) = Y + a \cdot \left(1 - e^{-b \cdot \varepsilon_{plas}}\right)$$

  with the **First Hardening Parameter** a and the **Second Hardening Parameter** b.

Isotropic and Kinematic Hardening

Isotropic and **Kinematic Hardening** describe the effect of the of the plastic deformation on the yield surface (see Wikipedia: Yield Surface for further reference).

In summary, the yield surface grows isotropically with isotropic hardening, whereas it moves with kinematic hardening. In real materials, the material behavior is usually a combination of both hardening types.

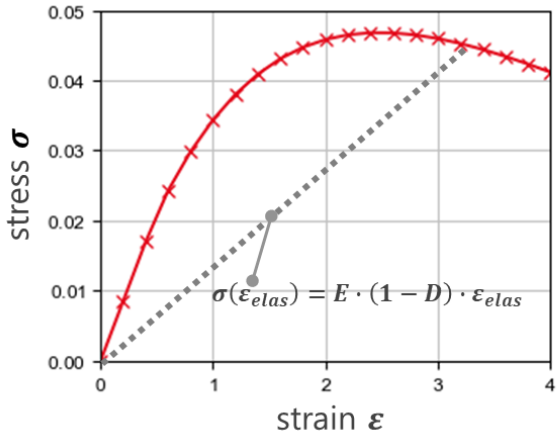
How to set up the hardening type for a material is expert knowledge and can only be analyzed by measuring multiple load cycles for a material. Nevertheless, if only tension or compression is applied to a material, the results for both hardening types are the same, and it is sufficient to keep the default **Isotropic Hardening** when setting up a material law.

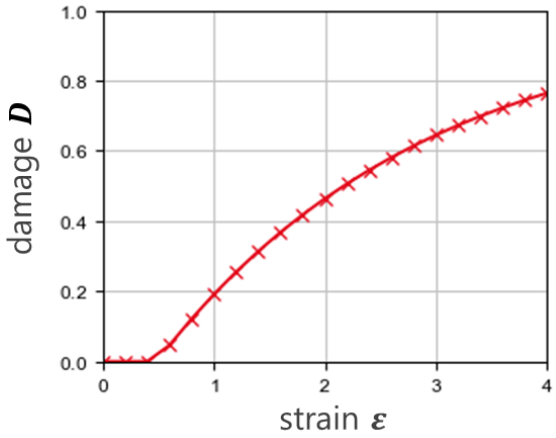
DAMAGE

With the damage models, the stiffness of the material is decreased with increasing material damage:

$$\sigma = (1 - D) \cdot E \cdot \varepsilon$$

with the damage variable D. The evolution of the damage D depends on the selected damage model, and the damage can only increase. The initial value is $D = 0$, and the maximal allowed value for the damage is $D = 0.99$. When unloaded, the material deforms elastically (with the decreased stiffness) back to its initial state.





Two damage models are available in GeoDict: The **Exponential Damage** model and **Mazars' Damage** model (See reference on page 81). Both models are very similar and differ only in the way they depend on the strain.

- **Mazars' Damage**: The damage depends on the strain, and the degradation begins as soon as the minimal strain for damage d_0 is reached:

$$D = 1 - \frac{d_0(1-d_2)}{\varepsilon} - \frac{d_2}{e^{d_1(\varepsilon - d_0)}}, \varepsilon > d_0$$

with d_0: minimal strain for damage, d_1: damage hardening modulus, d_2: damage evolution.

- **Exponential Damage**: The damage depends on the strain energy

$$U = U_{elas} + U_{plas} = \frac{E}{2} \cdot \varepsilon_{elas}^2 + \int_0^{\varepsilon_{plas}} (\sigma(\varepsilon_p) - Y) d\varepsilon_p$$

which is the sum of the elastic and plastic strain energies U_{elas} and U_{plas}. If no plastic deformations occur, the strain energy depends only on the elastic strains. The degradation begins as soon as the minimal energy for damage d_0 is reached:

$$D = 1 - \frac{d_0(1-d_2)}{U} - \frac{d_2}{e^{d_1(U - d_0)}}, U > d_0$$

with d_0: minimal energy for damage, d_1: damage hardening modulus, d_2: damage evolution.

The damage evolution formula is the same for both models, the significant difference is that the damage is driven by the strain for **Mazars' Damage** and driven by the elastic strain energy in the **Exponential Damage** model. In other words, the damage criterion for Mazars depends linearly on the strains, and a quadratic relation holds for the exponential damage model.

FAILURE

The **Failure** model in GeoDict is closely related to the damage models, but its approach is simpler. Instead of the continuous damage variable D, the failure model knows only two states: Failure or no failure. The material fails if the Failure Stress is exceeded, and the stiffness is degraded to 1% of the original stiffness.

The **Failure** model is available for isotropic and for transverse isotropic materials. In the isotropic case, the reference stress is the von Mises stress, and in the transverse isotropic case, the stress in the respective directions is checked.

Check the guidelines on page 81 for a comparison of the damage and failure models in GeoDict.

Guidelines for Plasticity, Damage and Failure models

The convergence for nonlinear materials can be bad if the simulation settings are not set up properly. Therefore, this section contains some best practices for these simulation types.

Boundary Conditions

*Don't use **Force** boundary conditions, if possible*:

With **Force** boundary conditions, it is possible to choose the applied load too high for the materials in the structure: For plastic materials and for the damage models, the maximal stress is limited by the material model. Therefore, applying a load which is higher than this maximal stress leads to unsolvable equations.

If it is important to use force boundary conditions (as e.g., in a cyclic load case, where the stresses should decrease to zero again), we recommend

- Do a first simulation with **Path** Boundary Conditions, to check out the maximal allowed stresses for the structure, *or*
- Check the materials carefully to estimate the maximum allowed load.

Nevertheless, even if the maximum allowed load is not reached, the convergence might be slow. For example, when using the exponential hardening model, a load slightly lower than the maximal allowed load might lead to strains near to infinity (which is also not realistic).

Damage models vs. failure model

The main difference between the damage models and the failure model is that the failure model decreases the stiffness suddenly, which introduces a discontinuity into the strain-stress relationship. The damage models lead to a gradual reduction of the stiffness. Thus, the damage models introduce no discontinuity, this means that the simulation is more stable and usually faster. Nevertheless, this gradual reduction of stiffness can be arbitrarily fast – this means that nearly the same results as with the failure model can be achieved. Additionally, the damage models can be combined with other models like e.g., plasticity.

The main advantage of the failure model is that it is easier to set up, since it contains less parameters. Additionally, the damage models are not available for the transverse isotropic case. Altogether, it is strongly recommended to use the damage models instead of the failure model, whenever possible.

Nonlinear material laws in GeoDict - References

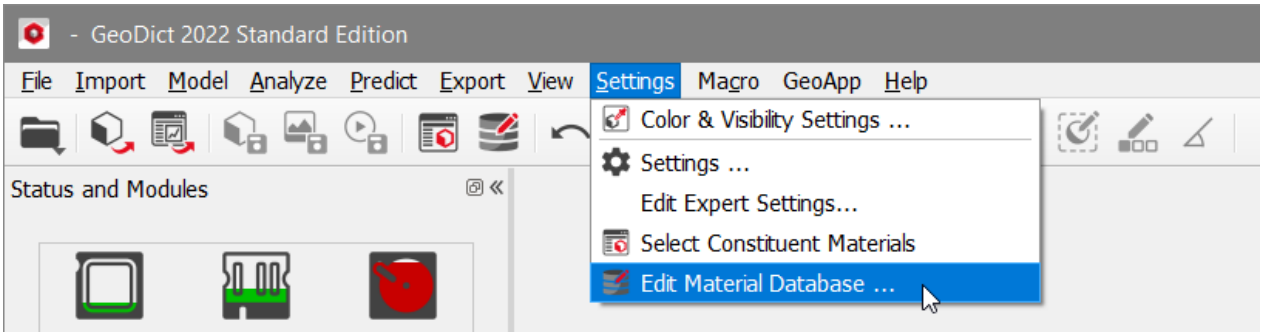
J. Mazars: **Mechanical damage and fracture of concrete structures**. *Advances in fracture research.* (1981) **4**, pp. 1499 – 1506.

G. Alfano, F. De Angelis and L. Rosati: **General solution procedures in elasto/viscoplasticity.** *Computer Methods in Applied Mechanics and Engineering*, **190(39)** (2001), pp. 5123 – 5147.

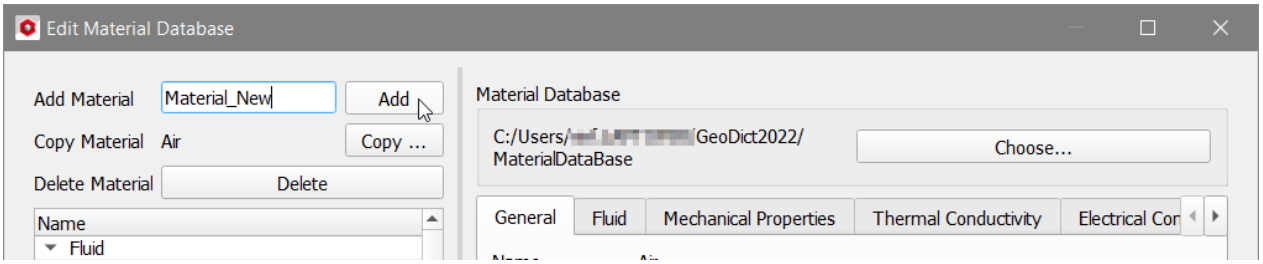
J-C. Michel and P. Suquet: **A model-reduction approach in micromechanics of materials preserving the variational structure of constitutive relations.** *Journal of the Mechanics and Physics of Solids*, **90** (2016), pp. 254 – 285.

SETTING UP THE INTERNAL MATERIAL LAWS

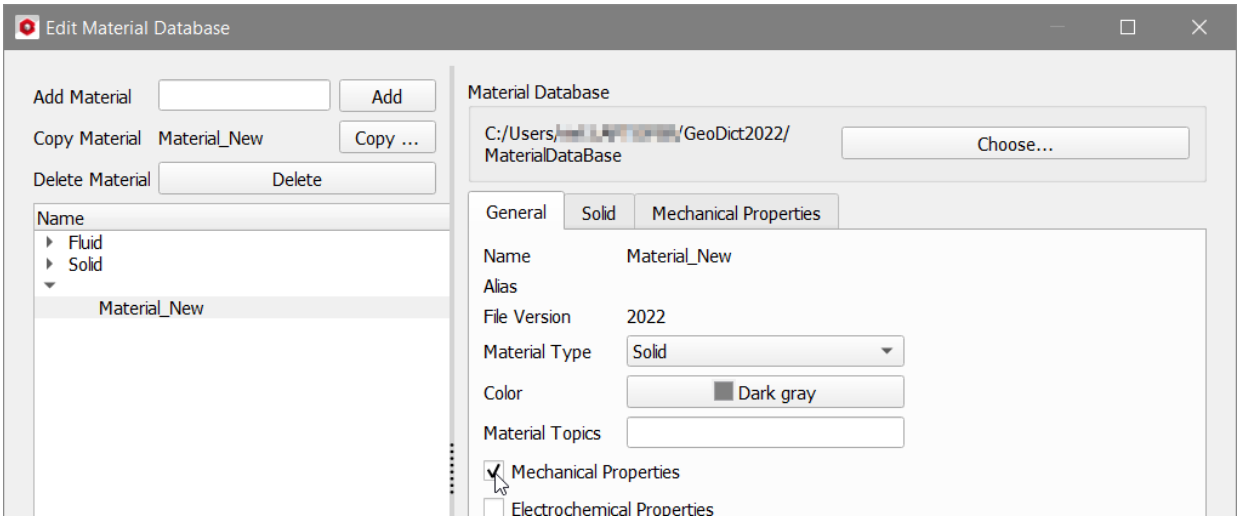
To set up a material law in GeoDict, first open the material data base via **Settings – Edit Material Data Base ...** in the menu bar:



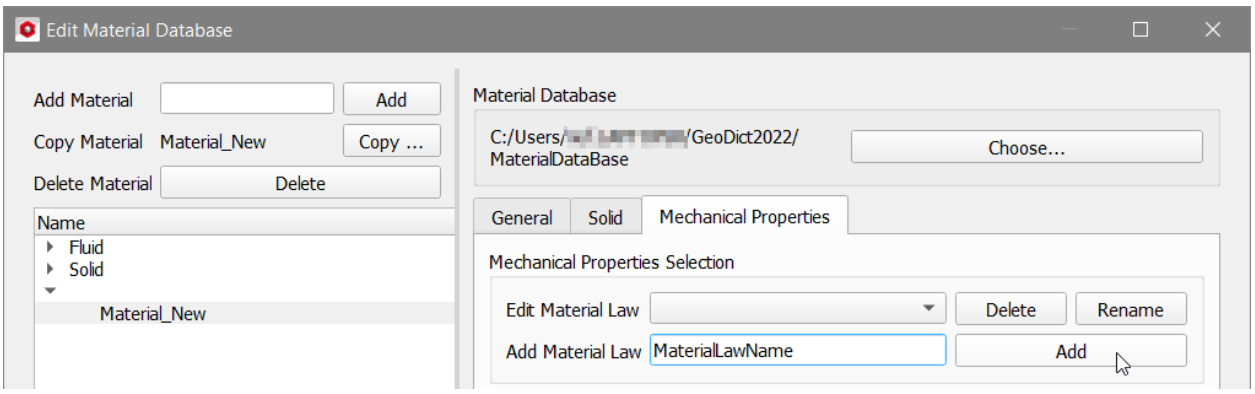
Then, either create a new material by entering a material name and clicking the **Add** button (as shown below), or open one of the materials in the database and add a material law to it.



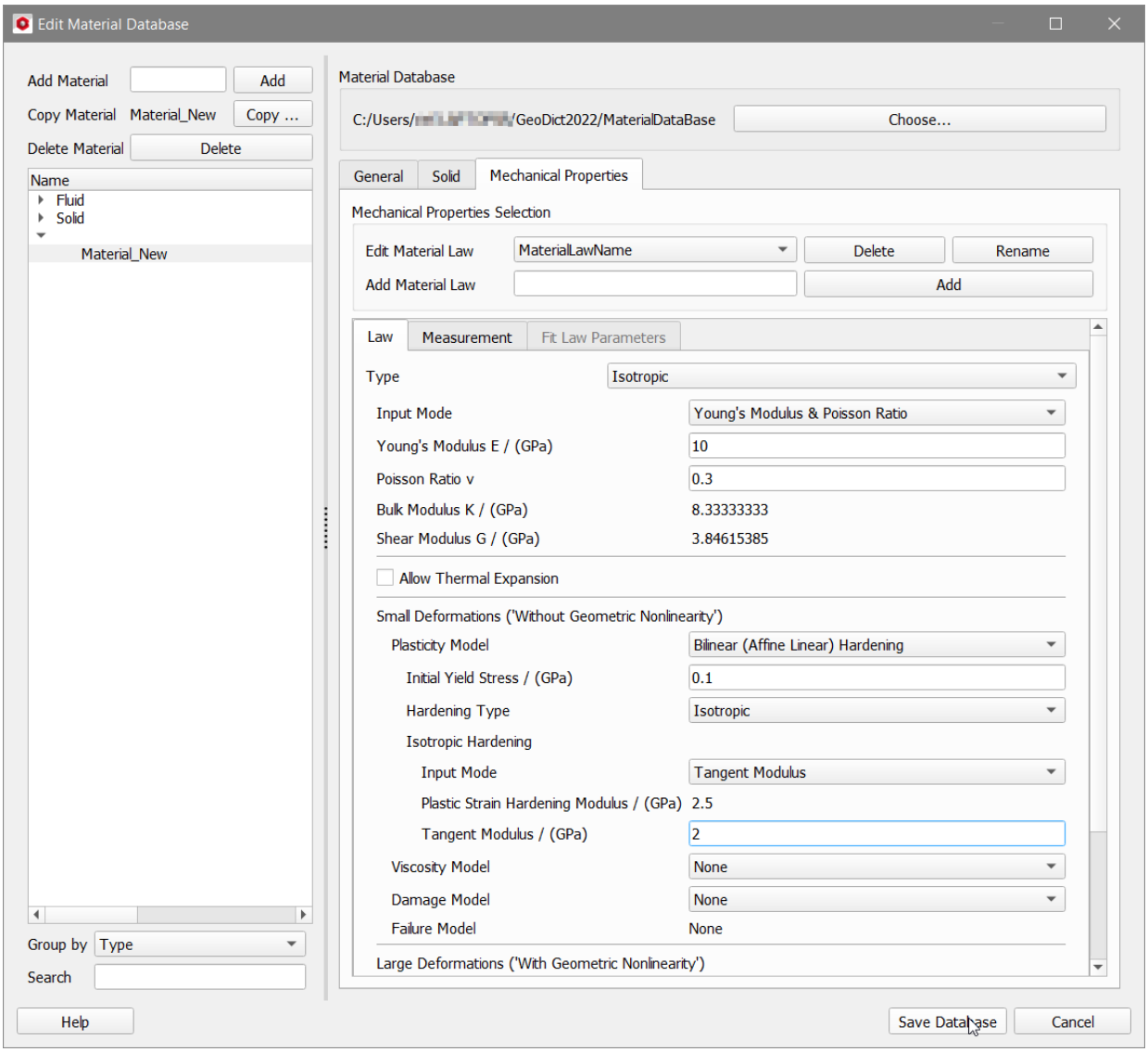
When creating a new material, make sure that the **Mechanical Properties** are activated under the **General** tab:



Switch to the **Mechanical Properties** tab. Here, existing material laws can be edited, or new material laws can be added. In the figure below, it is shown how to add a new material law: Enter the material law name in the field **Add Material Law** and click the **Add** button.



Then, the material parameters can be defined after selecting the material law. In the figure below, it is shown how to set up a material with Bilinear Hardening. Other material laws can be defined by selecting the corresponding fields in the interface. After all material parameters are defined, make sure to save the database with the **Save Database** button in the lower right corner.



Material Fitting for the internal material laws

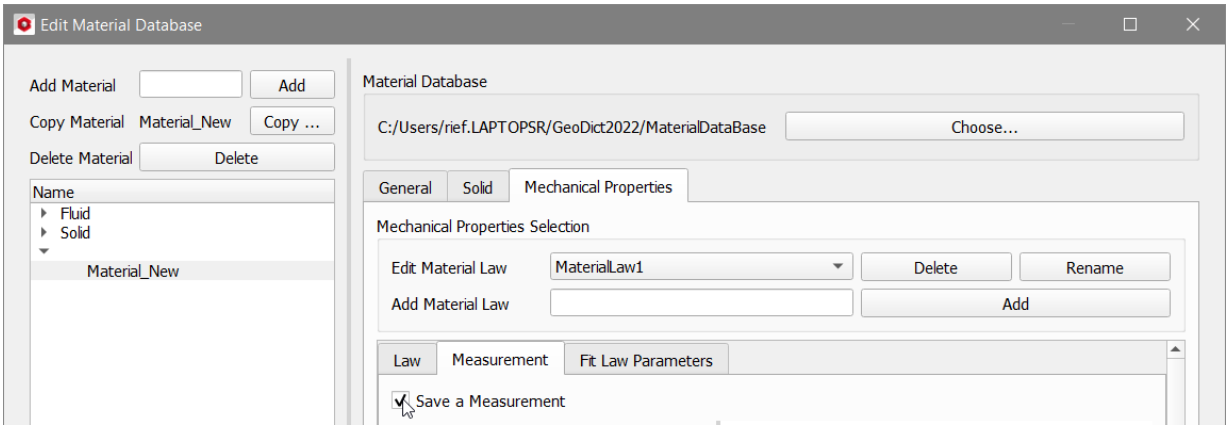
For nonlinear materials, finding the material parameters might be complicated. If measurement data for a given material is available, this data can be used to estimate the material parameters.

Material fitting is available for **Perfect Plasticity**, **Bilinear Hardening**, **Exponential Hardening** and both **Damage** models. For the material fitting, currently no combined material models are available.

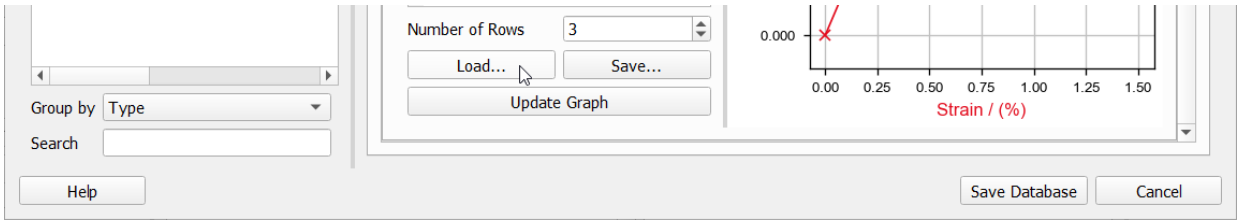
In GeoDict 2022, the material fitting routines are much faster than in previous versions. Now, the fitting relies on analytic formulas instead of repeated simulations – therefore the fitting finishes in several seconds instead of minutes as before.

Measurement

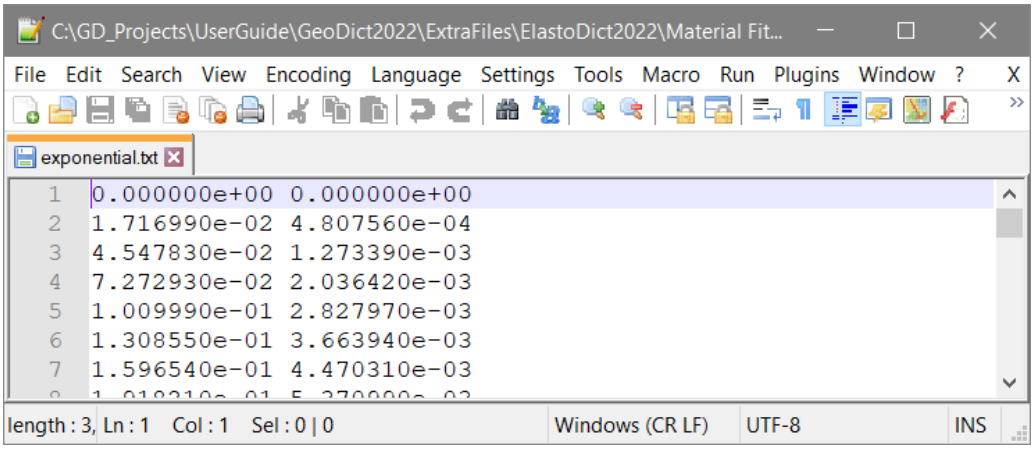
To fit a material law, a measurement must be loaded for the material. For this, check **Save a Measurement** under the **Measurement** tab of the current material law.



Material data can be loaded from a *.txt file with the **Load...** button.

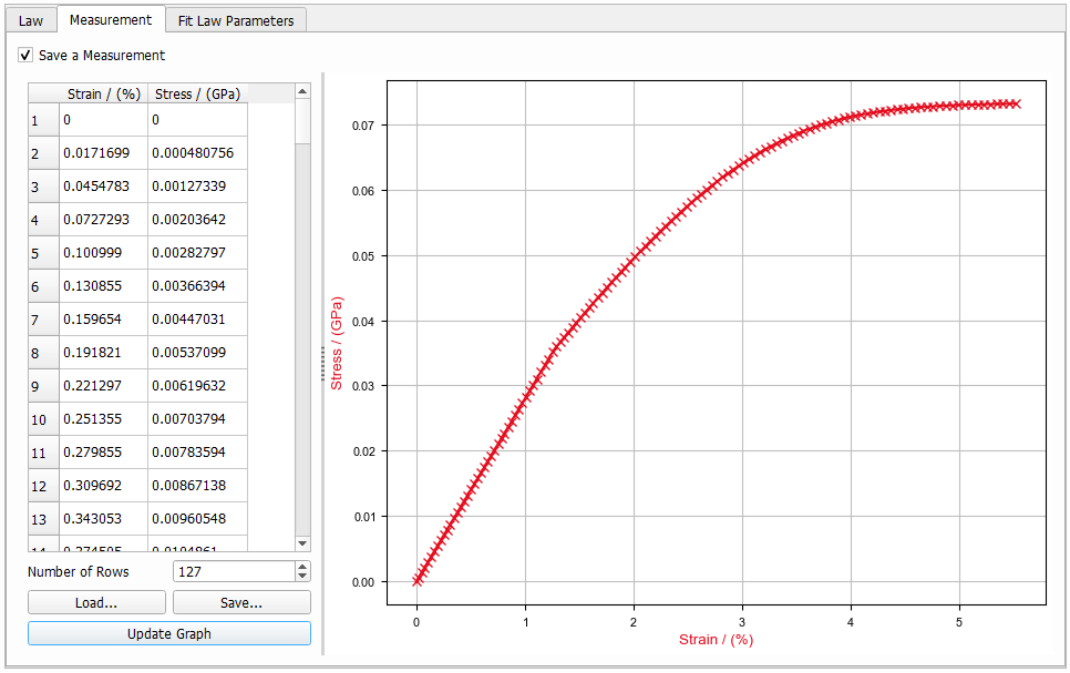


The data must be formatted in two columns, the first column represents the strain values in percent, and the second row contains the corresponding stress values in GPa. Both columns must be separated by spaces.



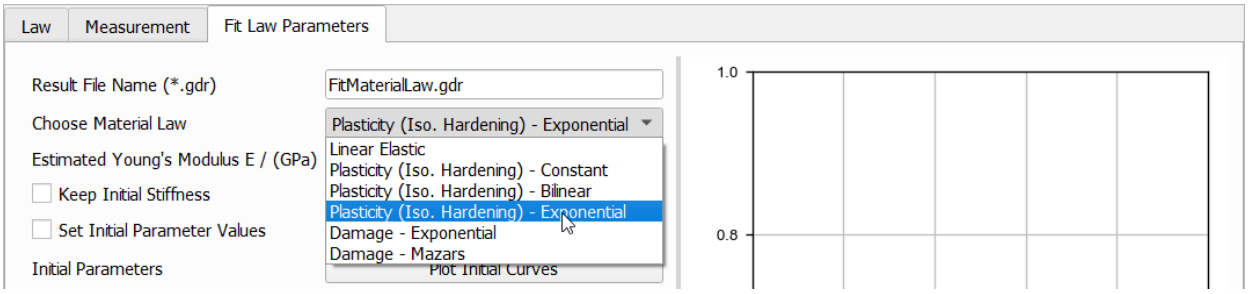
Alternatively, data can also be entered by copy-and-paste or manually.

To plot the data, click the **Update Graph** button.

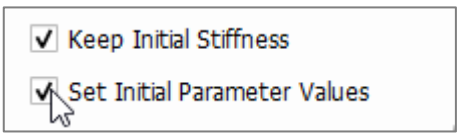


Fit Law Parameters

For fitting the material law, select the Fit Law Parameters tab under the current material law. Choose a material law from the pulldown menu:



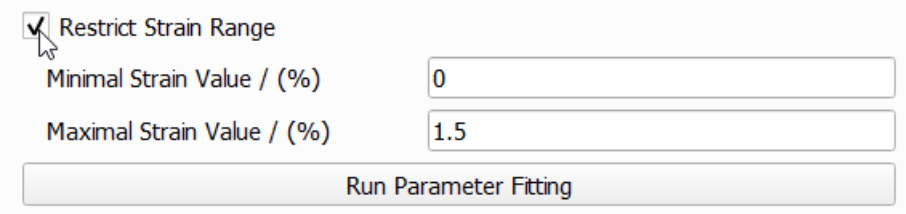
The result might be dependent on the start values for the fitting process. For this, the initial values can be user defined by checking **Set Initial Parameters**.

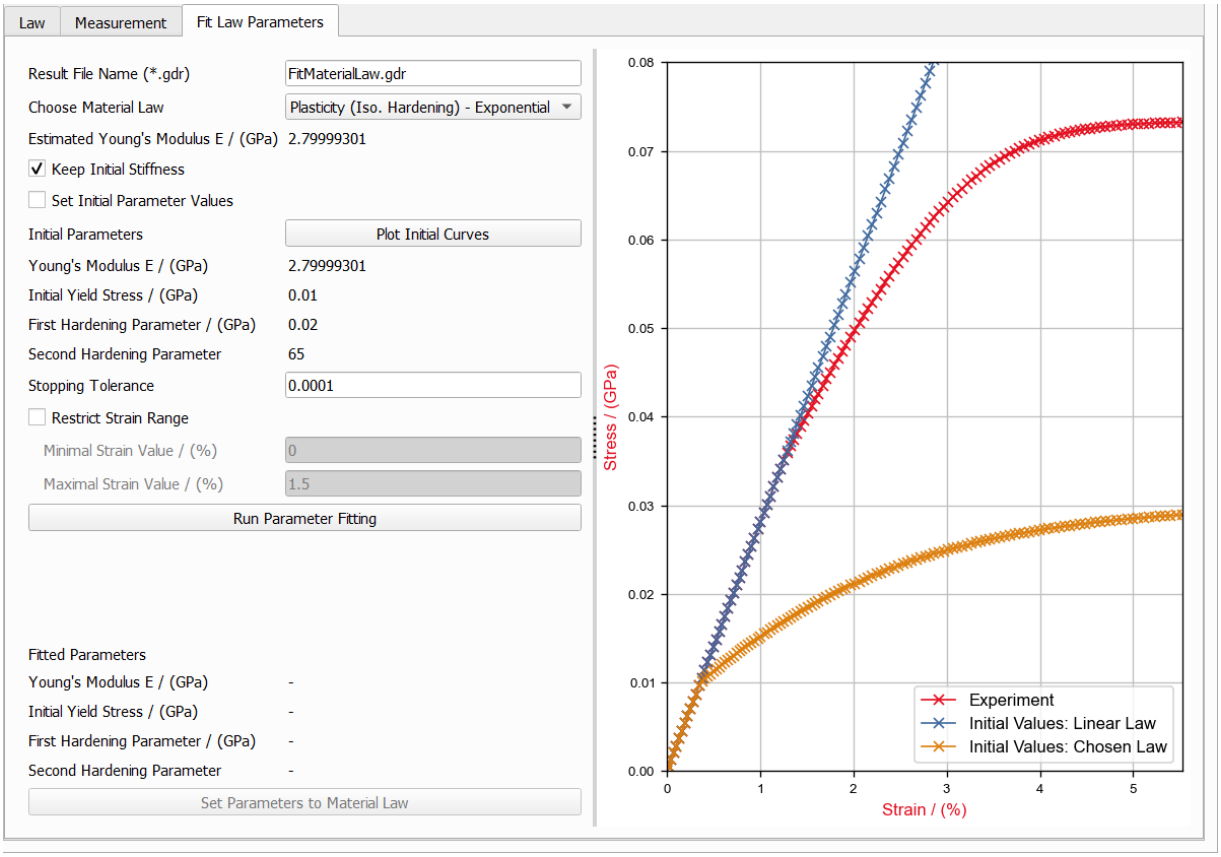


The quality of the initial values can be checked with **Plot Initial Curves**. It is recommended to try several combinations of initial values to find good start parameters for the material fitting algorithm. To edit the plot settings, right-click on the plot and choose **Edit Axis Settings**.

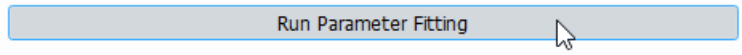
Restrict Strain Range

If only a part of the measurement data should be used for fitting the material laws, a strain range can be selected with **Restrict Strain Range**. This is especially useful if a part of the data contains effects which are not simulated by the selected material law, e.g., damage effects when fitting a material law for plasticity.

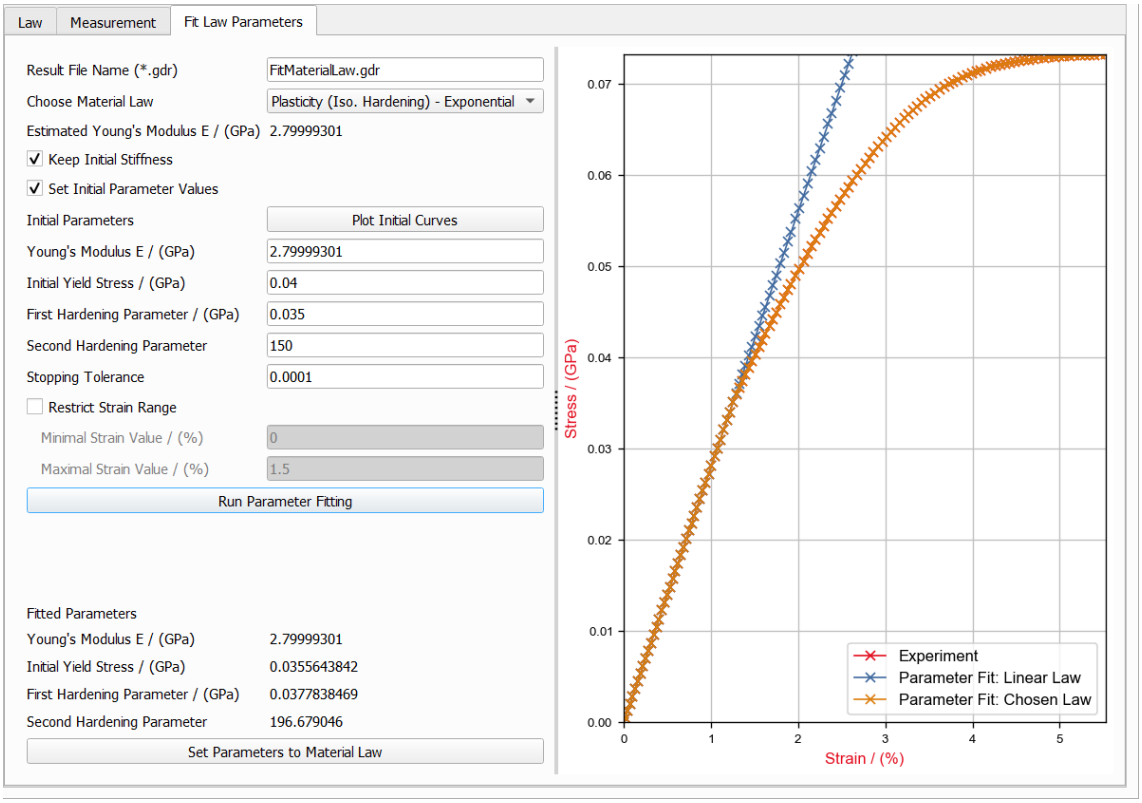


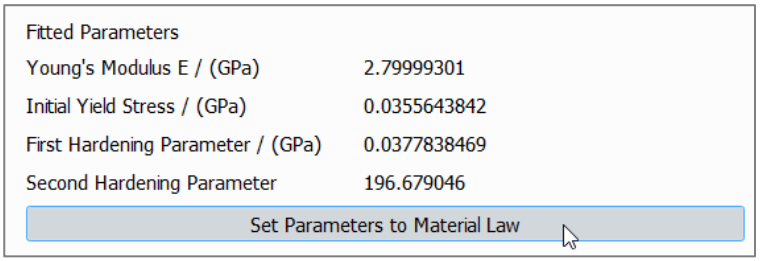


If the initial values are reasonable, the parameter fitting can be started with **Run Parameter Fitting**:

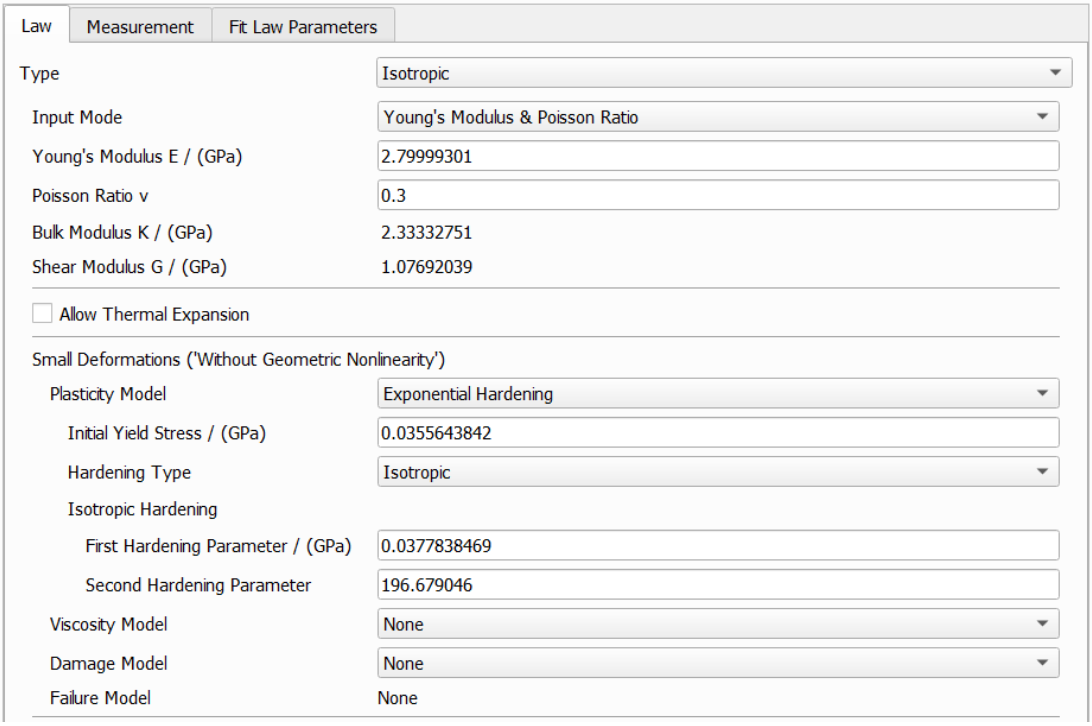


The fitting process will finish in several seconds, and the results are directly shown in the **Fitted Parameters** section and in the plot.

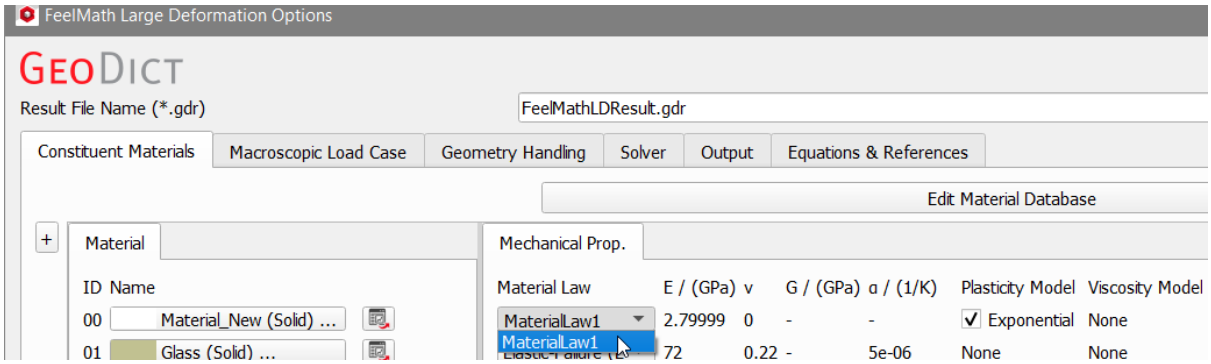




With the button **Set Parameters to Material Law**, the fitted parameters are copied to the material law under the **Law** tab.



Finally, save the changes to the material database with the **Save Database** button. Now, the new material law is saved and can be used in ElastoDict.



Select the material law (here Material Law1), and make sure that the nonlinear material model is enabled (here: Exponential under **Plasticity Model**).

USING UMATS FOR CUSTOM MATERIAL LAWS

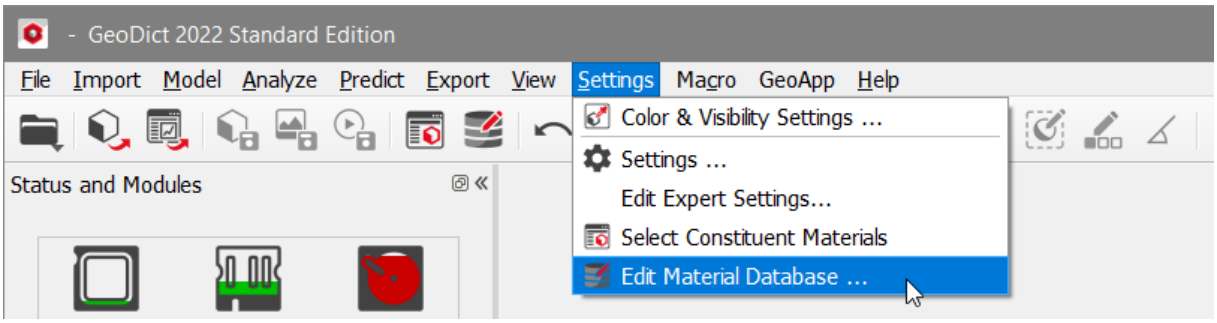
With the UMAT interface in GeoDict, the user can program his/her own user-defined material laws.

UMATs are a concept from the FEA software Abaqus, and the interface is compatible. This means that you can directly use your already existing user materials in GeoDict. If you want to get familiar with the syntax, some UMAT files are delivered with GeoDict (check page 89 for further information). UMATs are Fortran files, and GeoDict (*.f or *.f90), and it is also possible to directly use the compiled files (*.so). Nevertheless, *.so files from GeoDict 2020 and before cannot be used in GeoDict 2021 and later, since the required compiler version changed. Additionally, they might me incompatible between different computers. Therefore, it is important to always keep the source files (*.f or *.f90).

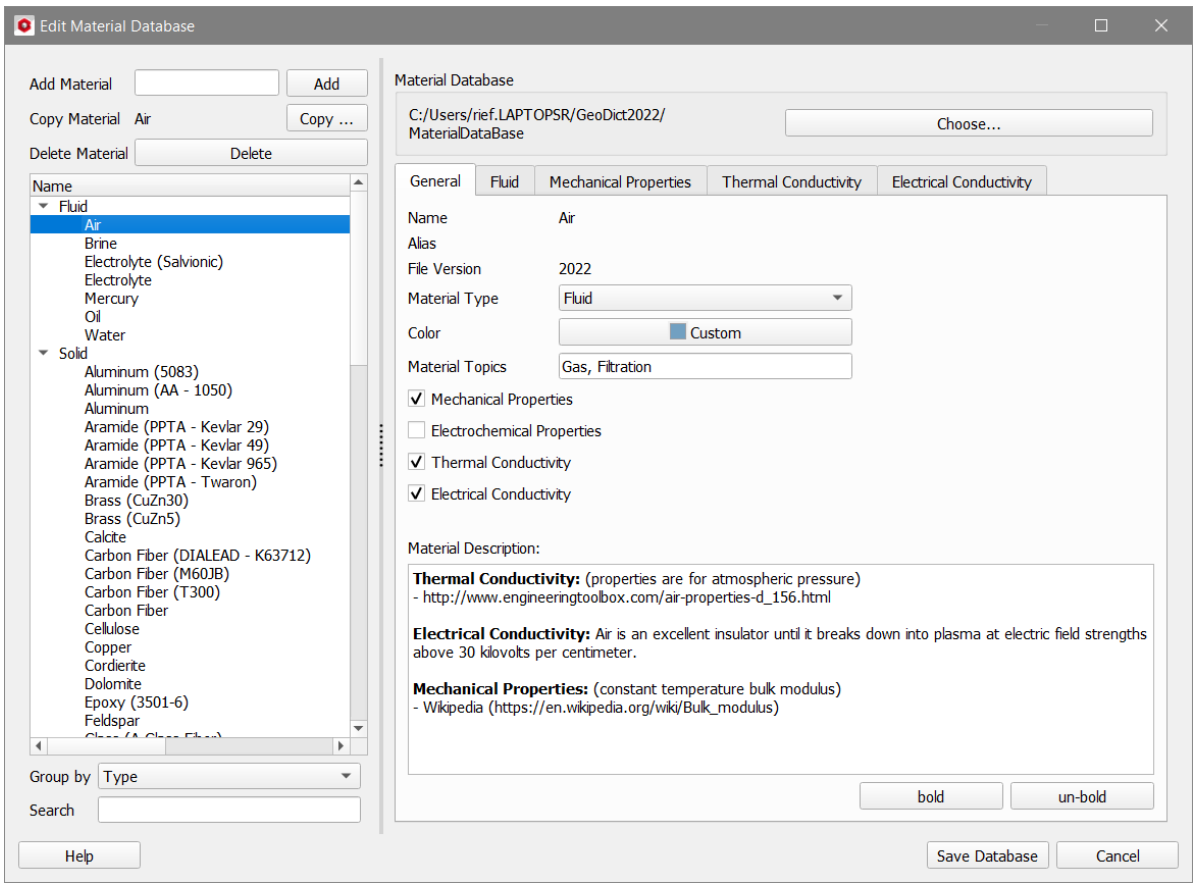
Nevertheless, if a material can be defined by using the internal material laws (See page 92), then we recommend using those instead of UMATs, since they are deeper integrated into GeoDict and easier to set up.

This section explains how to set up a material law using an UMAT in the GeoDict Material database.

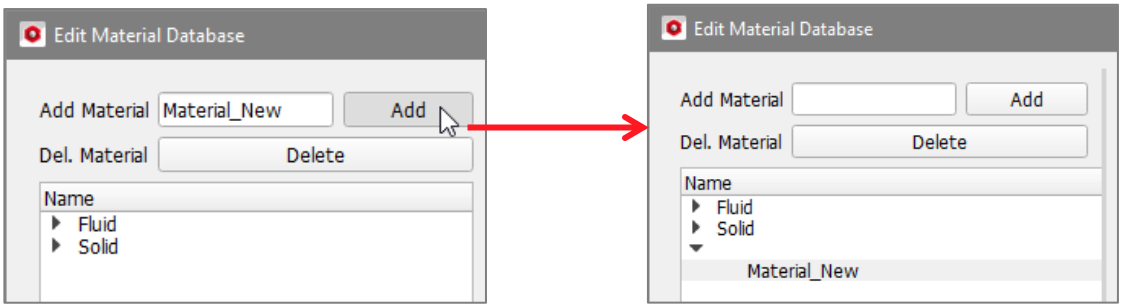
In the menu bar, go to **Settings** and select **Edit Material Data Base...** to access the GeoDict Material Database and add a new material to it.



After clicking **Edit Material Data Base...**, the Material Database dialog opens:



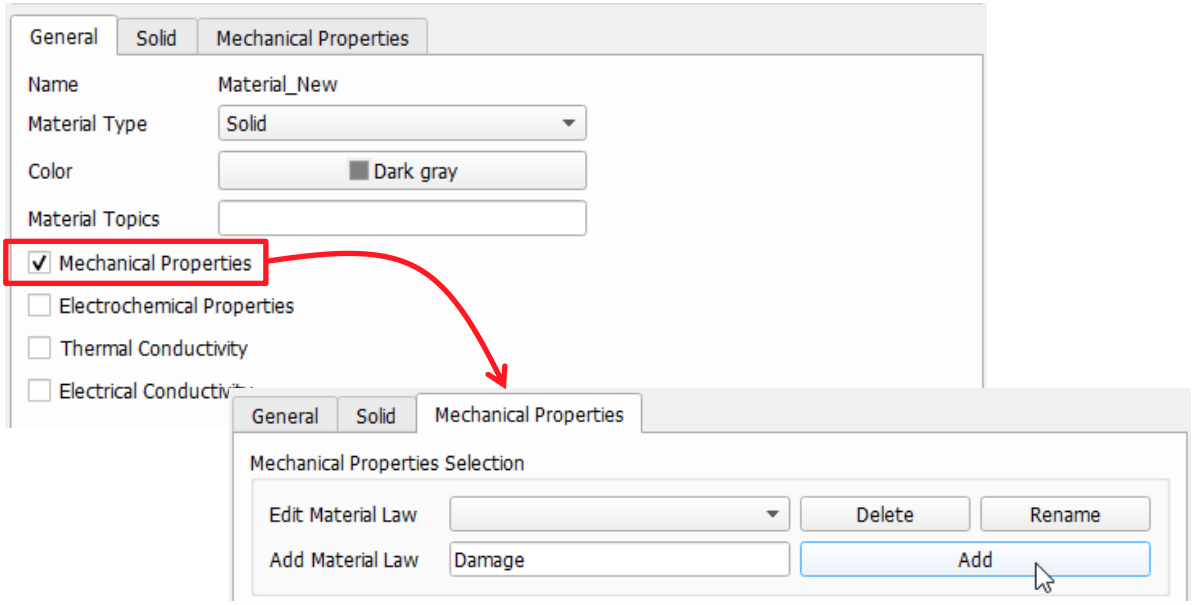
Through the upper left corner, a new material can be added to the database (or a material present in the database can be deleted). To do so, enter a name for the new material (e.g., **Material_New**) and click **Add**.



Material_New appears listed in the left panel and default values appear in the right panel.

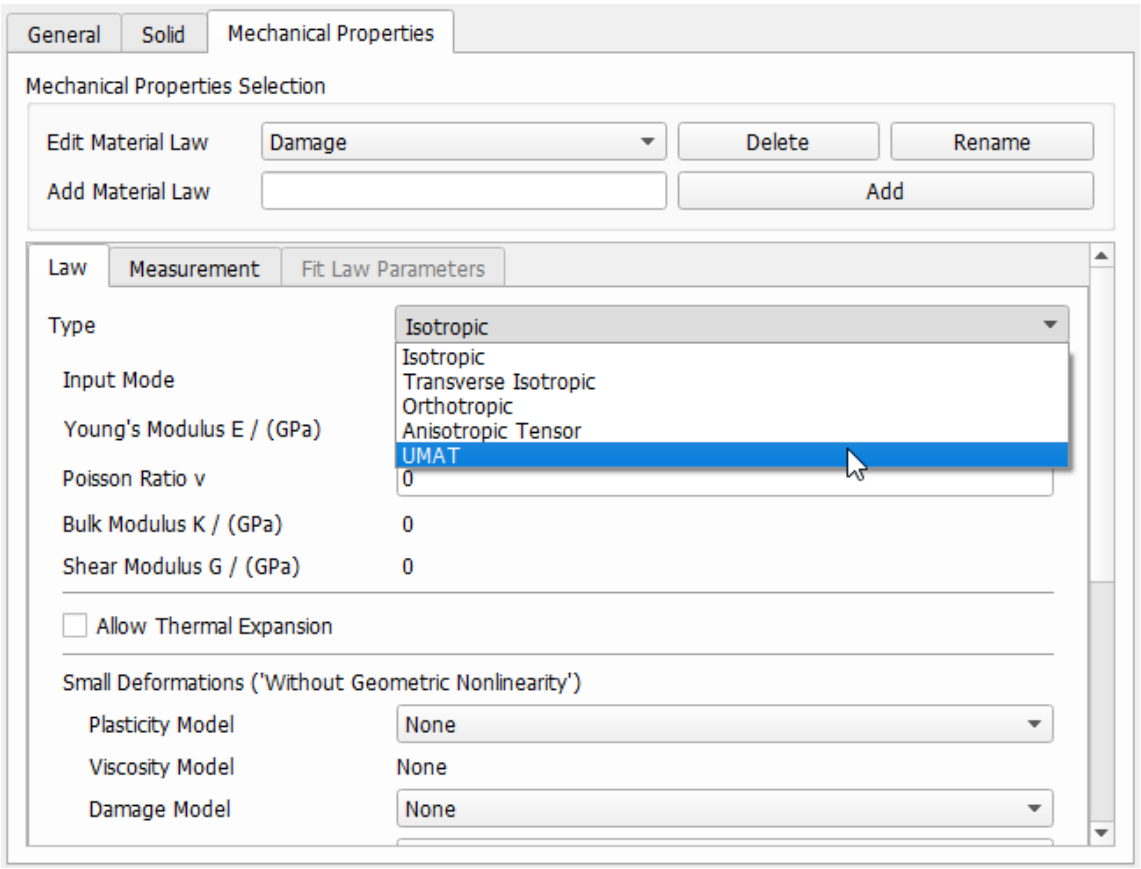
Under the **General** tab, check **Mechanical Properties** to define those for **Material_New**.

Under the newly appearing **Mechanical** tab, inside the **Mechanical Properties Selection** panel, enter **Damage** in the **Add Material Law** box, and click **Add**.



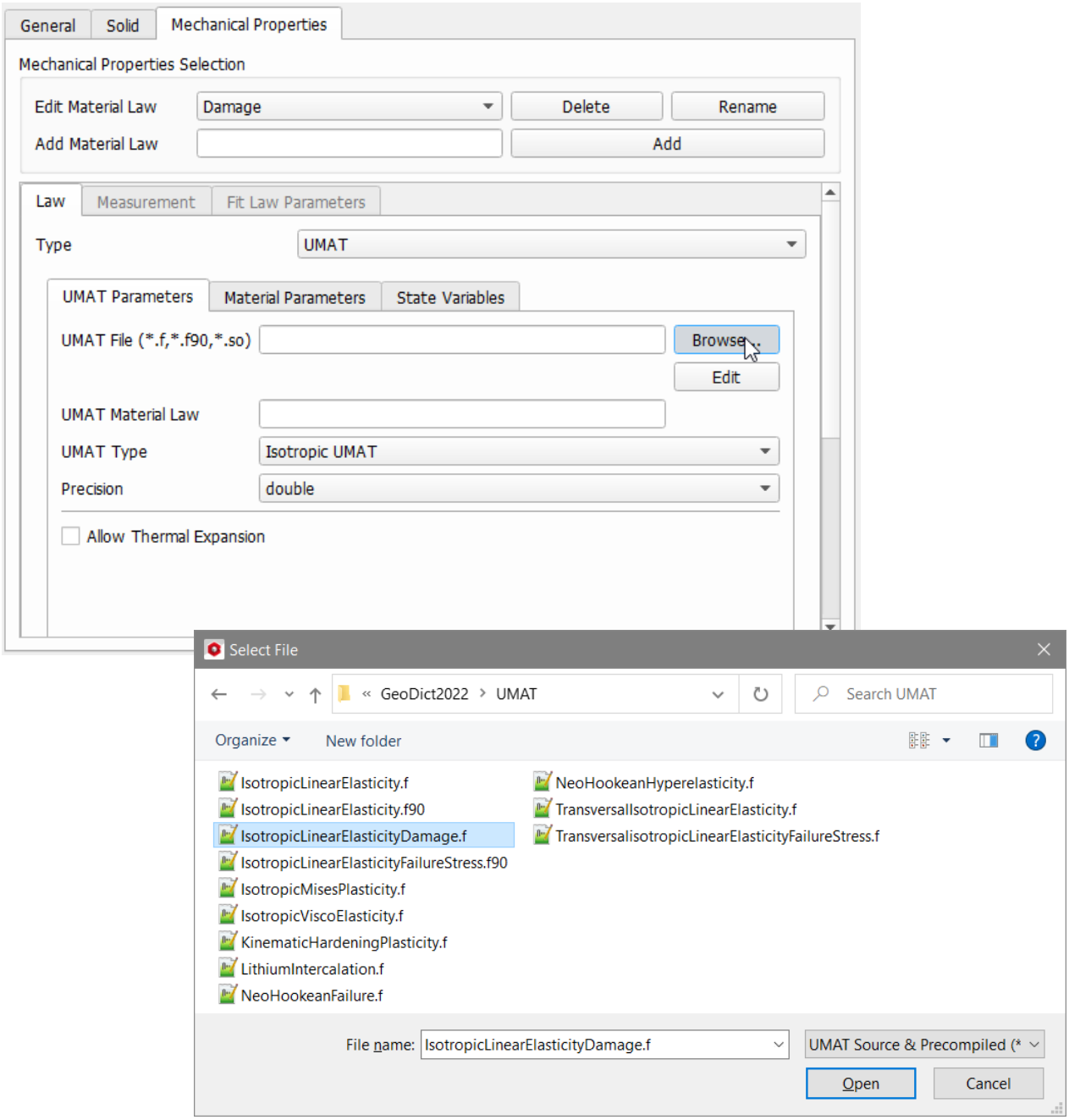
The parameters needed to define the mechanical properties of the new material, appear under the panel grouped under the **Law** tab.

From the **Type** pull-down menu, select **UMAT**.

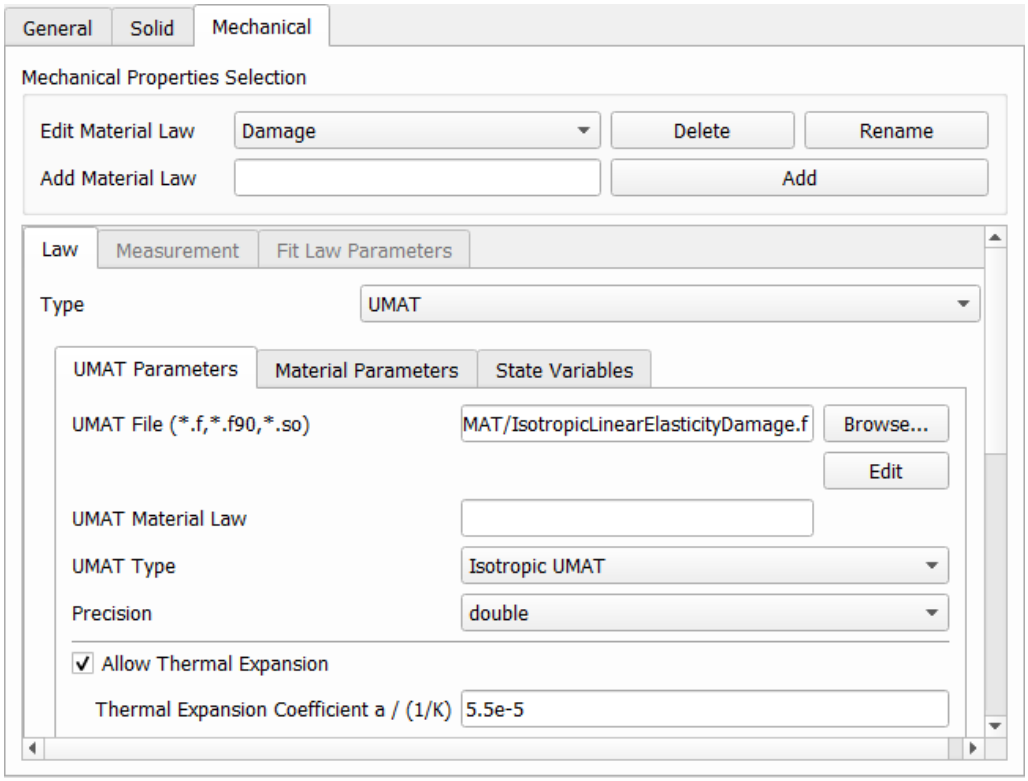


After selecting **UMAT**, a different panel opens below the **Type** pull-down menu, with the **UMAT Parameters**, **Material Parameters**, and **State Variables** tabs.

Under the UMAT Parameters tab, click **Browse** to find the UMATs for GeoDict 2022 in your user folder. UMATs are written in FORTRAN. Select the file `IsotropicLinearElasticityDamage.f` UMAT and click **Open**.

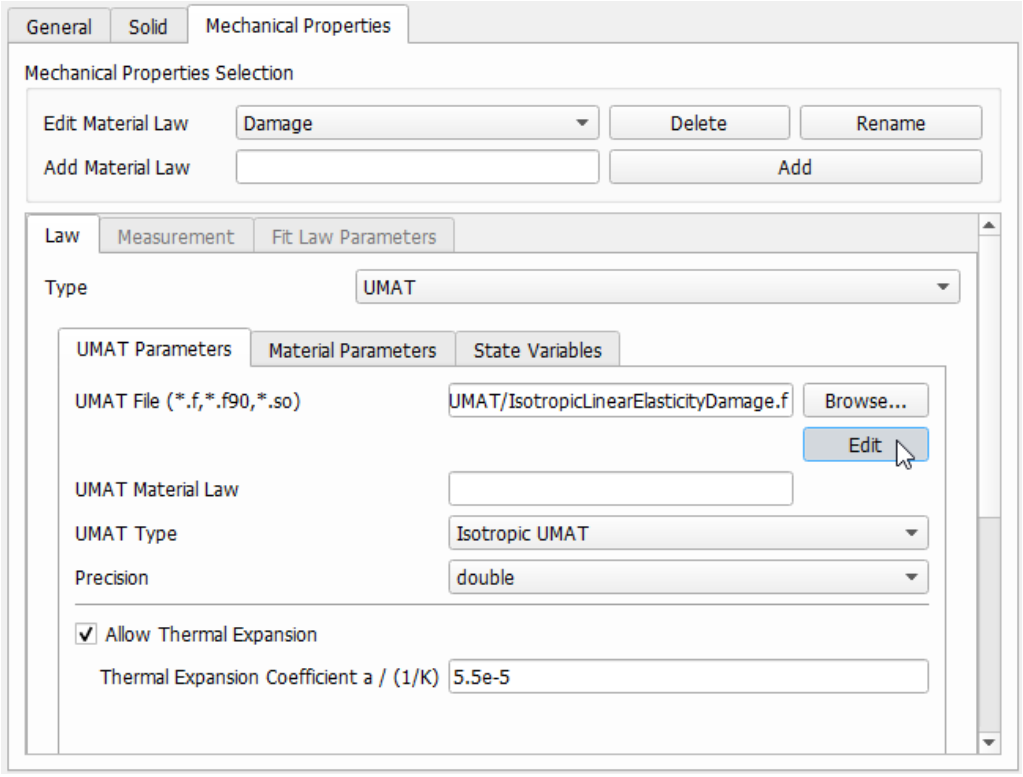


Alternatively, enter a path to the UMAT file relative to the user folder. For this example, this path would be *UMAT/IsotropicLinearElasticityDamage.f*. Relative paths have the advantage that they work independently from your username. Therefore, material database entries can be shared easily between different PCs, as long as the UMAT file is present in the UMAT folder.



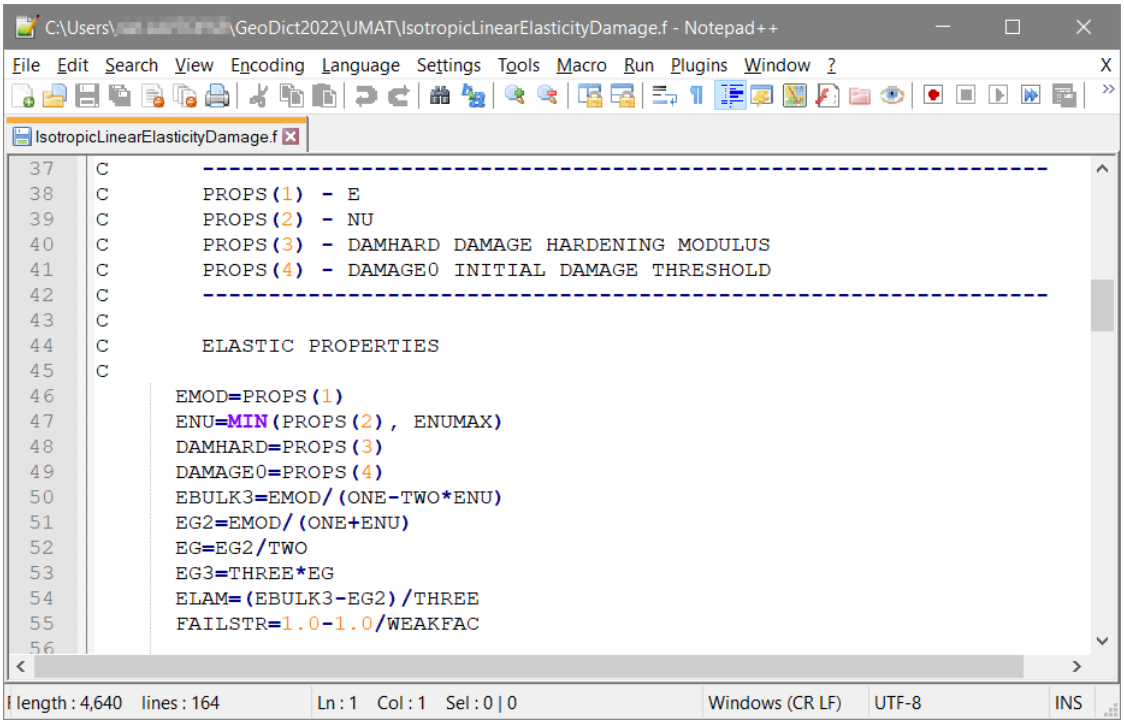
For the material law (defined in the UMAT) to be applied to the **Material_New**, some material parameters must be entered under the **Material Parameters** tab.

These material parameters, that the particular UMAT requires, can be found by opening the UMAT source file, if available (*.f or *.f90). To do so, simply click **Edit** under the **UMAT Parameters** tab and open it with a text editor (for example, with NotePad++).

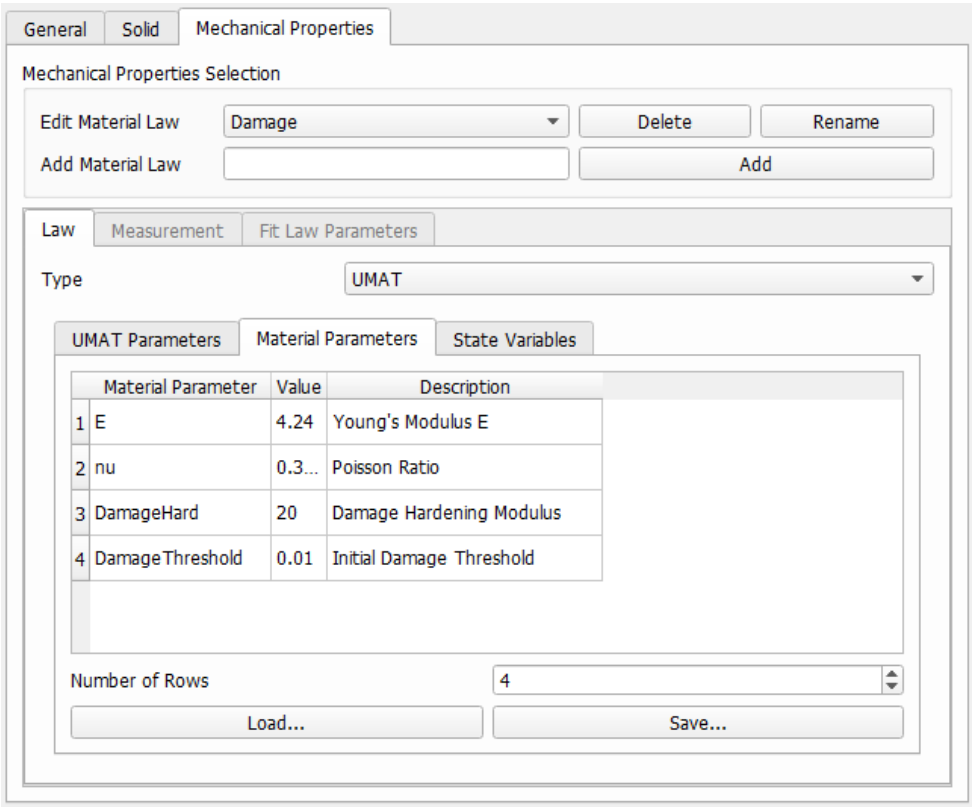


In the opened file, the text shows that applying the *IsotropicLinearElasticityDamage.f* UMAT to **Material_New** requires assigning the following material parameters or properties (PROPS):

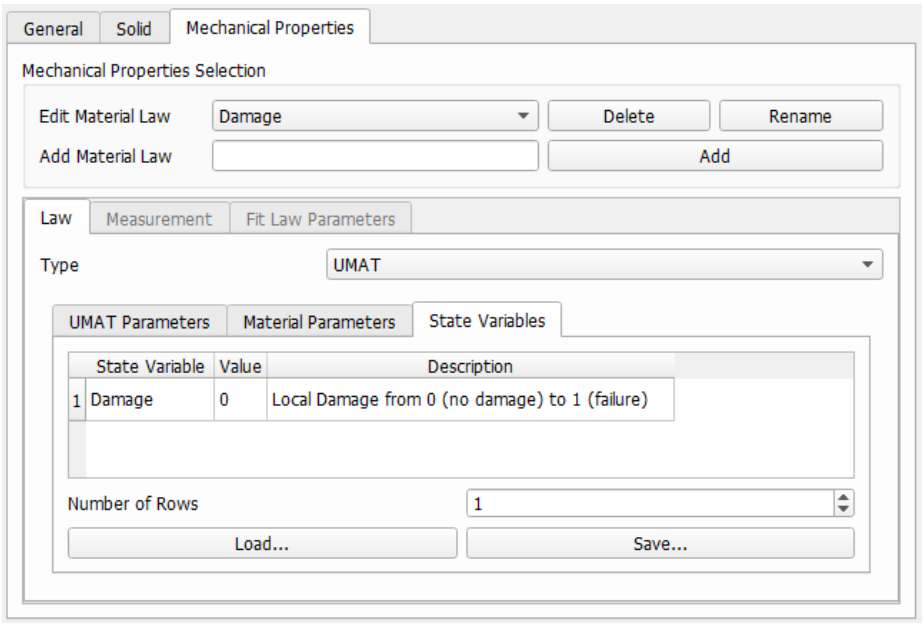
- Young's Modulus (E)
- Poisson's Ratio (NU)
- Damage Hardening Modulus (DAMHARD)
- Initial Damage Threshold (DAMAGE0).



Therefore, in the table under the **Material Parameters** tab, manually enter the needed parameters (Material Parameters), their values for **Material_New** (Value), and a brief parameter explanation (Description). For example, as follows:



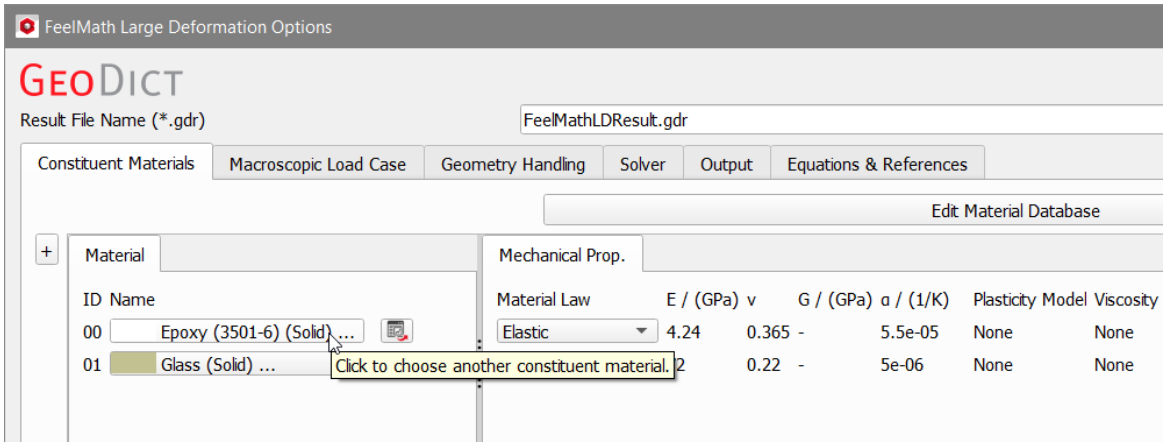
Next, go to the **State Variables** tab. State variables are internal variables of the UMAT, they store information which is used in the next iteration. When the State Variables are not properly defined, the UMAT does not work as intended, or it doesn't work at all.

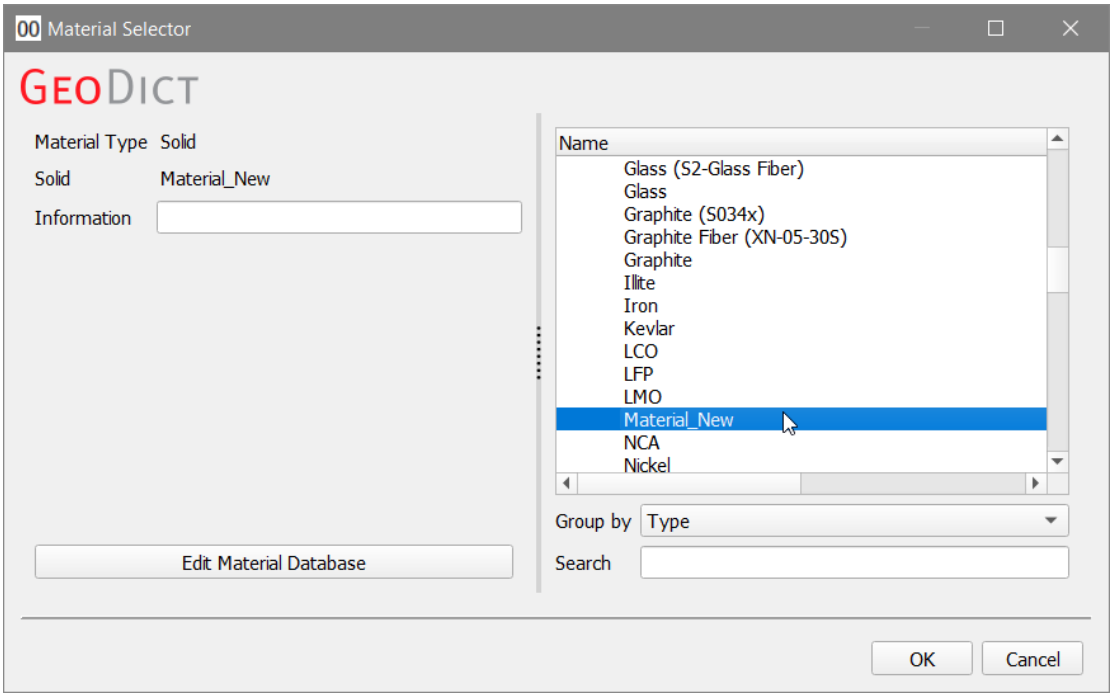


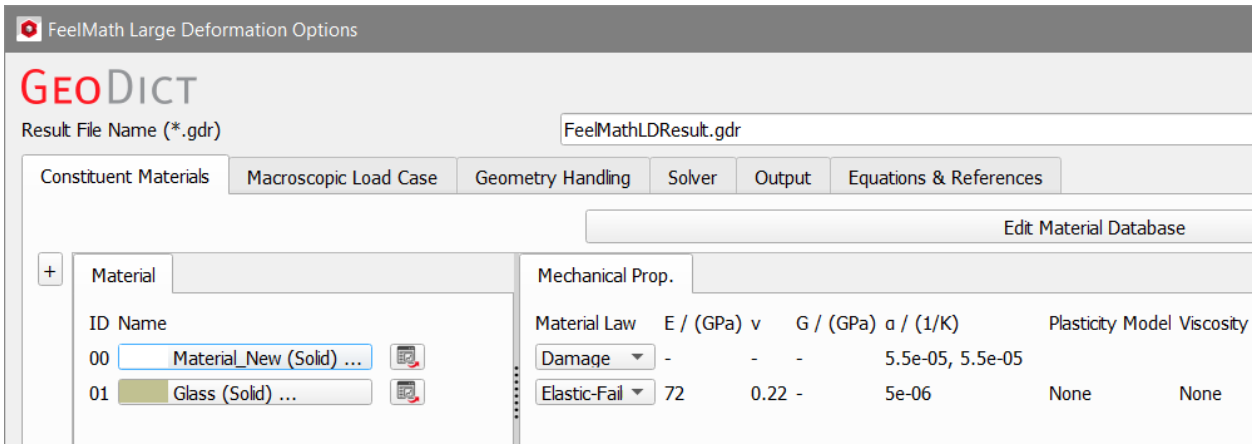
For the UMAT `IsotropicLinearElasticityDamage.f`, there is only one state variable which stores the damage value. It must be defined and initialized with 0, since there is no initial damage in the material. The number of state variables depends on the particular UMAT and is not always easy to find out. If you need more information about UMATs delivered with GeoDict, ask the GeoDict support for help.

Finally, click **Save Database** at the bottom right of the **Edit Material Data-Base** dialog.

After saving, the newly defined material **Material_New** can be chosen as constituent material when using ElastoDict.







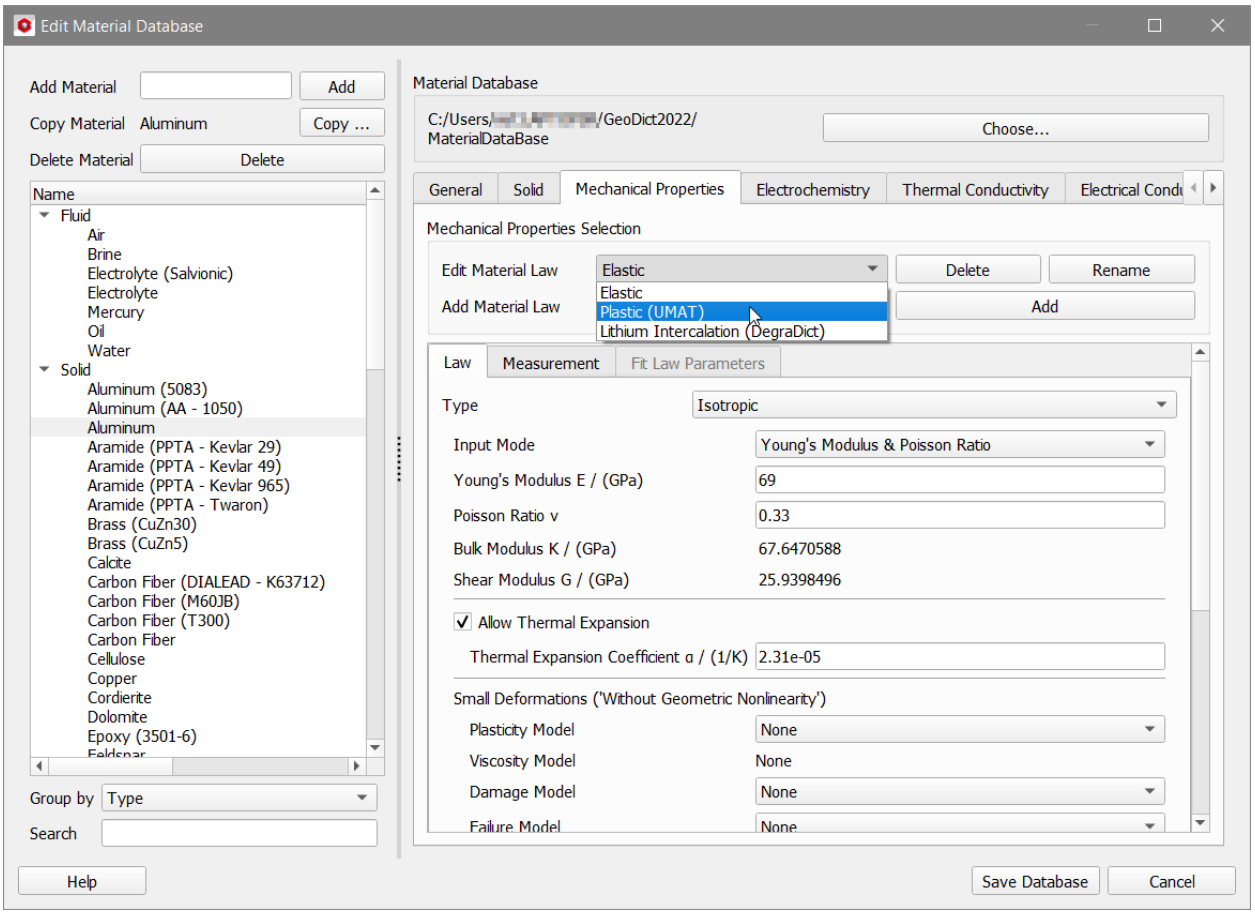
Make sure that the **Damage** material model is selected under Mechanical Properties tab. Now, the material law assigned to **Material_New** is applied in the ElastoDict calculations.

EXAMPLE: PLASTIC DEFORMATION WITH A UMAT

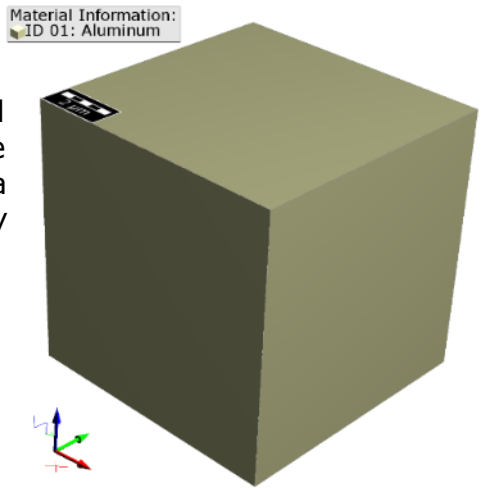
In this example, another UMAT included with GeoDict is used to simulate plastic deformation.

In the GeoDict Material Database, the UMAT *IsotropicMisesPlasticity.f* is contained in the database entry for **Aluminum** and appropriate parameters are already defined when choosing **Plastic (UMAT)** and **Type - UMAT** under the **Law** tab.

Besides the linear parameters (Young's Modulus, E; Poisson Ratio, ν), it includes a piecewise linear hardening curve that was entered beforehand under the **Mechanical Properties – Law - Material Parameters** tab.

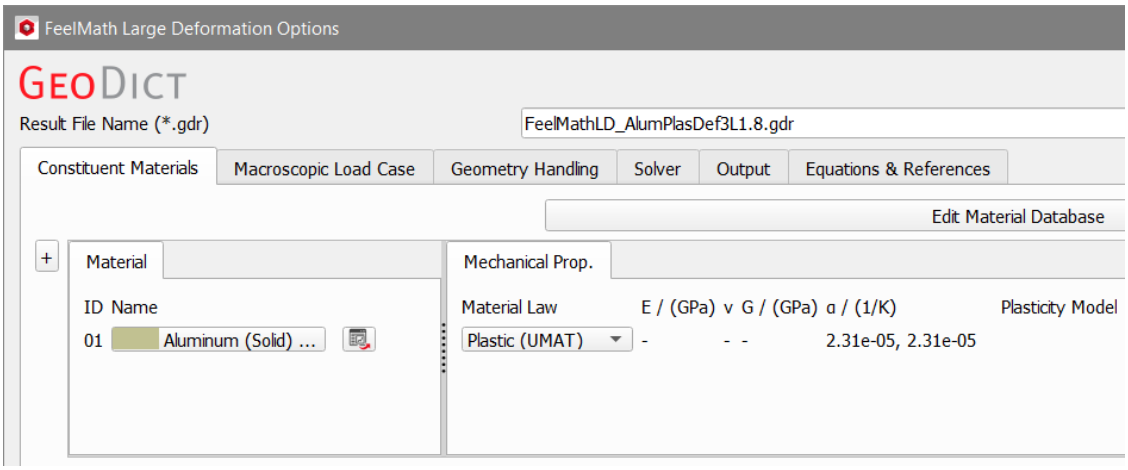


The plastic deformation of aluminum can be simulated in GeoDict using a solid block (generated through **Model** → **ProcessGeo** → **Create Empty Domain**, 1x1x1 voxels, and then, **Model** → **ProcessGeo** → **Invert**).

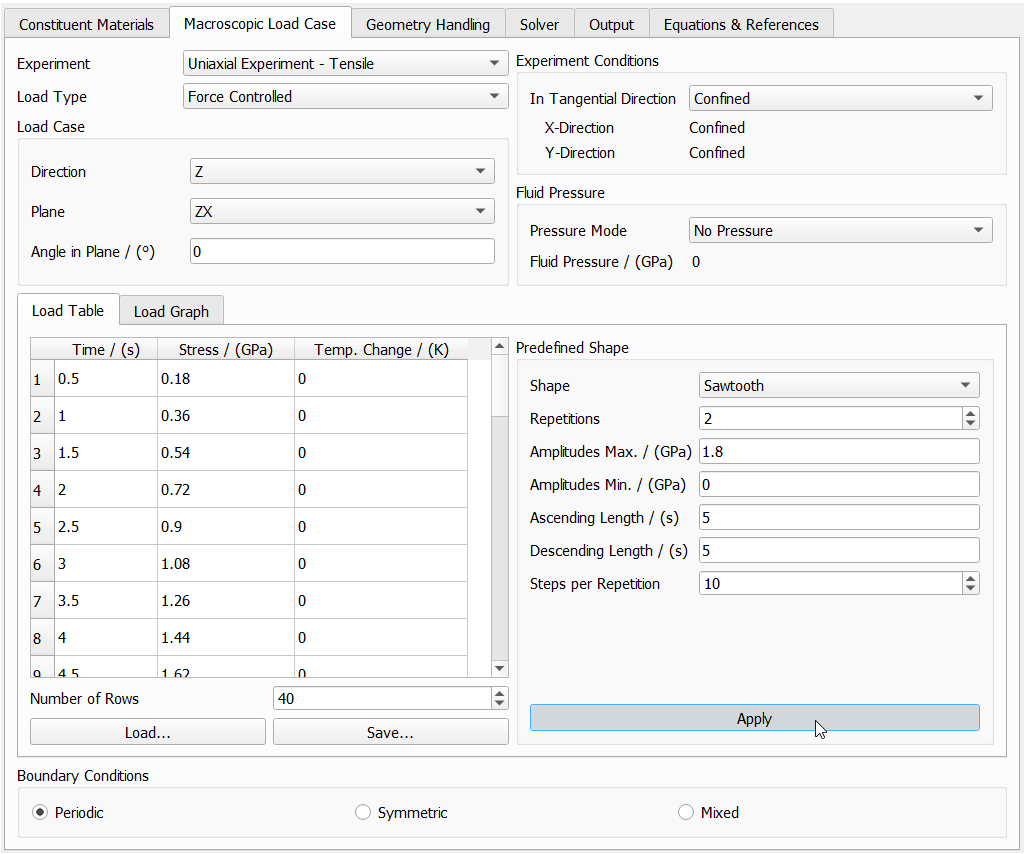


Generally, it is recommended to check the material behavior on small structures. If only a single constituent material must be investigated, a structure consisting of a single voxel is already enough.

In the menu bar, select **Settings** → **Select Constituent Materials**. Click the button for the solid block's material and, in the Material Selector dialog, select **Aluminum** from the list of available (Solid) constituent materials. The color of the constituent material (Aluminum) may be changed via **Settings** → **Color & Visibility Settings**.

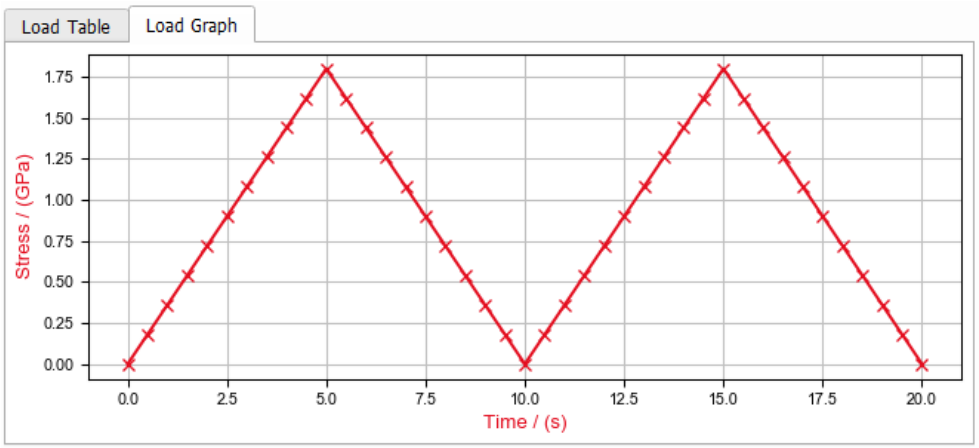


The plastic deformation can be examined during a cyclic stress experiment which can be set up in ElastoDict. In the menu bar, select **Predict** → **ElastoDict**. In the **ElastoDict** section, select **Deformations (FeelMath-LD)** and click the **Edit...** button. In the options dialog, choose to apply the load in Z-direction in a **Uniaxial Experiment-Tensile**, with **Confined** boundary conditions in tangential direction. Choose the **Load Type** as **Force Controlled**.

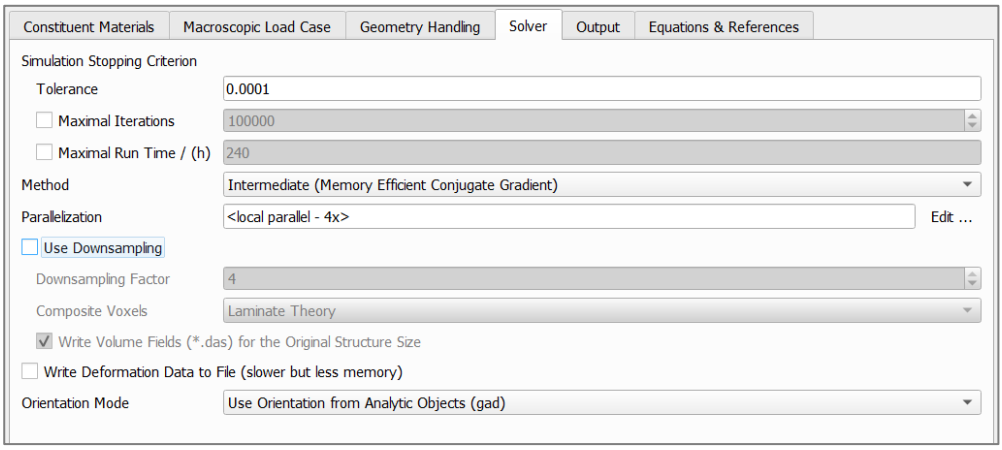


To define a cyclic load, use the **Predefined Shape** option to the right of the **Load Table** (screenshot above). Choose the **Shape** as **Sawtooth** and the settings a shown in the screenshot. By clicking **Apply**, the settings for the predefined shape are applied and the load table is defined automatically.

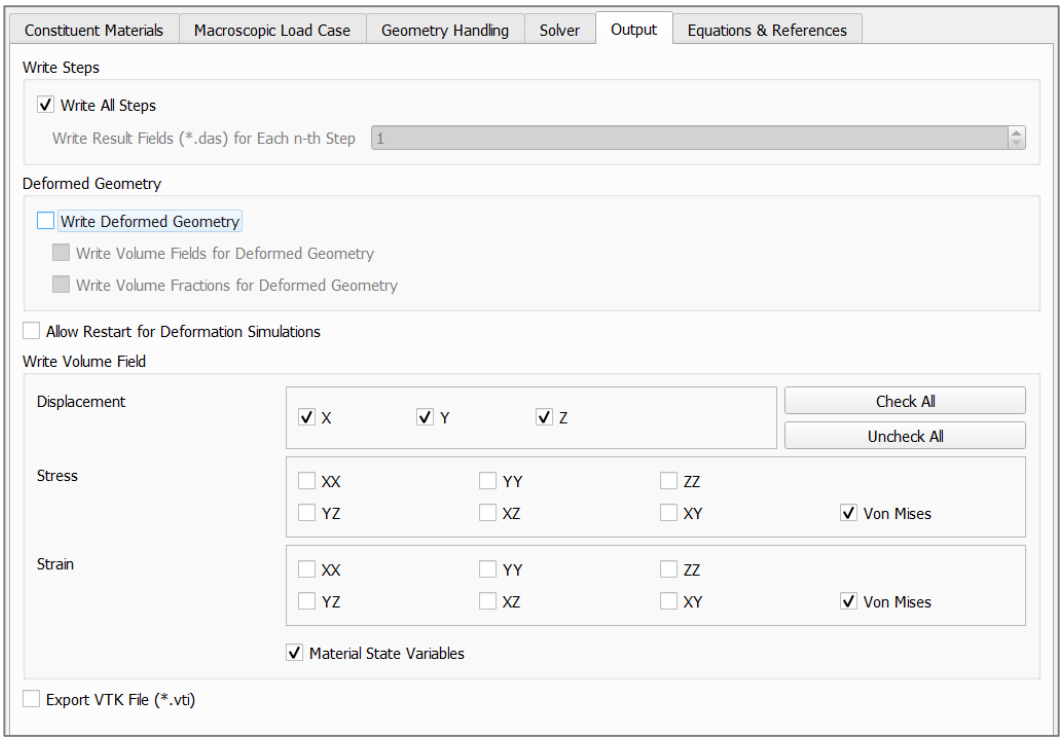
The graph of the load looks as follows:



Keep the default settings under the **Geometry Handling** tab. Under the **Solver** tab, keep the default settings as well: Before GeoDict 2022, it was necessary to select the **Memory Efficient (Neumann Series)** when using nonlinear material laws, but this is no longer necessary.

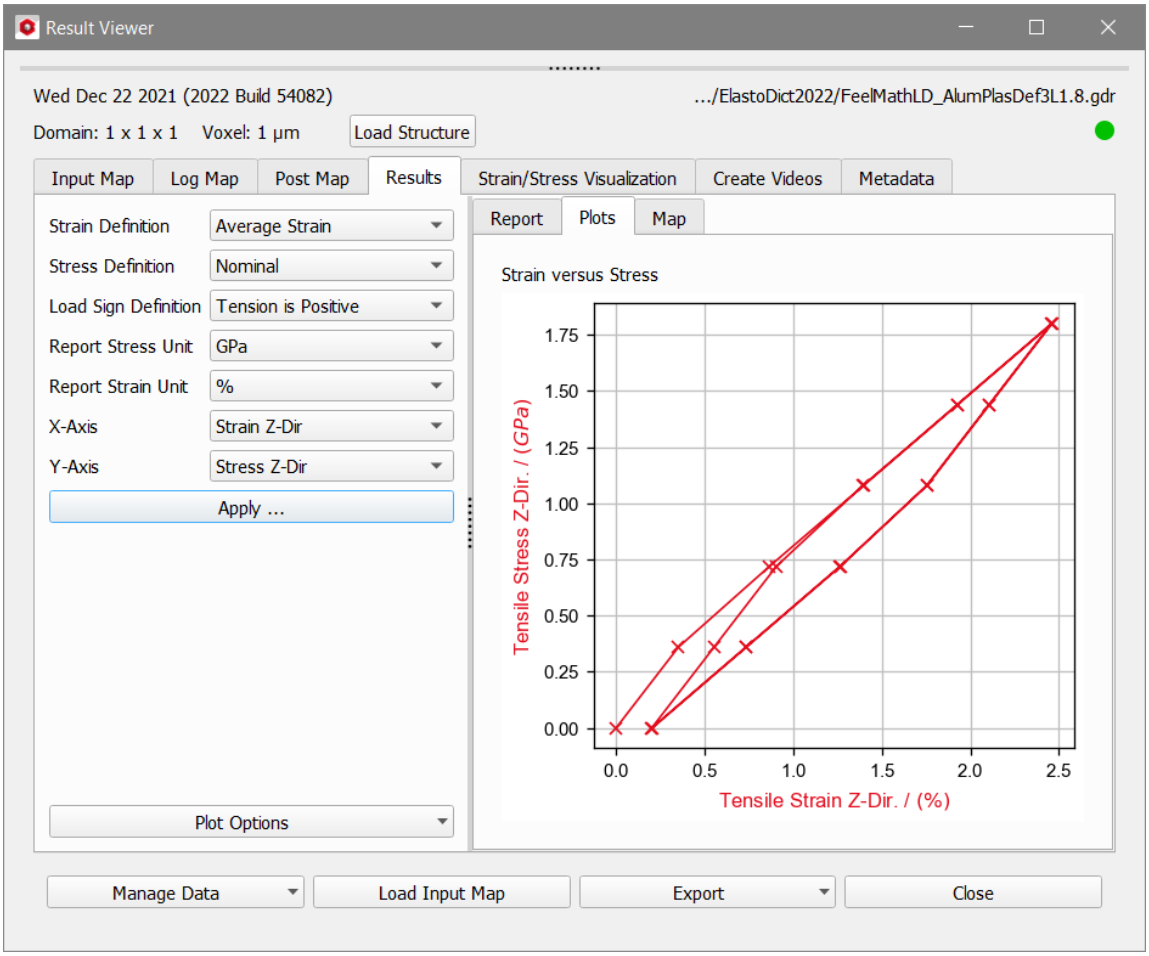


Under the Output tab, deselect **Write Deformed Geometry**. In this example, the simulation is done on a structure with only one voxel, and then the deformed geometry does not provide useful information.



After running the **ElastoDict** - **Deformations (FeelMath-LD)** computations, the Result Viewer of the result file (.gdr) opens at the **Results** tab. Under the **Results - Plots** subtab, choose to plot the Strain in Z-Direction (%) in the X-Axis against the resulting Stress in Z-Direction (GPa) in the Y-Axis, and click **Apply...**.

Observe that the strain does not return to zero after the first load cycle and the plastic deformation remains in the material.



APPENDIX III: ELASTICITY THEORY

A material is said to be elastic if it deforms under external forces (stress), but returns to its original shape when the stress is removed. For small deformations, the stress is roughly proportional to the strain in many solids. The constant of proportionality between stress and strain is given by the **Young's modulus (E)** which is a measure of *stiffness.* This linear relationship between stress and strain is called Hooke's law and is the basis for the *theory of linear elasticity*.

The general relationship (generalized Hooke's law) between multi-axial stress and strain is described by using 2nd order tensors for stress and strain and the 4th order *elasticity tensor* for their relation.

In solid mechanics, the **Young's modulus E** can be experimentally determined from the slope of a stress-strain curve created during tensile tests conducted on a test specimen of the material. Most metals and ceramics are isotropic. i.e., their mechanical properties are the same in all directions.

If e.g., metals are treated in a special way for example by deep drawing, they become anisotropic, so that the **Young's modulus** depends on the direction from which the force is applied. Some materials, which are composites of two or more constituents, such as wood or reinforced concrete, are strongly anisotropic materials and display widely different mechanical properties when load is applied in different directions. For example, they exhibit a higher Young's modulus (stiffness) when loaded parallel to the fibers. This is true under the assumption that the fibers have a higher **Young's modulus** than the surrounding matrix material.

Based on the input parameters, GeoDict solves six load cases or experiments (three compressions in x, y and z, and three shearing experiments) which are sequentially computed by the ElastoDict solver to predict the entries of the 6x6 effective elasticity tensor. Each of these six simulations is done by assigning load case-specific displacements on the boundaries of the structure and calculating the corresponding stresses. By averaging the stresses over the structure, the **Hooke's Law** in the general anisotropic case is obtained,

$$\sigma_{ij} = \sum_{r,s=1}^{3} c_{ijrs}\varepsilon_{rs}\,, \qquad i,j \in \{1,2,3\}$$

where *c* is a symmetric fourth order tensor, called also *elasticity tensor*. Usually, the elasticity tensor and the stresses and strains are written in *Voigt notation* (see https://en.wikipedia.org/wiki/Voigt_notation). This way, the elasticity tensor is reduced to a 6x6 matrix and the stresses and strains are written as 6x1 vectors. This leads to a more compact and readable notation.

Because of these symmetry properties, it is convenient to use the so-called *"reduced suffix notation"* (e.g., Chadwick et. al.) with the following index assignment:

Tensor notation Index ij	11	22	33	23, 32	31, 13	12, 21
denoted also by	*xx*	*yy*	*zz*	*yz*	*zx*	*xy*
Voigt notation index I	1	2	3	4	5	6

Then, taking into account also the symmetry of the elasticity tensor,

$$c_{ijkl} = c_{jikl} = c_{ijlk} = c_{klij}, \qquad i,j,k,l \in \{1,2,3\}$$

The stress tensor σ_{ij} can be written as σ_I in Voigt notation:

$$\sigma = \begin{pmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{31} \\ \sigma_{12} \end{pmatrix}$$

The strain tensor ε_{ij} can be written as ε_I in Voigt notation:

$$\varepsilon = \begin{pmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ \varepsilon_{23} \\ \varepsilon_{31} \\ \varepsilon_{12} \end{pmatrix}$$

With the Voigt notation, the symmetric fourth order elasticity tensor c_{ijkl} can be reduced to a symmetric matrix C_{IJ} with the following entries (coefficients):

$C_{11}=c_{1111}=c_{xxxx}$	$C_{12}=c_{1122}=c_{xxyy}$	$C_{13}=c_{1133}=c_{xxzz}$	$C_{14}=c_{1123}=c_{xxyz}$	$C_{15}=c_{1131}=c_{xxzx}$	$C_{16}=c_{1112}=c_{xxxy}$
	$C_{22}=c_{2222}=c_{yyyy}$	$C_{23}=c_{2233}=c_{yyzz}$	$C_{24}=c_{2223}=c_{yyyz}$	$C_{25}=c_{2231}=c_{yyzx}$	$C_{26}=c_{2212}=c_{yyxy}$
		$C_{33}=c_{3333}=c_{zzzz}$	$C_{34}=c_{3323}=c_{zzyz}$	$C_{35}=c_{3331}=c_{zzzx}$	$C_{36}=c_{3312}=c_{zzxy}$
	symmetric		$C_{44}=c_{2323}=c_{yzyz}$	$C_{45}=c_{2331}=c_{yzzx}$	$C_{46}=c_{2312}=c_{yzxy}$
				$C_{55}=c_{3131}=c_{zxzx}$	$C_{56}=c_{3112}=c_{zxxy}$
					$C_{66}=c_{1212}=c_{xyxy}$

Therefore, the generalized Hooke's law can be written as a matrix-vector product:

$$\sigma_I = \sum_{J=1}^{6} C_{IJ}\varepsilon_J, \qquad I = 1,\ldots,6$$

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{pmatrix} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_{xx} \\ \varepsilon_{yy} \\ \varepsilon_{zz} \\ 2\varepsilon_{yz} \\ 2\varepsilon_{xz} \\ 2\varepsilon_{xy} \end{pmatrix}$$

σ: stress tensor *C*: elasticity or stiffness tensor ε: deformation tensor

This elasticity or stiffness tensor describes the most general stress-strain relations for a linear elastic anisotropic solid (e.g., triclinic solid which has no material symmetry, *Nayfeh, A.H. 1995*).

According to Nayfeh, the constitutive relations for the different symmetry classes can be listed as follows:

Symmetry class	Number of parameters to define material	Form of elasticity tensor
Anisotropic (triclinic or general)	21 (C_{11}, C_{12}, C_{13}, C_{14}, C_{15}, C_{16}, C_{22}, C_{23}, C_{24}, C_{25}, C_{26}, C_{33}, C_{34}, C_{35}, C_{36}, C_{44}, C_{45}, C_{46}, C_{55}, C_{56}, C_{66})	$C_{\text{anisotropic}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{pmatrix}$
Monoclinic	13 (C_{11}, C_{12}, C_{13}, C_{16}, C_{22}, C_{23}, C_{26}, C_{33}, C_{36}, C_{44}, C_{45}, C_{55}, C_{56}, C_{66})	$C_{\text{monoclinic}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & C_{16} \\ C_{12} & C_{22} & C_{23} & 0 & 0 & C_{26} \\ C_{13} & C_{23} & C_{33} & 0 & 0 & C_{36} \\ 0 & 0 & 0 & C_{44} & C_{45} & 0 \\ 0 & 0 & 0 & C_{45} & C_{55} & 0 \\ C_{16} & C_{26} & C_{36} & 0 & 0 & C_{66} \end{pmatrix}$
Orthotropic	9 (C_{11}, C_{12}, C_{13}, C_{22}, C_{23}, C_{33}, C_{44}, C_{55}, C_{66})	$C_{\text{orthotropic}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{pmatrix}$
Transversely Isotropic	5 (C_{11}, C_{12}, C_{13}, C_{33}, C_{44})	$C_{\text{transversely isotropic}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{C_{11}-C_{12}}{2} \end{pmatrix}$
Cubic	3 (C_{11}, C_{12}, C_{66})	$C_{\text{cubic}} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{66} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{66} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{pmatrix}$
Isotropic	2 (C_{11}, C_{12})	$C_{\text{isotropic}} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{C_{11}-C_{12}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{C_{11}-C_{12}}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{C_{11}-C_{12}}{2} \end{pmatrix}$

The 6x6 matrix C_{IJ} for the homogeneous material "*nearest*" to the inhomogeneous original material is shown in the ***.gdr** result file after the solver has finished its computations.

When using ElastoDict with linear laws for the constituent materials, it is important to keep in mind that the elasticity solver is working in the range of linear elasticity. To compute large deformations, plastic yield, damage effects, possible crack initiation, crack growth, and other nonlinear effects one has to use nonlinear material laws, which describe the effects under consideration, for the constituent materials. For such cases, the Hooke's law does not hold.

A nonlinear material law can be described by an Abaqus UMAT. GeoDict contains examples for UMATs e.g., for plastic deformation and damage.

References

J.T. Browaeys and S. Chevrot: **Decomposition of the elastic tensor and geophysical applications.** *Geophys. J. Int.* (2004) **159**, pp. 667-678.

P. Chadwick, M Vianello and S.C. Cowin: **A new proof that the number of linear elastic symmetries is eight.** *Journal of Mechanics and Physics of Solids*, **49** (2001), pp. 2471 – 2492.

A.H. Nayfeh: **Wave propagation in layered anisotropic media with applications to composites.** *Elsevier Science, North-Holland series in Applied Mathematics and Mechanics*, Vol. 39, 1995.

V. Rutka and A. Wiegmann: **Explicit Jump Immersed Interface Method for virtual material design of the effective elastic moduli of composite materials.** *Technical Report of the Fraunhofer ITWM,* No. 73 (2005).

V. Rutka, A. Wiegmann, and H. Andrä: **EJIIM for Calculation of effective Elastic Moduli in 3D.** *Technical Report of the Fraunhofer ITWM* No. 93 (2006)

Wikipedia: Hooke's law. https://en.wikipedia.org/wiki/Hooke's_law

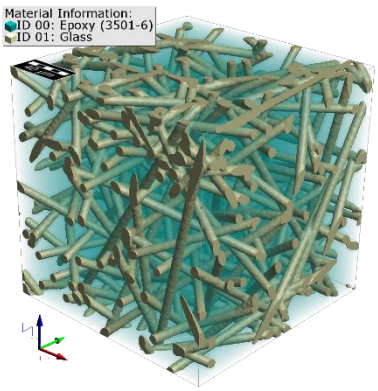
APPENDIX IV: EFFECTIVE ELASTIC PROPERTIES

To understand what ElastoDict computed effective elastic properties mean, FeelMath-VOX computations are run on two fiber-reinforced composite structures, generated using the FiberGeo module with previously known isotropic and transverse isotropic fiber orientation.

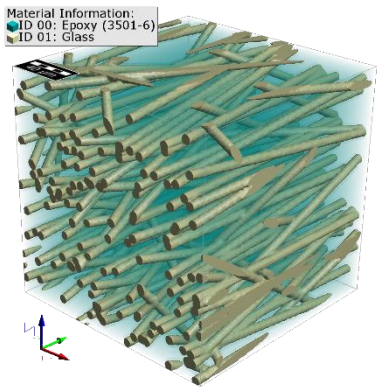
Both composite structures contain the same type of fiber (curved elliptical, diameter 6 µm), at the same solid volume percentage, but differ in their fiber orientation. Iso.gad is isotropic. The transverse isotropic TransvIso.gad has been generated with *Anisotropy 1* = 1 and *Anisotropy 2* = 10.

For more information on generating isotropic and anisotropic structures, see the FiberGeo handbook of this User Guide.

Isotropic structure



Transverse isotropic structure

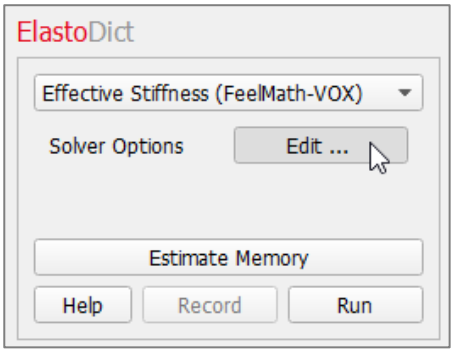


Here, already knowing that the fibers in the structure are isotropic or anisotropic helps explaining how to interpret the results obtained with ElastoDict. However, the true power of the ElastoDict analysis lies in cases where the orientation of the media is not known in advance, such as imported segmented 3D-images obtained from CT (Computed Tomography) scans.

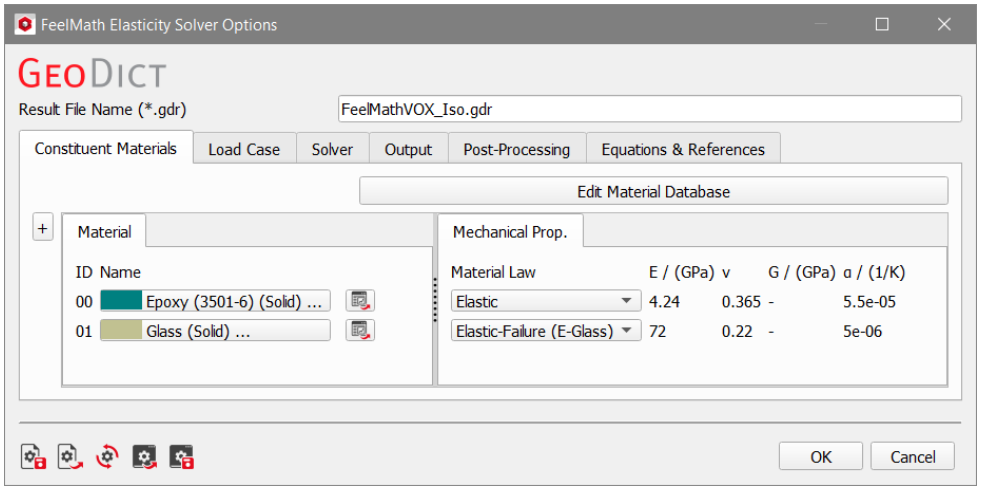
Load the two composite structures generated with FiberGeo, provided with the documentation, by selecting **File** → **Open *.gad File...** in the menu bar.

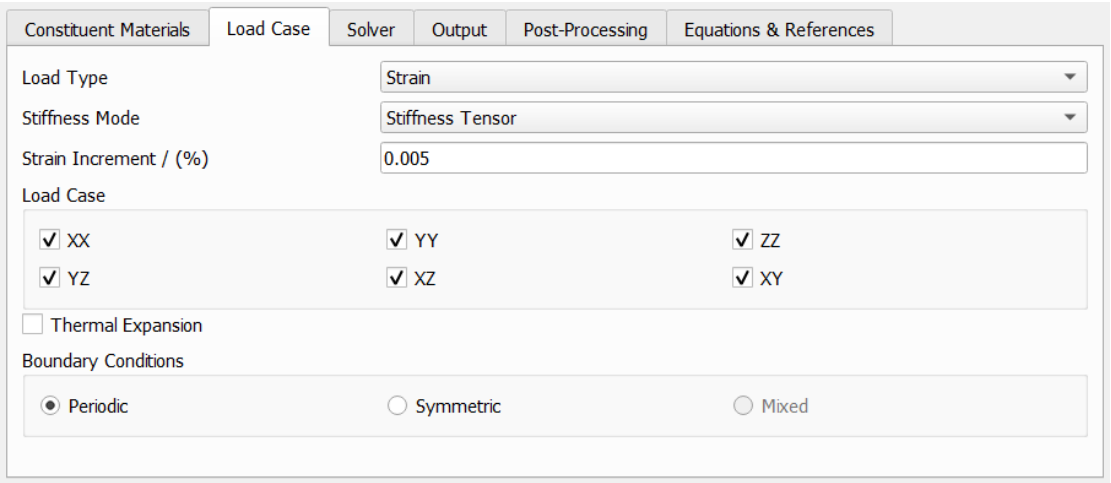
Start ElastoDict (**Predict** → **ElastoDict** in the menu bar). For both structures, the options and parameters need to be set to run a computation and obtain the predicted effective elastic properties of these two structures.

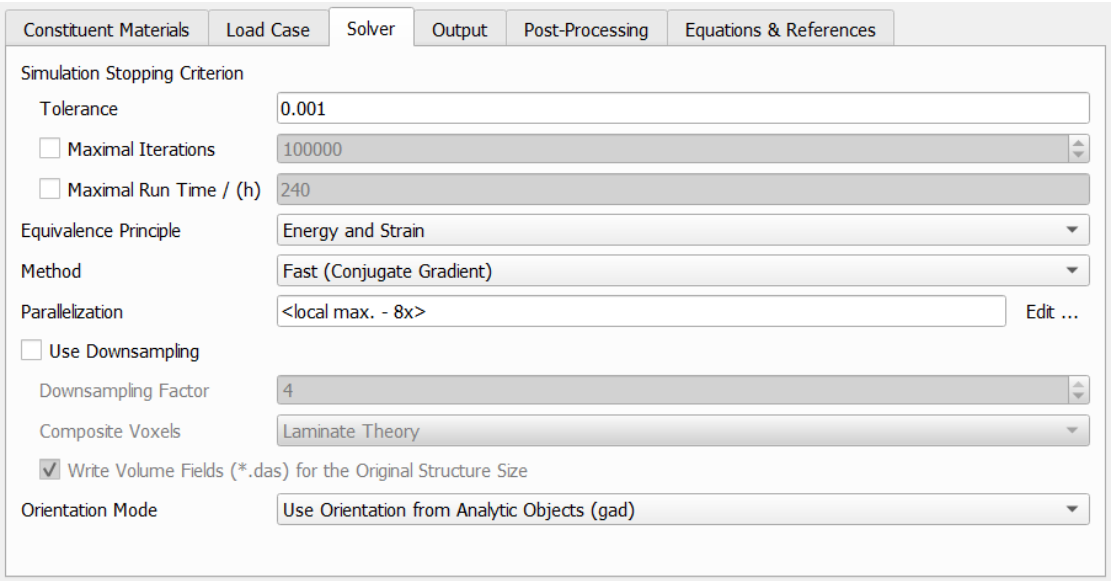
For each of the two runs, select Effective Stiffness (FeelMath-VOX) from the pull-down menu, and click the **Solver Options' Edit...** button.

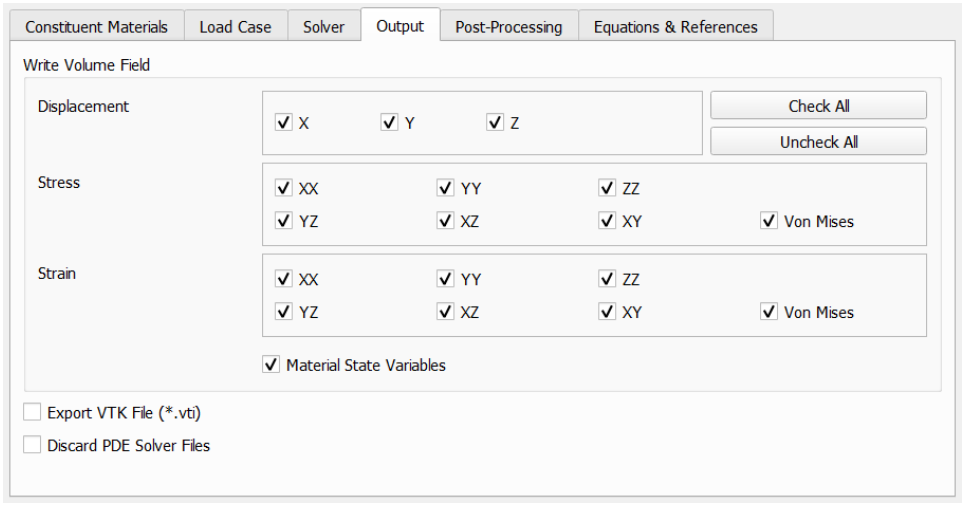


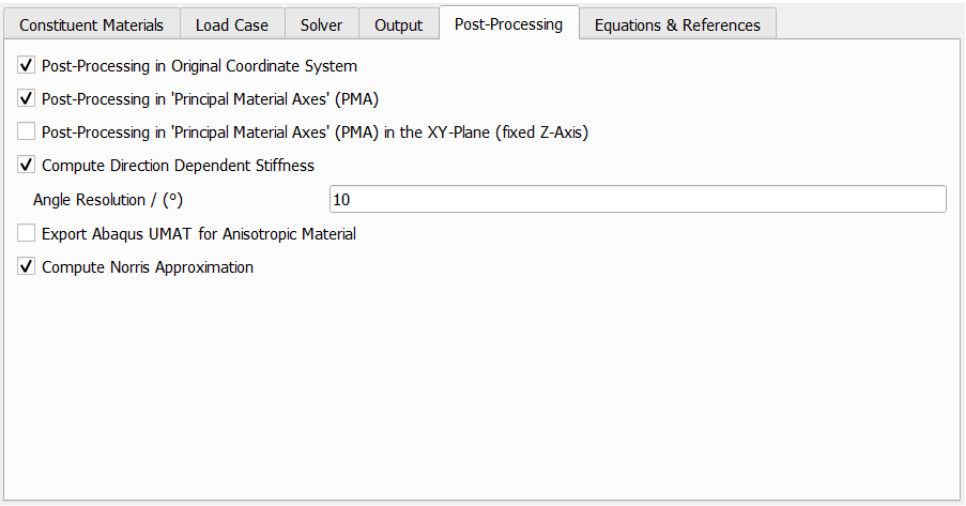
In the **FeelMath Elasticity Solver Options** dialog, the values under the tabs are adjusted as seen below. For example, under the Constituent Materials tab, the values are adjusted to the mechanical properties values of **Epoxy 3501-6 – Elastic** and **Glass – Elastic-Failure (E-Glass)**.



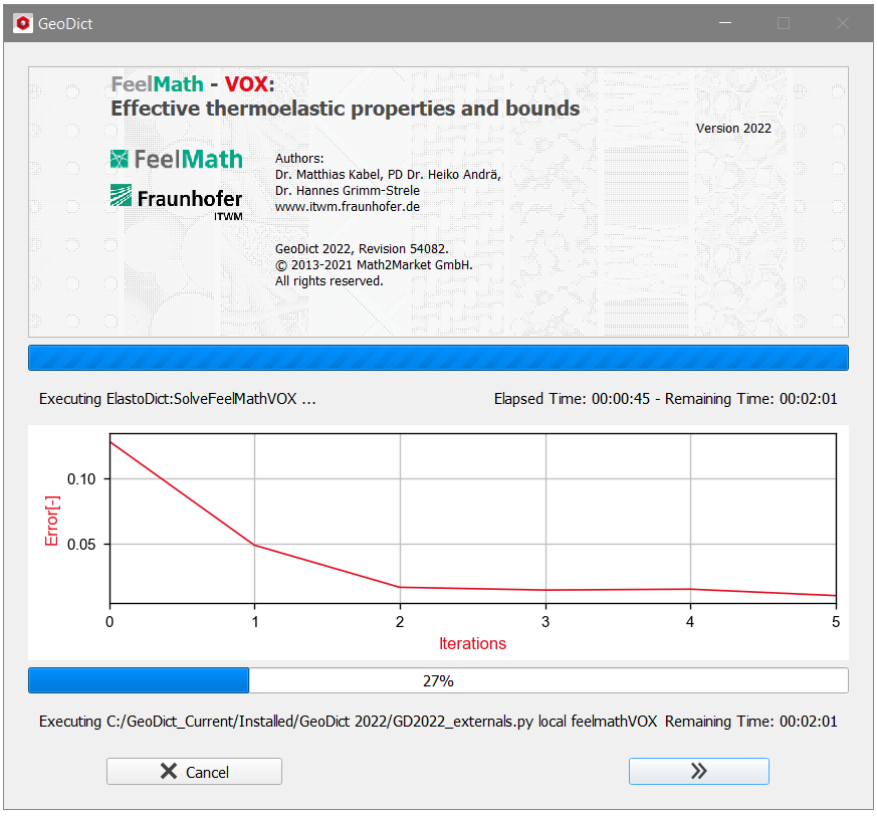




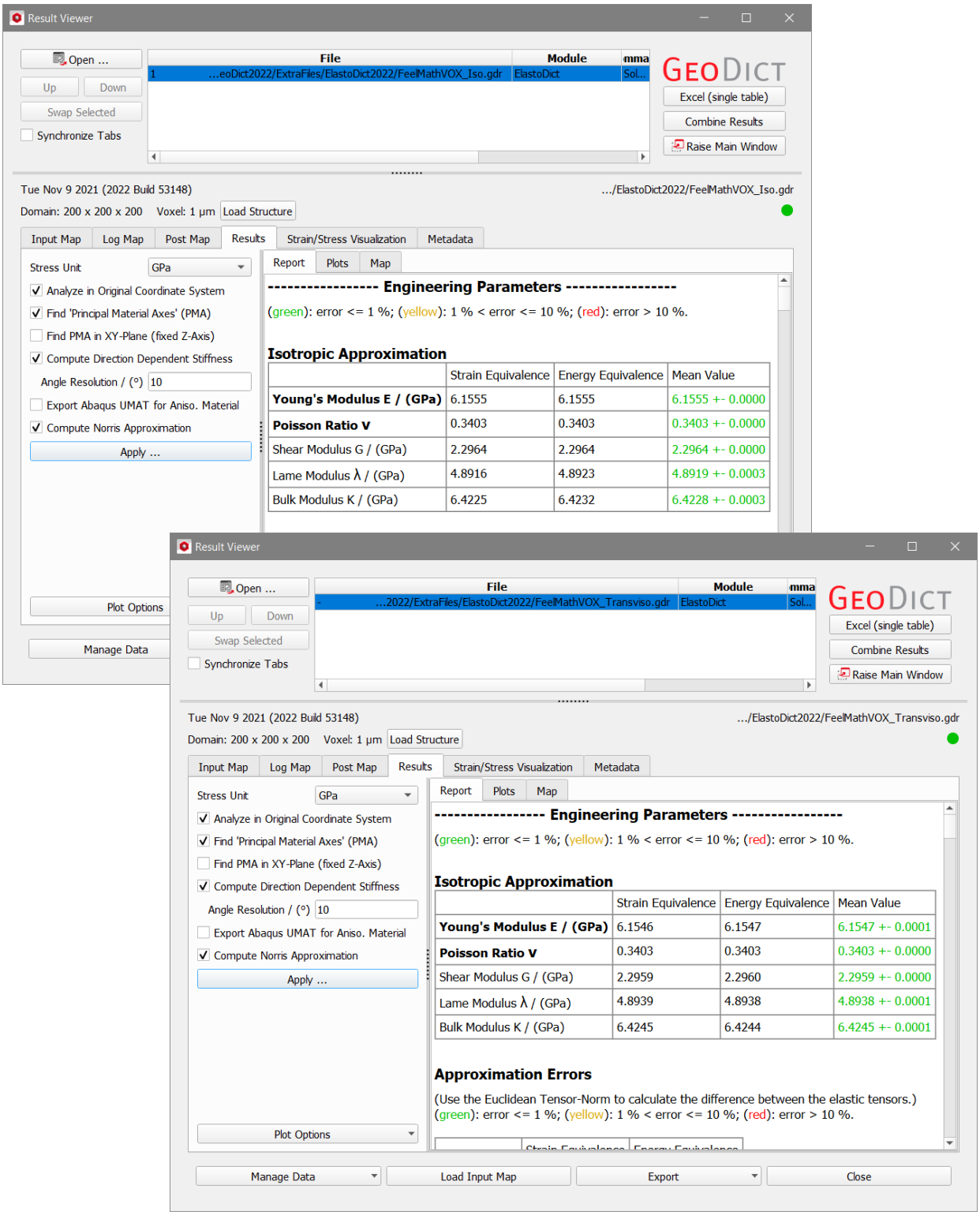




Click **OK** to close the solver options dialog and return to the **ElastoDict** section. Click **Run**. The calculations run and the iterations can be followed in the console window.



At the end of each of the two computations, the Result Viewer of the result files open (*FeelMathVOX_Iso.gdr* and *FeelMathVOX_TransvIso.gdr*).



Under the **Results - Report** subtab, several outputs or approximations of the result are provided. These approximations correspond to the different symmetry classes mentioned in page 103.

In the following analysis of some of these result values, only two decimal digits of the result are shown for better readability. The symmetrical part of the elasticity tensor is left out for the same reason.

ANISOTROPIC ELASTICITY TENSOR

The Stiffness Formulation for Strain Equivalence (GPa) is the first matrix displayed for the **Anisotropic Elasticity tensor** It is the direct result of the numerical computation and the starting point for all other approximations. This tensor is important if you are not interested in engineering parameters (Lamé parameters) but instead need the most accurate relationship between the stress and the strain. A fully anisotropic material requires 21 distinct parameters to describe it.

For the isotropic and the anisotropic composite structures being compared here, this tensor looks as follows:

FeelMathVOX_Iso.gdr

Anisotropic Elasticity Tensor

Stiffness Formulation for Strain Equivalence [GPa]

9.3178	**4.8731**	**4.8482**	-0.019358	0.067698	0.0074325
4.8734	**9.4706**	**4.9037**	-0.036231	0.011258	0.0051064
4.8483	**4.9035**	**9.3589**	-0.060116	0.081232	0.019734
-0.019443	-0.036252	-0.060062	**2.2592**	0.010641	0.0058032
0.066444	0.011262	0.080351	0.010641	**2.195**	-0.03232
0.006986	0.0046492	0.019773	0.0057625	-0.032347	**2.223**

FeelMathVOX_TransvIso.gdr

Anisotropic Elasticity Tensor

Stiffness Formulation for Strain Equivalence [GPa]

8.4888	**4.6584**	**4.6739**	0.0045115	-0.0026477	0.01679
4.6577	**12.438**	**4.7086**	0.076857	0.0049453	0.067074
4.6733	**4.7078**	**8.486**	0.023056	0.006048	0.0055766
0.0045339	0.074703	0.023056	**2.1225**	0.0066694	-0.012618
-0.0027528	0.0054416	0.0060128	0.0065934	**1.9188**	0.0062245
0.01679	0.065703	0.0055545	-0.012533	0.006286	**2.0607**

The values obtained for the coefficients defining the relationship between stress and strain can be compared to the matrix for the general elasticity tensor.

$$C_{\text{general}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{pmatrix}$$

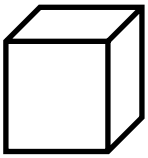
The other approximations of this general elasticity tensor are shown when scrolling down in the result file. The user can extract common physical quantities and check for differences between the other approximations and the general elasticity tensor. A large difference could mean that:

- The representative volume element is too small, and a larger structure should be used for computations.
- The chosen approximation principally does not hold. For example, it could be that assuming that a certain material is isotropic is false.

Isotropic approximation for Strain Equivalence (GPa)

Isotropy means independence of direction. An isotropic material can be simply described with two distinct parameters, the Young's modulus, and the Poisson's ratio, which are the same in all directions. In the isotropic case there are only two independent elastic coefficients e.g., E, ν or Lamé parameters λ, μ. An isotropic material is also transverse isotropic, with repetition of parameter values.

For this approximation, the full 6x6 elasticity tensor is matched against the matrix for the isotropic symmetry class (see the section about Elasticity theory, page 101 ff.).



$$C_{\text{isotropic}} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{C_{11}-C_{12}}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{C_{11}-C_{12}}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{C_{11}-C_{12}}{2} \end{pmatrix}$$

The Lamé parameters μ (Shear Modulus) and λ (Lamé Modulus) are found by calculating:

$$\mu = \frac{C_{11}-C_{12}}{2} \text{ and } \lambda = C_{12}$$

From the values of μ and λ, the estimates for the effective **Young's modulus** (E) and effective **Poisson's ratio** (ν) are computed as:

$$E = \frac{\mu(2\mu + 3\lambda)}{\mu + \lambda}$$

and

$$\nu = \frac{\frac{\lambda}{2}}{\mu + \lambda}$$

Other engineering constants can also be obtained by transformation formulas (given e.g., by the Wikipedia page on Hooke's Law).

For the isotropic (Iso.gad) and transverse isotropic (TransvIso.gad) structures, the Isotropic Approximation for Strain Equivalence look as follows:

FeelMathVOX_Iso.gdr

Isotropic Approximation for Strain Equivalence [GPa]

9.36	4.8862	4.8862	0	0	0
4.8862	9.36	4.8862	0	0	0
4.8862	4.8862	9.36	0	0	0
0	0	0	2.2369	0	0
0	0	0	0	2.2369	0
0	0	0	0	0	2.2369

FeelMathVOX_TransvIso.gdr

Isotropic Approximation for Strain Equivalence [GPa]

9.3818	4.8914	4.8914	0	0	0
4.8914	9.3818	4.8914	0	0	0
4.8914	4.8914	9.3818	0	0	0
0	0	0	2.2452	0	0
0	0	0	0	2.2452	0
0	0	0	0	0	2.2452

To compare these to the Anisotropic Elasticity Tensor in PMA Coordinates, we calculate the absolute value of the difference for both example structures:

0.00	**0.04**	**0.01**	0.01	0.01	0.01
	0.16	**0.00**	0.02	0.01	0.01
		0.26	0.01	0.01	0.00
symmetric			**0.01**	0.00	0.00
				0.00	0.01
					0.04

0.89	**0.22**	**0.23**	0.00	0.01	0.00
	0.90	**0.18**	0.01	0.01	0.00
		3.06	0.02	0.01	0.01
symmetric			**0.12**	0.01	0.00
				0.19	0.00
					0.33

Observe that the maximal absolute value of the difference (marked in red) for the transverse isotropic structure is much higher than for the isotropic structure when comparing the isotropic approximation tensor to the anisotropic elasticity tensor.

This means that the transverse isotropic structure does not fit the isotropic approximation, which is hardly surprising, given that the transverse isotropic structure behaves differently along the fibers than perpendicular to the fibers.

Estimated Principal material Axes (PMA)

For non-isotropic materials, an appropriate coordinate system is given by the so-called **principal material axes**. While the Cartesian coordinates are the direction of computation (and experiment e.g., taking CT and applying loads), the structure material has its own symmetries e.g., the plane perpendicular to the mean direction of the fibers. These intrinsic symmetries may not be aligned with the Cartesian coordinates yet define another orthonormal coordinate system. The estimation of principal axes is a means to find these intrinsic symmetries.

The principal material axes are fitted following Browaeys and Chevrot (See references on page 104). They are shown in the results file and are used for approximations of the elasticity tensors.

FeelMathVOX_Iso.gdr

—— Elasticity Tensor Approximation in the Principal Material Axes (PMA) ——

Stiffness Formulation for Strain Equivalence

Estimated Principal Material Axes (PMA)

-0.654992	-0.241376	**0.716043**
-0.578936	**0.769283**	-0.270243
-0.485612	-0.591559	-0.643624

(The columns of the table give the PMA in the original coordinate sy

FeelMathVOX_TransvIso.gdr

—— Elasticity Tensor Approximation in the Principal Material Axes (PMA) ——

Stiffness Formulation for Strain Equivalence

Estimated Principal Material Axes (PMA)

-0.999247	-0.0319282	0.0220892
0.0228533	-0.0255342	**0.999413**
-0.0313467	**0.999164**	0.0261842

(The columns of the table give the PMA in the original coordinate system.)

If we denote by *U* the matrix with the new coordinate vectors:

$$U = \begin{pmatrix} u_1 & v_1 & w_1 \\ u_2 & v_2 & w_2 \\ u_3 & v_3 & w_3 \end{pmatrix}$$

Then, the coordinates of the elasticity tensor c_{ijkl} in the new coordinate system are

$$c'_{\gamma\delta kl} = U_{\alpha\gamma}U_{\beta\delta}U_{jk}U_{jl}c_{\alpha\beta ij}$$

See the section about the elasticity theory, page 101 ff., for the relationship between the elasticity tensor as 4th order tensor and the matrix notation.

Anisotropic Elasticity Tensor in PMA Coordinates

The second matrix displayed for the **Stiffness Formulation for Strain Equivalence** shows the Anisotropic Elasticity Tensor (GPa) in PMA Coordinates. In particular, the difference from this tensor can be used to estimate the quality of the Orthotropic Approximation, Transverse Isotropic Approximation, Cubic Approximation (all in PMA coordinates), and Isotropic Approximation shown also in the result file.

The Anisotropic Elasticity Tensor in PMA Coordinates looks similar to the **Anisotropic Elasticity Tensor**, but it has been transformed to another coordinate system. The off-diagonal coefficients are smaller, so that setting them to zero would lead to smaller errors. For our examples, we obtain:

FeelMathVOX_Iso.gdr

Anisotropic Elasticity Tensor [GPa] in PMA Coordinates

9.3603	**4.9281**	**4.8968**	-0.0074016	0.007665	0.0059868
4.9286	**9.5156**	**4.8823**	0.019955	0.0059887	-0.0063053
4.8984	**4.8828**	**9.1047**	-0.012581	-0.012973	0.0010513
-0.0075401	0.020033	-0.012503	**2.2515**	-0.00071437	0.004678
0.0074531	0.0061223	-0.012585	-0.00072685	**2.2323**	-0.007016
0.005827	-0.0063215	0.00015478	0.0043397	-0.0068508	**2.2767**

FeelMathVOX_TransvIso.gdr

Anisotropic Elasticity Tensor [GPa] in PMA Coordinates

8.4872	**4.6739**	**4.6585**	0.0049817	-0.011101	0.0025668
4.6733	**8.4836**	**4.7071**	0.010077	-0.0061002	-0.0044453
4.6577	**4.7078**	**12.443**	-0.015351	0.014274	-0.0056108
0.0050136	0.010051	-0.017473	**2.1228**	0.011491	-0.0027658
-0.01112	-0.0060637	0.01568	0.01142	**2.0596**	0.0025143
0.0026886	-0.0043965	-0.0061351	-0.002677	0.0024391	**1.9189**

$$C_{\text{anisotrope}} = \begin{pmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{pmatrix}$$

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