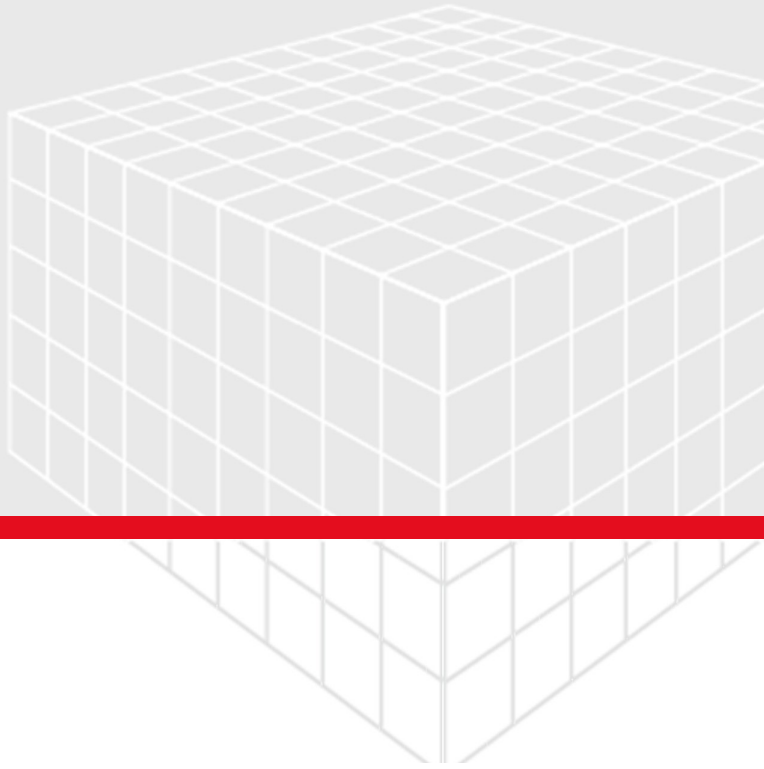
ConductoDict

User Guide



GEODICT Release 2026

Published: June 2026

GeoDict

https://doi.org/10.30423/userguide.geodict

ConductoDict

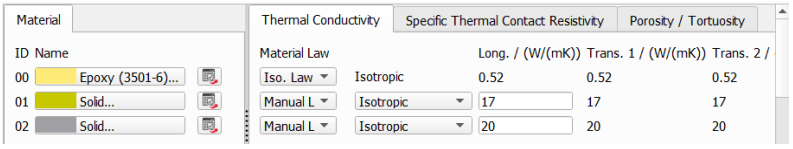
1 ConductoDict

The ConductoDict module computes effective conductivity of porous and composite materials through the following commands:

- **Compute Thermal Conductivity** calculates the effective (homogenized) thermal conductivity with constituent materials which have isotropic, transverse isotropic or orthotropic conductivity. The input parameters include the thermal conductivity of the constituent materials, the direction(s) of conduction, and the specific contact resistivity between different materials in contacts when they exist. By solving one partial differential equation per direction of interest, it computes how the spatial distribution of these different heat conduction capacities influences the overall heat conduction capacity of the composite material in the specified direction(s) of conduction.

As output, the computation assigns a single effective heat conduction tensor to the whole data set.

Input



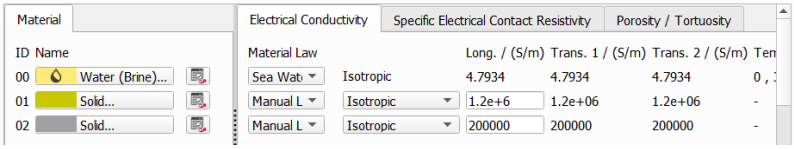
Output

Thermal conductivity tensor / (W/(mK))

1.04146	-0.0134277	-0.00311726
-0.0134238	**1.04878**	-0.0080366
-0.00311958	-0.0080206	**1.01225**

- **Compute Electrical Conductivity** computes the effective (homogenized) electrical conductivity from the isotropic, transverse isotropic or orthotropic electrical conductivity of the constituent materials.

Input

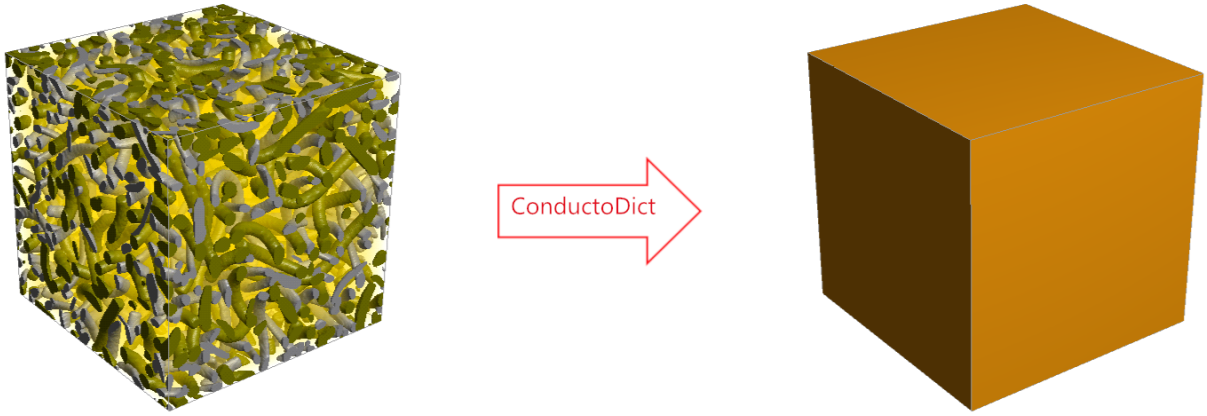


Output

Electrical conductivity tensor / (S/m)

167.327	0	0
0	**59.7615**	0
0	0	**57.1621**

As illustrated in the figure below, we address the conduction problem within the detailed microstructure (left) to derive an overall effective thermal or electrical conductivity that represents the material as a whole (right).



Learn to use ConductoDict

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  Computes effective thermal of porous and composite materials.
- Compute Electrical Conductivity 38
  Computes effective electrical conductivity of porous and composite materials.
- References 47
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Find illustrative application examples on the website.
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Send your Support Request to our technical Support.

1.1 Theoretical Background

Governing equations and explanations

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  The governing equations for calculating electrical conductivity and how they are solved.
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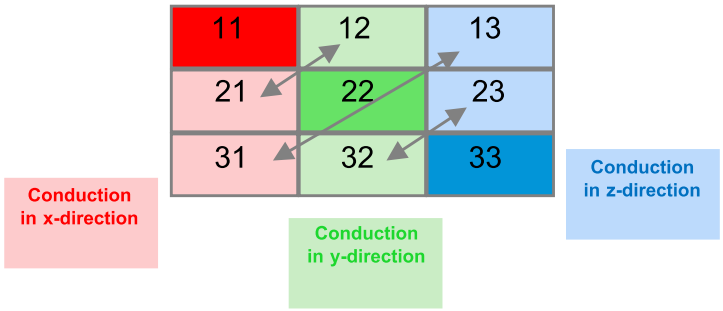
1.1.1 Conductivity Tensor

The conductivity tensor, included in the result file after running ConductoDict, contains **diagonal** values and **off-diagonal** values.

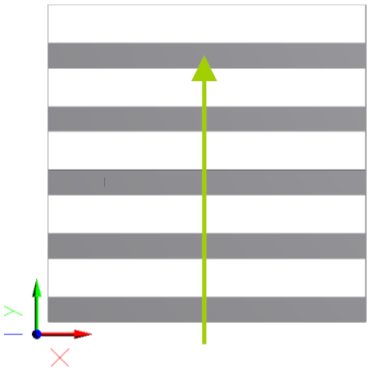
The diagonal values (11, 22, and 33) correspond to the calculated conductivity values for the **X-direction**, the **Y-direction**, and the **Z-direction**. These values are the same when conduction is equal in all directions. When one of these directions has not been selected and is not calculated, instead of a value, the word **unknown** appears.

The off-diagonal tensor values reflect the symmetry of the composite material and the orientation with respect to the direction of conduction.

11	12	13
21	22	23
31	32	33



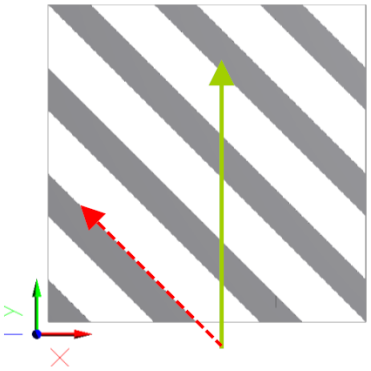
The off-diagonal values correspond to the component of conduction in a certain Cartesian direction. Theoretically, they have pairwise the same value (i.e. 12 and 21, 13 and 31, and 23 and 32). A minor difference within a pair of values is possible and is due to the limitations of accuracy when solving the equations. An increase of the accuracy of the solver decreases this difference. For example, when calculating conduction in the Y-direction (and not in the X-, or the Z-direction) the following may occur:



Thermal conductivity tensor / (W/(mK))

unknown	0	unknown
unknown	**1.25**	unknown
unknown	0	**unknown**

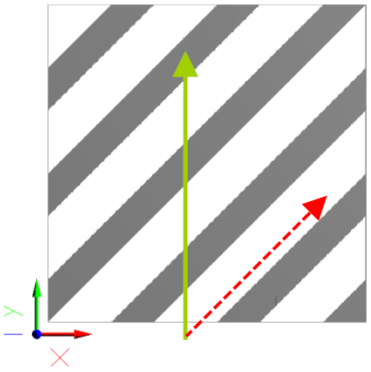
The off-diagonal values are zero when the conduction in the Y-direction does not have a component in another direction, i.e. no conduction occurs in the secondary direction due to the conductivity of the constituent materials and/or their orientation in the structure.



Thermal conductivity tensor / (W/(mK))

unknown	-0.0739899	unknown
unknown	**1.32399**	unknown
unknown	0	**unknown**

Off-diagonal values are non-zero when the conduction in the Y-direction has a component in another direction, i.e. conduction also occurs in the X-direction.



Thermal conductivity tensor / (W/(mK))

unknown	0.0739899	unknown
unknown	**1.32399**	unknown
unknown	0	**unknown**

The sign of the off-diagonal non-zero value indicates the sense of the component (towards X+ or X-).

1.1.2 Thermal Conductivity

Thermal conductivity represents the rate at which heat is transferred by conduction through a given unit area of a given material when the temperature difference or gradient is normal to the cross-sectional area. The coefficient of thermal conductivity can be defined as the quantity of heat that travels through a unit volume of a material structure at a given time when the temperature gradient is one degree.

In physics, the thermal conductivity κ is the property of a material's ability to conduct heat, primarily as in Fourier's Law for heat conduction. Heat transfer across materials of high thermal conductivity occurs at a higher rate than across materials of low thermal conductivity. The law of heat conduction, also known as Fourier's law, states that the time rate of heat transfer through a material is proportional to the negative gradient in the temperature and to the area, at right angles to that gradient, through which the heat is flowing.

$$Q = -\mathrm{K}\nabla T \tag{1}$$

where Q is the heat flux, T is the temperature, and K is the effective thermal conductivity [W/mK, Watts per meter Kelvin]. When the temperature at inlet T^{in}, at outlet T^{out}, also the thickness of the material L, are known, the effective thermal conductivity is expressed as

$$\mathrm{K} = Q\frac{L}{T^{\mathrm{in}} - T^{\mathrm{out}}} \tag{2}$$

In general, the effective thermal conductivity is a second order tensor

$$\mathrm{K} = \begin{pmatrix} \kappa_{11} & \kappa_{12} & \kappa_{13} \\ \kappa_{21} & \kappa_{22} & \kappa_{23} \\ \kappa_{31} & \kappa_{32} & \kappa_{33} \end{pmatrix} \quad (3)$$

If the material is isotropic, that is, its properties are the same in all directions, instead of the tensor K, a scalar constant can be used.

Compute Thermal Conductivity determines the effective (homogenized) thermal conductivity tensor of a structure. To achieve this, the Poisson equation

$$-\nabla \cdot (\kappa \nabla T) = 0 \quad (4)$$

is solved in the 3D structure model. Each material within the structure is characterized by its local thermal conductivity κ. The constituent materials can be with **isotropic**, **transverse isotropic**, or **orthotropic** conductivity.

The resulting material is in general anisotropic, and a conductivity tensor is needed to prescribe complete thermal behavior. To reduce computational time, it is also possible to limit calculations to certain columns of the conductivity tensor, if heat flux in only one direction is of interest.

1.1.3 Electrical Conductivity

Electrical conductivity σ measures a material's ability to conduct an electric current. Ohm's Law relates the electric potential φ and the magnitude of current density J:

$$J = -\sigma \nabla \varphi \quad (5)$$

Ohm's law is the electrical analogue of Fourier's law. When the electrical potential at inlet ϕ^{in}, at outlet ϕ^{out}, also the thickness of the material L, are known, the effective thermal conductivity is expressed as

$$\sigma = J \frac{L}{\phi^{\mathrm{in}} - \phi^{\mathrm{out}}} \quad (6)$$

Like the thermal conductivity, the electrical conductivity for isotropic materials is constant in all directions and can be characterized by a scalar. For anisotropic materials, σ is a tensor.

The effective electrical conductivity σ is determined by solving the Poisson equation

$$\nabla \cdot (\sigma_c \nabla \varphi) = 0 \quad (7)$$

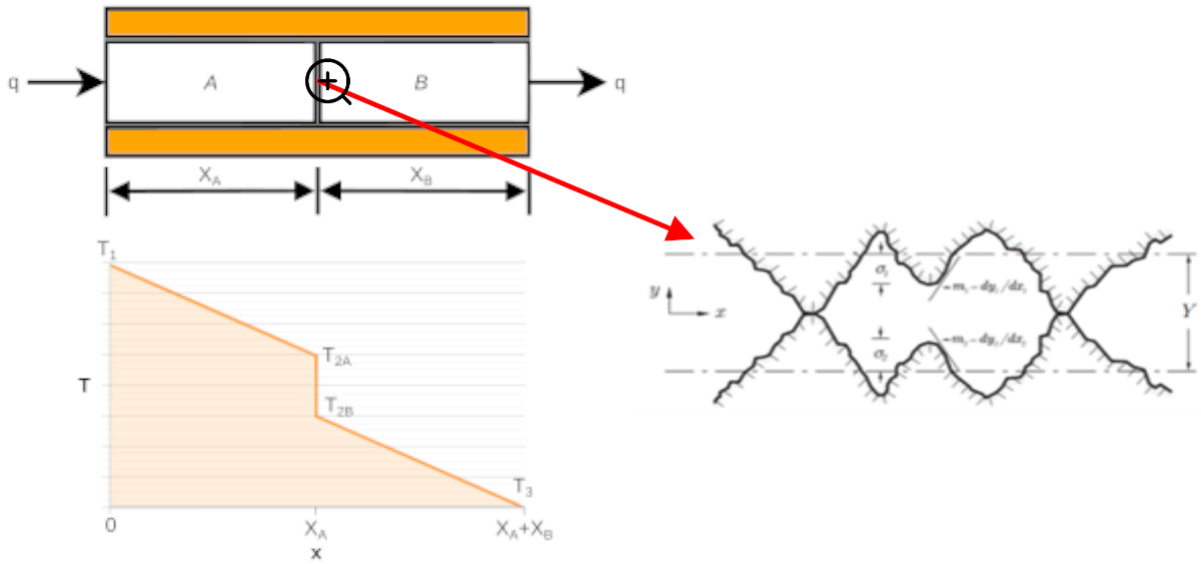
in the 3D structure model, where σ_c denotes the local electrical conductivity of the constituent materials.

The algorithm in ConductoDict (Wiegmann and Zemitis, 2006) has been used for many applications, in industrial settings (e.g., thermal insulation) and for academic purposes. Publications include heat transfer properties of medium density fiberboard (MDF) samples (Thoemen et al., 2008), of cast iron microstructures (Velichko, 2008, Velichko et al., 2009), of the gas diffusion layer in fuel cells (Schulz et al., 2007, Becker et al., 2008, Becker et al., 2009, Zamel et al., 2010, Veyret and Tsotridis, 2010, Pfrang et al., 2010) and electrical conductivity of Ag/SnO_2 (Jeanvoinea et al., 2010).

1.1.4 Contact Resistance

Although most surfaces seem flat, on a microscopic level all of them are found to possess micro asperities. This effectively reduces the contact area, and a temperature drop is observed at the interface between the two surfaces in contact Holman, 1997, Hasselström and Nilsson, 2012.

One way to solve this problem is to resolve the microscopic zig-zag interfaces (the right picture in the following) with very small voxels and result in a large computational domain. The more attractive way, however, is to introduce contact resistance to the simulation. The rough surface of two different materials in contacts does not need to be resolved, but a contact resistance is assigned to it.



The heat flow at the interface is expressed as

$$q = h_c \Delta T_c \,, \tag{8}$$

where h_c is contact conductance, in W/(m²·K), ΔT_c is the temperature difference across the interface. And the specific contact resistivity is defined as

$$R_c = \frac{1}{h_c} \tag{9}$$

From considerations of energy conservation, the heat flow between the two bodies in contact, bodies A and B, is found as:

$$q = \frac{T_1 - T_3}{\frac{\Delta x_A}{\kappa_A} + R_c + \frac{\Delta x_B}{\kappa_B}} \quad (10)$$

1.1.5 Mixing Rules

When a constitute material in a structure is pure solid or fluid, the intrinsic thermal or electrical conductivity of the material is needed to compute the effective conductivity of the structure. However, when the material is unresolved and is composed of both solid and fluid, the effective conductivity should be given. You can obtain it from laboratory measurements, or by simulating a resolved structure by using higher resolution. Besides those, mixing rules are widely used to express the effective properties of porous media.

Since GeoDict 2025, the following mixing rules are possible in Constituent Materials for porous media to find the effective thermal / electrical conductivity that can take porosity and tortuosity factors into account.

Single Phase

Single Phase is applicable for pure material of solid, fluid or porous. Also, if you know the effective property of the porous medium and do not need the mixing rules, you can just give the value for the porous medium by choosing Single Phase.

Parallel Model

In general there are two models for a rule of mixtures, one for axial loading, and one for transverse loading. The axial-loading case is described by the parallel model, also known as the Upper Bound or Voigt model. The transverse-loading case is represented by the series model, also referred to as the Lower Bound or Reuss model. For parallel model, solid and fluid are assumed to be distributed parallel in the conduction direction and the effective conductivity is the weighted arithmetic mean of the conductivity of the solid and fluid

$$\kappa_{eff} = \kappa_s \cdot \phi + \kappa_f \cdot (1 - \phi)\,, \quad (11)$$

where κ_s and κ_f are the conductivity for solid and fluid, respectively. ϕ is the solid volume fraction.

Series Model

Here, solid and fluid are connected in series and the effective conductivity is the weighted harmonic mean of the conductivity of the two substances.

$$\frac{1}{\kappa_{eff}} = \frac{\phi}{\kappa_s} + \frac{1-\phi}{\kappa_f} \tag{12}$$

Hill's Average

The Parallel Model and the Series Model represent the upper and lower bound, respectively, of the quantity of the effective properties. Hill's average is the middle value of them.

Tortuosity Model

The tortuosity model finds the effective conductivity based on the increased path length

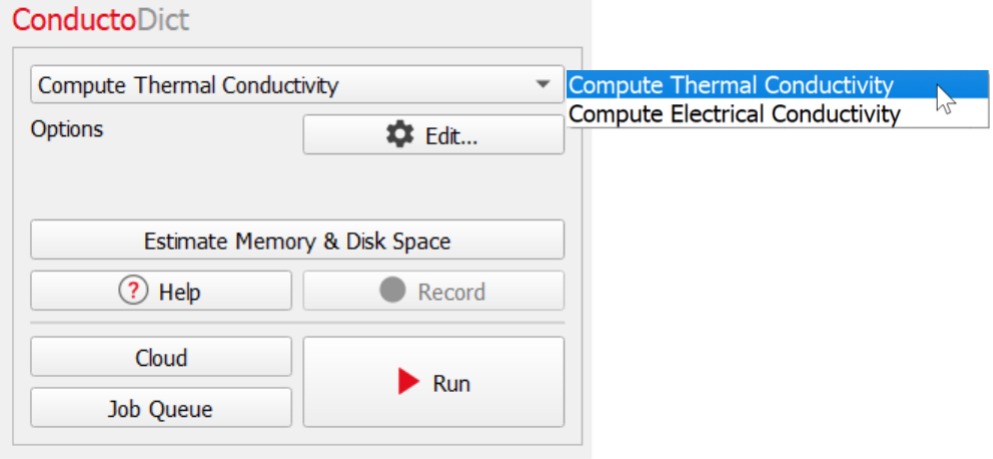
$$\kappa_{eff} = \left(\frac{\kappa_s}{\tau_s} + h_i\right) \cdot \phi + \left(\frac{\kappa_f}{\tau_f} + h_i\right) \cdot (1-\phi), \tag{13}$$

where τ_s and τ_f are the tortuosity factor for solid and fluid, and h_i is interfacial conductance, which is zero as the default at the moment in ConductoDict.

1.2 Compute Thermal Conductivity

Use **Compute Thermal Conductivity** to compute the thermal properties of composite or porous media, given the thermal conductivity of each constituent of the material.

To compute the thermal conductivity of a material, choose **Compute Thermal Conductivity** from the dropdown menu in the ConductoDict GUI.

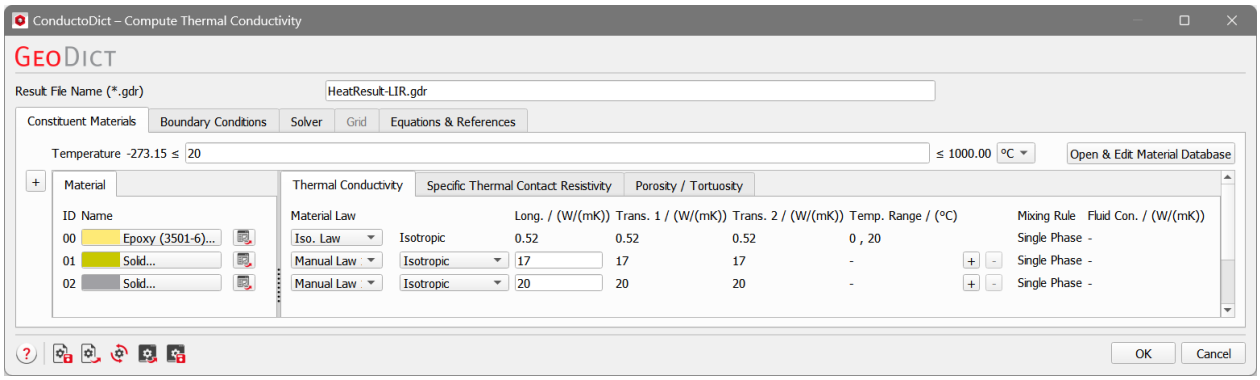


The Compute Thermal Conductivity command

- Input Parameters 12
  How to set the input parameters for Compute Thermal Conductivity command.
- Results 33
  How to understand the computed results.
- Data Visualization 36
  How to visualize the computed results.

1.2.1 Input Parameters

When **Compute Thermal Conductivity** is selected from the pull-down menu, clicking the **Edit...** button opens the **Conductivity- Compute Thermal Conductivity** dialog.



Choose a name for the files containing the results of the computations according to your current project. The result files are saved in the project folder (**File** → **Choose Project Folder**, in the Menu bar).

An additional directory with this name is created to keep the intermediate computation files (PDE solver files) and the temporary computation files.

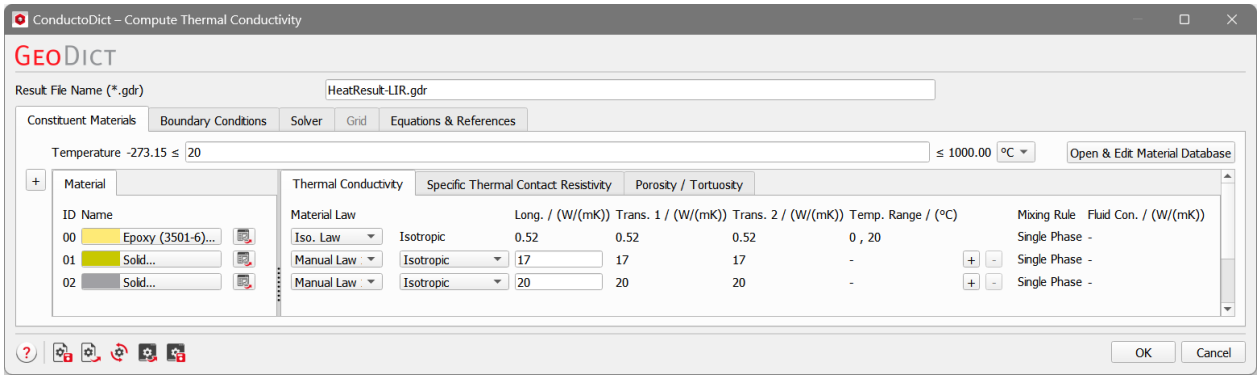
The parameters are organized under the **Constituent Materials**, **Boundary Conditions**, **Solver**, **Grid**, and **Equations & References** tabs.

Tabs of the Compute Thermal Conductivity dialog

- Constituent Materials 13
  Specify the thermal properties of the constituent materials.
- Boundary Conditions 18
  Set the conditions at the boundaries of the structure.
- Solver 20
  Set the options used to control how the heat problem is solved.
- Grid 32
  Decide whether voxels or boxels are used.

Constituent Materials

Under this tab, the constituent materials of the pore space/matrix and the structure material(s) can be set or chosen from the GeoDict Material Database.

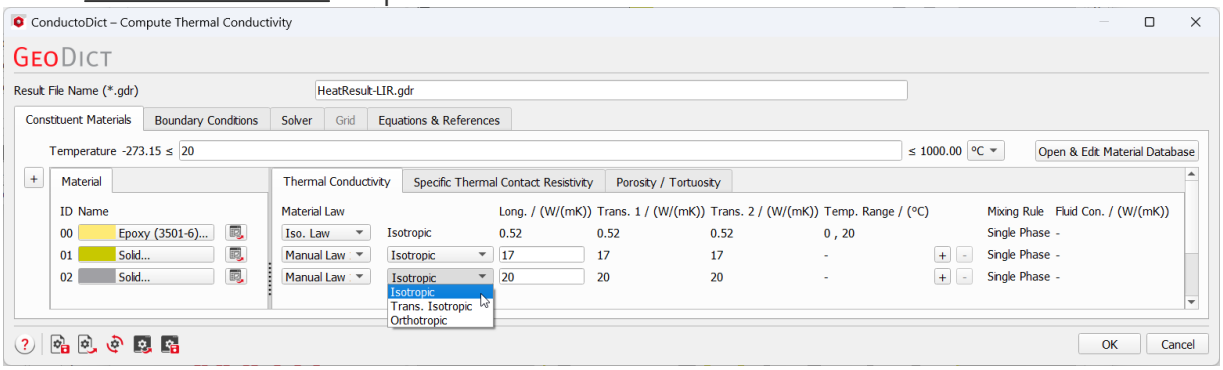


The parameters for each material are subdivided into **Thermal Conductivity**, **Specific Thermal Contact Resistivity**, and **Porosity / Tortuosity**.

Thermal Conductivity

The thermal conductivity for each of the constituent materials needs to be specified for **Compute Thermal Conductivity**. More information on constituent materials can be found

in the Material Database chapter.



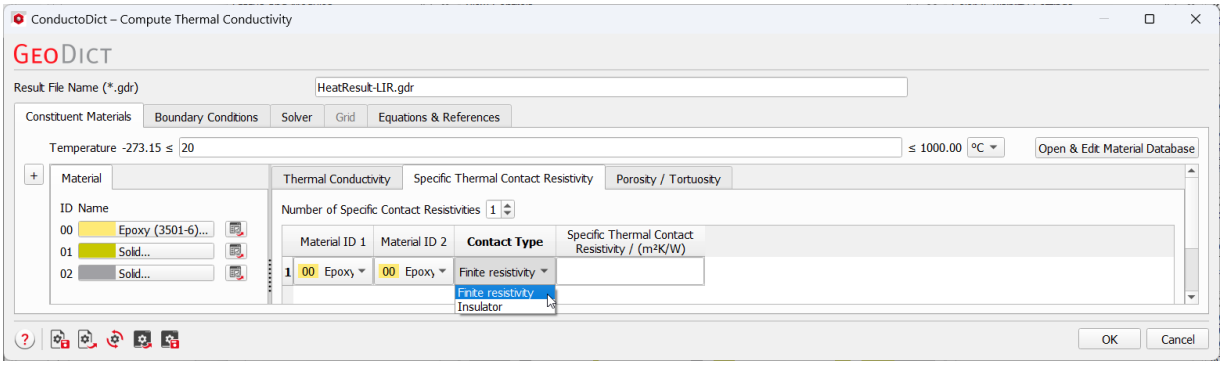
For every material, one of the material laws defined in the material database must be selected. For **Manual** defined materials, **Isotropic**, **Transverse Isotropic** or **Orthotropic** conductivity can be chosen from the pull-down menus. When **Transverse Isotropic** or **Orthotropic** is chosen, the EJ solver cannot be selected in the **Solver** tab, and the LIR becomes the only choice of the solver.

A **Mixing Rule** is only available for porous media. The different mixing rules can be chosen to find the effective thermal / electrical conductivity. The details of the mixing rules are described in the Porosity / Tortuosity tab 15.

Specific Thermal Contact Resistivity

When contact resistances exist between different materials, enter the parameters in the **Specific Thermal Contact Resistivity** subtab.

First, choose the **Number of Specific Contact Resistivities**. This creates the desired number of rows in the input tab. There, select the materials for **Material ID 1** and **Material ID 2**, and set the value of the specific thermal contact resistivity between these two materials.



If the contact resistivity between the two materials has a finite value, then **Finite resistivity** should be chosen as the **Contact Type**. The contact can also be an insulator, which means the resistivity is infinite. Then **Insulator** is chosen and no value for **Specific Thermal Contact Resistivity** column is needed for the input.

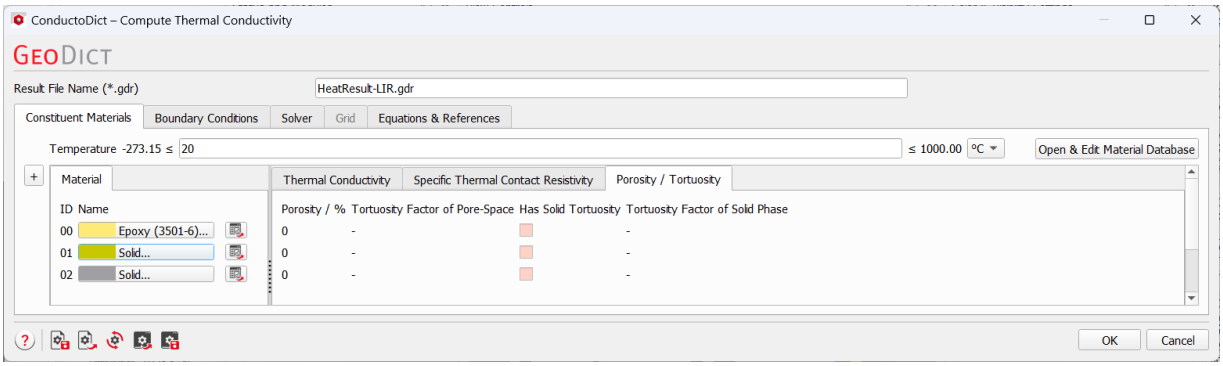
Contact resistances can be applied between the same Material IDs, as well as between different material IDs.

If the same material ID is chosen for **Material ID 1** and **Material ID 2**, the contact resistance is applied only between different objects of the same color. There are two different ways how objects can be defined, for this see the description of the Object Mode 28 of this user guide chapter.

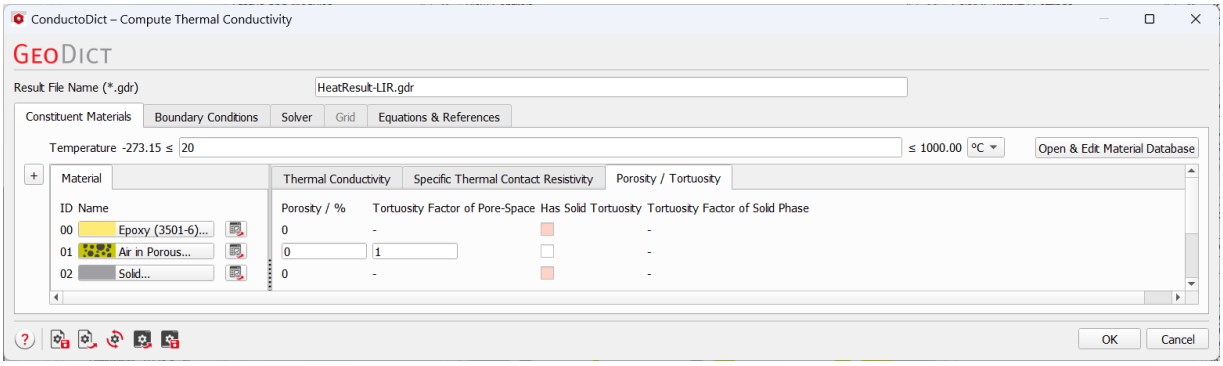
If there are no contact resistances, just leave the **Number of Specific Contact Resistivities** to be 0.

Porosity / Tortuosity

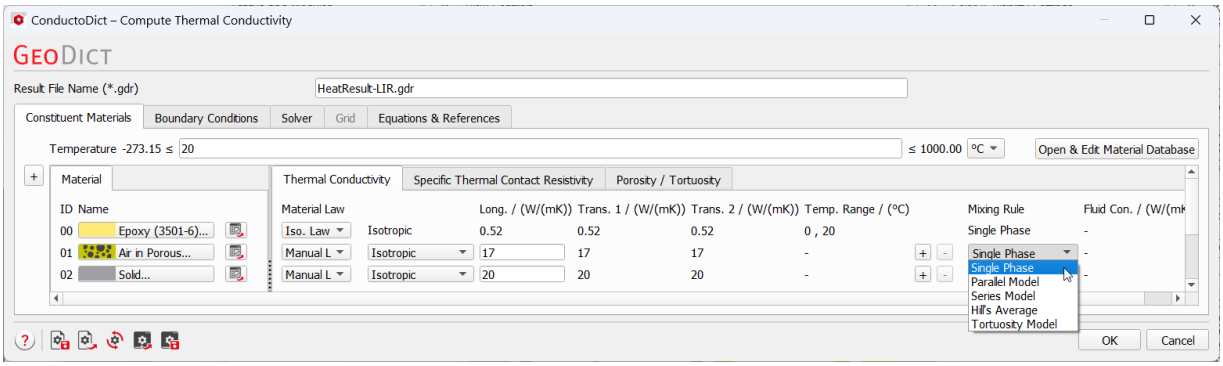
If there is no porous material in the structure, but only pure solid or fluid materials, you do not need to set any parameters in the **Porosity / Tortuosity** tab.



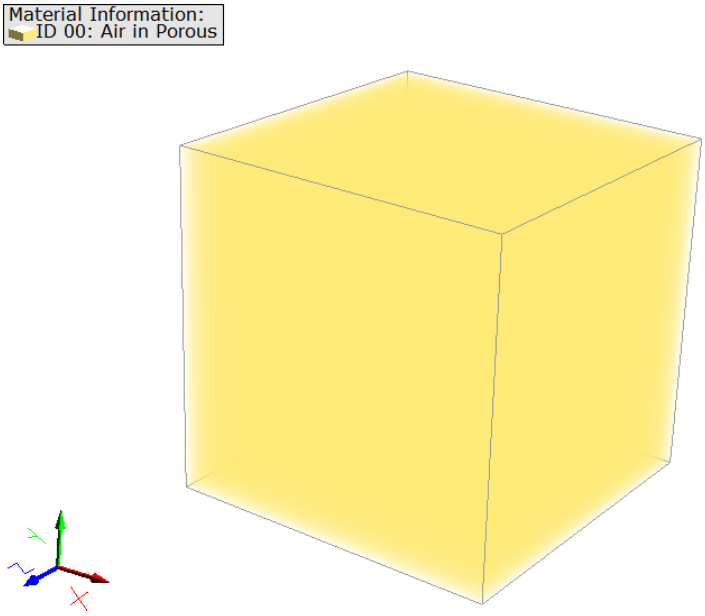
When the current structure contains a porous material, the parameters **Porosity**, **Tortuosity Factor of Pore-Space**, and **Has Solid Tortuosity** become selectable. When you select **Has Solid Tortuosity**, you can also enter a value for the **Tortuosity Factor of Solid Phase**.

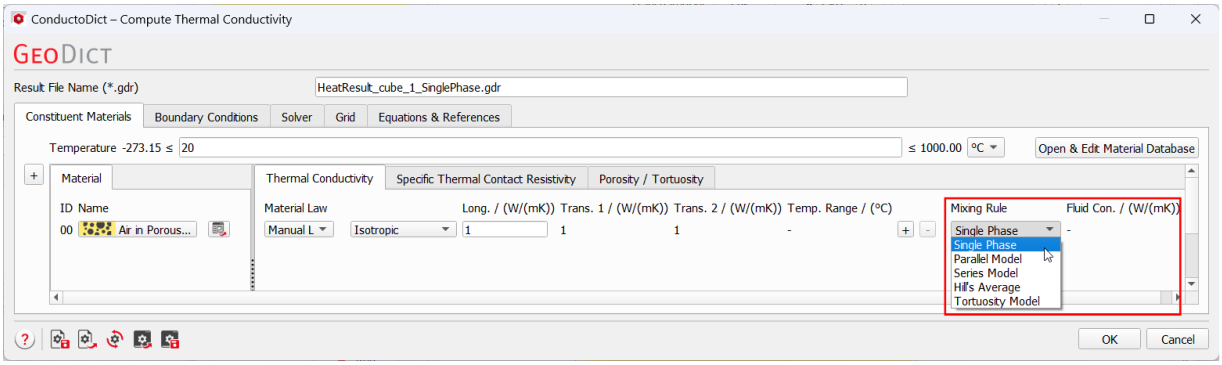


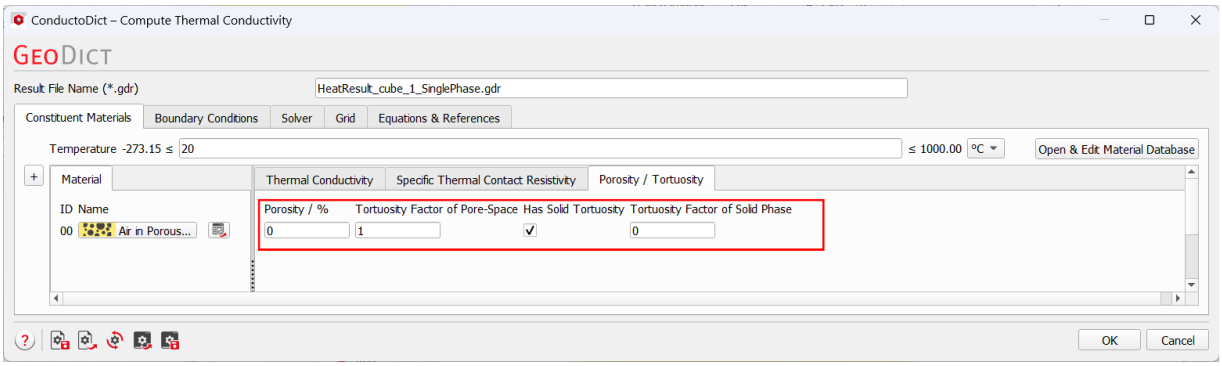
For each porous material, select the applied **Mixing Rule** on the **Thermal Conductivity** tab. The different rules are described on the Mixing Rules page 10.



To illustrate how the mixing rule works, we create a 1 x 1 x 1 structure and show what the effective conductivity would be when different rules are chosen.





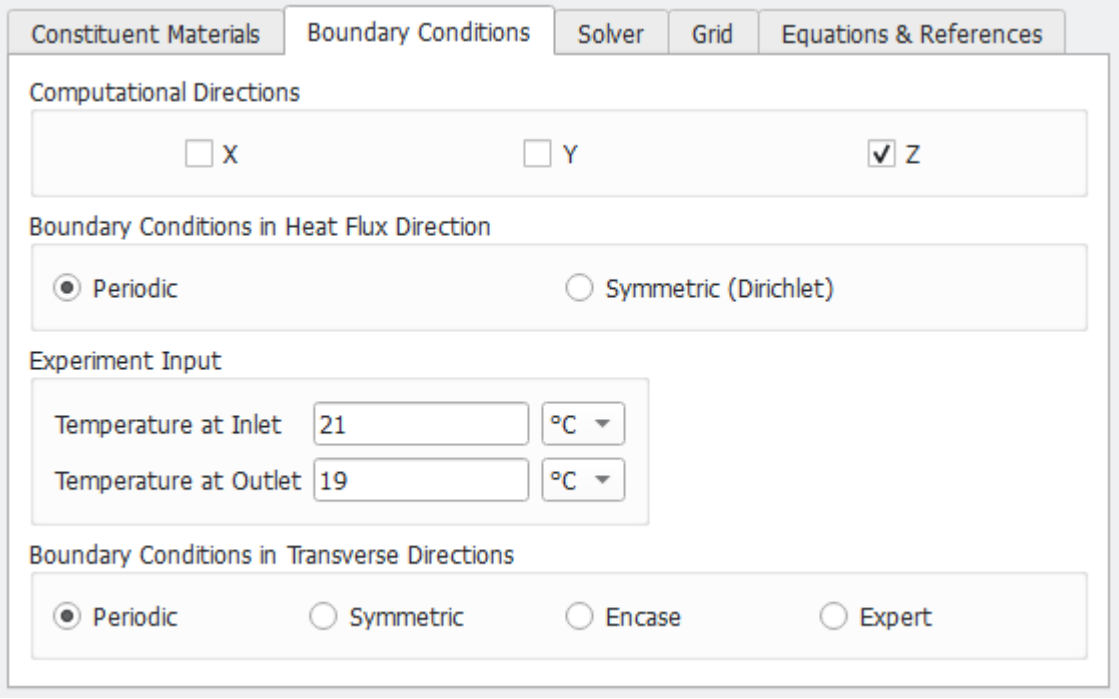


We set the thermal conductivity 1 W/(mK) for the material 00. By choosing the different mixing rules, the parameters including the fluid conductivity, porosity, tortuosity of pore space and solid phase may matter. The table shows the results in the last column for the given parameters in the first 6 columns. When a table cell is empty, the value does not take effects on the result. The results can be validated easily with the formulas given on the Mixing Rules section 10.

Mixing Rule	Fluid Con. / (W/mK)	Porosity / %	Tortuosity Factor of Pore-Space	Has Solid Tortuosity	Tortuosity Factor of Solid Phase	Effective Thermal Conductivity / (W/mK)
SinglePhase						1
Parallel Model	9	100				9
Parallel Model	9	50				5
Series Model	9	50				1.8
Hill's Average	9	50				3.4
Tortuosity Model	9	50	1.5	True	2	3.25

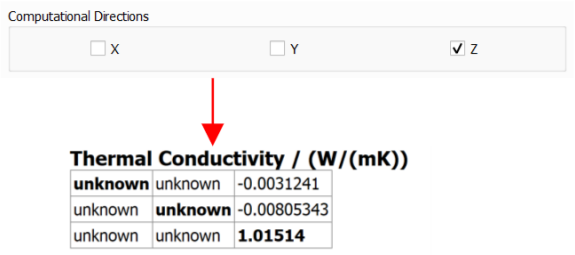
Boundary Conditions

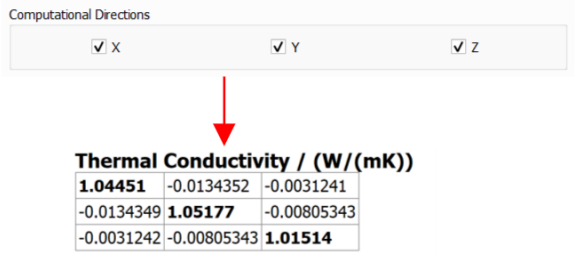
The **Boundary Conditions** tab contains four panels: **Computational Directions**, **Boundary Conditions in Heat** (or **Potential**) **Flux Direction**, **Experiment Input**, and **Boundary Conditions in Transverse Directions**.



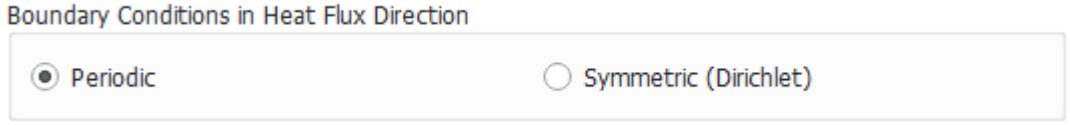
For the **Computational Directions**, choose the direction for the conductivity to be computed.

To obtain the whole 3x3 conductivity tensor (for each direction) in the result file, it is necessary to choose all three directions. Checking all directions prolongs the computational time of the solver.





The choice of **Boundary Conditions in Heat Flux Direction** depends on the morphology of the structure and the field of application.

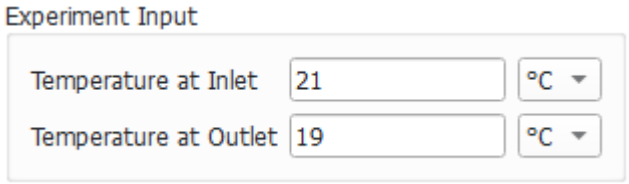


If **Periodic** is selected, the conductivity is computed assuming that the structure is periodically repeated in the flux direction. If **Symmetric (Dirichlet)** is checked, constant temperature or potential is assumed along both border planes in the heat flux or the potential flux direction.

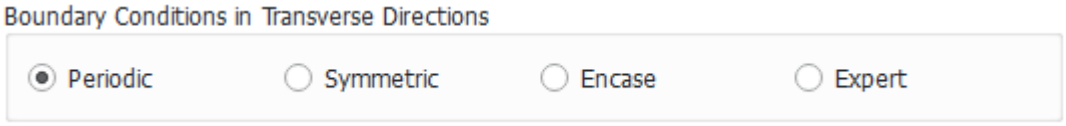
For non-periodic structures, **Symmetric (Dirichlet)** boundary conditions give more accurate results than **Periodic** boundary conditions.

For most applications, the difference between these two cases is insignificant and can be compared with a computational error.

An arbitrary temperature can be set as boundary conditions in the **Experiment Input** panel to define the temperature difference or the potential difference across the material structure.



Besides the boundary conditions chosen for the main conduction direction, the **Boundary Conditions in Transversal Directions** can also be chosen to be **Periodic, Symmetric**, **Encase**, or any combinations of those boundary conditions in two tangential directions with the choice of **Expert**.



With **Periodic** boundary conditions, the structure is repeated in the tangential directions. With **Symmetric** boundary conditions, the structure is flipped and then repeated.

Periodic boundary conditions

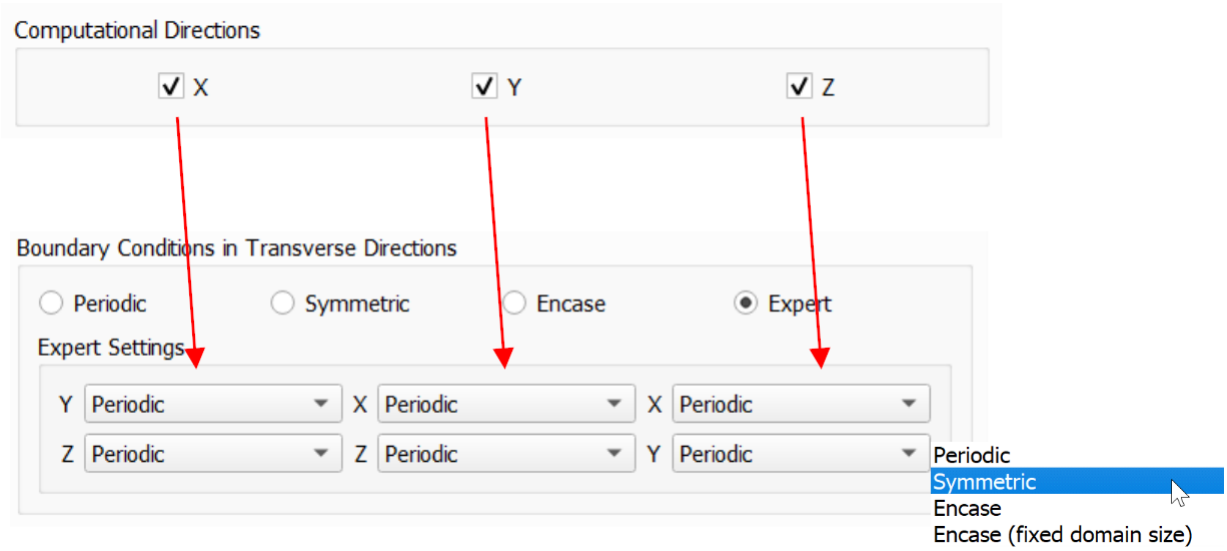
Symmetric boundary conditions

In both cases, the numerical solution can be computed without flipping or repeating the structure in memory. Therefore, the memory and runtime costs for all boundary conditions are comparable.

When **Encase** is chosen, the structure is encased by two non-conducting plates added in the two tangential directions.

Choose **Expert** when different boundary conditions need to be specified for the two tangential directions. When **Expert** is checked, more choices appear.

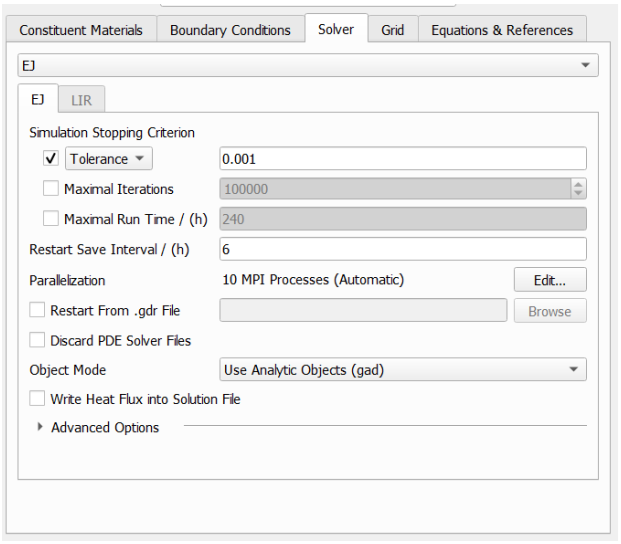
For each selected computation direction, the boundary conditions in the two transverse directions must be selected. For each tangential direction, you have the choice of **Periodic**, **Symmetric**, **Encase**, and **Encase (fixed domain size)**.

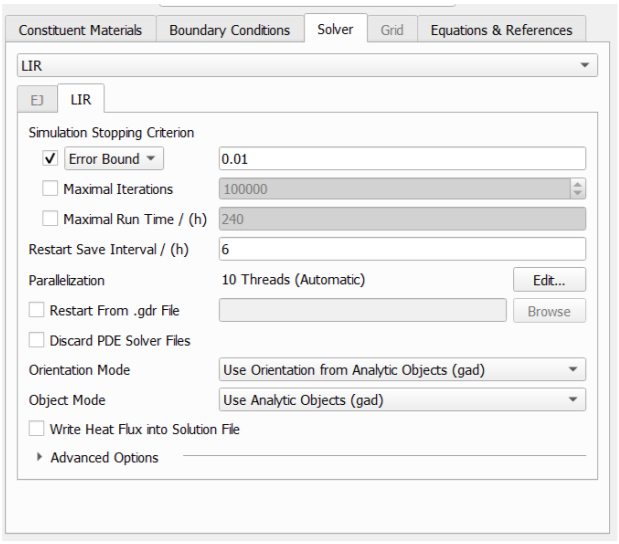


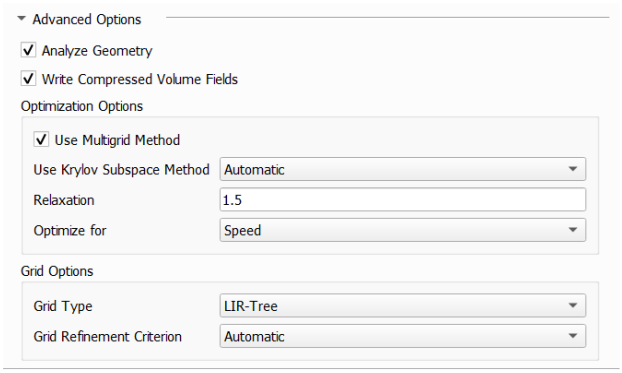
When **Encase** is used, the solver internally adds a one-voxel layer in the required direction and solves with periodic boundary condition. That effectively is equivalent to solving the structure with casing in two ends in the direction of interest. So, the size of computation in this direction becomes n+1. However, if changing the computational size is not preferable, using **Encase (fixed domain size)** can avoid that, then the first layer of the structure is replaced by a non-conducting material.

Solver

Two solvers, **EJ** and **LIR** can be chosen to solve the thermal or electrical conductivity problem. However, when transverse isotropic or orthotropic thermal or electrical conductivity materials are chosen, the **LIR** must be used.







The best solver choice for isotropic cases depends very much on the ratio of the largest and smallest conductivity (i.e., high contrast) within the structure. For structures with high contrast (e.g., $>10^6$) or high contact resistivity it is recommended to use the EJ solver, or choose **Automatic** or **Enabled** for **Use Krylov Subspace Method** in the LIR solver.

Simulation Stopping Criterion

Both LIR and EJ solve the Poisson equations by an iterative approach. The basic idea of an iterative method is to:

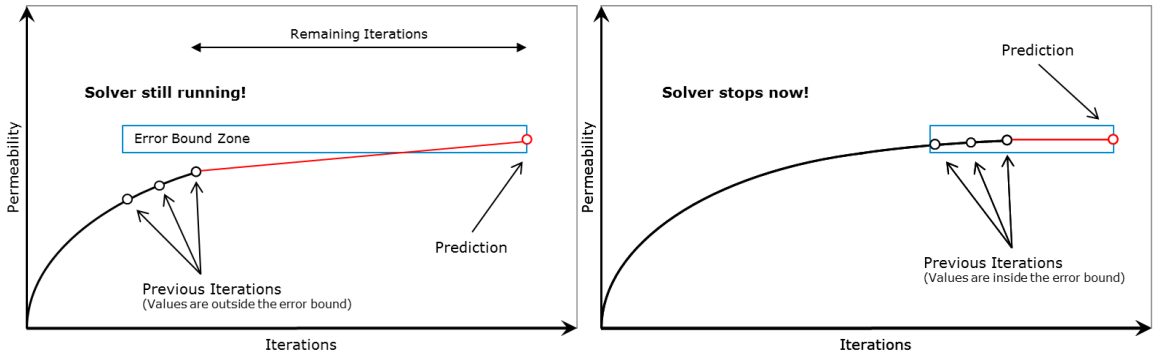
1. Start with some initial guess for the unknown values.
2. Improve the current values in each iterative step.
3. Repeat the iterative process until one of the stopping criteria (**Error Bound**, **Tolerance**, **Residual**, **Maximal Iterations** or **Maximal Run Time**) occurs.

For the EJ solver, select either **Tolerance** (recommended default) or **Residual** as stopping criterion. For the LIR solver, select **Error Bound** (recommended default) or **Tolerance** as stopping criterion.

Tolerance detects if the iterative process becomes stationary. This occurs when the change in the conductivity value from iteration to iteration becomes extremely small. If the relative change is smaller than the value entered for **Tolerance** the iteration is stopped.

When the **Residual** stopping criterion is used, the iteration is stopped if the solution satisfies the equation up to the required accuracy.

The default stopping criterion of the LIR solver, **Error Bound**, uses the result of previous iterations, and predicts the final solution based on linear and quadratic extrapolation. The solver stops if the relative difference regarding the prediction is smaller than the specified error bound. The stopping criterion recognizes oscillations in the convergence behavior and prevents premature stopping at local minima or maxima. A damped convergence curve is fit through the oscillating curve and the solver stops then regarding the damped convergence curve.



When the solver stops because the **Maximal Iterations** value or **Maximal Run Time** has been reached, no guarantee on the quality of solution can be given. Following possibilities might help:

- Check the corresponding .log file to see how large the residual values and conductivity increase are. If these values are already very close to the desired result, you may decide to use the current result.
- Double check the structure and parameter values. Unphysical parameters or too rough resolution of the structure (leading, e.g., to artificial unconnected components) can cause an iterative solver to fail.

Which stopping criterion has occurred, can be seen in the Result Viewer of the GeoDict result file (*.gdr) under the **Results Map** tab.

Restart Save Interval

The calculations run by the solvers can be restarted from saved intermediate result files and the interval between auto-saves can be configured from the value entered in **Restart Save Interval (h)**.

Parallelization

Depending on the purchased license, the simulation process can be parallelized.

The **Parallelization Options** dialog box opens when clicking the **Edit...** button, to choose between **Sequential**, **Parallel (Shared Memory)**, **Automatic Number of Threads**, and **Cluster** for EJ, and **Sequential**, **Parallel (Shared Memory)**, and **Automatic Number of Threads** for LIR.

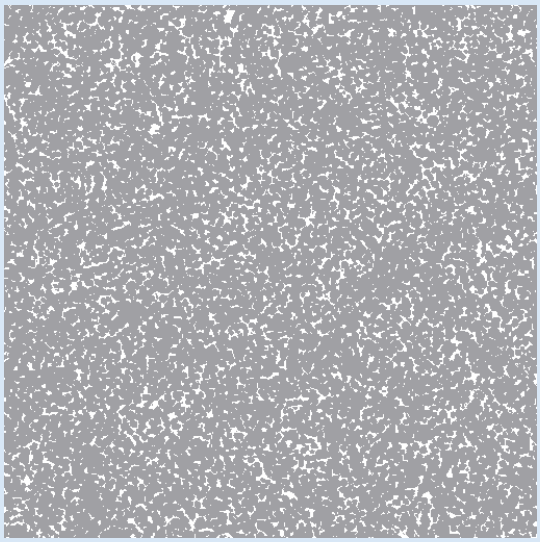
For details on how to set up und run parallel computations, consult the High Performance Computing chapter.

Parallelization Benchmark Results

Two examples of parallelization benchmark results for ConductoDict are shown here. Both benchmark computations were run on a server with 2xIntel E5-2697A v4 processors with 16 cores each, running with a maximum of 3.60 GHz, and 1024 GB RAM.

The first example is the computation of the electrical conductivity through a synthetic X-ray tomography data of a sandstone structure (Mattila et al. 2016 [47]).The structure has a porosity of 13.6% and a size of 2048x2048x2048 voxels.

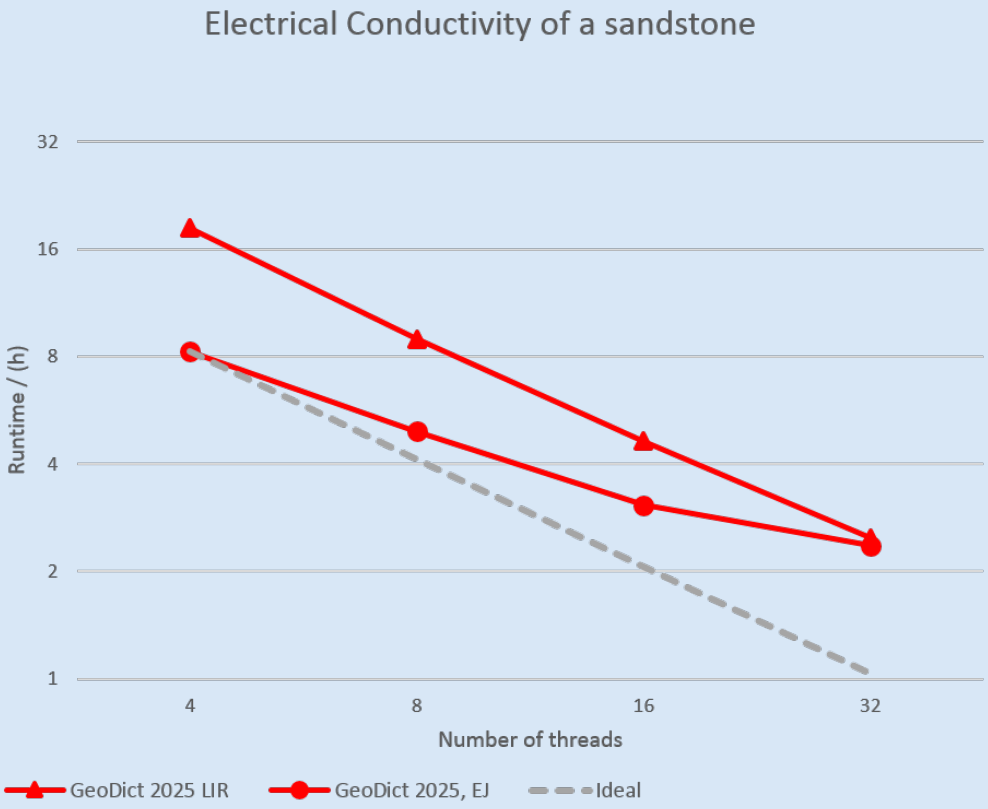
The electrical conductivity of the structure, for pores filled with brine, is computed with the EJ and the LIR solver. For sandstone, an electrical conductivity of 1e-08 S/m and for the brine of 5 S/m is used as input values.



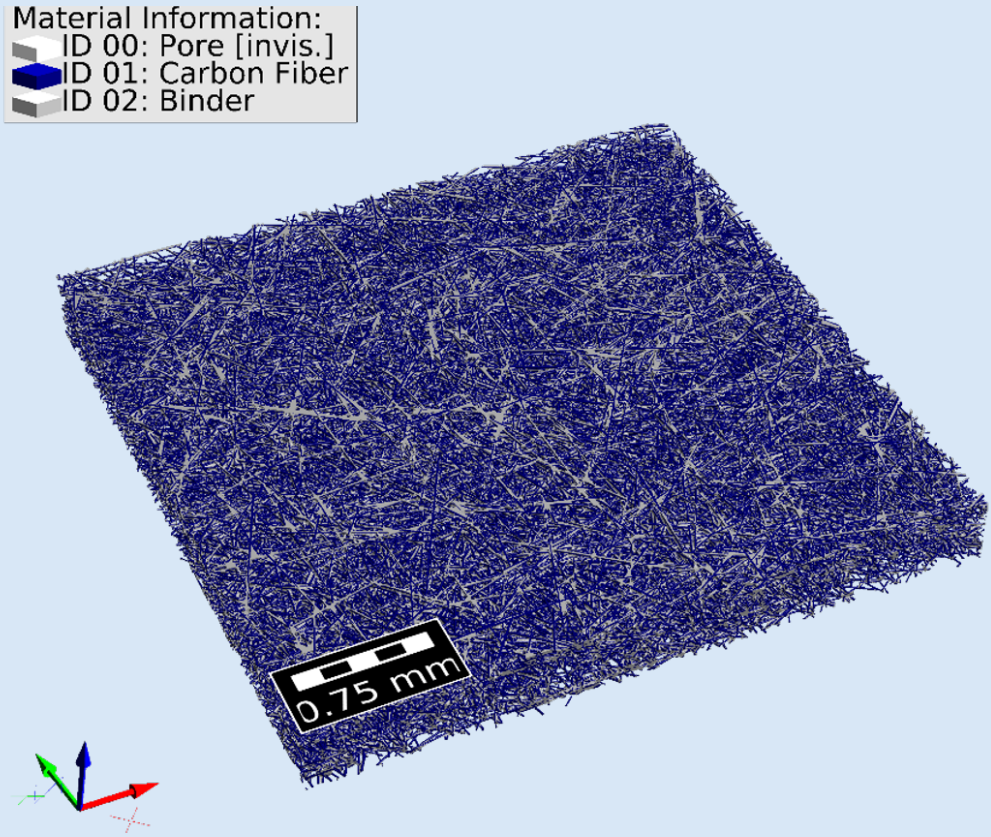
The following figure shows the runtime for a different number of processes to compute the electrical conductivity of the structure of 0.1137 S/m with an error bound of 0.001 for LIR and of 0.1135 S/m with a tolerance of 0.001 with EJ solver.

For both solvers, the ideal speedup, i.e., getting half of the runtime for twice the number of processes, is also shown. The speedup for LIR solver is close to the ideal one, which is usually not possible to reach for real life examples. The speedup of EJ differs more from the ideal one.

For both EJ and LIR, the performance in GeoDict 2025 is comparable to the one in GeoDict 2024. The memory requirement for this example is 233 GB when LIR is used with the option of speed optimization, and is 239GB when EJ is used.



The second benchmark is the computation of transverse isotropic thermal conductivity in a gas diffusion layer (GDL). The structure size is 4096x4096x512. A portion of the structure, of size 512x512x512 voxels, is shown in the figure below.



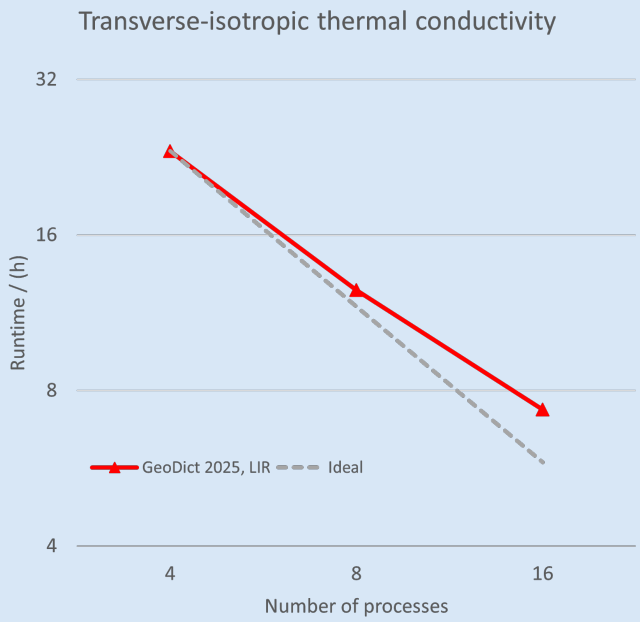
The synthetic GDL, created with GeoDict, consists of 7% carbon fibers and 4% binder.

The transverse isotropic thermal conductivity of 0.3 W/(mK) in both in-plane directions of the GDL and of 0.053 W/(mK) in through-plane direction is computed with the LIR solver with an error bound of 0.01.

The following thermal conductivities for the different materials of the structure where used as input for the computation.

Material	Thermal Conductivity W/(mK)
Fibers, in fiber direction	10
Fibers, orthogonal to fiber direction	2
Binder	1
Air	0.0257

Runtimes for a different number of processes are shown in the following figure. Again, the speedup of the LIR solver is close to the ideal one. For this example, LIR requires 259 GB memory.



Restart from *.gdr File

In some situations, it may be useful to re-use previously computed results and save a great amount of time by restarting the process from an existing GeoDict result file (*.gdr). Typical examples would be

- non-sufficient accuracy of some computation, when it is suspected that more iterations may improve the quality of the result,
- trying another boundary condition (e.g., Dirichlet instead of Periodic or other way around),
- continuing an iteration process,
- or using similar parameter values for the computation.

To restart and initialize the solver from a result file (*.gdr), check **Restart from .gdr File** and enter the name of a file, or **Browse** for it in the project folder.

When using **Restart From .gdr File** only the volume field (*.hht file) associated to the loaded *.gdr file will be used to continue the simulation.

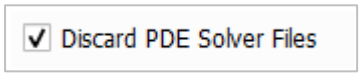
Important! The *.hht file is saved in the result folder of a previous run. Make sure that this file was not deleted from the results folder. If the *.hht file is not available the restart option cannot be used.

No other parameters from the options dialog will be loaded from the *.gdr file, but it is possible to load them by clicking **Load Parameters** in the Result Viewer. This way the simulation can be continued while using the same settings as in the initial simulation.

Important! The structure from the run of which you want to use the result file must be loaded into GeoDict. If this is not the case, an error message is displayed.

Discard PDE Solver Files

Checking **Discard PDE Solver Files** causes the deletion of all intermediate computation files, such as log files and flow field files.



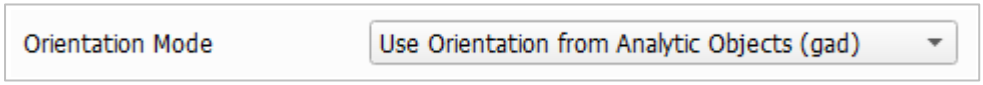
Only the content of the final GeoDict result file (*.gdr) is stored.

While having the benefit of saving hard disk storage place, discarding intermediate solver files has also the effect of disabling the 3D visualization of the results.

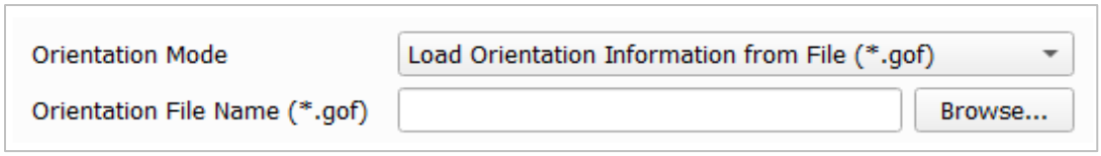
Orientation Mode (LIR only)

If one of the constituent materials has a non-isotropic material law, a local orientation is needed to compute the conductivity. There are three different choices how to determine the local orientation.

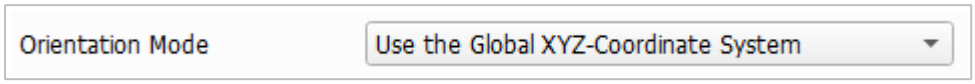
The standard case is to use the orientation defined by the local orientation of the GAD objects, e.g., the direction of a fiber (**Use Orientation from Analytic Objects (gad)**).



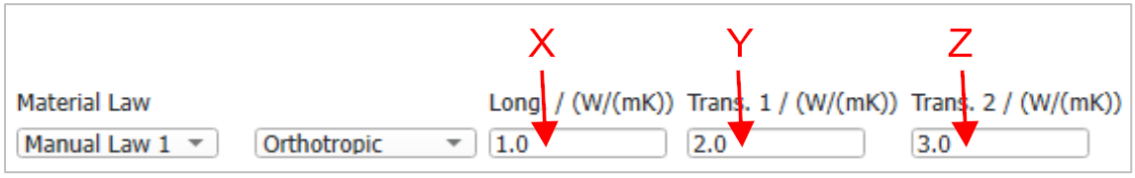
However, if the current structure was not generated using one of the structure generation modules, but imported from a 3D scan, GAD object information is not available. In such a case, the local orientation must be estimated from the image first, e.g., by using FiberFind or GrainFind. It is then possible to load the local orientation from a file generated by one of those modules, by selecting **Load Orientation Information from File (*.gof)**.



The last option is to simply **Use the Global XYZ-Coordinate System**.



In this case, the conductivities entered in the Constituent Materials tab are the conductivities in the X-, Y-, and Z-directions.

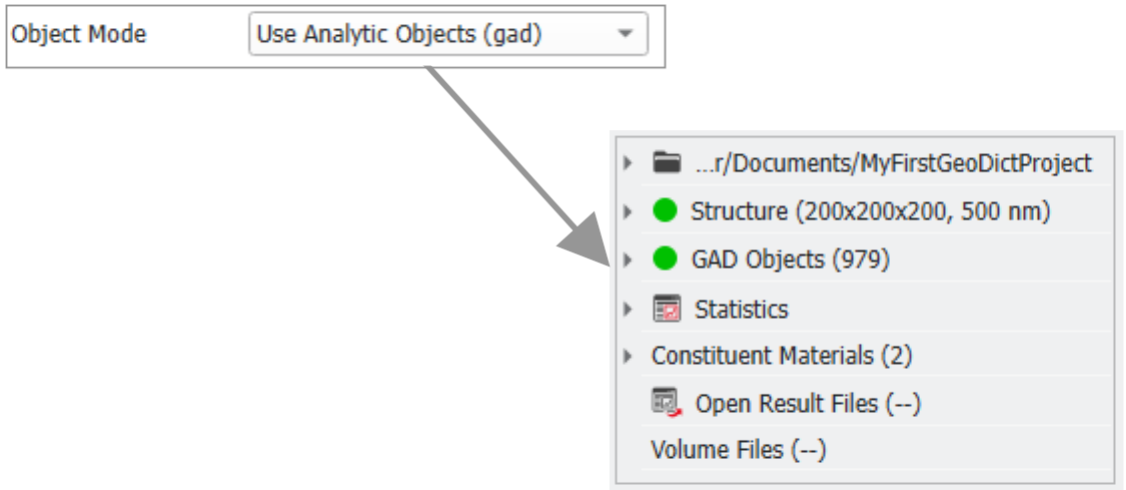


Object Mode

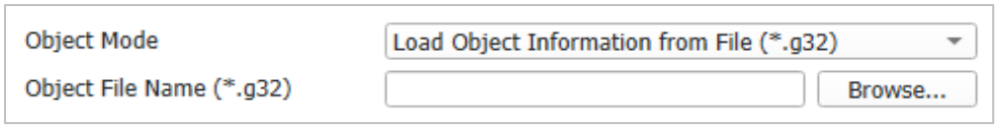
If contact resistances between objects of the same material have been set in the **Constituent Materials** tab, GeoDict must be able to distinguish between different objects of the same type. This can be done in two different ways.

The standard approach is to use the GAD information available for the current structure:

Such information is available if a green dot is shown in front of **GAD Objects** in the Project Status section (left side of the GUI).



A red dot might be shown if the current structure was not generated using one of the structure generation modules but imported from a 3D image. Then, GAD object information is not available, and the structure must be segmented into separate objects first, e.g., by using FiberFind or GrainFind. It is then possible to load the segmentation results from a file generated by one of those modules:



Note! The Object Mode is only required when the contact resistance is between the same Material IDs. No object information is necessary if all the contact resistances are between different Material IDs.

Write Heat Flux into Solution File

Additional 3D data can be added to the solution *.hht files for visualization or later analysis. With **Write Heat Flux into Solution File** the Heat Flux in the three coordinate directions is saved, allowing a detailed analysis of the field. The size of the result files and the memory requirements increase when selecting this option.

Advanced Options: Analyze Geometry

Checking **Analyze Geometry** performs an analysis of the geometry before the solver computations.

If no percolation path through the structure is found, the partial differential equation does not need to be solved, and a conductivity of 0.0 is directly reported as the solution.

Furthermore, the solver operates on the whole structure, regardless of which parts are connected or unconnected. However, unconnected components are not transport relevant, thus the effort of solving in these parts is not necessary.

For these reasons, a geometrical analysis is routinely run to determine whether a through path exists. After the analysis is finished, unconnected components are removed from the computational grid.

This may speed up the computations but requires some time for the geometrical analysis, especially for very large structures. So if you know beforehand that there are no unrelevant parts or that the structure has been processed to eliminate them, the geometry analysis can be switched off by unchecking **Analyze Geometry**.

Advanced Options: Write Compressed Volume Fields

The LIR solver uses a very memory efficient adaptive grid structure for the simulations.

If the option **Write Compressed Volume Fields** is checked, then the adaptive grid is used

as compression method for writing out *.hht files. This option allows to save 80-90% space on hard drive. The runtime for writing *.hht files is also reduced significantly. But the runtime for loading and uncompressing of compressed *.hht is increased by the amount of runtime that was saved for writing out compressed *.hht files.

If the option **Write Compressed Volume Fields** is not checked, then a usual regular grid is used for writing out *.hht files.

Advanced Options: Optimization Options

The **Multigrid Method** (see, e.g., Wesseling, 2004) was introduced to speed-up the computation and reduce the runtime significantly. The main idea of **Multigrid** is the usage of multiple coarser adaptive grids to speed up convergence behavior but requires only little more memory.

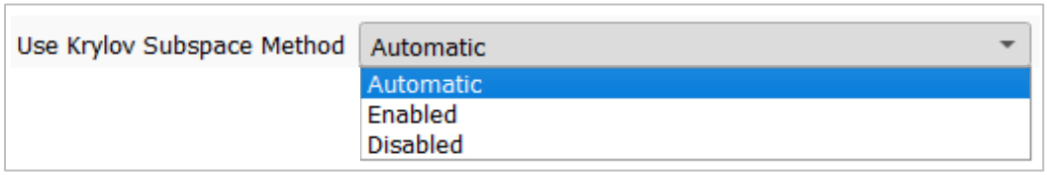
The method is available to solve the Stokes and Stokes–Brinkman equations as well as for solving mechanics, diffusion, thermal, and electrical conduction and is enabled by default.

Another speed-up option to accelerate the convergence behavior of the LIR solver is called **Krylov Subspace Method**.

The runtime of the LIR solver depends on many different properties of the structure and the simulation parameters. The BiCGStab algorithm is used, which can reduce the runtime for challenging simulation very drastically.

Note! Using the BiCGStab method approximately doubles the amount of RAM needed for the computation.

Unfortunately, the Krylov method is not always faster than a simulation without the Krylov method and therefore we introduced an **Automatic** mode which uses some heuristics to choose the most efficient method based on structure, material parameters, and boundary conditions automatically. Of course, it is possible to explicitly enable (**Enabled**) or disable (**Disabled**) the method.

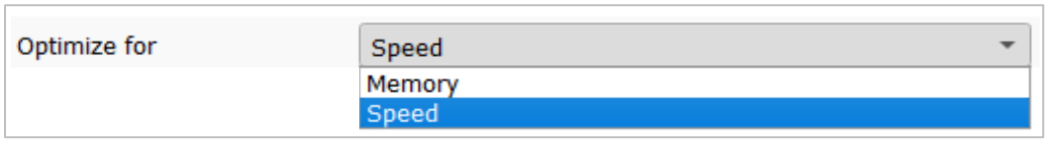


Note! In case that the Krylov subspace method (BICGStab) is used, the **Relaxation** may also be adapted automatically.

Depending on the material parameters and geometry of the structure, the underlying mathematical problem can vary in complexity, thus influencing the behavior of the solver. The more complex the problem is, the more stable the solver settings should be.

With the **Relaxation** number, the solver is adjusted from **Stable** (which results in higher number of iterations, slower time stepping, and longer solver run times), to **Fast**, which makes the solver run less iterations but implies the risk that the solver does not converge. The **Relaxation** is a parameter of the SOR method and must be between 0 and 2 to ensure convergence. For relaxation values smaller than one (<1.0), the simulation is more stable. For relaxation values larger than one (>1.0), the simulation converges faster.

The **LIR** solver can **Optimize for Speed** or **Memory**.



- If **Speed** is chosen, the solver constructs additional optimization structures. The runtime is decreased by up to 30% but requires up to 50% more memory compared to the other option.
- If **Memory** is chosen, the runtime is increased by up to 40% but the solver requires up to 50% less memory.

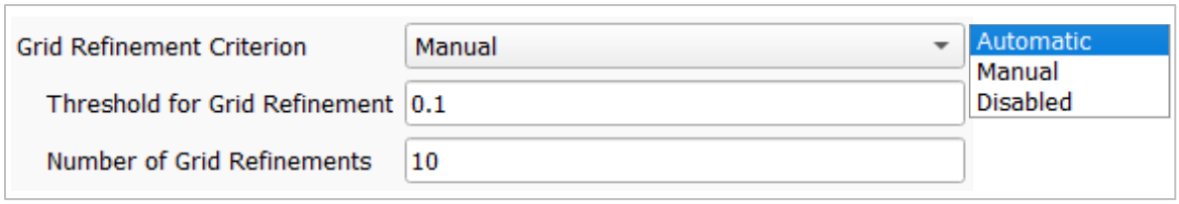
Advanced Options: Grid Options

The **Grid Type** decides what kind of tree structure is used for the simulation.

The default option is **LIR-Tree** and should always be used. The solver uses an adaptive grid structure called LIR-tree and needs up to 10 times less runtime and memory compared to the **Regular Grid** option.

The solver can analyze the result field during the computation and improves the adaptive grid in places where more accuracy is needed. The LIR solver splits cells where a high gradient occurs.

The solver refines the adaptive grid based on the computed fields. New cells are introduced at locations where higher accuracy is needed. Three settings are available here:

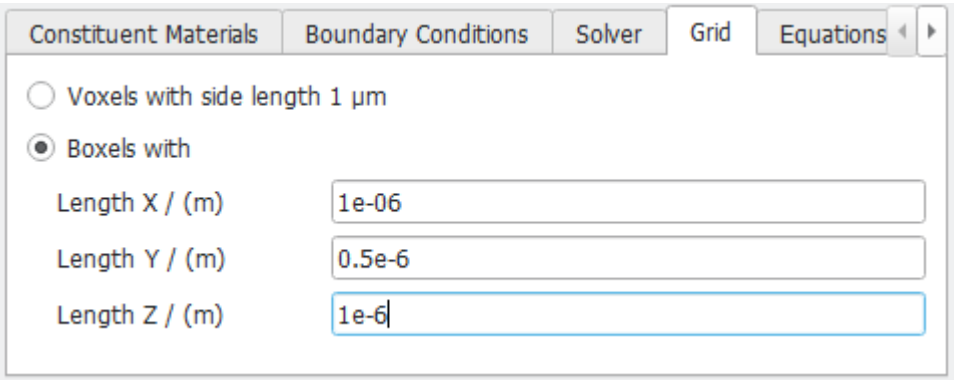


- **Automatic**: The computational cells are split when the difference in values between neighboring cells exceeds an automatically determined threshold. The solver automatically chooses all internal parameters based on the structure and simulation settings.
- **Manual**: The computational cells are split when the difference in values between neighboring cells exceeds the specified threshold. With this option you can specify the parameters **Threshold for Grid Refinement** and the **Number of Grid Refinements** manually. The **Threshold for Grid Refinement** must be between 0.0 and 1.0, while the recommended value range is between 0.05 and 0.1. The solver refines the grid at regions with high gradients and thus, the accuracy of the grid is enhanced in areas where it is necessary. Cells are split where the current gradient exceeds the **Threshold** multiplied by the maximum gradient. The **Number of Grid Refinements** is the maximum number of grid refinements that the solver can perform and should be between 1 and 10. The gradient-based grid refinement can increase the number of iterations, runtime, and memory requirements.
- **Disabled**: The grid refinement is turned off.

Know how! Grid Refinement can be neglected in most of the cases but should be used if a flow simulation is done on a structure with a very long inlet and outlet, for pleated filter structures, or for Navier-Stokes simulations.

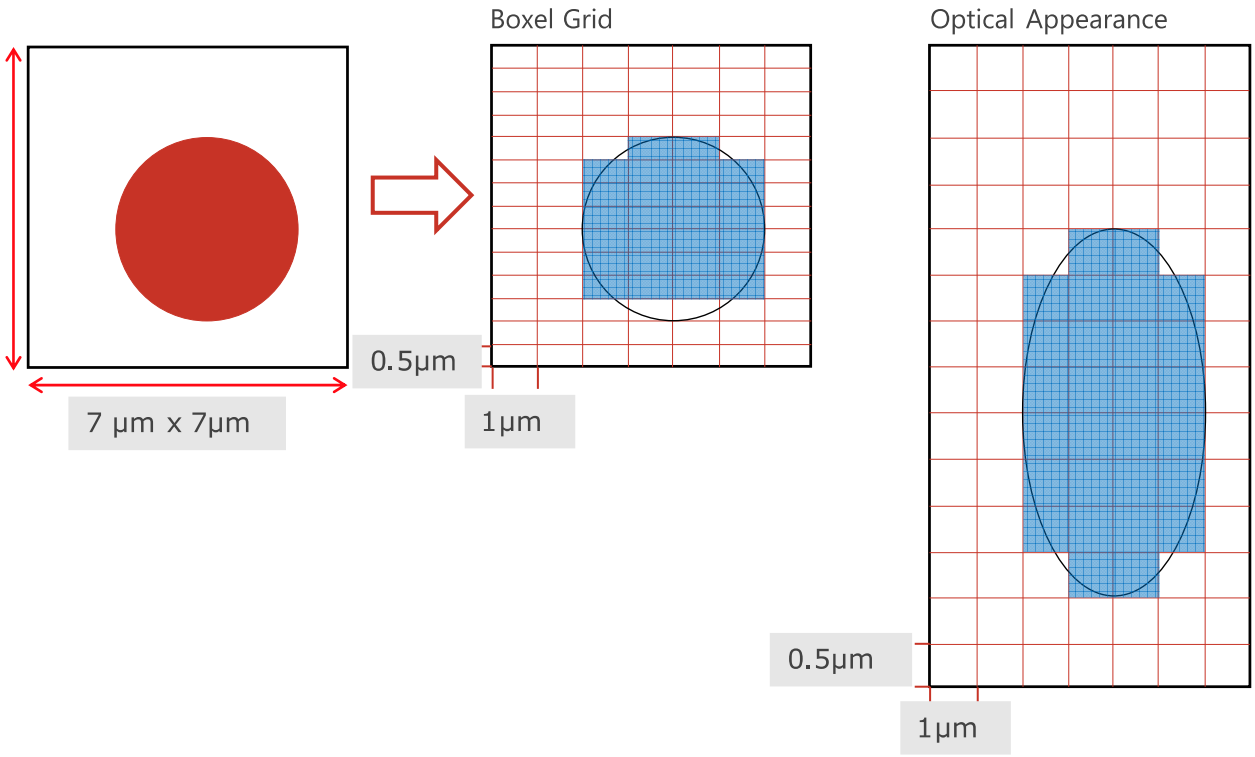
Grid

If **Boxels** (cuboid) instead of **Voxels** (cube) are used to resolve the structure, the boxel lengths can be set in the **Grid** tab.



Sometimes, grid lengths may be different in each direction, e.g., for Focused Ion Beam (FIB) images, the grid size in Z-direction is often different from the size in X- and Y-directions.

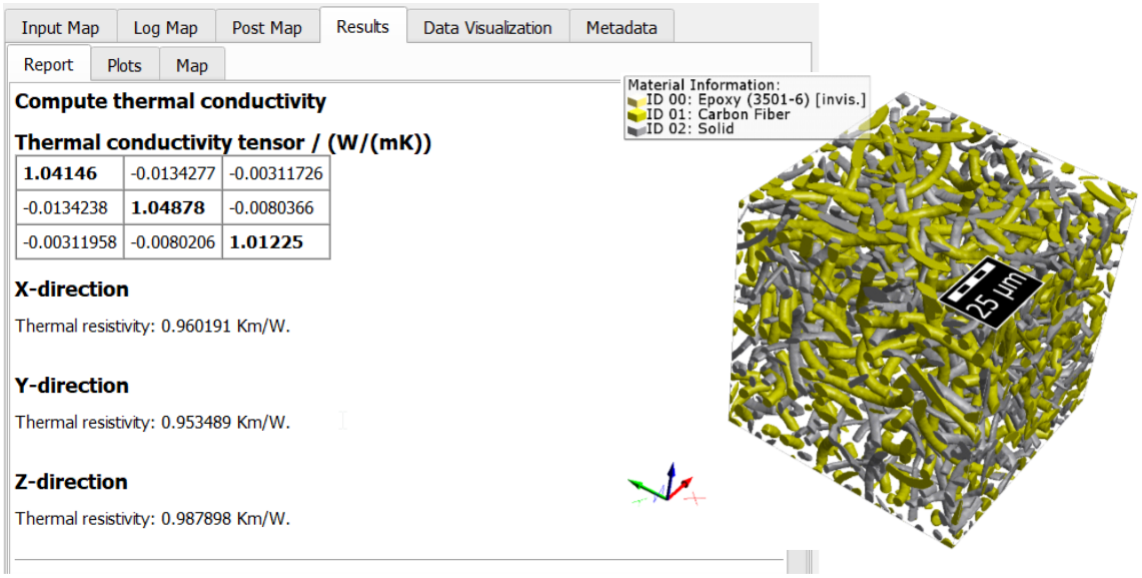
For example, a structure is sampled in a computational grid with different lengths in X- and Y-direction (e.g., LX = 2*LY). When the structure is loaded in GeoDict, each grid cell gets assigned 1 voxel and the visual representation of the structure looks stretched. To correct this effect, boxels set as, e.g., LX = 1 µm and LY = 0.5 µm, need to be chosen in the **Grid Size** panel.



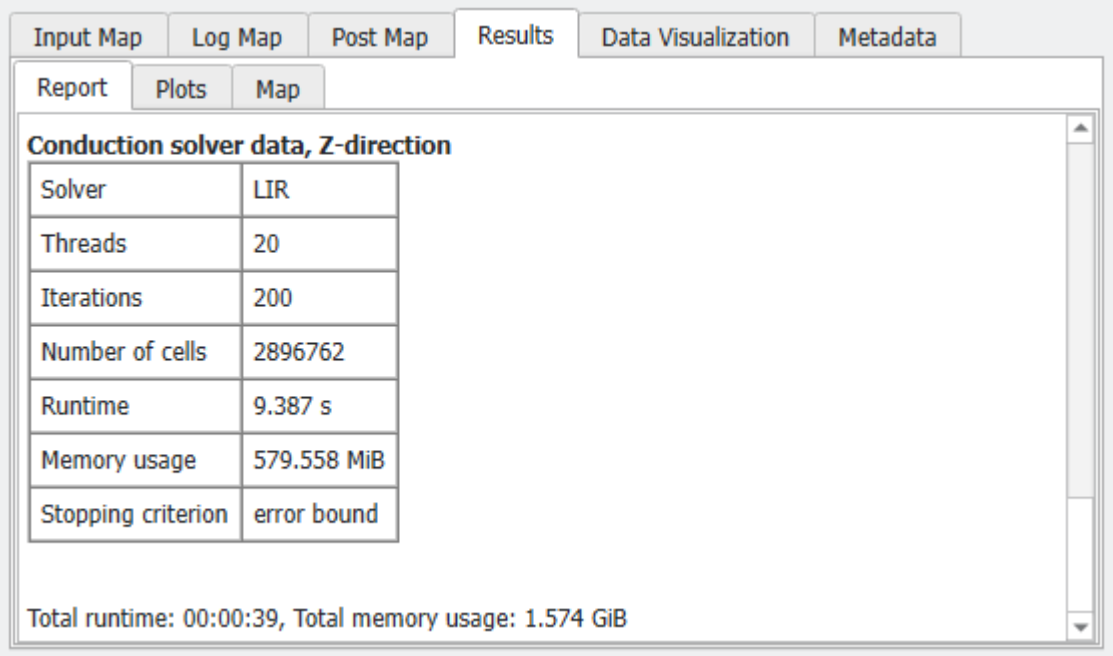
1.2.2 Results

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

The **Results - Report** sub-tab displays the computed Thermal Conductivity tensor.

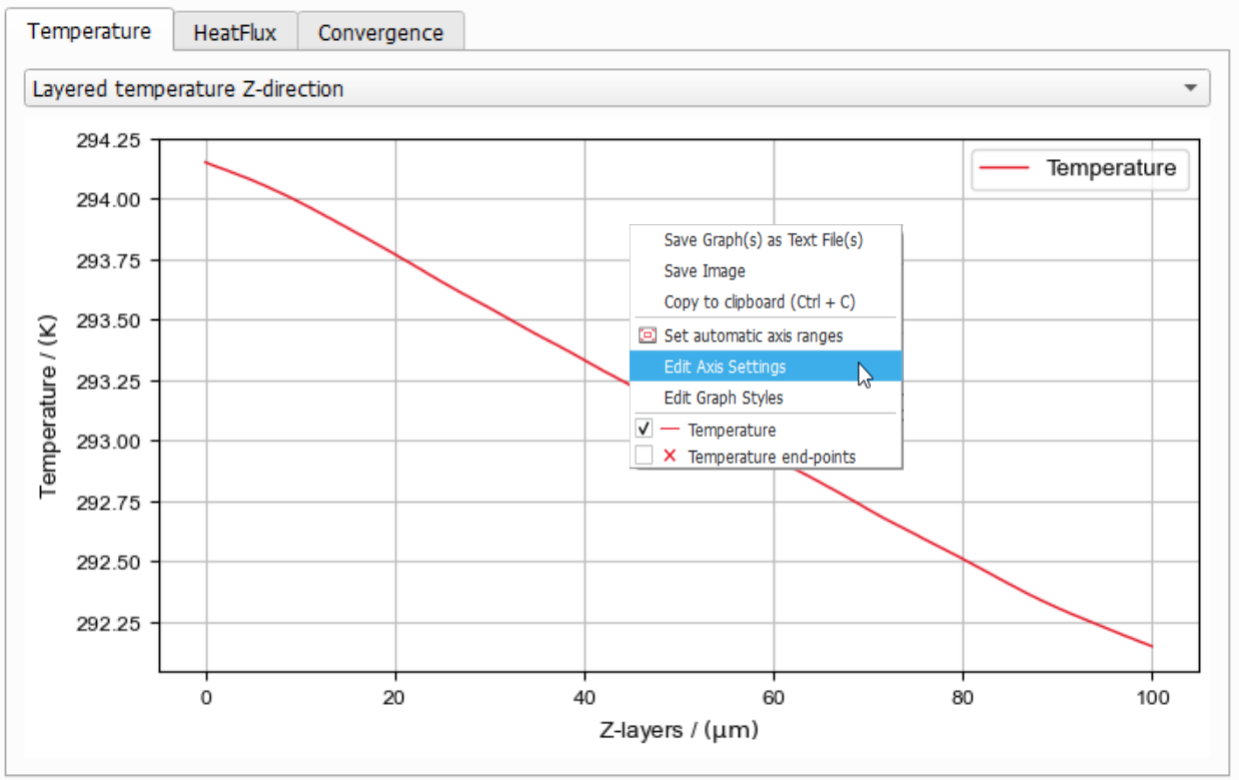


Also, for each computation, the solver, number of threads, number of iterations, number of cells (only for LIR), runtime, and stopping criterion are reported.



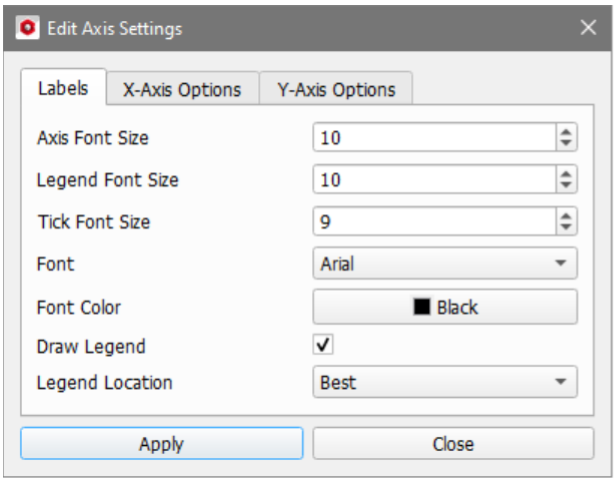
The **Results - Plots** sub-tab allows choosing different plots.

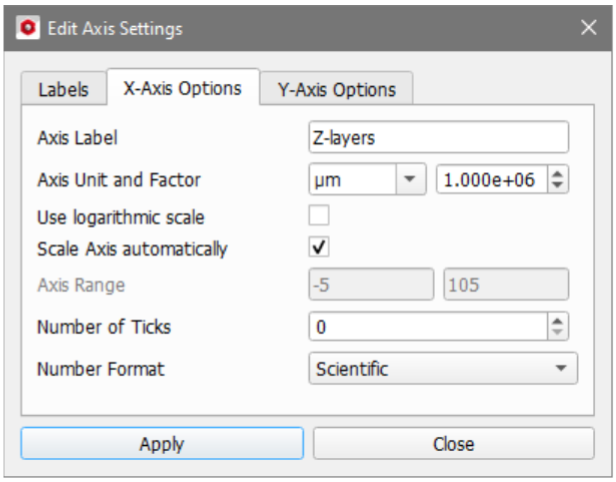
Under **Temperature**, the temperature gradient across the structure can be plotted. The plot shows on the y-axis the computed average temperature on each voxel layer.



Right clicking on the plot opens a small dialog box where you may choose to **Edit Axis Settings**.

In the dialog that appears, you may change the scale, ticks and labels of the X- and Y-axis manually, and set the position of the legend in the chart.

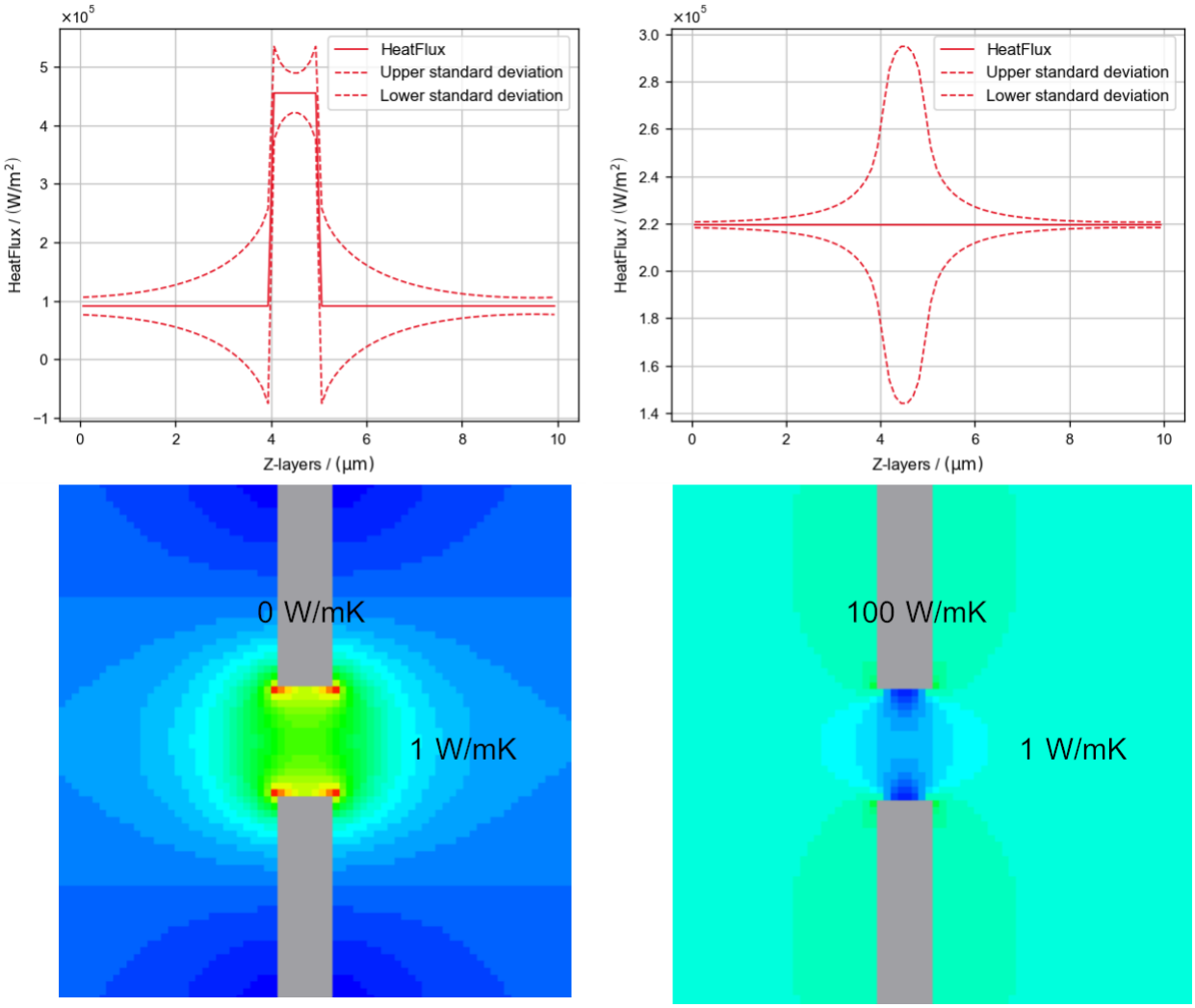




Under **HeatFlux,** the mean heat flux and the standard deviation in each layer is plotted.

When all parts of the structure are conducting (example on the right hand side), the mean current density is constant, and the standard deviation shows in which parts of the structure material with higher conductivity is accumulated.

If non-conducting materials are present (example on the left-hand side), the mean current density varies and shows where the bottlenecks are.



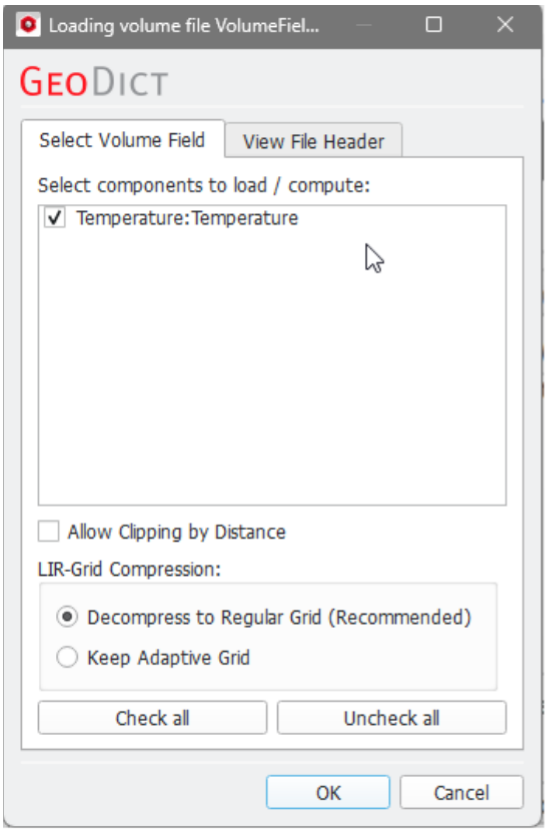
Under **Convergence**, the plot of the **Conductivity** at given **Iteration** values is charted for the selected directions. Selecting the direction from the pull-down menu, it is possible to see graphs of the convergence of the iterative solver for each of the computed directions.

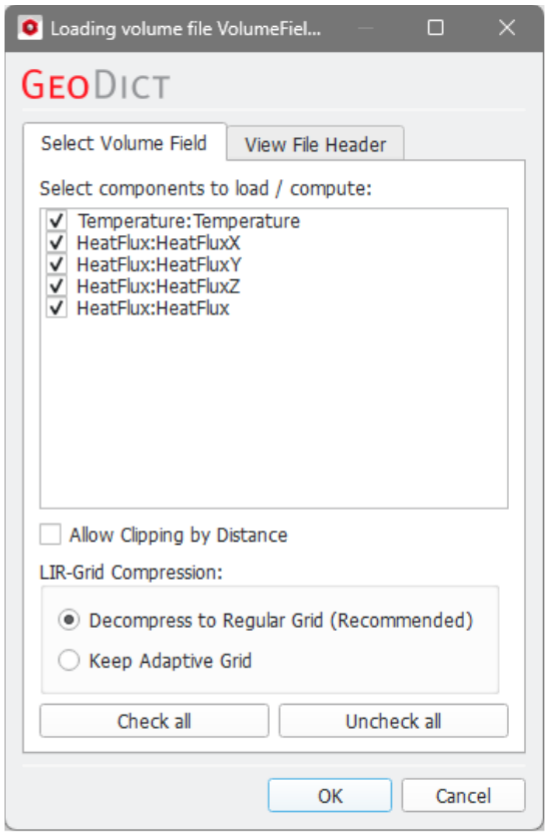
1.2.3 Data Visualization

Under the **Data Visualization** tab, the results of the thermal conductivity calculations can be graphically visualized in 2D-Cross section view or 3D-Rendering.

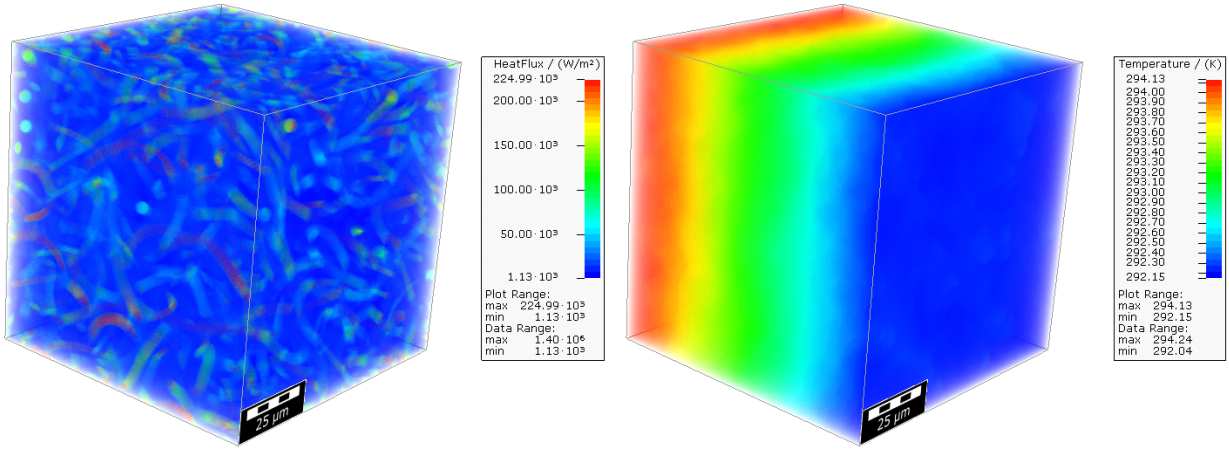
Directions that were selected when setting up the simulation were computed, and, thus, are available for visualization. Otherwise they are grayed out.

Click **Load** to load the computed temperature or heat flux field. If Write Heat Flux into Solution File 29 was not checked, only the **Temperature** volume field is available. Otherwise, the heat flux components can be loaded, too.





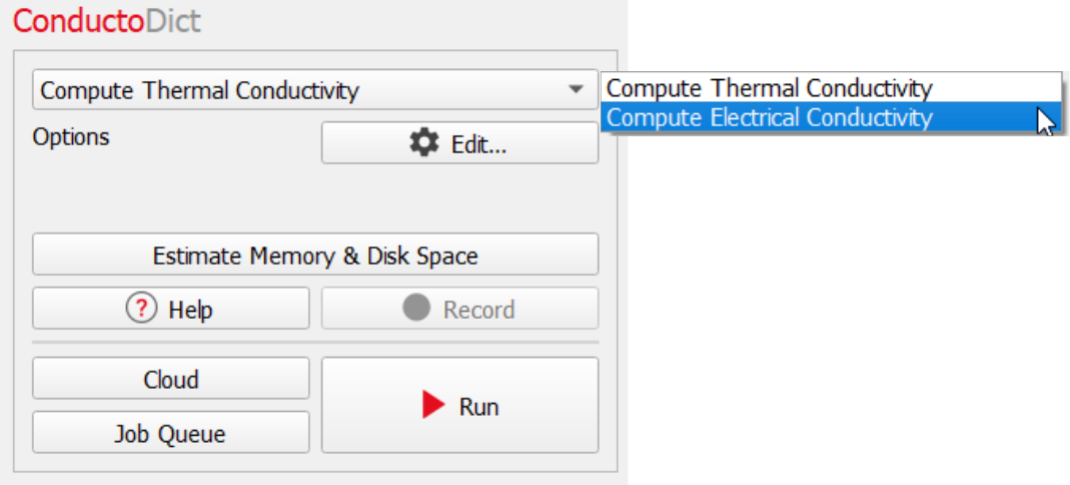
The loaded volume field then can be visualized. The options available for visualization of 3D scalar or vector fields are explained in detail in the Visualization chapter of this User Guide.



1.3 Compute Electrical Conductivity

Use **Compute Electrical Conductivity** to compute the electrical properties of composite or porous media, given the electrical conductivity of each constituent of the material.

To compute the electrical conductivity of a material, choose **Compute Electrical Conductivity** from the dropdown menu in the ConductoDict GUI.

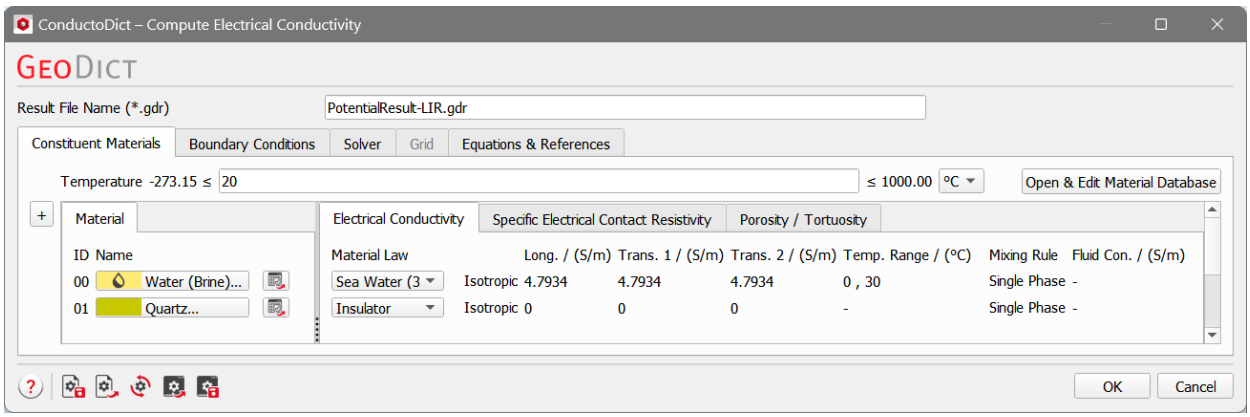


Topics of this section

- Input Parameters 38
  How to set the input parameters for Compute Electrical Conductivity command.
- Results 41
  How to understand the computed results.
- Data Visualization 45
  How to visualize the computed results.

1.3.1 Input Parameters

When **Compute Electrical Conductivity** is selected from the pull-down menu, clicking the **Edit...** button opens the **ConductoDict - Compute Electrical Conductivity** dialog.



Choose a name for the files containing the results of the computations according to your current project. The result files are saved in the project folder (**File** → **Choose Project Folder**, in the Menu bar).

An additional directory with this name is created to keep the intermediate computation files (PDE solver files) and the temporary computation files.

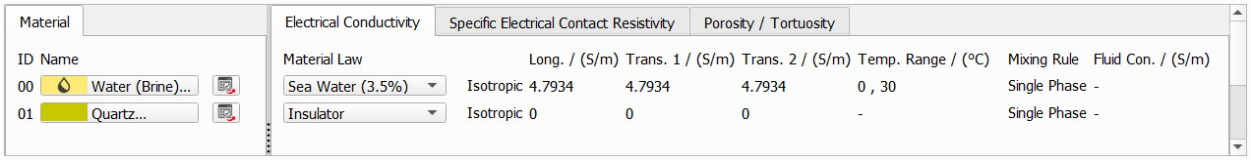
The parameters are organized under the **Constituent Materials**, **Boundary Conditions**, **Solver**, **Grid**, and **Equations & References** tabs.

Tabs of the ConductoDict-Compute Electrical Conductivity dialog

- Constituent Materials 39
  Specify the electrical properties of the constituent materials.
- Boundary Conditions 40
  Set the conditions at the boundaries of the structure.
- Solver 41
  Set the options used to control how heat problem is solved.
- Grid 41
  Decide whether voxels or boxels are used.

Constituent Materials

Under this tab, the constituent materials of the pore space/matrix and the structure material(s) can be chosen from the GeoDict Material Database or set by the users.



The parameters for **Constitute Materials** are divided into **Electrical Conductivity**, **Specific Electrical Contact Resistivity**, and **Porosity / Tortuosity**.

Electrical Conductivity

The electrical conductivity for each of the constituent materials needs to be specified for **Compute Electrical Conductivity**. More information on constituent materials can be found in the Material Database chapter.

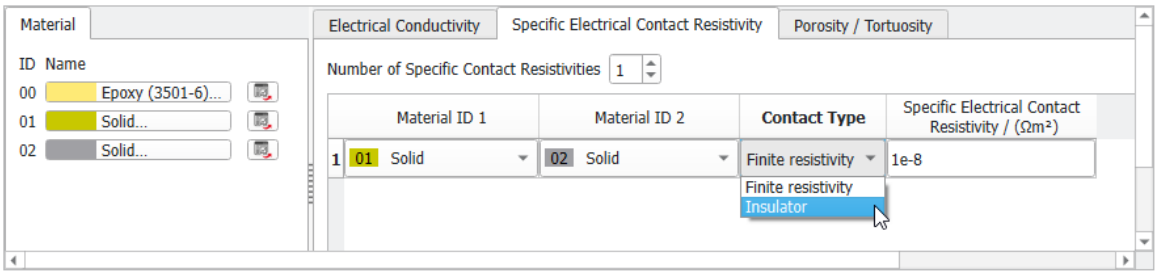
For every material, one of the material laws defined in the material database must be selected. For **Manual** defined materials, Isotropic, Transverse Isotropic or Orthotropic conductivity can be chosen from the pull-down menus. When Transverse Isotropic or Orthotropic is chosen, the EJ solver cannot be selected in the **Solver** tab, and the LIR becomes the only choice of the solver.

Specific Electrical Contact Resistivity

When contact resistances exist between different materials, enter the parameters in the **Specific Electrical Contact Resistivity** sub-tab.

First, choose the **Number of Specific Contact Resistivities**. This creates the desired number of rows in the input tab. There, select the materials for **Material ID 1** and **Material ID 2**, and set the value of the specific thermal contact resistivity between these two materials.

If the contact resistivity between the two materials has a finite value, then **Finite resistivity** should be chosen as the **Contact Type**. The contact can also be an insulator, which means the resistivity is infinite. Then **Insulator** is chosen and no value for **Specific Electrical Contact Resistivity** column is needed for the input.



Contact resistances can be applied between the same Material IDs as well as between different material IDs. If the same material ID is chosen for **Material ID 1** and **Material ID 2**, the contact resistance is applied only between different objects of the same color. There are two different ways how objects can be defined, for this see the description of the Object Mode 28 of this user guide chapter.

If there are no contact resistances, just leave the **Number of Specific Contact Resistivities** to be 0.

Porosity / Tortuosity

If there is no porous material present in the structure, but only pure solid or fluid, you do not need to set any parameters on the **Porosity / Tortuosity** tab. When there is porous material, the **Porosity**, **Tortuosity Factor of Pore-Space**, and **Has Solid Tortuosity** become selectable. When **Has Solid Tortuosity** is checked, the value of **Tortuosity Factor of Solid Phase** can also be given. When you go back to the **Electrical Conductivity** tab, the different options for **Mixing Rule** are visible to choose for the porous medium, too. The description of the different rules are found in Mixing Rules for Effective Properties of Porous Media 10.

The results of different mixing rules on an example of 1 x 1 x 1 structure is found in Porosity / Tortuosity 15 in the Compute Thermal Conductivity 12 section.

Boundary Conditions

The parameters have the same meaning as described on the Boundary Conditions 18 page of the **Compute Thermal Conductivity** command.

Solver

The parameters have the same meaning as described on the Solver 20 page of the **Compute Thermal Conductivity** command.

Grid

The parameters have the same meaning as described on the Grid 32 page of the **Compute Thermal Conductivity** command.

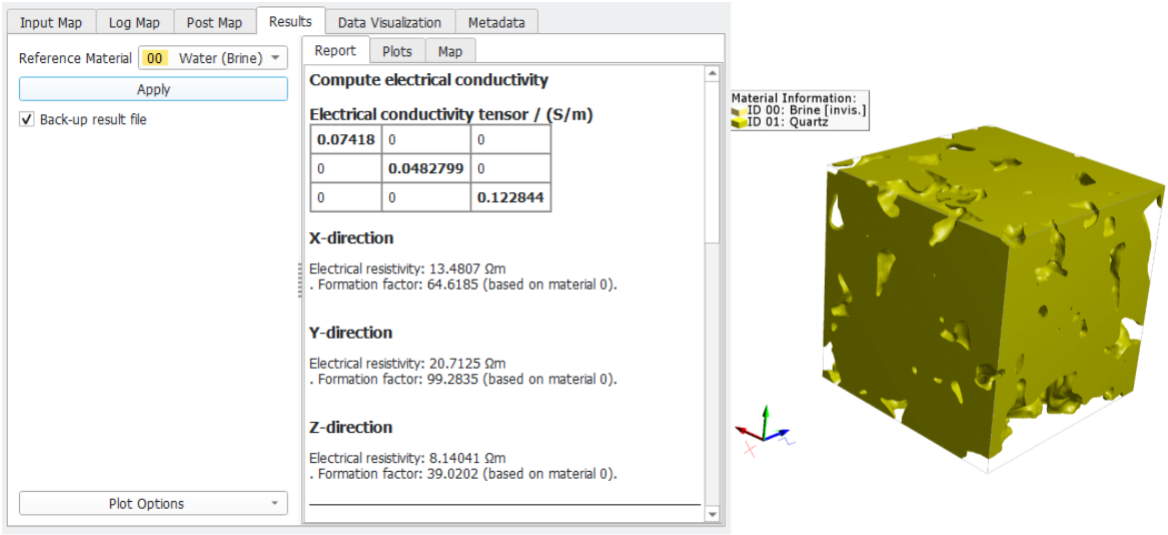
1.3.2 Results

The **Results - Report** subtab displays the computed Electrical Conductivity tensor.

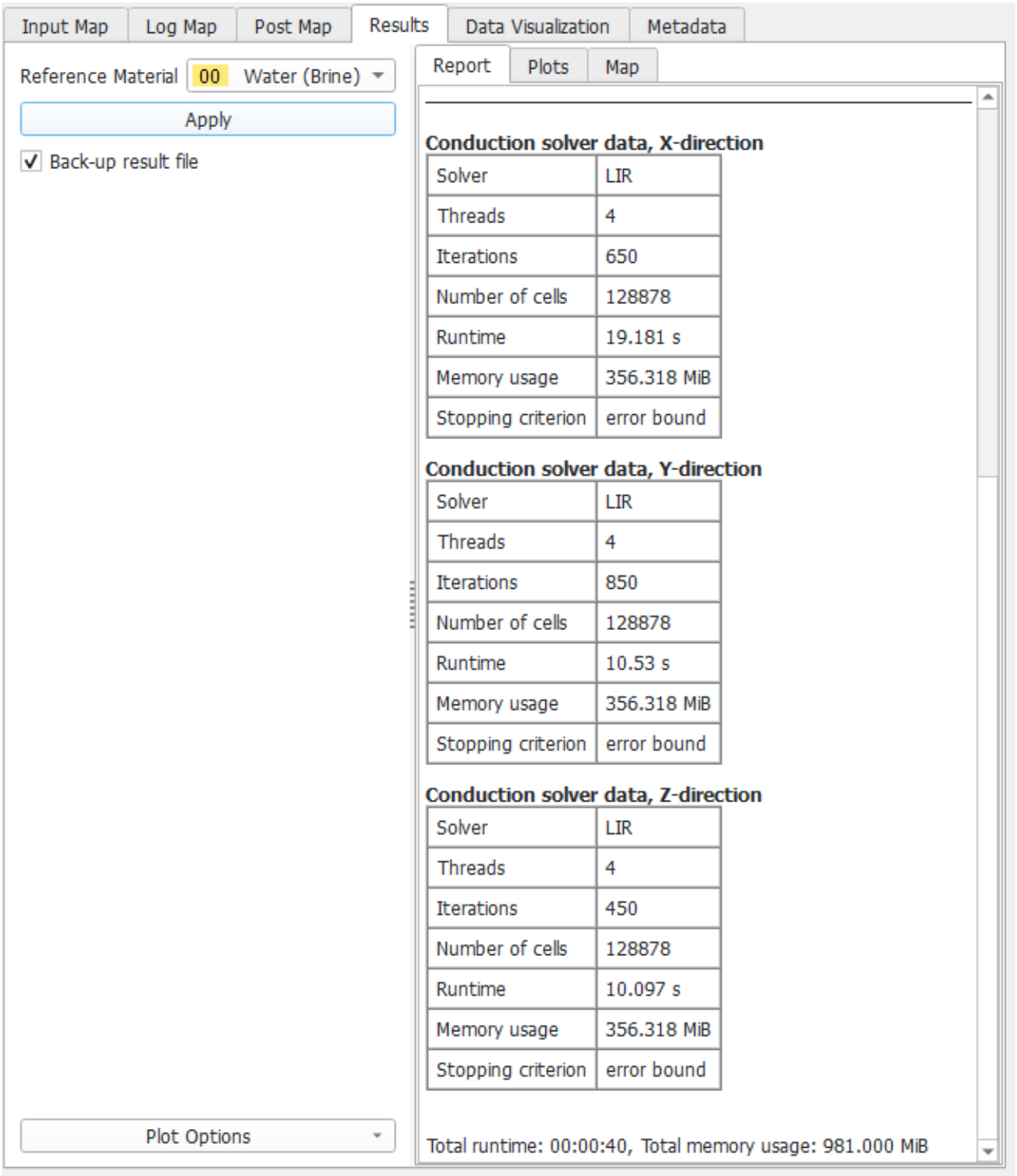
For each space direction, also the electrical resistivity is reported. It is the inverse of the electrical conductivity value in that space direction.

The formation factor is the conductivity of the **Reference Material** (brine in this example) divided by the computed conductivity in this space direction. The reference material can be set in the left part of the dialog.

For the computation of resistivities and formation factors only the diagonal entries of the tensor are taken into account.

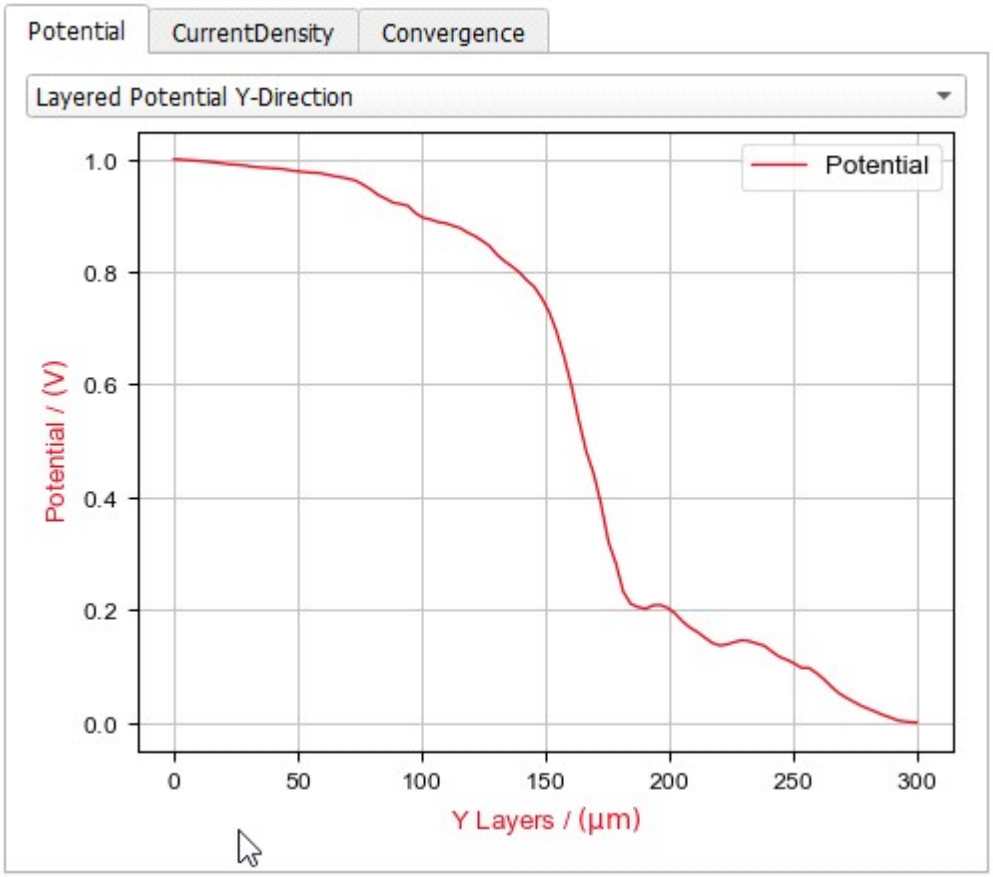


Additionally, for each computation, the number of iterations, runtimes, and stopping criteria applied are reported.

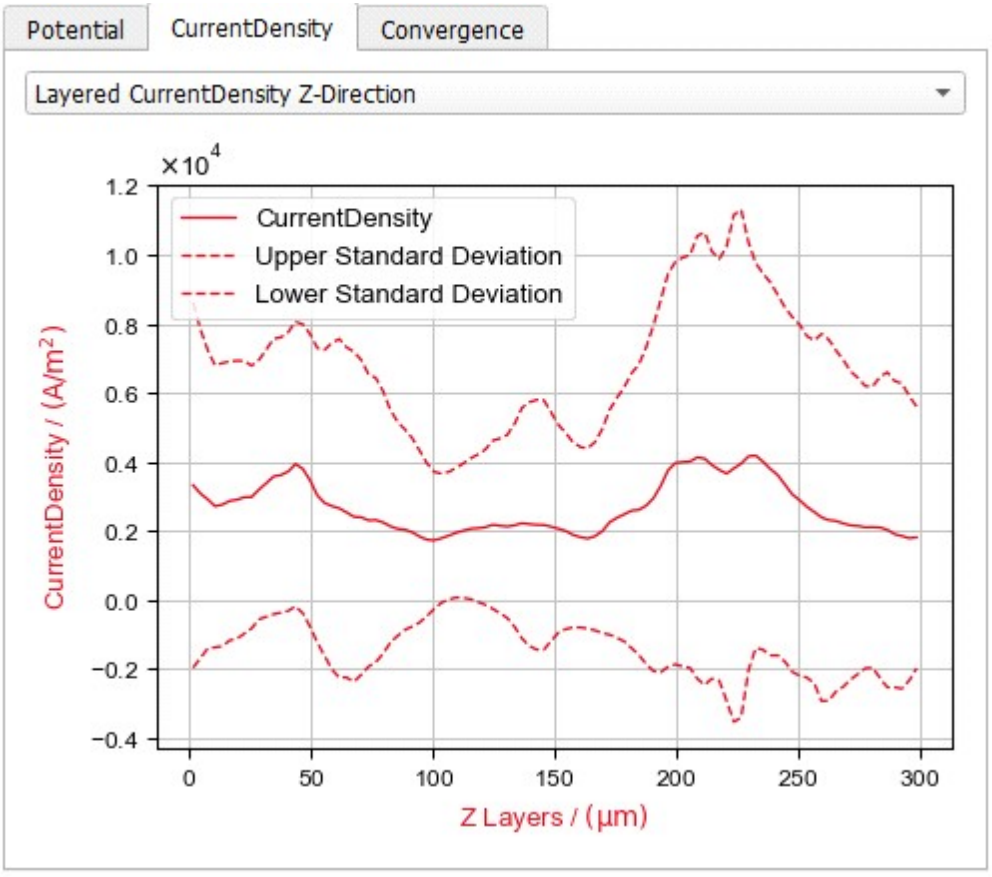


The **Results - Plots** subtab displays different graphs under tabs:

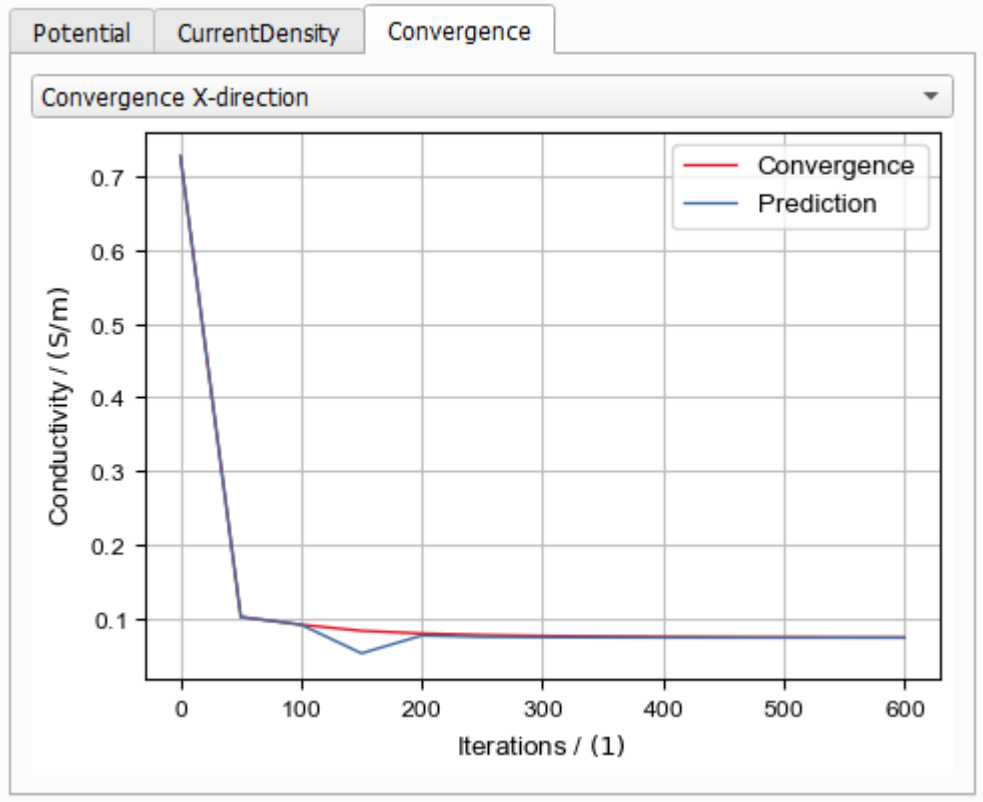
First, the **Potential** gradient across the structure (**Layered Potential X/Y/Z-Direction**).



Second, the mean **Current Density** with the standard deviation in each voxel layer. If non-conducting materials are present, the mean current density varies and shows where the bottlenecks are.



Third, under **Convergence**, the plot of the **Conductivity** at given **Iteration** values is charted for the selected directions. If the **LIR** solver is used, and **Error Bound** is used as stopping criterion, also the predicted conductivity is shown.

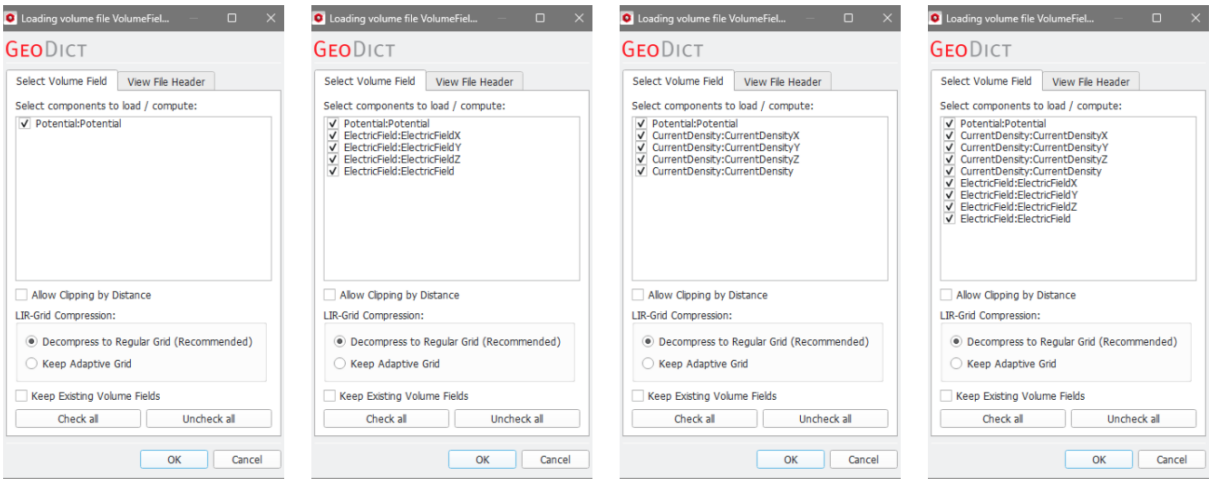


1.3.3 Data Visualization

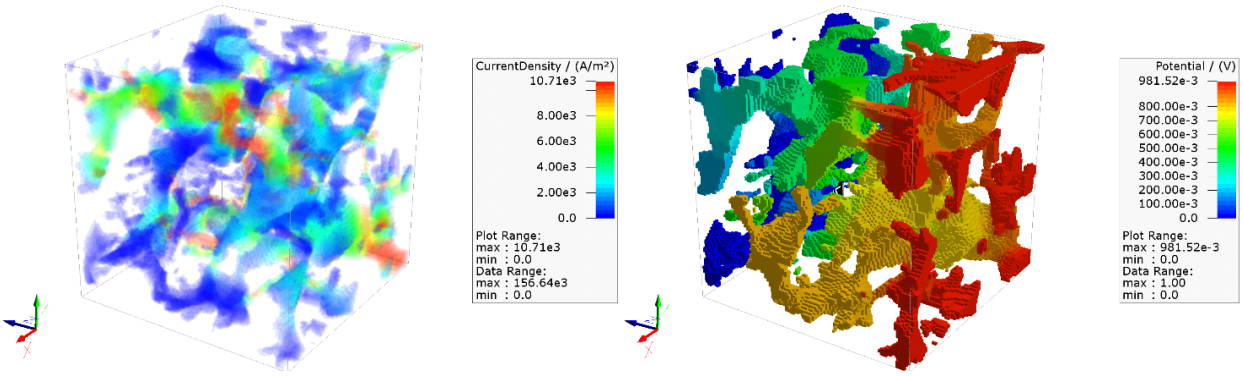
Under the Data Visualization tab, the results of the electrical conductivity calculations can be graphically visualized in 2D-Cross section view or (as shown here) in 3D-Rendering.

Directions that were selected when setting up the simulation were computed, and, thus, are available for visualization. Otherwise they are grayed out.

Click **Load** to load the computed potential or flux field. When **Write Electric Field into Solution File** and **Write Current Density into Solution File** were not checked prior to computation, only the volume field for **Potential** is available for loading. If one of them are chosen, the volume field for electric field or current density are shown below the potential. When both are selected, all the volume field components can be loaded.



The loaded volume fields can be visualized. The options available for visualization of 3D scalar or vector fields are explained in detail in the Visualization chapter of this User Guide.



1.4 References

J. Becker, R. Flückiger, M. Reum, F. Büchi, F. Marone, and M. Stampanoni, *Determination of Material Properties of Gas Diffusion Layers: Experiments and Simulations Using Phase Contrast Tomographic Microscopy*, Journal of The Electrochemical Society, Vol. 156, No 10, pp B1175-B1181 (2009), https://dx.doi.org/10.1149/1.3176876

J. Becker, V. Schulz, and A. Wiegmann, *Numerical Determination of Two-Phase Material Parameters of a Gas Diffusion Layer Using Tomography Images*, Journal of Fuel Cell Science and Technology, No. 2, Vol. 5, pp 21006-21014 (2008), https://doi.org/10.1115/1.2821600

A.K. Hasselström, and U.E. Nilsson, *Thermal Contact Conductance in Bolted Joints* (2012)

J.P. Holman, *Heat Transfer*, 8th Edition (1997)

N. Jeanvoinea, A. Velichko, C. Selzner, and F. Mücklich, *Nanotomography of electrical contacts - new insights by high resolution 3D analysis of local material degradation*, Eur. Phys. J. Appl. Phys. 49, 22907 (2010), https://doi.org/10.1051/epjap/2009210

Mattila et al., *A prospect for computing in porous material research: very large fluid flow simulations*, Journal of Computational Science 15, pp. 62-76 (2016)

A. Pfrang, D. Veyret, F. Sieker, and G. Tsotridis, *X-ray computed tomography of gas diffusion layers of PEM fuel cells: Calculation of thermal conductivity*, International Journal of Hydrogen Energy, 35, No.8, pp 3751-3757 (2010), https://doi.org/10.1016/j.ijhydene.2010.01.085

V.P. Schulz, P.P. Mukherjee, J. Becker, A. Wiegmann, and C.Y. Wang, *Modeling of Two-phase Behavior in the Gas Diffusion Medium of Polymer Electrolyte Fuel Cells via Full Morphology Approach*, Journal of the Electrochemical Society, Issue 4, Vol. 154, pp B419-B426 (2007), https://dx.doi.org/10.1149/1.2472547

H. Thoemen, T. Walther, and A. Wiegmann, *3D Simulation of Macroscopic heat and mass transfer properties from the microstructure of wood fibre networks*, Composites Science and Technology, No. 3-4, Vol. 68, pp 608-616 (2008), https://doi.org/10.1016/j.compscitech.2007.10.014

A. Velichko, *Quantitative 3D characterization of graphite morphologies in cast iron using FIB microstructure tomography*, Dissertation, Saarland University (2008), http://dx.doi.org/10.22028/D291-22506

A. Velichko, A. Wiegmann, and F. Mücklich, *Estimation of the effective conductivities of complex cast iron microstructures using FIB-tomographic analysis*, Acta Materialia, Vol. 57, pp 5023-5035 (2009), https://doi.org/10.1016/j.actamat.2009.07.004

D. Veyret and G. Tsotridis, *Numerical determination of the effective thermal conductivity of fibrous materials. Application to proton exchange membrane fuel cell gas diffusion layers*, Journal of Power Sources Vol. 195, No. 5, pp 1302-1307 (2010), https://doi.org/10.1016/j.jpowsour.2009.09.028

A. Wiegmann and A. Zemitis, *EJ-HEAT: A Fast Explicit Jump Harmonic Averaging Solver for the Effective Heat Conductivity of Composite Materials*, Report of the Fraunhofer ITWM, Nr. 94 (2006)

N. Zamel, X. Li, J. Shen, J. Becker, and A. Wiegmann, *Estimating effective thermal conductivity in carbon paper diffusion media*, Chemical Engineering Science, Vol 65, Issue 13, pp 3994-4006 (2010), https://doi.org/10.1016/j.ces.2010.03.047

Citation: Math2Market GmbH, 2026: GeoDict 2026 User Guide, ConductoDict, Math2Market GmbH, Germany, doi.org/10.30423/userguide.geodict

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