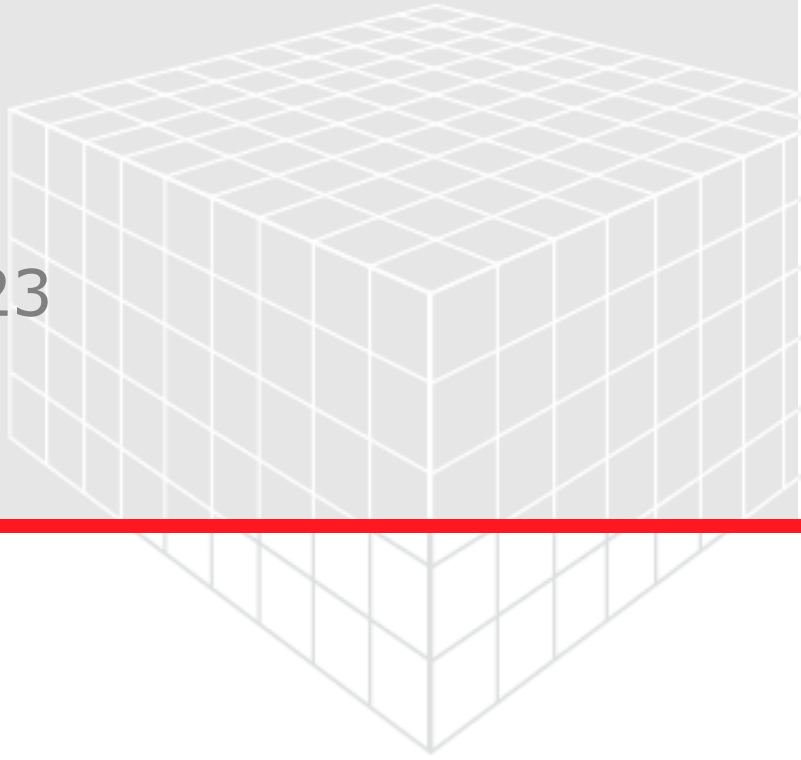
ConductoDict



User Guide

GeoDict release 2023

Published: November 28, 2022

GeoDict

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

Citation:
Jürgen Becker, Liping Cheng, Barbara Planas. GeoDict 2023 User Guide. ConductoDict Handbook. Math2Market GmbH, Germany, doi.org/10.30423/userguide.geodict

The handbooks in the User Guide series of Math2Market GmbH can be obtained from:

Math2Market GmbH
Richard-Wagner-Strasse 1
67655 Kaiserslautern
Germany

Phone: +49 631 205 605 0
Fax: +49 631 205 605 99
Email: info@math2market.de
Web: www.math2market.de

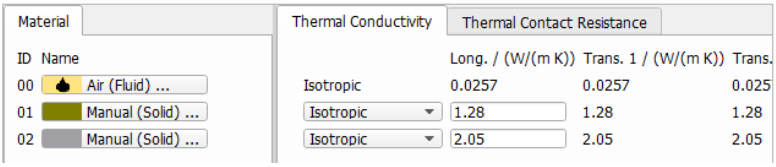
COMPUTING EFFECTIVE THERMAL AND ELECTRICAL CONDUCTIVITY

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 user enters the thermal conductivity of the constituent materials, the direction(s) of conduction, and the contact resistances 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



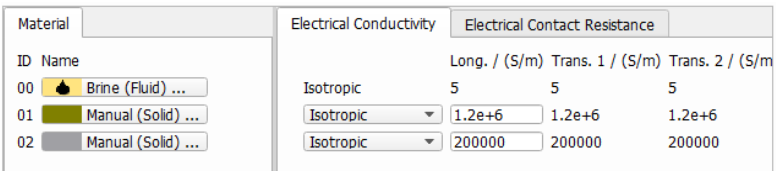
Output

Thermal Conductivity / (W/mK)

0.062441	-0.00110252	-0.000350964
-0.00110252	**0.0632144**	-0.000674321
-0.000350963	-0.000674323	**0.0604864**

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

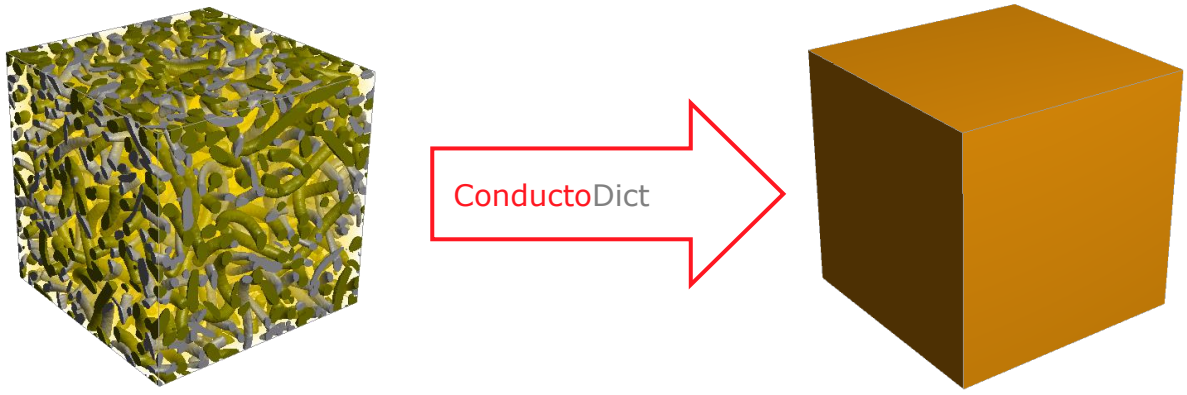
Input



Output

Electrical Conductivity / (S/m)

237.698	4.65782	0.843868
4.84093	**194.342**	26.0438
3.119	40.4392	**321.997**



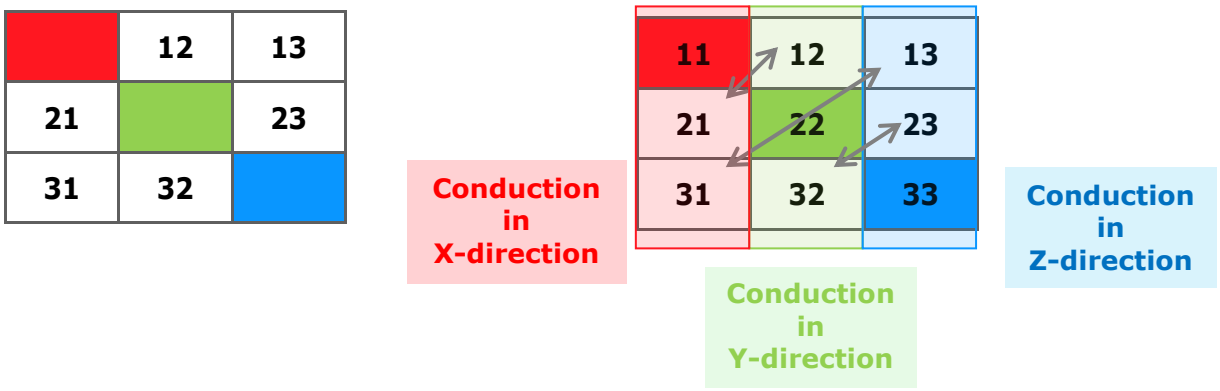
UNDERSTANDING THE CONDUCTIVITY TENSOR VALUES

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.

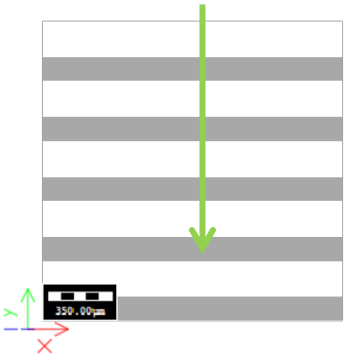
The off-diagonal tensor values reflect the symmetry of the composite material and the orientation with respect to the direction of conduction.



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.

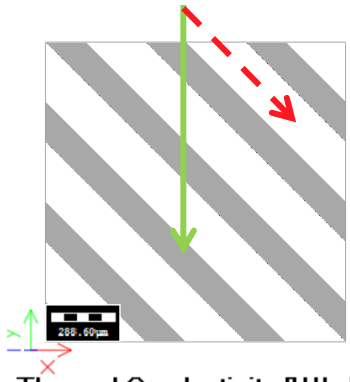
For example, when calculating conduction in the Y-direction (and not in the X-, or the Z-direction) the following may occur:



Thermal Conductivity [W/mK]

unknown	0	unknown
unknown	**1.15385**	unknown
unknown	0	**unknown**

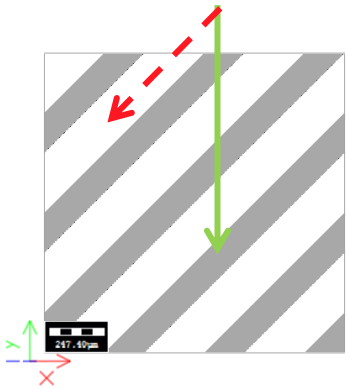
The off-diagonal values are zero when the conduction in the Y-direction does not have a component in another direction, i.e. no conduction occurs in the secondary direction due to the conductivity of the constituent materials and/or their orientation in the structure.



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 [W/mK]

unknown	0.0227739	unknown
unknown	**1.17662**	unknown
unknown	0	**unknown**



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

Thermal Conductivity [W/mK]

unknown	-0.0227739	unknown
unknown	**1.17662**	unknown
unknown	0	**unknown**

Theoretical basis of Effective Conductivity computation

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 k 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.

$$\dot{\boldsymbol{q}} = -K\nabla T \tag{1}$$

where $\dot{\boldsymbol{q}}$ is the heat flux, T is the temperature, and K is the thermal conductivity [W/mK, Watts per meter Kelvin]. In general, thermal conductivity is a second order tensor

$$K = \begin{pmatrix} k_{11} & k_{12} & k_{13} \\ k_{21} & k_{22} & k_{23} \\ k_{31} & k_{32} & k_{33} \end{pmatrix} \tag{2}$$

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 computes the effective (homogenized) thermal conductivity tensor of a structure. Each material within the structure is characterized by a scalar thermal conductivity. The resulting material is in general anisotropic and a conductivity tensor is needed to prescribe complete thermal behavior. The constituent materials can be with **isotropic**, **transverse isotropic** or **orthotropic** conductivity.

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.

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 $\boldsymbol{j}$:

$$\boldsymbol{j} = -\sigma\nabla\varphi \tag{3}$$

See: Electrostatics

Ohm's law is the electrical analogue of Fourier's law. Similar to the thermal conductivity and for isotropic materials, the electrical conductivity is constant in all

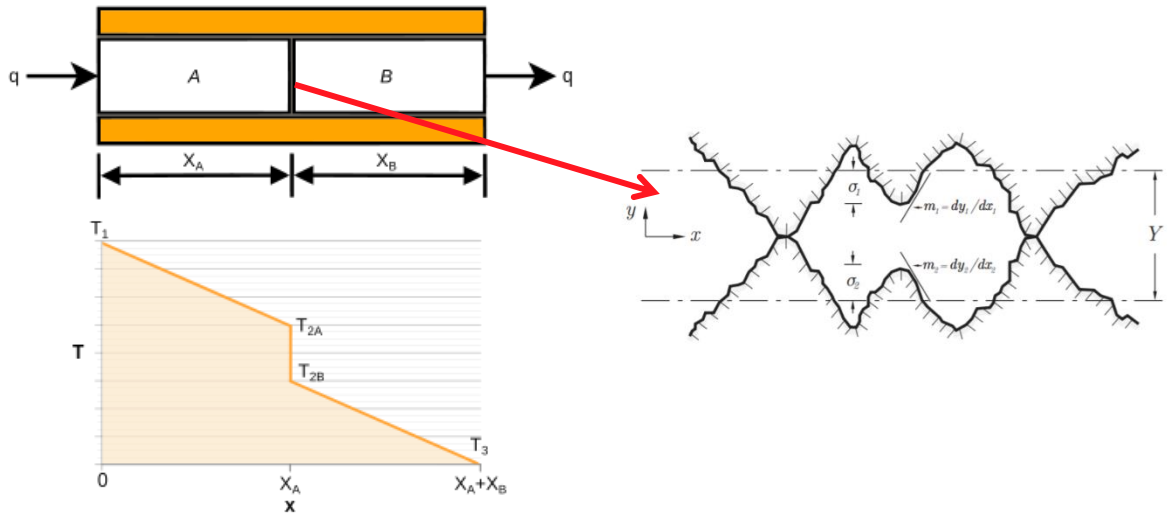
directions and can be characterized by a scalar. For anisotropic materials, σ is a tensor.

The algorithm in ConductoDict [1] 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 [2] , of cast iron microstructures ([5], [6]), of the gas diffusion layer in fuel cells ([3], [4], [7], [8], [10], [11]) and electrical conductivity of Ag/SnO_2 [9].

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 [12], [13].

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:

$$q = h_c \Delta T_c \tag{4}$$

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

$$R_c = \frac{1}{h_c} \tag{5}$$

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

$$q = \frac{T_1 - T_3}{\frac{\Delta x_A}{k_A} + R_c + \frac{\Delta x_B}{k_B}} \tag{6}$$

CONDUCTODICT COMPUTATIONS

ConductoDict computes the thermal or electrical properties of composite or porous media, given the thermal or electrical conductivity of each constituent of the material.

The computation of effective conductivity properties of a material with ConductoDict is done following these steps:

1. Generate a 3D-material model of a structure with a GeoDict generator or use a 3D-material model obtained from importing µCT or FIB/SEM 3D-image data.
2. Select ConductoDict from the menu bar (**Predict** → **ConductoDict**) and
   a. Choose the appropriate command (Compute Thermal Conductivity or Compute Electrical Conductivity),
   b. Set the solver options,
   c. Run the effective thermal or electrical conductivity properties computation,
   d. Analyze the results.

MATERIAL STRUCTURES FOR CONDUCTODICT

A variety of materials can be used as input for ConductoDict computations.

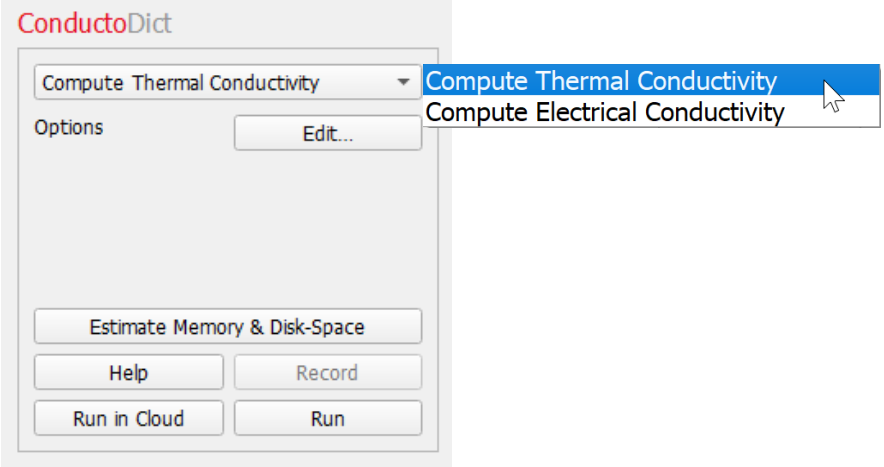
The constituent materials can be isotropic, transverse isotropic or orthotropic. Including the matrix or pore material, GeoDict handles structures with up to 256 different constituents. Specific constant resistivity can be used for both **Compute Thermal Conductivity** and **Compute Electrical Conductivity**.

Porous materials with one or more phases having zero conductivity (insulating materials) can also be used for ConductoDict computations.

For more examples of structures, see References, in particular [1], [8], and [11].

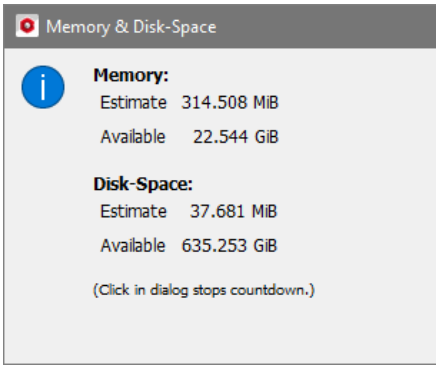
CONDUCTODICT GRAPHICAL USER INTERFACE

Start ConductoDict by selecting **Predict** → **ConductoDict** in the Menu bar. The **ConductoDict** section contains a pull-down menu to switch between the commands **Compute Thermal Conductivity** and **Compute Electrical Conductivity**.



The **Options** for the selected command from GeoDict can be modified through the **Edit...** buttons.

When the **Estimate Memory & Disk-Space** button is clicked, the RAM needed for the computation is estimated based on the size of the structure and the parameters entered in the solver options. The estimated computational memory and disk space requirements are shown in a **Memory & Disk-Space** pop-up message.



After that, clicking the **Run** button in the **ConductoDict** section starts the computations. If recording a macro, the **Record** button becomes active and the **Run** button changes to **Run & Record.**

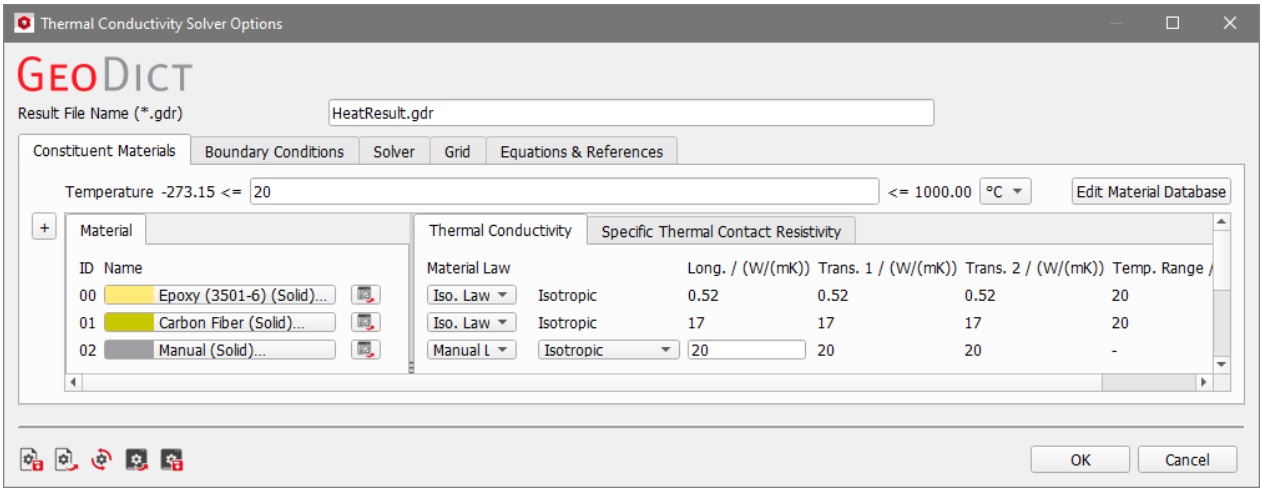
Click **Run in Cloud** to run it in the Kaleidosim cloud, see the High Performance Computing chapter of the GeoDict User Guide for details.

After clicking **Run**, the computations start but the solver process can be cancelled or stopped when clicking **Cancel** or **Stop** in the progress dialog box. The difference between them is that **Stop** writes a result GDR file and give the intermediate result while **Cancel** terminates the simulation without giving GDR. Depending on the solver's internal processes and actual memory usage, cancelling or stopping the computation may not be instantaneous.

Compute Thermal Conductivity

Input Parameters

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

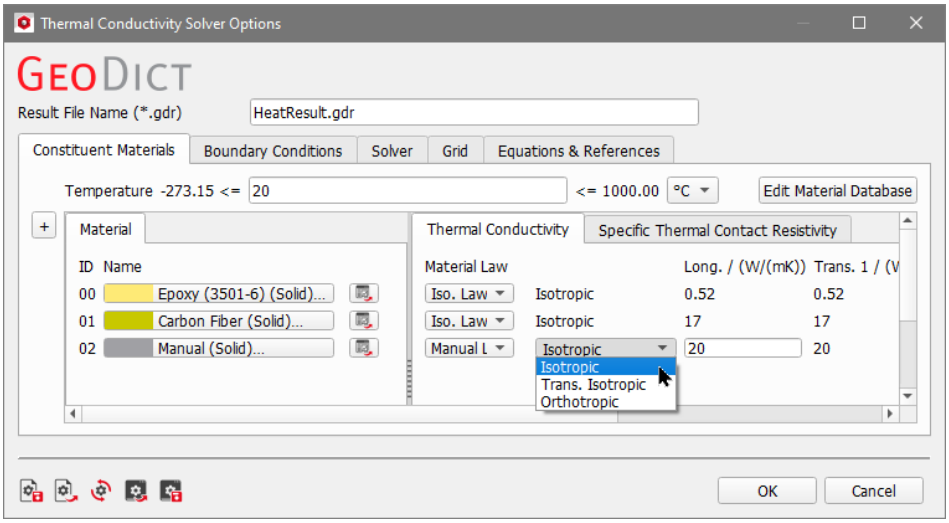
An additional directory with this name is created to keep the intermediate computation files (PDE solver files) and the temporary computation files.

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

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.

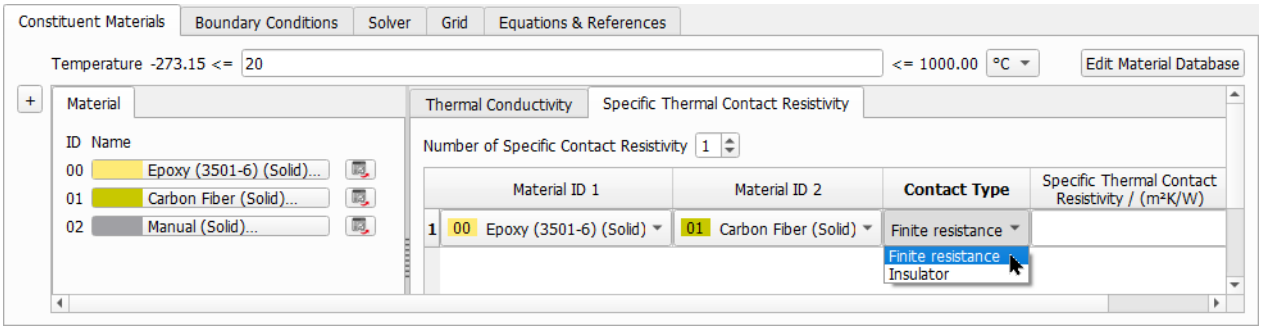
The thermal conductivity for each of the constituent materials needs to be specified for **Compute Thermal Conductivity**. More information on constituent materials can be found in the Material Database 2023 handbook of this User Guide.



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.

When contact resistances exist between different materials when they contact with each other, they are to be entered 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.

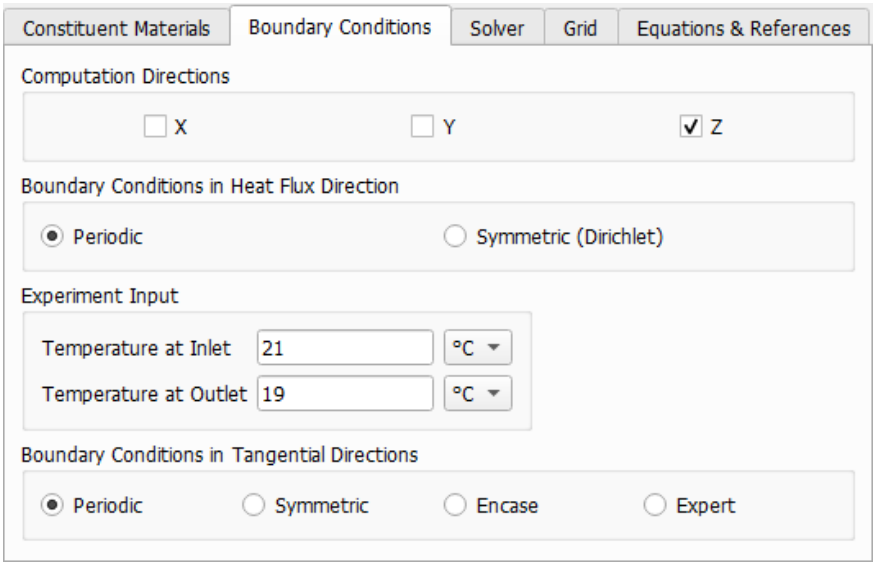
Contact resistances can be applied between the same Material IDs, as well as between different material IDs.

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 on page 18 of this user guide chapter.

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

Boundary Conditions

The **Boundary Conditions** tab contains three panels: **Computation Directions**, **Boundary Conditions in Heat** (or **Potential**) **Flux Direction**, **Experiment Input**, and **Boundary Conditions in Tangential Directions**.

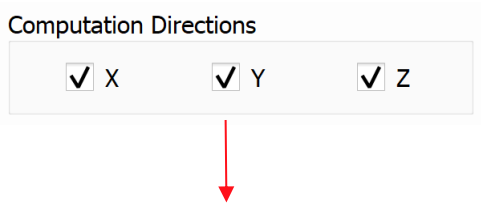


For the **Computation Directions**, choose the direction for the computed conductivity.

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.

Thermal Conductivity / (W/(mK))

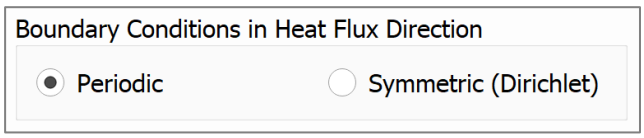
unknown	unknown	-0.0031241
unknown	**unknown**	-0.00805343
unknown	unknown	**1.01514**



Thermal Conductivity / (W/(mK))

1.04451	-0.0134352	-0.0031241
-0.0134349	**1.05177**	-0.00805343
-0.0031242	-0.00805343	**1.01514**

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



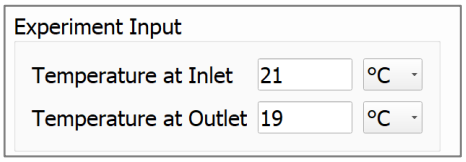
If **Periodic** is selected, the conductivity is computed assuming that the structure is periodically repeated in the flux direction. If **Symmetric (Dirichlet)** is checked, constant temperature or potential is assumed along both border planes in the heat flux or the potential flux direction. For non-periodic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

(Dirichlet) boundary conditions give more accurate results then **Periodic** boundary conditions.

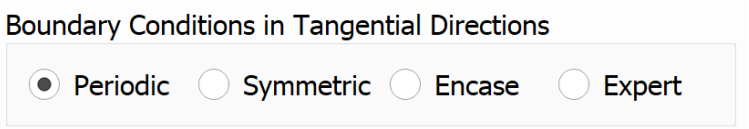
In previous versions of GeoDict, the computational memory requirements for **Symmetric (Dirichlet)** boundary conditions case were almost two times higher and therefore, the computational time were longer. This is no longer the case since GeoDict 2022.

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 Tangential 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

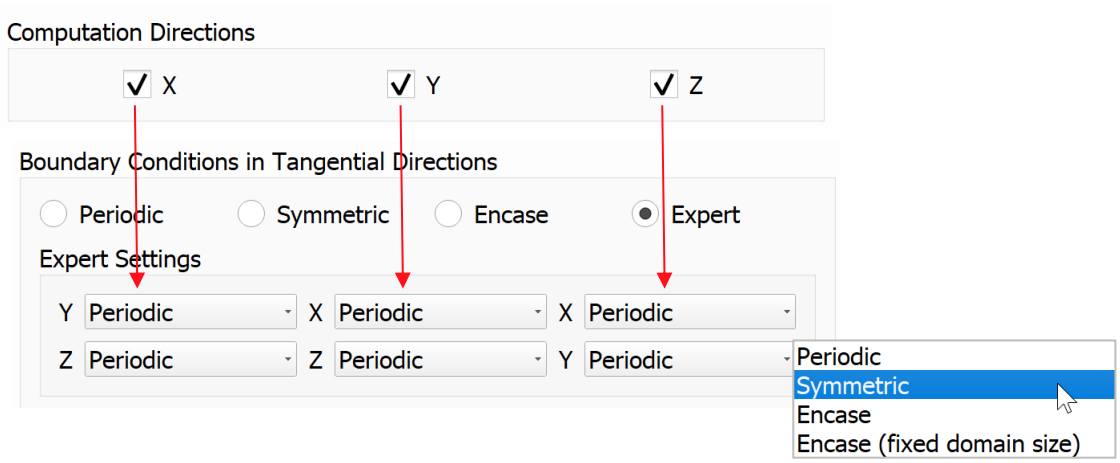
Symmetric boundary conditions

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.

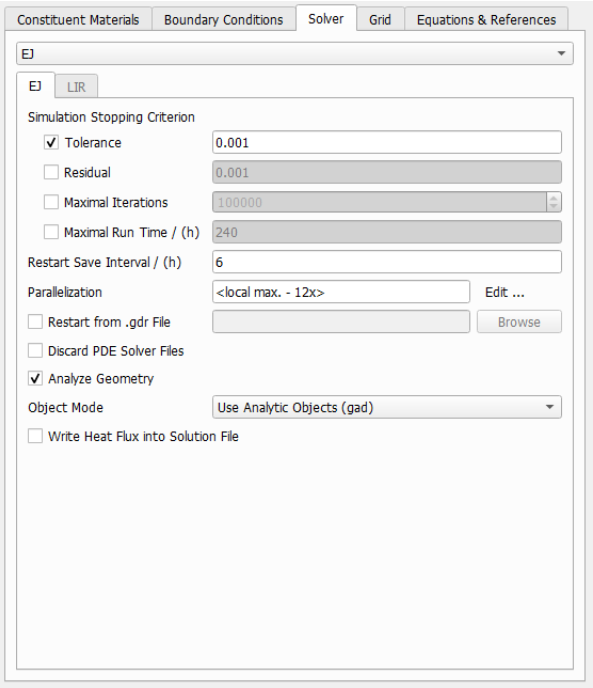
For each selected computation direction, the boundary conditions in the two tangential directions have to be selected. For each tangential direction, you have the choice of **Periodic**, **Symmetric**, **Encase**, and **Encase (fixed domain size)**.

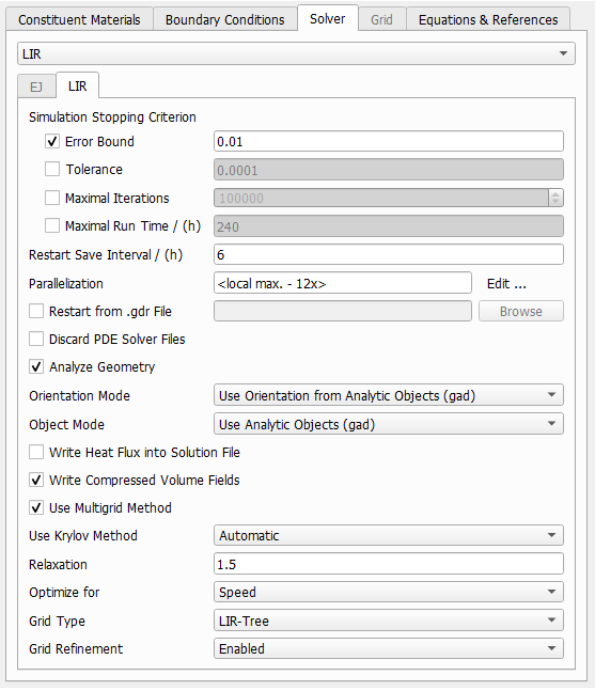


When **Encase** is used, the solver internally adds a one-voxel layer in the required direction and solves with periodic boundary condition. That effectively is equivalent to solve the structure with casing in two ends in the direction of interest. So, the size of computation in this direction becomes 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 structure. For structures with high contrast (e.g. $>10^6$) or high contact resistivities it is recommended to use the EJ solver or enable the option of **Use Krylov Method** in LIR solver.

Simulation Stopping Criterion

Compute Thermal Conductivity solves the underlying partial differential equations by using an iterative solver.

The basic idea of an iterative method is to:

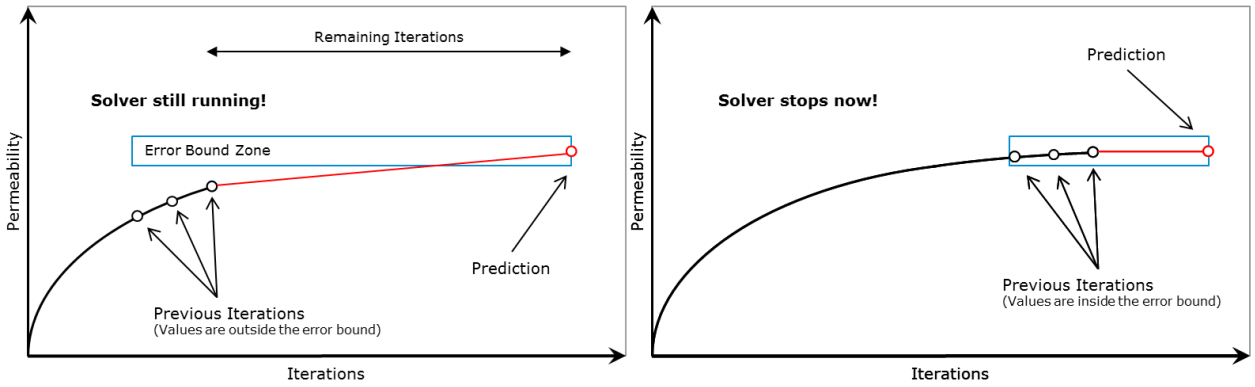
1. Start with some initial guess for the unknown values.
2. Improve the current values in each iterative step.
3. Repeat the iterative process until one of the stopping criteria (**Error Bound**, **Tolerance**, **Residual**, **Maximal Iterations** or **Maximal Run Time**) occurs.

The default stopping criterion of the EJ solver, **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.

$$\frac{\text{[new conductivity – previously computed conductivity]}}{\text{previously computed conductivity}}$$

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. **Error Bound** is not available for the **EJ** solver.



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

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 intermediate results, 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.

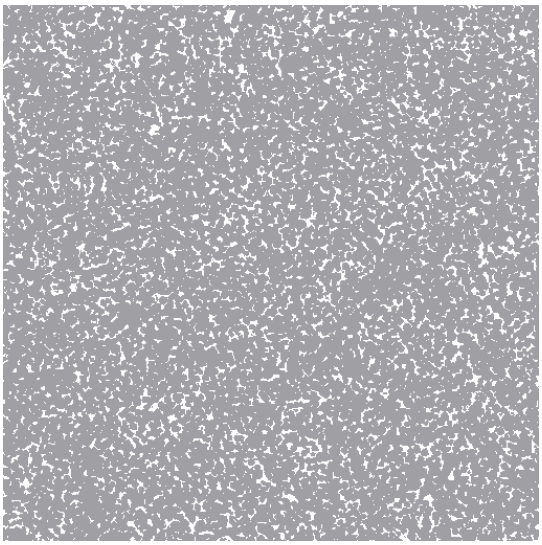
The **Parallelization Options** dialog box opens when clicking the **Edit...** button, to choose between **Local, Sequential**, **Local, Parallel**, **Local, Maximum**, and **Cluster** for EJ, and **Local, Sequential**, **Local, Parallel** and **Local, Maximum** for LIR.

For details on how to set up und run parallel computations, consult the High-performance Computing for GeoDict handbook of this User Guide.

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.

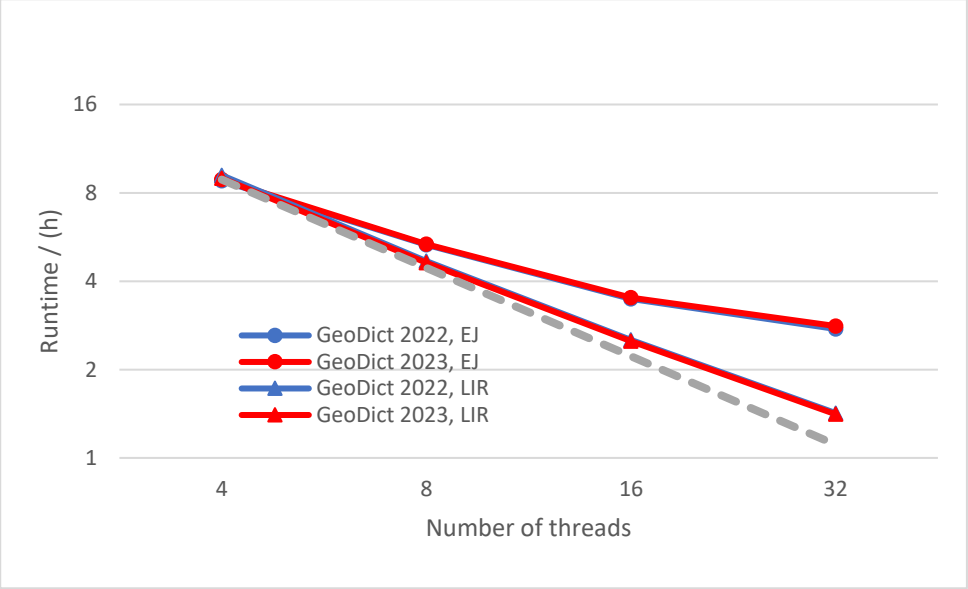
The first example is the computation of the electrical conductivity through a synthetic X-ray tomography data of a sandstone structure [14].The structure has a porosity of 13.6% and a size of 2048x2048x2048 voxels.



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 0.01 for LIR and of 0.1135 S/m with a tolerance of 0.001 with EJ solver.

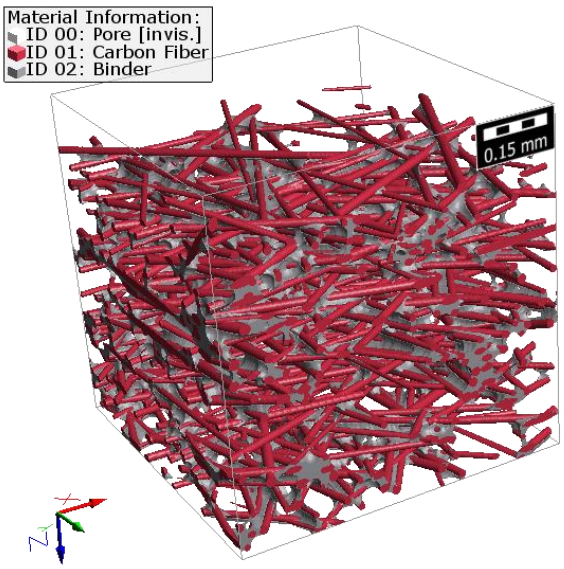
For both solvers, the ideal speedup, i.e. getting half of the runtime for twice the number of processes, is also shown. The speedup for LIR solver is close to the ideal one, which is usually not possible to reach for real life examples. The speedup of EJ differs more from the ideal one. For both EJ and LIR, the performance in GeoDict 2023 is the same as in GeoDict 2022.



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.

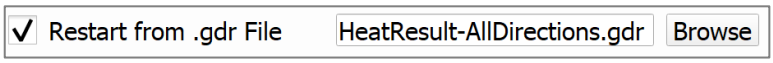
Memory requirements for both examples and for the first example for both solvers, are listed in the following table:

Microstructure	Memory for computation with LIR (speed optimized)	Memory for computation with EJ
Sandstone	264 GB	239 GB
GDL	259 GB	-

Restart from *.gdr File

In some situations, it may be useful to re-use previously computed results and, thus, reduce the runtime of the conductivity computation. Typical examples would be non-sufficient accuracy of some computation, when it is suspected that more iteration may improve the quality of the result.

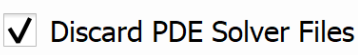
To use some previously computed result, **Restart from .gdr File** can be checked and **Browse** used to search for the file.



Note that the structure used for restarting for both the current and the restart result file, must be the same. If this is not the case, an error message is displayed.

Discard PDE Solver Files.

Checking the **Discard PDE Solver Files** box causes the deletion of all intermediate computation files. While having the benefit of saving storage place, discarding *.pde solver files has also the side effect of disabling the 3D visualization of the results.



Of course, the contents of the result file (*.gdr) are not discarded even in this case.

Analyze Geometry

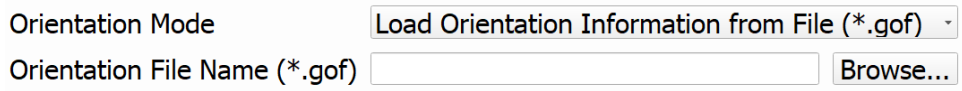
Analyze Geometry is checked by default to enable a geometry analysis before the solver runs to know if a through path exists.

Orientation Mode (for LIR)

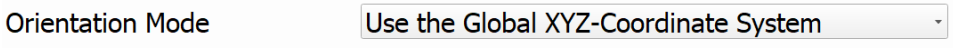
If one of the constituent materials has a transverse isotropic or orthotropic material law, a local orientation is needed to compute the conduction. There are three different choices how to determine the local orientation.

The standard case is to use the orientation defined by the local orientation of the GAD objects, e.g. the direction of a fiber.

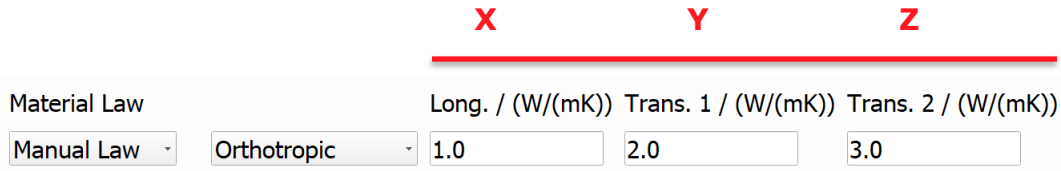
However, if the current structure was not generated using one of the structure generation modules, but imported from a 3D image, GAD object information is not available. In such a case, the local orientation must be estimated from the image first, e.g. by using FiberFind or GrainFind. It is then possible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



Last, one can simply use the coordinate system:



In this case, the entered conductivities are the conductivities in the X, Y, Z space directions:

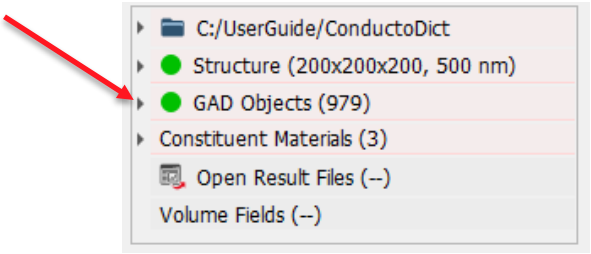


Object Mode

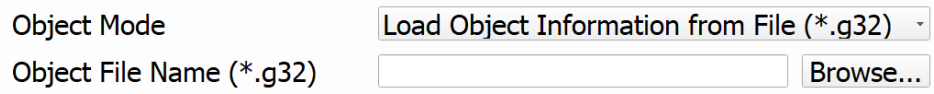
If contact resistances between objects of the same material have been set in the **Constituent Materials** tab, GeoDict must be able to distinguish between different objects of the same type. This can be done in two different ways.

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).



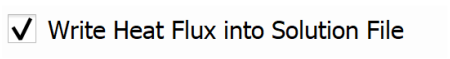
A red dot might be shown if the current structure was not generated using one of the structure generation modules but imported from a 3D image. Then, GAD object information is not available, and the structure must be segmented into separate objects first, e.g. by using FiberFind or GrainFind. It is then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



Please note that 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 Field into Solution File

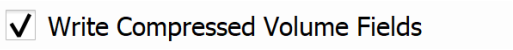
Additional 3D data can be added to the solution .hht files for visualization or later analysis. For thermal conductivity computations, **Write Heat Flux into Solution File** stores the flux in the three coordinate directions, allowing a detailed analysis of the flux field.



The memory requirements increase when selecting this option.

Write Compressed Volume Fields (for LIR)

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

Use Multigrid Method (for LIR)

The Multigrid method 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 in FlowDict as well as for solving diffusion, thermal and electrical conduction in DiffuDict and ConductoDict and is enabled by default.

Use Krylov Method (for LIR)

Depending on the structure and the corresponding material parameters, a significant speedup of the LIR can be achieved by using the BiCGstab method to compute the solution. Using the BiCGstab method approximately doubles the amount of RAM needed for the computation.

When **Use Krylov Method** is set to **Automatic**, GeoDict decides based on structure, material parameters and boundary condition which method is expected to be faster and uses this method. In case that the Krylov subspace method (BICGstab) is used, the **Relaxation** is also chosen automatically.

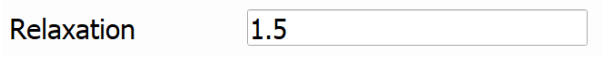
Alternatively, the user may also explicitly enable or disable this method.

If the ratio of the largest and smallest conductivity within the structure (i.e. high contrast) is large (approx. $>10^6$), usage of the Krylov method is recommended.

For structures without a high conductivity contrast, the usage of this option is not recommended.

Relaxation (for LIR)

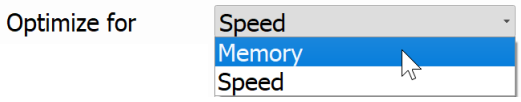
Depending on the material parameters and geometry of the structure, the underlying mathematical problem can vary in complexity, thus influencing the behavior of the solver. The iterative method uses the relaxation number to adjust it from **Stable** (with smaller number chosen, which results in higher number of iterations, slower time stepping, and longer solver run times), to **Fast** with higher number chosen, which makes the solver run less iterations but implies the risk that the solver does not converge.



For the LIR solver, this balance is managed through the **Relaxation**. The value should be between 0 and 2. For relaxation values smaller than one (<1.0), the simulation is more stable. For relaxation values larger than one (>1.0), the simulation is faster.

Optimize for (for LIR)

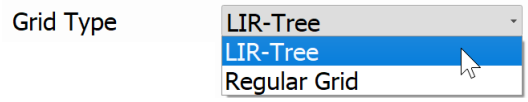
The **LIR** solver can **Optimize for** speed or memory.



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, then the runtime is increased by up to 40% but the solver requires up to 50% less memory.

Grid Type (for LIR)

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

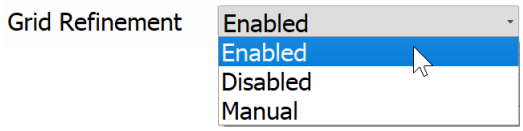


The default option is **LIR-Tree** and should always be used. The solver uses an adaptive tree structure called LIR-tree and needs up to 10 times less runtime and memory compared the **Regular Grid** option.

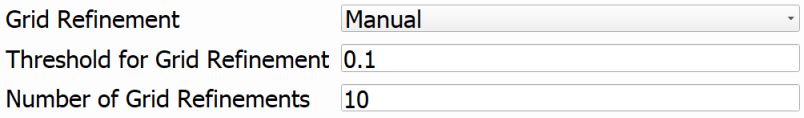
Grid Refinement (for LIR)

The solver can analyze the velocity and pressure field during the computation and improves the adaptive grid in places where more accuracy is needed. The LIR solver splits cells where a high velocity-gradient or high pressure-gradient occurs. The analysis is enabled if the **Grid Refinement** option is set to **Enabled** or **Manual**.

If the **Grid Refinement** is set to **Enabled**, the solver chooses the **Number of Grid Refinements** and **Threshold for Grid Refinement** automatically.



If the **Grid Refinement** is set to **Manual**, the user can enter the parameters manually.



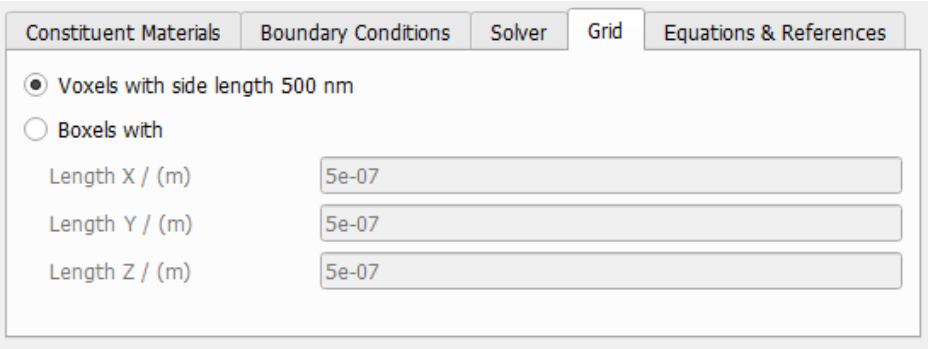
The **Number of Grid Refinement** controls how many velocity-based and pressure-based grid refinements are allowed during the simulation. The value should be between 0 and 10. Velocity-based and pressure-based grid refinements may increase the number of iterations, runtime and memory requirements.

The **Number of Grid Refinement** can be zero in most of the cases and should be greater than zero 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.

Refinement is done at regions with high-velocity gradient or high-pressure gradient. Cells are split where the current velocity gradient (or pressure gradient) is greater than the **Threshold for Grid Refinements** times the maximal velocity gradient (or pressure gradient). This threshold must be between 0.0 and 1.0. The recommended value range is between 0.05 and 0.1.

GRID (FOR EJ)

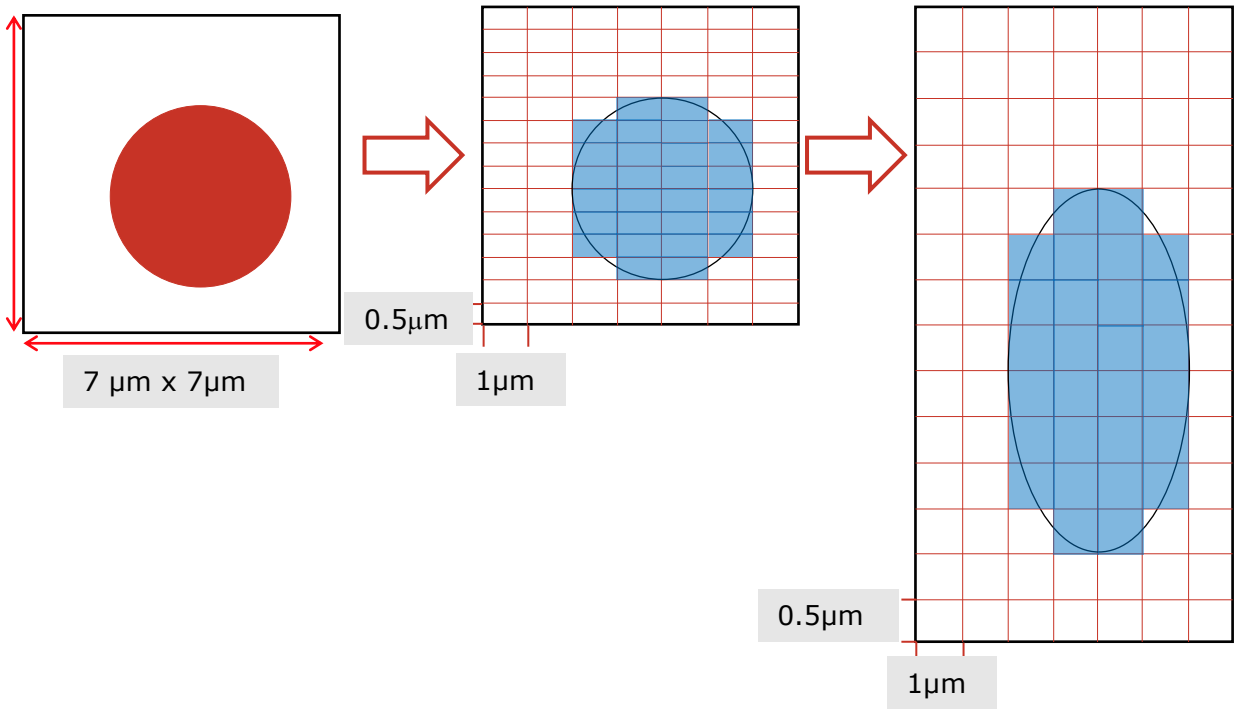
If boxels (cuboid) instead of voxels (cube), are used to resolve the structure, the boxel lengths can be set in the **Grid** tab.



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.

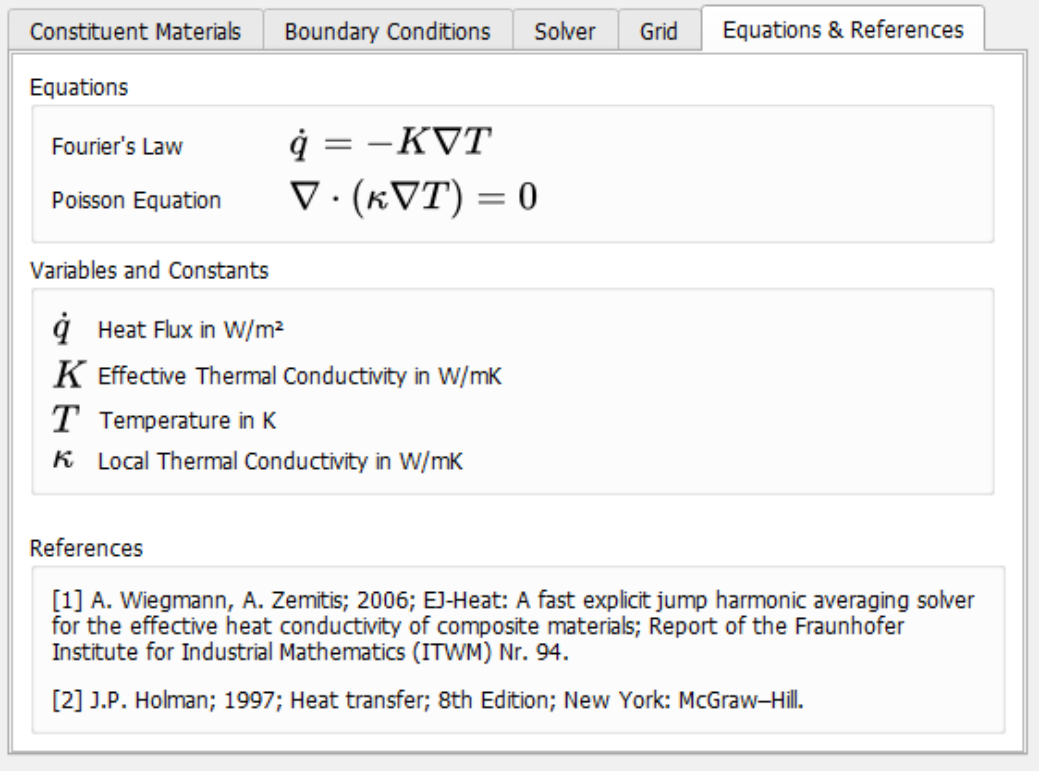
For example, a structure is sampled in a computational grid with different lengths in X- and Y-direction (e.g. LX = 2*LY).

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.



EQUATIONS & REFERENCES

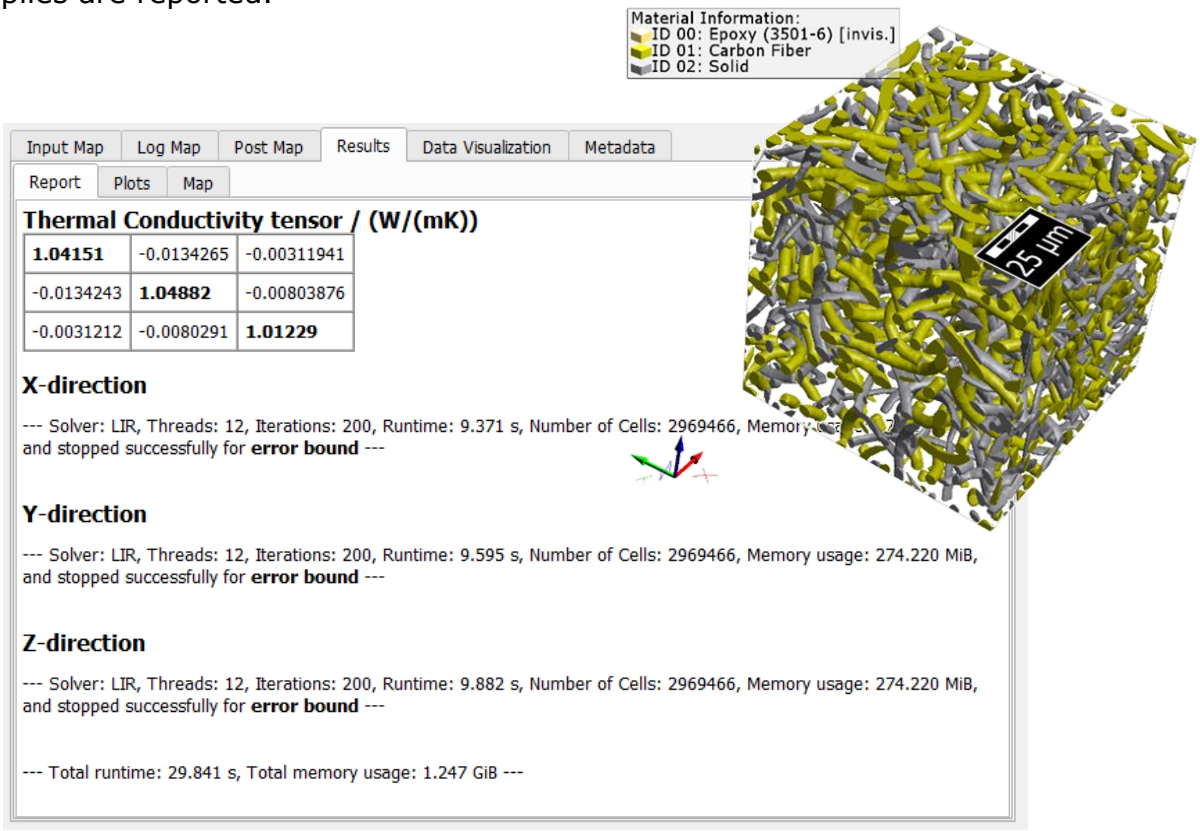
The **Equations & References** tab shows the formulas that are used for the solver. To **Compute Thermal Conductivity**, the Poisson Equation is solved on the whole domain and Fourier's Law is used to obtain the effective thermal conductivity.



RESULTS

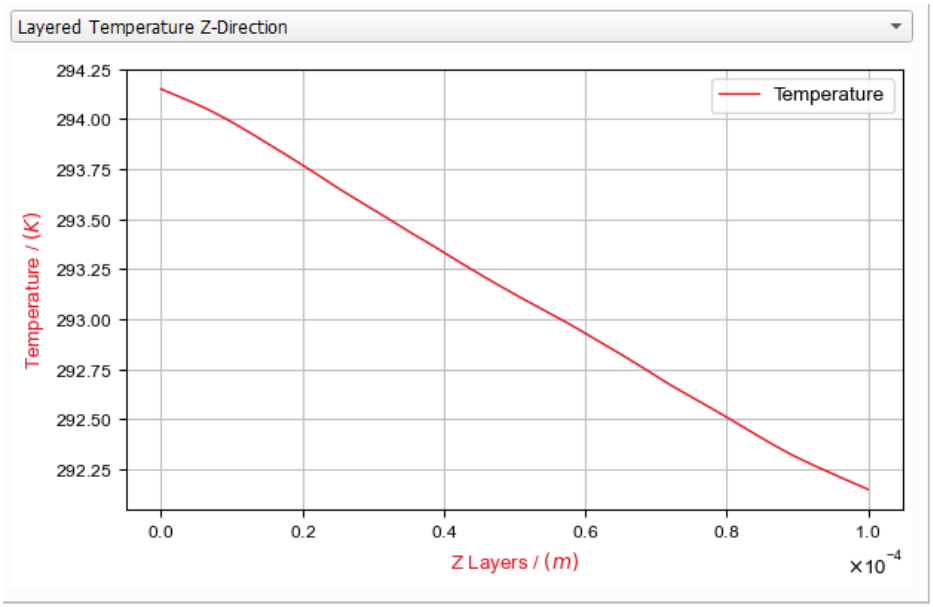
Click **OK** to input the entered parameters, and then click **Run** in the ConductoDict section to start the command. The results are immediately shown in the opening Result Viewer after the process is finished.

The **Results - Report** sub-tab displays the computed Thermal Conductivity tensor. Also, for each computation, the number of iterations, runtimes, and stopping criteria applies are reported.

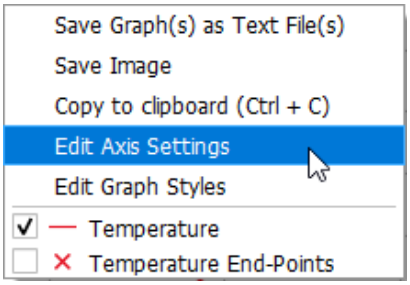


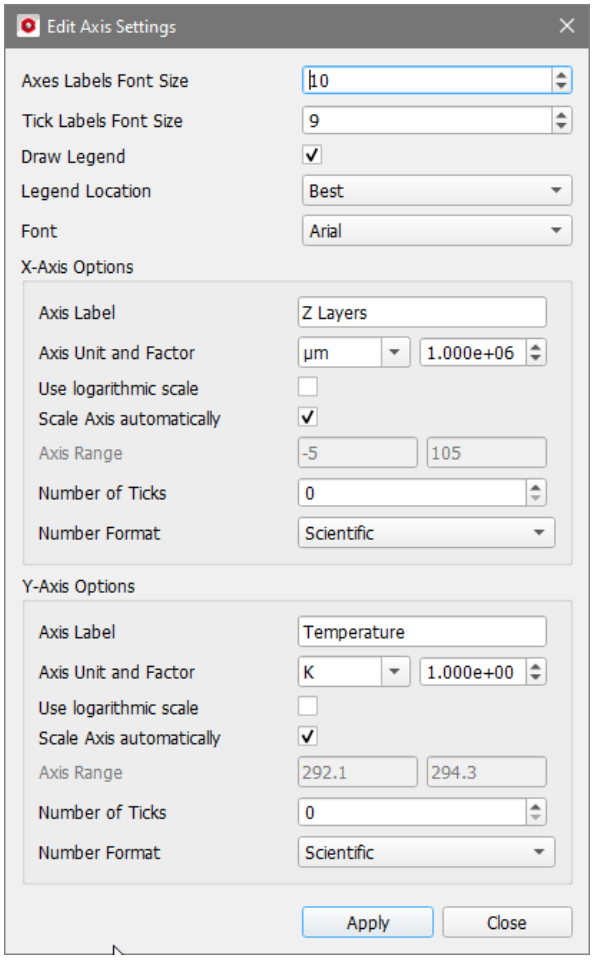
The **Results - Plots** subtab allows choosing different plots.

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.



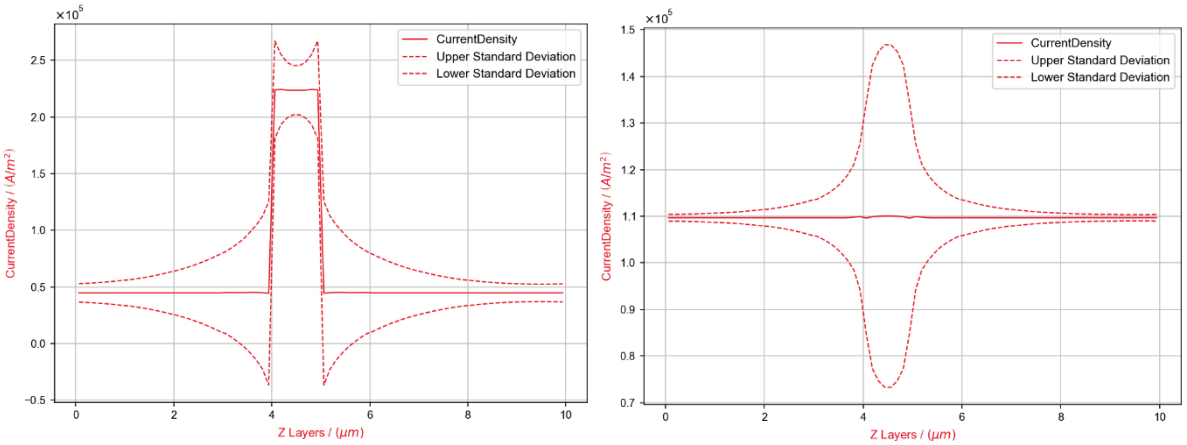
Right clicking on the plot opens a small dialog box where you may choose to **Edit Axis Settings**.

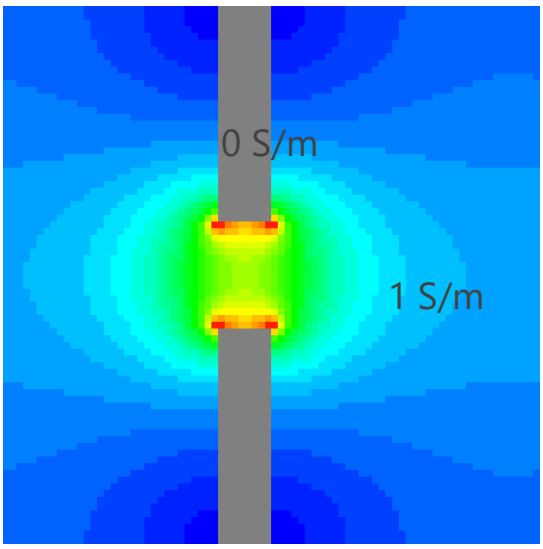


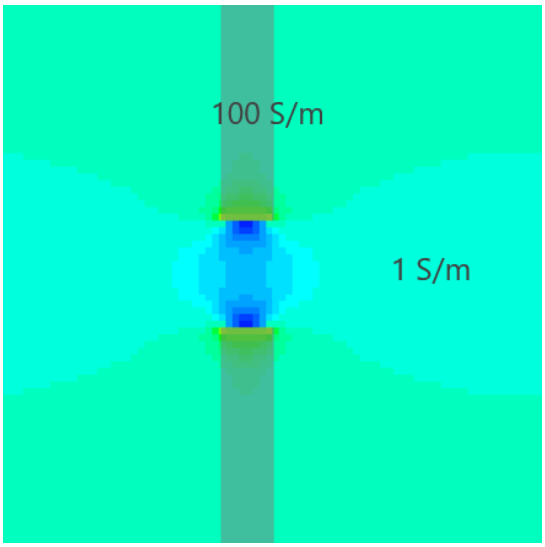


In the dialog that appears, you may change the scale, ticks and labels of the X- and Y-axis manually, and set the position of the legend in the chart.

Under **HeatFlux,** the mean current density 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.



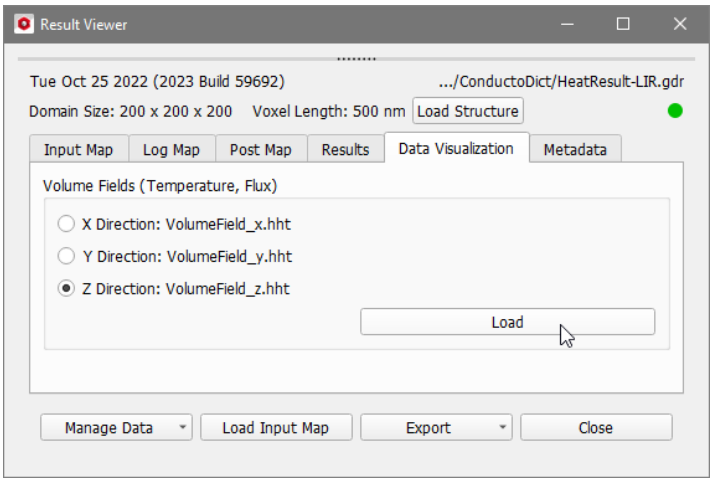




Under **Convergence**, the plot of the **Conductivity** at given **Iteration** values is charted for the selected directions. Selecting the direction from the pull-down menu, it is possible to see graphs of the convergence of the iterative solver for each of the computed directions.

Data Visualization

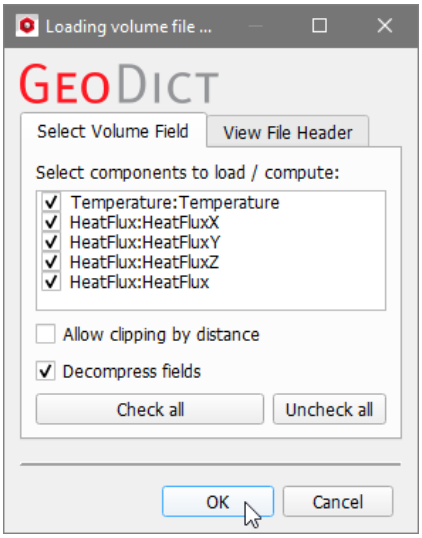
Under the **Data Visualization** tab, the results of the thermal conductivity calculations can be graphically visualized in 2D-Cross section view or 3D-Rendering.

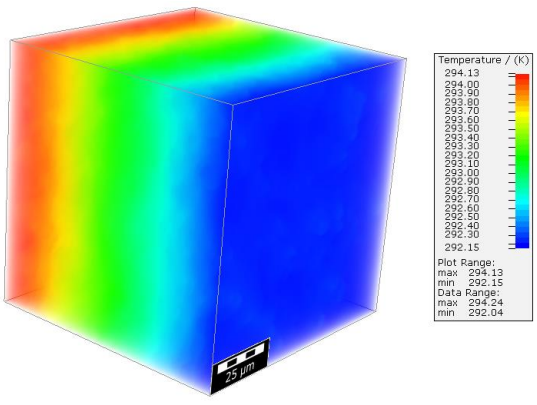


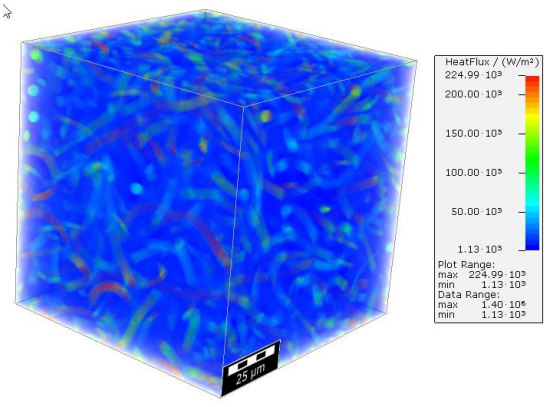
Click **Load** to load the computed temperature field.

Directions that were not selected when setting up the simulation were not computed, and, thus, are unavailable for visualization.

When before the computing, **Write Heat Flux into Solution File** was checked, the available components to be loaded includes the heat flux, too.







The options available for visualization of 3D scalar or vector fields are explained in detail in the Visualization in GeoDict handbook of this User Guide.

Compute Electrical Conductivity

Input Parameters

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

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

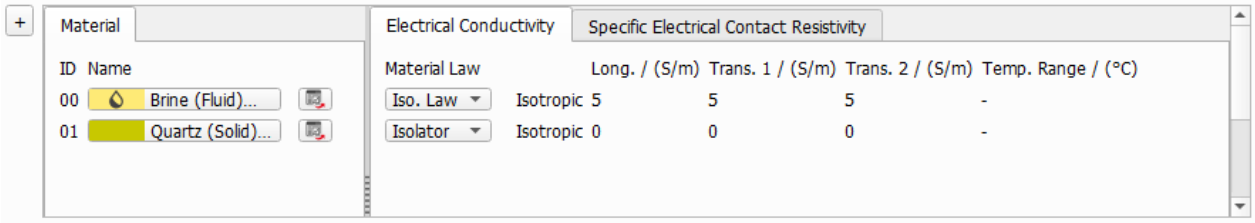
Choose a name for the files containing the results of the computations according to your current project. The result files are saved in the project folder (**File** → **Choose Project Folder**, in the Menu bar).

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

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 electrical 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 2023 handbook of this User Guide.



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.

When contact resistances exist between different materials when they contact with each other, they are to be entered in the **Specific Electrical 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 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 on page 18 of this user guide chapter.

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

Boundary Conditions

The parameters have the same meaning as described for the **Compute Thermal Conductivity** command on page 10ff.

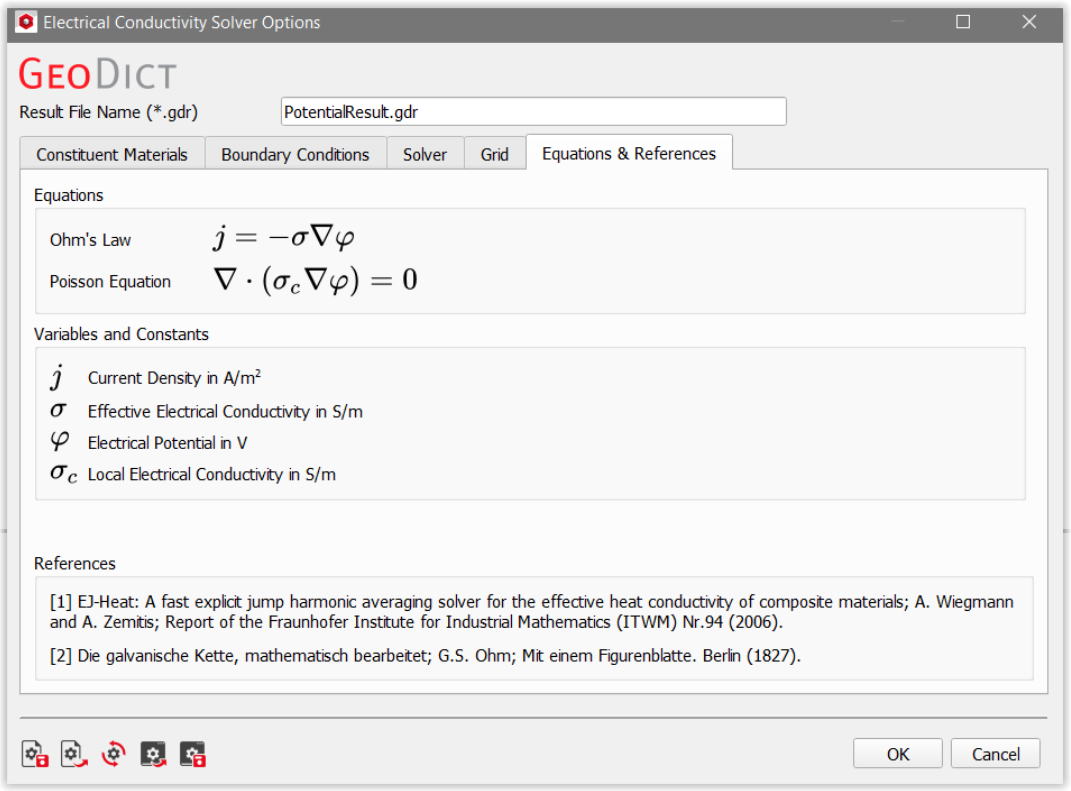
Solver and Grid

The parameters have the same meaning as described for the **Compute Thermal Conductivity** command on page 13ff.

Equations and References

The **Equations & References** tab shows the formulas that are used for the solver.

To **Compute Electrical Conductivity**, the Poisson Equation is solved on the whole domain and Ohm's Law is used to obtain the effective electrical conductivity.



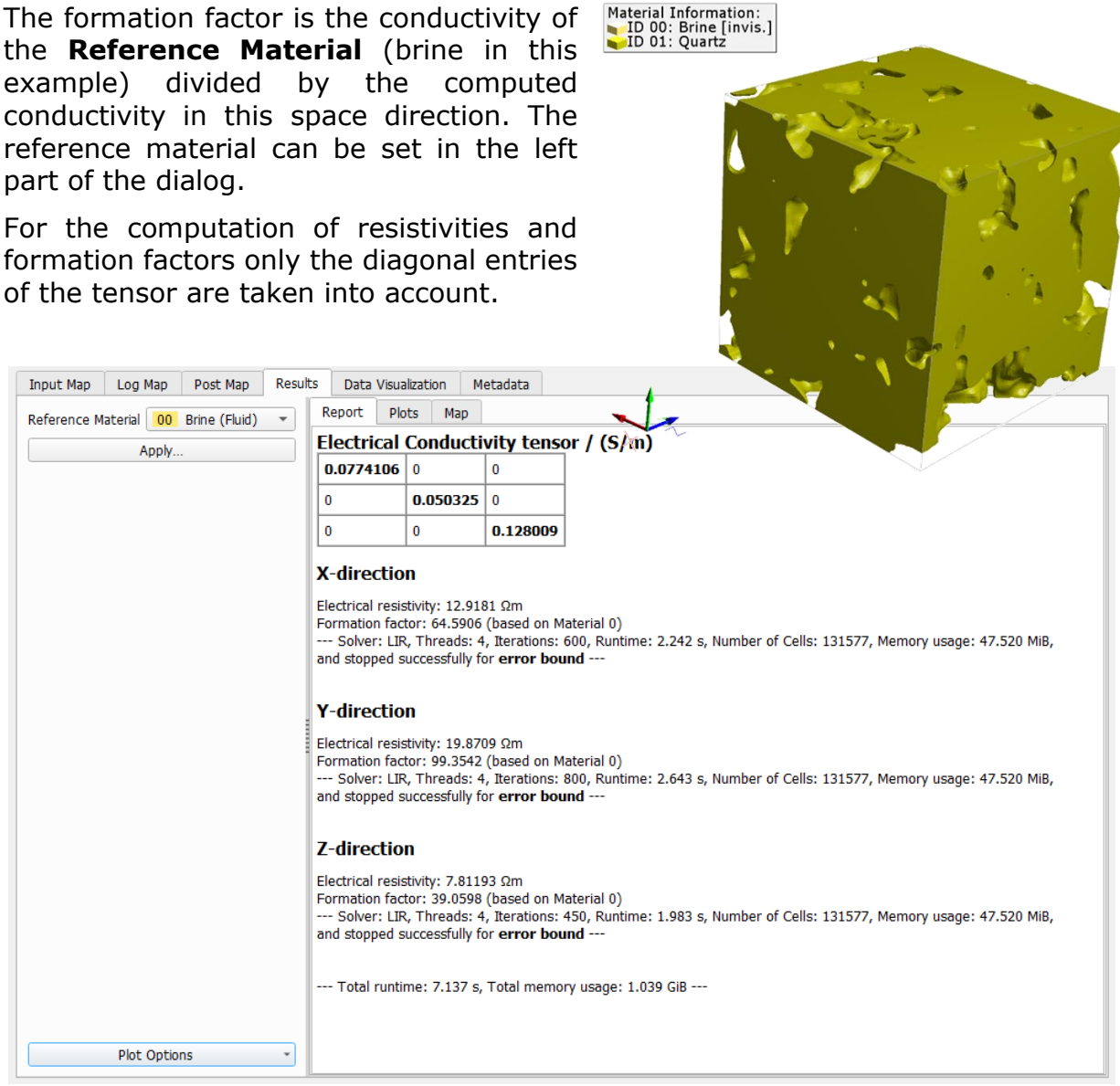
RESULTS

The **Report** sub-tab 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.

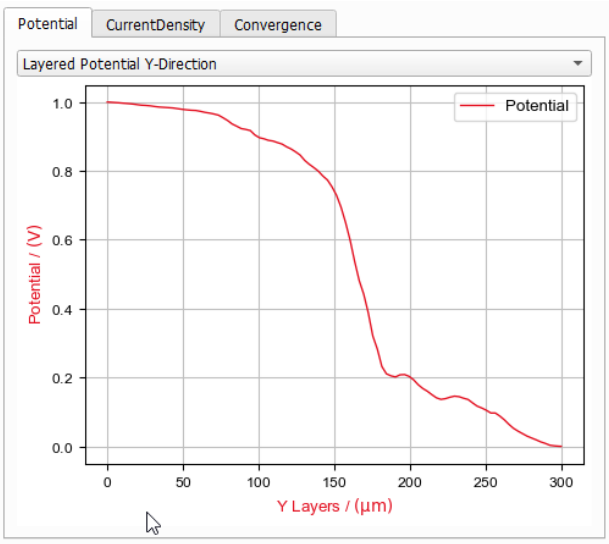
The formation factor is the conductivity of the **Reference Material** (brine in this example) divided by the computed conductivity in this space direction. The reference material can be set in the left part of the dialog.

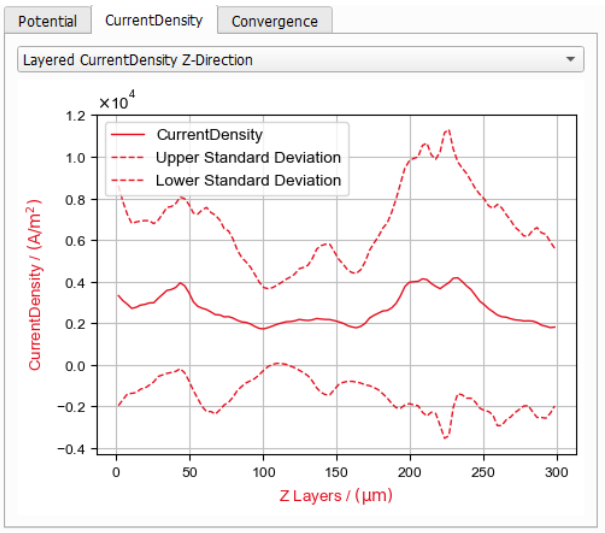
For the computation of resistivities and formation factors only the diagonal entries of the tensor are taken into account.



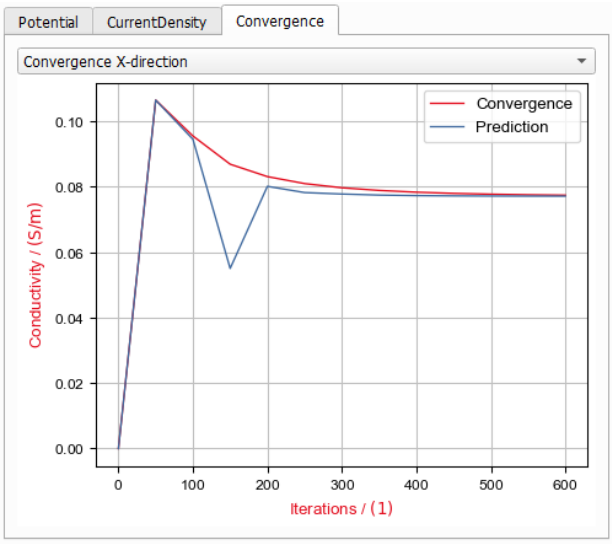
Additionally, for each computation, the number of iterations, runtimes, and stopping criteria applied are reported.

The **Plots** subtab depicts three different graphs: First, the potential gradient across the structure (**Layered Potential X/Y/Z-Direction**). Second, the mean current density and the standard deviation in each voxel layer. If non-conducting materials are present, the mean current density varies and shows where the bottlenecks are.



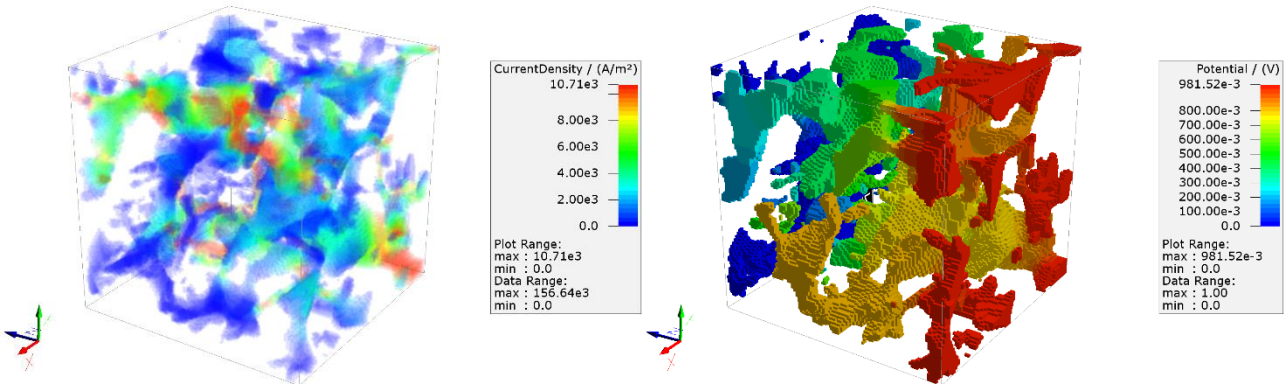


Under **Convergence**, the plot of the **Conductivity** at given **Iteration** values is charted for the selected directions. If the **LIR** solver is used, and **Error Bound** is used as stopping criterion, also the predicted conductivity is shown.



DATA VISUALIZATION

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



The options available for visualization of 3D scalar or vector fields are explained in detail in the Visualization in GeoDict handbook of this User Guide.

References

[1] 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.

[2] 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, 2008, pp 608-616.

[3] 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, 2007, pp B419-B426.

[4] 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, 2008, pp 21006-21014.

[5] A. Velichko, Quantitative 3D characterization of graphite morphologies in cast iron using FIB microstructure tomography, Dissertation, Saarland University, 2008.

[6] 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, 2009, pp 5023-5035.

[7] 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, 2009, pp B1175-B1181.

[8] 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, 2010, pp 3994-4006.

[9] 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, 2010, p. 22907.

[10] 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, 2010, pp 1302-1307.

[11] 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, 2010, pp 3751-3757.

[12] J.P. Holman, Heat Transfer, 8th Edition, 1997.

[13] A.K. Hasselström, and U.E. Nilsson, Thermal Contact Conductance in Bolted Joints, 2012.

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

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

Technical documentation:

Jürgen Becker

Liping Cheng

Barbara Planas

Math2Market GmbH

Richard-Wagner-Str. 1, 67655 Kaiserslautern, Germany
www.geodict.com