COMSOL MULTIPHYSICS

MATERIAL LIBRARY

USER'S GUIDE

VERSION 3.4

COMSOL

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Material Library User's Guide

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1

Introduction

Welcome to the Material Library. This optional package extends the COMSOL Multiphysics® modeling environment with data for more than 2500 materials. The entry for a given material can contain data for as many as 27 different material properties with a focus on elastic and thermal properties. Each of these material properties is described as a function of some variable, typically temperature. In all, the Material Library contains a total of almost 20,000 property functions.

Although the data is specified in the SI unit system, COMSOL Multiphysics can automatically convert it to other unit systems.

Most of the properties are available as functions of temperature, which makes the Material Library ideal for multiphysics couplings such as electrical-thermal analysis and structural-thermal analysis. In some cases, data is given for a material's solid, liquid, and vapor phases.

The properties are analytic functions over a given interval of the argument. COMSOL Multiphysics makes use of smoothing to interpolate the values of the properties between different intervals. You can choose the smoothing settings in order to obtain continuous first and second derivatives of the property functions.

It is possible to copy the materials to a user-defined library where you can add and edit their properties. You can also plot and inspect the definition of a function.

The Material Library stores the material data in groups and subgroups, thus making it easy to find the material you are looking for. In addition, a flexible search feature lets you look for materials by name, UNS number, or DIN number. A reference provides the source of the function that defines each property.

The material property data in the Material Library is based on the Material Property Database (MPDB) from JAHM Software, Inc.

Typographical Conventions

All COMSOL manuals use a set of consistent typographical conventions that should make it easy for you to follow the discussion, realize what you can expect to see on the screen, and know which data you must enter into various data-entry fields. In particular, you should be aware of these conventions:

- A **boldface** font of the shown size and style indicates that the given word(s) appear exactly that way on the COMSOL graphical user interface (for toolbar buttons in the corresponding tooltip). For instance, we often refer to the **Model Navigator**, which is the window that appears when you start a new modeling session in COMSOL; the corresponding window on the screen has the title **Model Navigator**. As another example, the instructions might say to click the **Multiphysics** button, and the boldface font indicates that you can expect to see a button with that exact label on the COMSOL user interface.
- The names of other items on the graphical user interface that do not have direct labels contain a leading uppercase letter. For instance, we often refer to the Draw toolbar; this vertical bar containing many icons appears on the left side of the user interface during geometry modeling. However, nowhere on the screen will you see the term "Draw" referring to this toolbar (if it were on the screen, we would print it in this manual as the **Draw** menu).
- The symbol **>** indicates a menu item or an item in a folder in the **Model Navigator**. For example, **Physics>Equation System>Subdomain Settings** is equivalent to: On the **Physics** menu, point to **Equation System** and then click **Subdomain Settings**. **COMSOL Multiphysics>Heat Transfer>Conduction** means: Open the **COMSOL Multiphysics** folder, open the **Heat Transfer** folder, and select **Conduction**.

- A `Code` (monospace) font indicates keyboard entries in the user interface. You might see an instruction such as "Type `1.25` in the **Current density** edit field." The monospace font also indicates COMSOL Script codes.
- An *italic* font indicates the introduction of important terminology. Expect to find an explanation in the same paragraph or in the Glossary. The names of books in the COMSOL documentation set also appear using an italic font.

Overview of the Material Library

The Material Library incorporates mechanical, thermal, and electrical properties primarily for solid materials. It is organized in groups and subgroups according to the components of the material or its application. These groups and subgroups are contained in corresponding folders in the user interface as outlined here:

FOLDER	SUBFOLDERS	NUMBER OF MATERIALS
Elements	-	97
Fe and Ni Alloys	Iron Alloys	231
	Nickel Alloys	117
Al and Cu Alloys	Aluminum Alloys	104
	Copper Alloys	84
Mg and Ti Alloys	Magnesium Alloys	32
	Titanium Alloys	19
Oxides	Simple Oxides	86
	Complex Oxides	206
Carbides, Cermets, and Tool Steels	Carbides	39
	Cermets	16
	Tool Steels	51
Carbons and Thermal Insulators	Carbons	24
	Thermal Insulators	29
Intermetallics, TBC, and Refractory Metals	Intermetallics & TBC (thermal barrier coatings)	93
	Refractory Metal Alloys	84
Polyamides and Polyesters	Nylons and Polyamides	88
	Polyethers and Polyesters	8
Acetal, PVDF, and EVA	Acetal Resins	20
	PVDF (polyvinylidene fluoride)	9
	EVA (ethylene-vinyl Acetate)	12
Elastomers and epoxies	Miscellaneous Polymers	25
	Epoxies	25

FOLDER	SUBFOLDERS	NUMBER OF MATERIALS
Misc. Polymers and Polymer Composites	Polymer Composites	21
	Elastomers	7
Minerals, Rock, Soil, and Woods	Minerals, Rocks, and Soils	70
	Woods	18
Polypropylenes and PET	Polypropylenes	7
	PET Compounds	21
Controlled Expansion and Thermocouple Alloys	Controlled Expansion Alloys	33
	Thermocouple Alloys	5
Semiconductors, Optical, and Other Materials	Semiconductors and Optical Materials	106
	Other Materials	27
Solders, dental, and Co Alloys	Solders, Low-Melting, and Dental Materials	35
	Cobalt Alloys	19
Resistance and Magnetic Alloys	Resistance Alloys	49
	Magnetic Alloys	25
Metal-Matrix and Ceramic-Matrix Composites	Metal-Matrix Composites	23
	Ceramic-Matrix Composites	63
Salts, Fuel-cell, Battery, and Electroceramic Materials	Salts	30
	Fuel-cell, Battery, and Electroceramic Materials	117
Silicides and Borides	Silicides	57
	Borides	38
Glasses, Metallic Glasses, Nitrides, and Beryllides	Glasses and Metallic Glasses	122
	Nitrides and Beryllides	21
Cast Irons and Mold Materials	Cast Iron	116
	Mold Materials	15

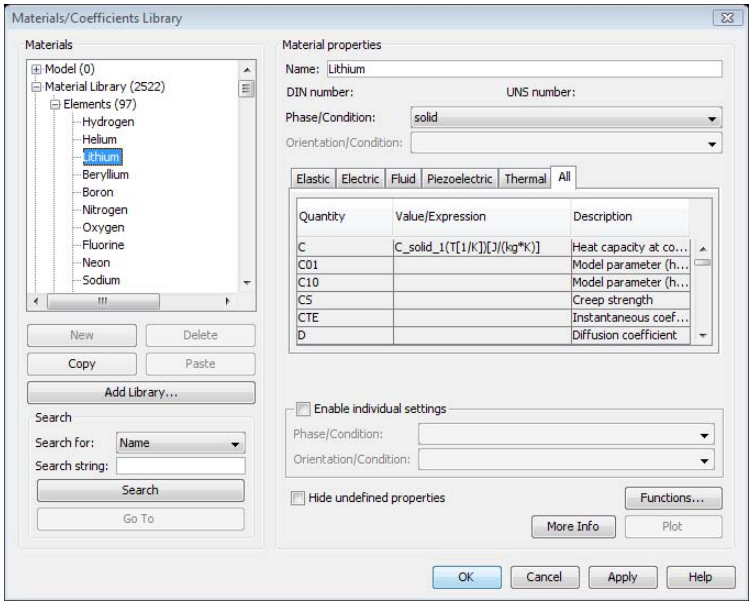
Each material can have at most 27 properties defined, each of which is available as a function of temperature or another appropriate argument. The following table lists these property functions:

PROPERTY NAME	DESCRIPTION	SI UNIT	ARGUMENT
dL	Linear expansion	-	Temperature
CTE	Instantaneous coefficient of thermal expansion	1/K	Temperature
alpha	Coefficient of thermal expansion	1/K	Temperature
k	Thermal conductivity	W/(m·K)	Temperature
HC	Molar heat capacity	J/(mol·K)	Temperature
C	Heat capacity	J/(kg·K)	Temperature
eta	Dynamic viscosity	Pa·s	Temperature
TD	Thermal diffusivity	m^2/s	Temperature
VP	Vapor pressure	Pa	Temperature
E	Young's modulus	Pa	Temperature
kappa	Initial bulk modulus	Pa	Temperature
mu	Initial shear modulus	Pa	Temperature
nu	Poisson's ratio	-	Temperature
res	Electric resistivity	ohm·m	Temperature
sigma	Electric conductivity	S/m	Temperature
epsilon	Emissivity	-	Temperature
nemiss	Normal total emissivity	-	Temperature
Syt	Tensile strength	Pa	Temperature
Sys	Yield strength level	Pa	Temperature
elong	Elongation	-	Temperature
rho	Density	kg/m^3	Temperature
SR	Stress rupture	Pa	Time
CS	Creep strength	Pa	Time
FSN	Fatigue S-N curve	Pa	Number of cycles
mur	Relative permeability	-	Norm of H field
normfB	Nonlinear magnetic flux density, norm	T	Norm of H field
normfH	Nonlinear magnetic field, norm	A/m	Norm of B field

Quick Start

To access the Material Library, open the **Materials/Coefficients Library** dialog box.

1 Go to the **Options** menu and select **Materials/Coefficients Library**.



The Material Library appears as an additional node in the **Materials** tree, just beneath the **Model** node listing the materials available in your current model. You can browse the different material groups to find the desired one, for example **Lithium** in the nearby figure.

2 Double-click on **Elements** (or click the plus sign to the left of **Elements**) to see all the elements, then select **Lithium**.

You can review all the properties defined for **Lithium** in the **Material properties** area. For example, the function representing its thermal conductivity, k, appears in the **Value/Expression** column on the **Thermal** and **All** pages of the table:

`k_solid_1(T[1/K])[W/(m*K)]`.

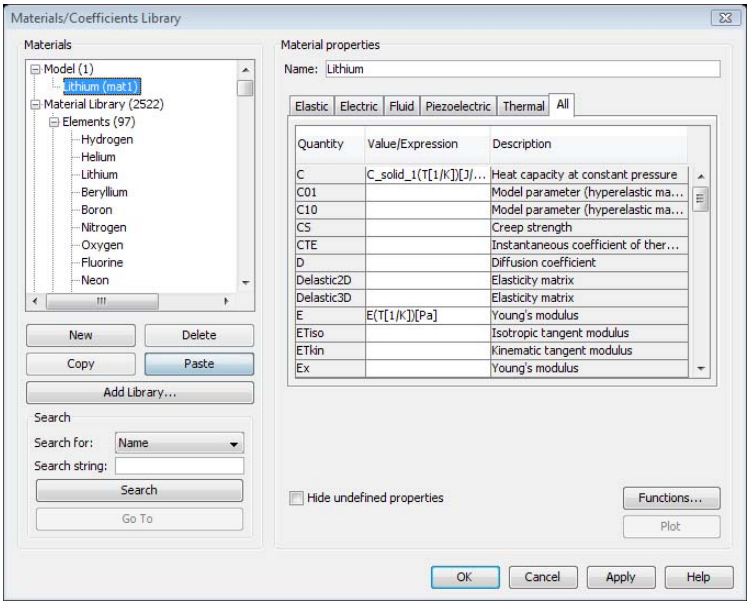
`k_solid_1` is defined as a continuous and piecewise analytic function of its argument. This argument must be the numeric value of the temperature, T, when expressed in the SI unit kelvin; the conversion factor `[1/K]` extracts this numeric

value from the temperature variable, `T`, independently of which base unit system you are using. The resulting numeric function value, `k_solid_1(T[1/K])`, is the thermal conductivity expressed in the SI unit W/(m·K); appending `[W/(m*K)]` to the function value thus gives the complete, dimensionally correct expression for the thermal conductivity.

Note: The unit conversion factors appear as a result of how the material property functions are defined, producing expressions that are independent of the choice of unit system. Thus, no matter what the current base unit system setting in your model is, you do not need to alter these factors.

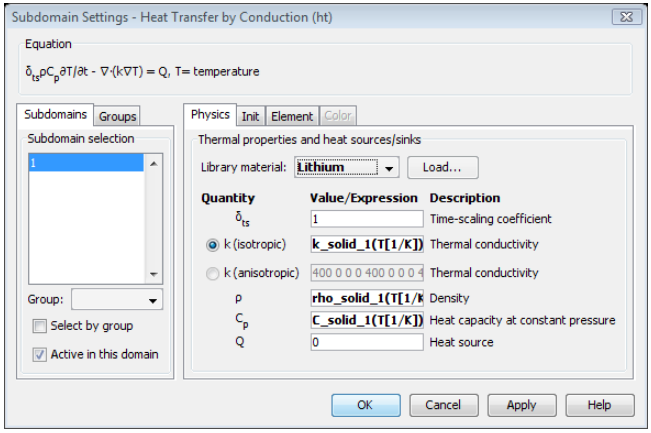
You incorporate a material into a model using the following procedure:

1. Click the **Copy** button beneath the **Materials** tree to copy **Lithium**.
2. Click on the **Model** node (the top node in the **Materials** tree) and click the **Paste** button.



Note that pasting a material transfers only the properties of one phase, orientation, or condition into the model.

Once you have incorporated a material into a model, you can access it from the different physics settings dialog boxes in the user interface. The following figure shows the **Subdomain Settings** dialog box for the Heat Transfer by Conduction application mode. Here you can select **Lithium** from the **Library material** list.



The Subdomain Settings dialog box for the Heat Transfer by Conduction application mode where Lithium is selected from the Library Material list.

Note that you can also open the **Materials/Coefficients Library** dialog box by clicking the **Load** button in the **Subdomain Settings** dialog box shown in the previous figure. When you select a material through this procedure, the **Materials/Coefficients Library** dialog box opens in read-only mode.

2

Using the Material Library

This chapter provides a detailed description of how to use the Material Library. This optional product adds the **Material Library** node to the **Materials** tree in the **Materials/Coefficients Library** dialog box, giving you access to more than 2500 materials with their corresponding 20,000 property functions.

This discussion guides you through the process of selecting a material, adding it to a model, editing and adding properties, creating your own material library, and using material library properties in COMSOL Multiphysics models. The chapter ends by describing the material properties in detail.

Working with the Material Library

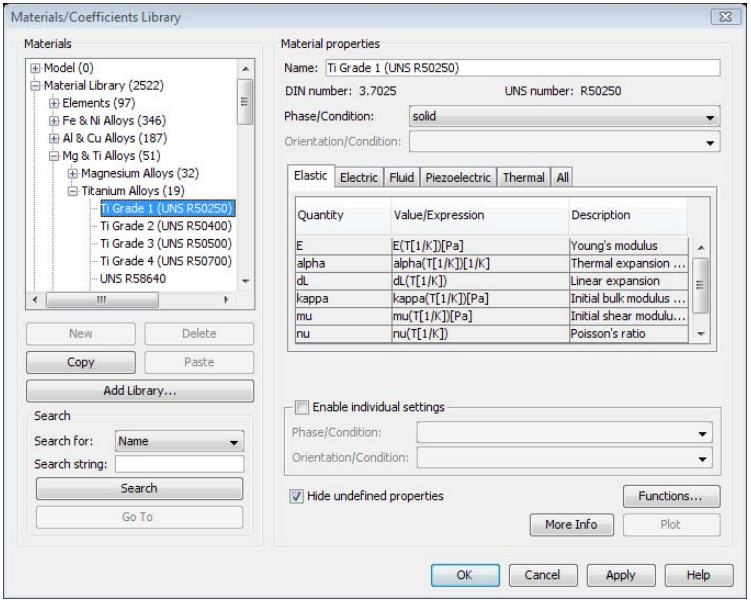
You can access the Material Library in two ways:

- Through the **Materials/Coefficients Library** dialog box, which you open from the **Options** menu in COMSOL Multiphysics.
- Through the **Load** library material button in the **Subdomain Settings** dialog box in an application mode. This opens the Material Library in read-only mode.

When using the Material Library, you typically work through the following steps:

1. Select or search for a specific material or material property
2. Review the selected properties with respect to the conditions in the model
3. Add materials to models and create a custom library
4. Edit or add property functions in a model or library
5. Include properties from a library in the physics settings of your models

You can perform Steps 1 to 4 from the **Materials/Coefficients Library** dialog box (see the following figure). A glance at it gives you a hint about the steps just mentioned.



For the first step, start with the **Materials** list, which groups materials in an intuitive fashion. In addition, a **Search** button makes it possible to search materials by name, UNS (Unified Numbering System) number, or DIN (Deutsches Institut für Normung e.V., the German Institute for Standardization) number. Once you have selected a material, you can search for specific properties organized in several groups, which you access by clicking the **Elastic**, **Electric**, **Fluid**, **Piezoelectric**, or **Thermal** tabs.

Next, review material properties. For this step, the **Plot** button at the bottom of the dialog box graphs a property over the relevant temperature range. The nearby **Functions** button gives you access to the corresponding analytic function expressions and intervals of validity. The **More Info** button provides information about the source of the material property consisting of a literature reference, the material's composition, and the conditions for the property function's estimation or measurement.

You can then add materials to models or create a custom library through the **Copy**, **Paste**, and **Add Library** buttons. The **New** button makes it possible to define materials from scratch.

Once you have added a material to a library or a model, you can edit its properties or add new properties. To do so click the **Functions** button. In the case where you need to enhance the Material Library with a new property function, go to the **Materials/Coefficients Library** dialog box and type the function name in the **Value/Expression** column in the relevant **Quantity** row.

The following discussion presents several examples how to use the Material Library according to the five steps listed above. These examples assume that you have opened COMSOL Multiphysics using, in this case, the Conductive Media DC application mode.

Selecting and Searching the Material Library

Even though the Material Library is organized in an intuitive fashion with folders and subfolders, the search function can still be an efficient tool when you know a material's name, UNS number, or DIN number. Note that the search engine examines only the material's name string.

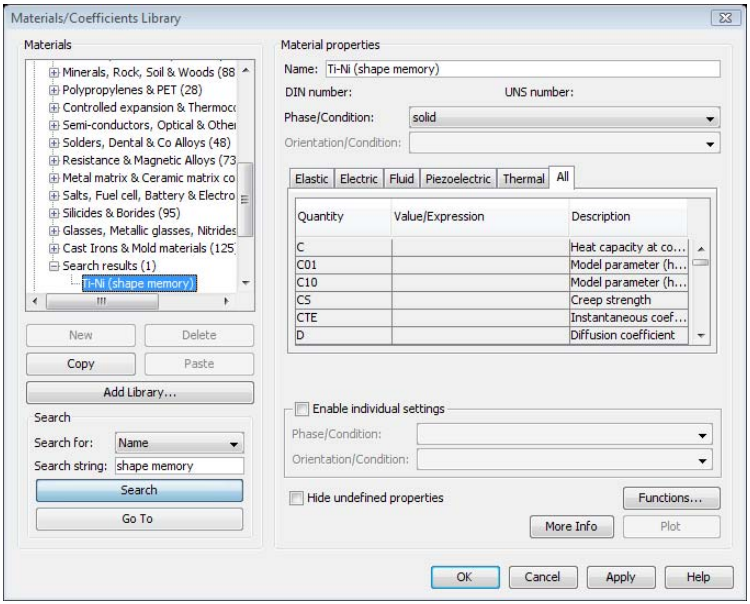
Assume that you are looking for a shape memory alloy. You can search for materials with the word "shape" or "memory" in their name in this way:

1. From the **Options** menu open the **Materials/Coefficients Library** dialog box.
2. Select the **Material Library** node in the **Materials** tree.

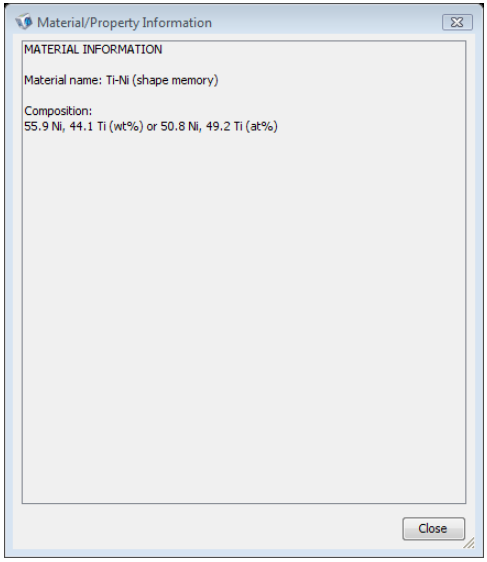
3 Select **Name** from the **Search for** list.

4 Enter `shape memory` in the **Search string** edit field.

5 Click the **Search** button. All materials meeting the search criteria are listed at the **Search result** node, in this case one material: a Ti-Ni shape memory alloy.



6 Click the **More Info** button. This displays some general information about the material. Click **Close** to close just the **Material/Property Information** dialog box.

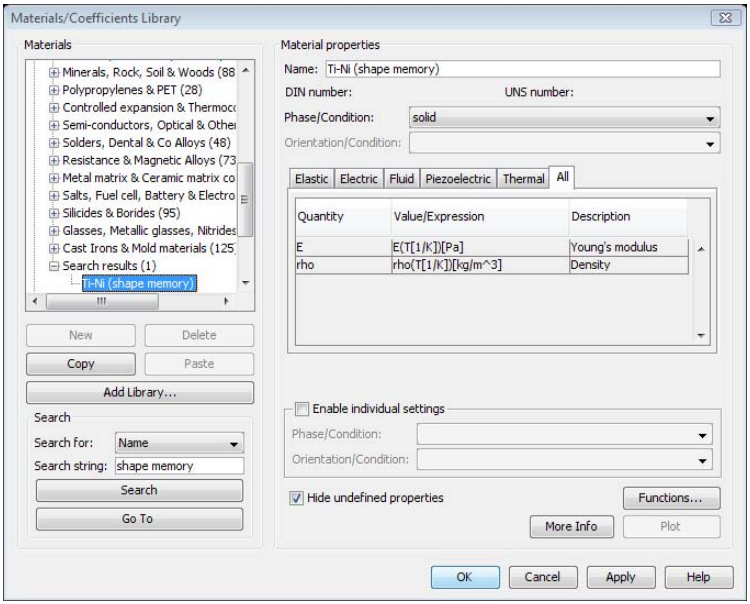


By clicking the **Go To** button when a material in the Search node is selected you move from the search tree to the node where the material is organized. Use this to find similar materials of the same group.

Reviewing Material Properties

Assume that you have found the desired material. You can then quickly list its property functions:

1 With the **All** page displayed, select the **Hide undefined properties** check box at the bottom of the dialog box.

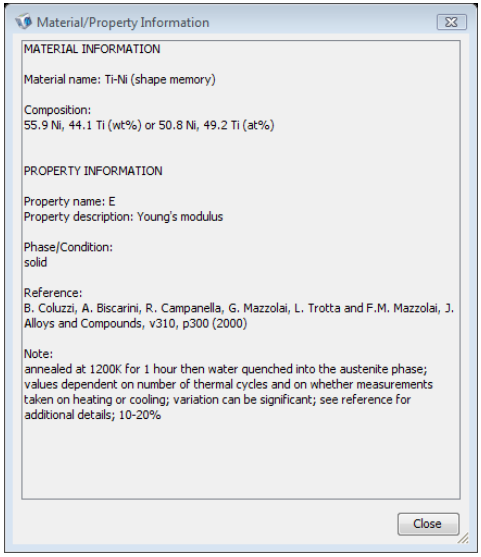


The only property functions available for this material are the Young's modulus and the density in the solid phase (the material can only be solid in this specific case). You can also select the **Enable individual settings** check box to list all properties regardless of phase, orientation, or condition. Ti-Ni (shape memory) properties are available only in one orientation or condition, so this procedure does not change this particular list.

Proceed by reviewing the Young's modulus for the material.

2 Click the **Young's modulus** row on the **All** page.

3 Click the **More Info** button and examine the resulting dialog box.

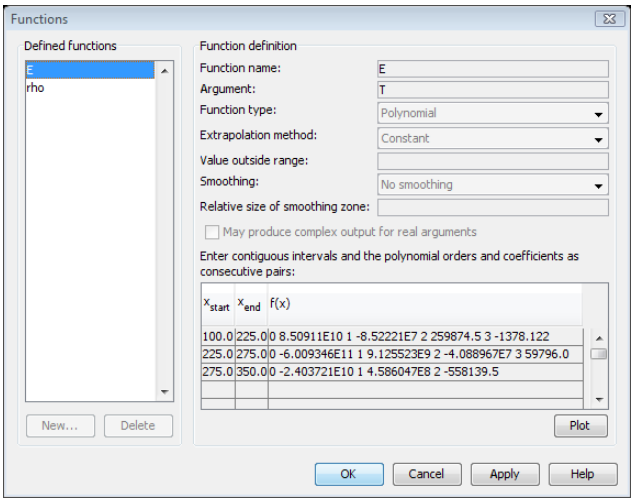


In addition to the material information, you can review the property information including references and notes about the evaluation and measurements of this specific property.

4 Click **Close**.

Continue by reviewing the property functions.

5 Click the **Functions** button.



The **Functions** dialog box displays the expressions used in the different intervals for the **Argument**, which here is temperature, **T**. Note that a different polynomial defines each interval. The coefficients for the terms in the polynomial are entered in pairs, where the first term denotes the order and the second term represents the coefficient. For example, the pair `0 8.50911E10` specifies a constant (order `0`) with the value `8.50911E10`; the next pair, `1 -8.5221E7`, specifies the coefficient for the linear term (order `1`); and so on, defining the polynomial

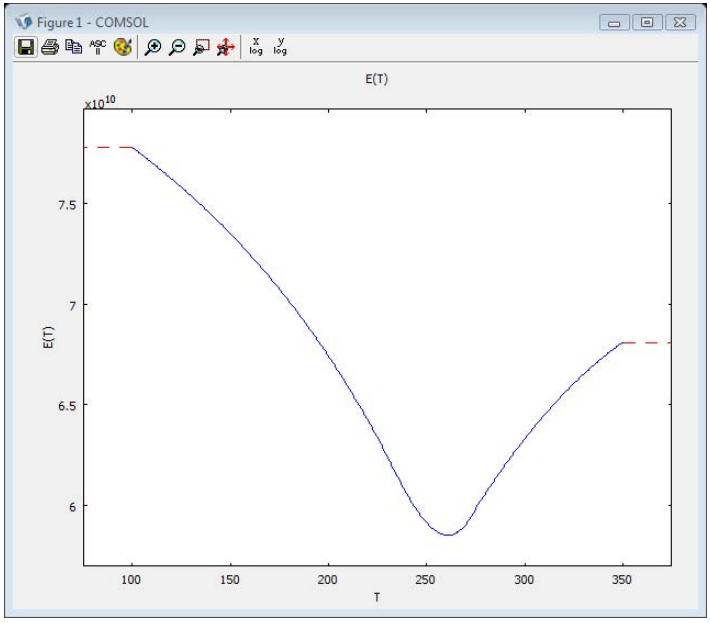
$$8.50911 \cdot 10^{10} - 8.5221 \cdot 10^{7} T + \ldots$$

The $\mathbf{x_{start}}$ and $\mathbf{x_{end}}$ rows define the intervals for the functions.

6 Click **Cancel** to close the **Functions** dialog box.

Next plot the Young's modulus over all intervals for which it is defined.

7 Click the **Plot** button. This plot then appears in a separate figure window:



Adding Materials to Models and Creating Your Own Library

Once you have selected a material and reviewed its properties, you can add it to the current model and include it in a custom material library. There is a good reason for creating your own library, specifically, the ability to add and change property functions. In contrast, the Material Library and the Material/Coefficients files included in the basic package or any of the optional modules contain read-only properties and materials.

Start by adding the selected material, Ti-Ni (shape memory), to the model.

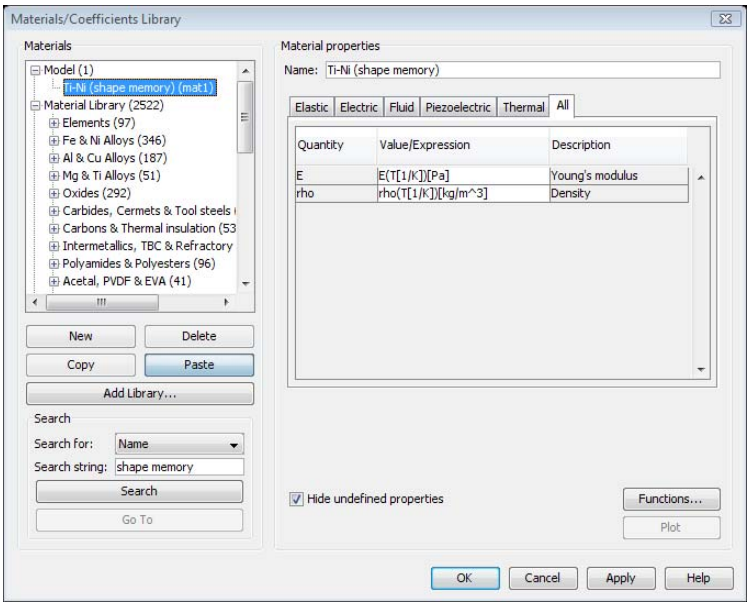
1 Select the **Materials/Coefficients Library** dialog box.

2 Go to the **Materials** list and verify that **Ti-Ni (shape memory)** is still selected.

3 Click **Copy**.

4 Click the **Model** node in the **Materials** list.

5 Click **Paste**.



If you need only the material's Young's modulus and density, close the dialog box and continue modeling. However, assume that you later want to edit the material properties or add new property functions to this material. You can then save the material in a custom library for later manipulation of its properties:

6 Click the **Add Library** button.

7 Enter `my_own_lib` in the **Name** edit field, click **OK**.

8 Select the new **my_own_lib** node in the **Materials** list.

9 Click **Paste**.

An alternative is to store your edited material in the **User Defined Materials** library shipped with COMSOL Multiphysics.

Editing and Adding Property Functions

Continuing on the previous discussion, edit one of the material's property functions. For example, for the Young's modulus change the lower range of the temperature interval from 100 K to 90 K:

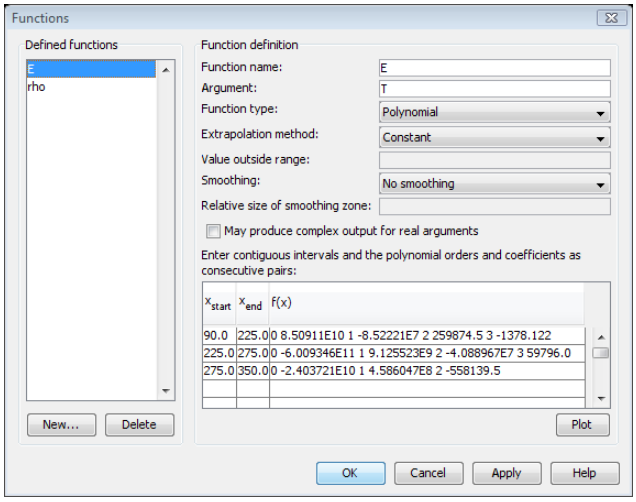
1 Click the **Young's modulus** row in the **Materials/Coefficients Library** dialog box.

2 Click the **Functions** button.

3 Select **E** in the **Defined functions** list.

4 Click the first row in the $\mathbf{x_{start}}$ column.

5 Replace `100` with `90` in the corresponding cell.



6 Click **OK**.

7 In the **Materials/Coefficients Library** dialog box, click the **Young's modulus** row if it is not already selected.

8 Click **Plot**.

The resulting plot appears in a new figure window. You can compare this to the original property function that should still be displayed in the **Figure 1** window.

Note that this is a convenient way of changing material properties in an existing model. Assume that you have used the material `Ti-Ni (shape memory)` in several subdomains. By applying a change to the property function, you change the property of this material in all subdomains and application modes referring to the material without the need to open the **Subdomain Settings** dialog box.

Continue by adding a new property to this material, for example, electric conductivity.

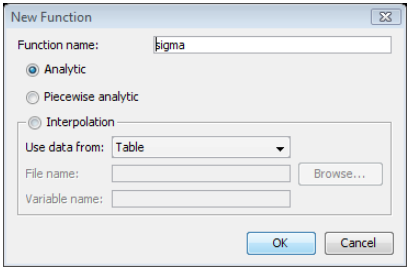
1 Click the **Materials/Coefficients Library** dialog box.

2 Click the **Function** button.

3 Click the **New** button below the **Defined functions** list.

4 Type `sigma` in the **Function name** edit field.

5 Click the **Interpolation** button.

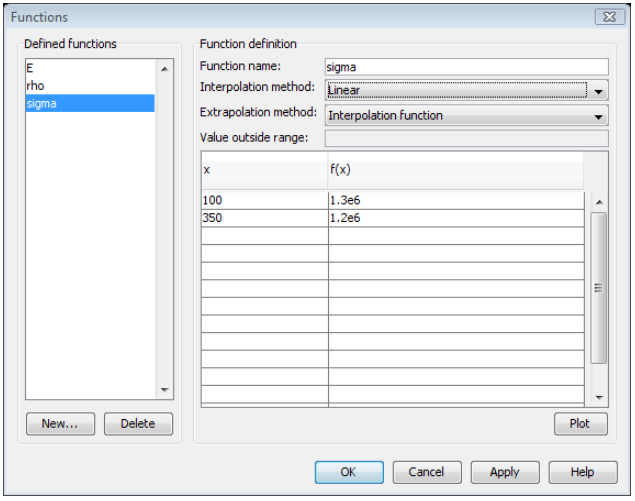


6 Click **OK**.

7 While in the **Functions** dialog box find the **Interpolation method** list and select **Linear**.

8 Type `100` in the first row in the **x** column, then enter `1.3e6` in the first row in the **f(x)** column.

9 Type `350` in the second row in the **x** column, then enter `1.2e6` in the corresponding **f(x)** column.



10 Click **OK**.

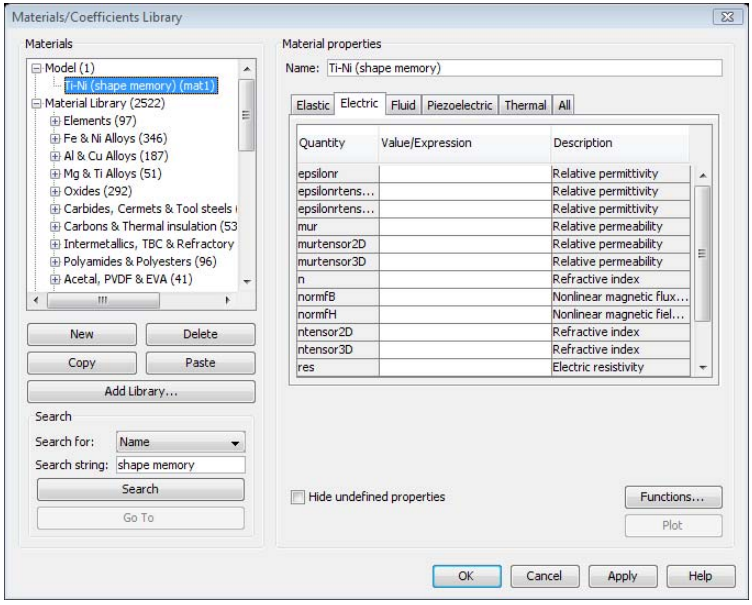
11 Return to the **Materials/Coefficients Library** dialog box.

12 In the **Material properties** area click the **Electric** tab.

13 Clear the **Hide undefined properties** check box.

I4 Click in the **sigma** row for the electric conductivity.

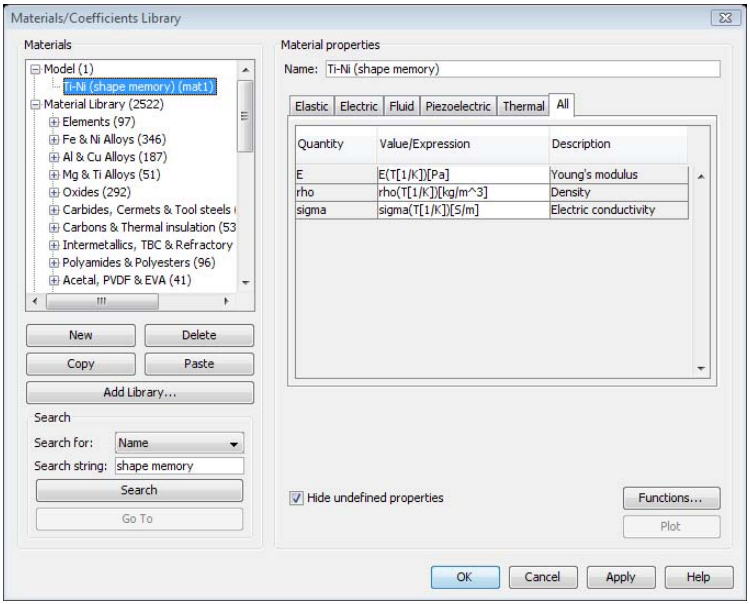
I5 Type `sigma(T[1/K])[S/m]` in the corresponding **Value/Expression** edit field. This gives access to the already defined function `sigma` with the argument T automatically transformed to kelvin and the function value given in S/m.



I6 Click **Apply**.

I7 In the **Material properties** area click the **All** tab.

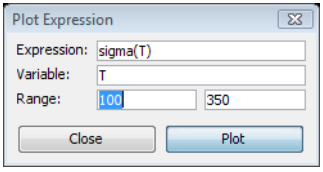
18 Select the **Hide undefined properties** check box. You have three defined properties.



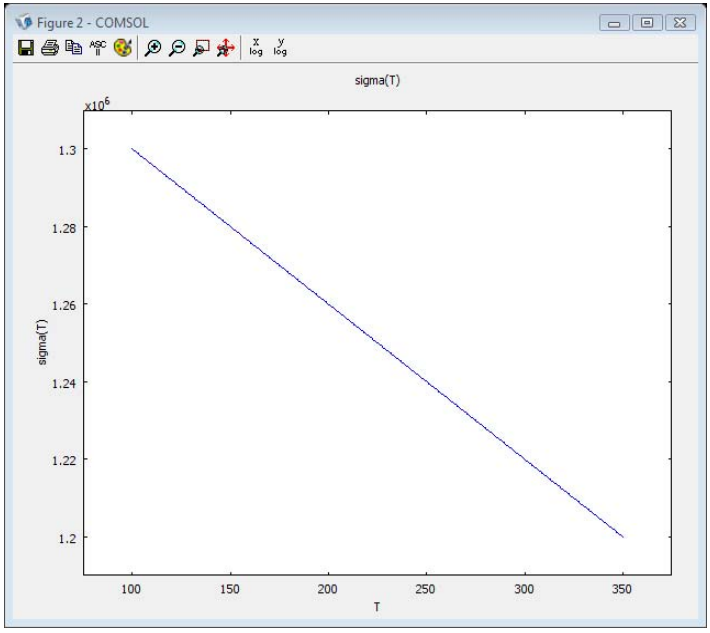
19 Click the row for **Electric conductivity**.

20 Click **Plot**.

21 Type 100 and 350 in the **Range** edit fields.



22 Click **Plot**.



23 Select the **Plot Expression** dialog box and click **Close**.

24 Click **OK** to close the **Materials/Coefficients Library** dialog box.

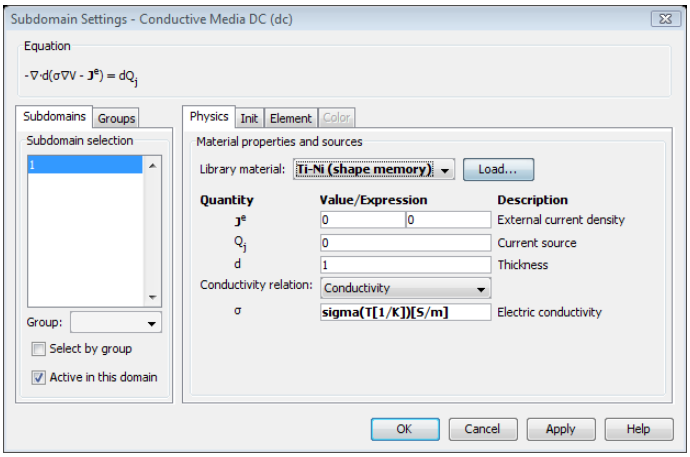
Including Properties in the Physics Settings of Models

Another way to access the Material Library is from the **Subdomain Settings** dialog boxes in the physics modes and in the optional COMSOL modules. If you do not have a geometry defined in the current model, define the simplest possible one, such as an arbitrary rectangle in 2D or a sphere in 3D, in order to follow this discussion. Then follow these steps:

1 From the **Physics** menu open the **Subdomain Settings** dialog box.

2 Click the **Physics** or **Material** tab depending on the application mode. This example uses the **Subdomain Settings** dialog box for the Conductive Media DC application mode.

3 Select **Ti-Ni (shape memory)** from the **Library material** list.

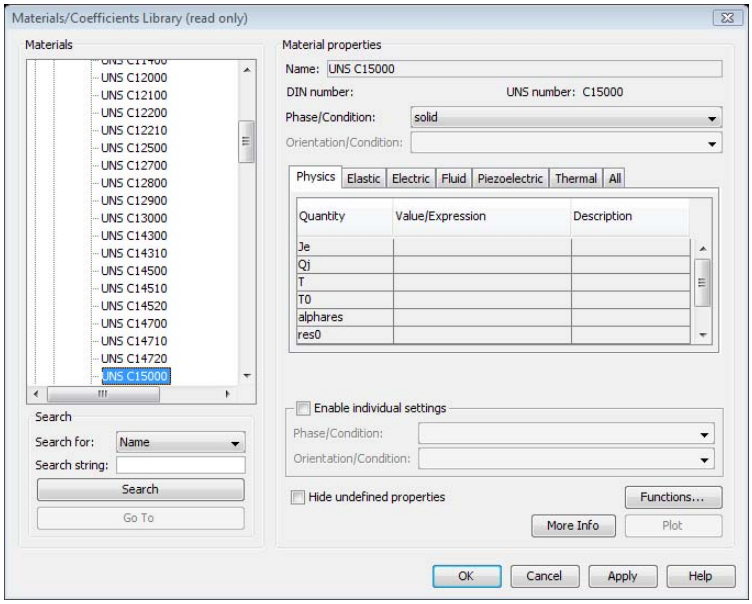


Note that you have now selected the property for the electric conductivity that you defined earlier.

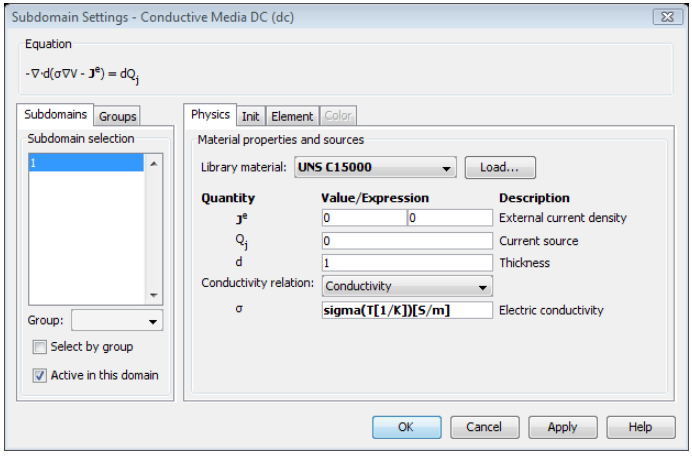
In case you want to load a new material from the Material Library without first editing it, you do not need to go to the **Options** menu. Instead, load it directly from the **Subdomain Settings** dialog box in this way:

1 In the **Subdomain Settings** dialog box click the **Load** button. This step opens the **Materials/Coefficients Library** in read-only mode. You can, for example, select the copper alloy UNS C15000, which is an excellent conductor.

2 Select the **Material Library>Al & Cu alloys**>**Copper alloys** node and then select **UNS C15000**.



3 Click **OK**.



This replaces the Ti-Ni (shape memory) alloy with the properties of the copper alloy in the selected subdomain.

As this example shows, the Conductive Media DC application mode has direct support for the Material Library. This means that once you have selected a material, the application mode automatically places the correct properties in the proper edit fields. Be aware, though, that this is not the case for all application modes. However, you can still manually access any property function from the materials that you have incorporated in a model by typing its function call in the desired edit field. For example, typing `mat1_rho(T[1/K])` in any edit field calls the density function of the material that you first incorporated in the model, in this case Ti-Ni (shape memory), while `mat2_rho(T[1/K])` calls the corresponding function for the second material, the copper alloy UNS C15000.

Material Properties

COMSOL Multiphysics and its modules cover a wide range of disciplines in applied physics modeling, thus involving a large number of material properties. The user interfaces for different physics modeling, our so-called application modes, require more than 50 material properties.

The Material Library contains 27 specific material properties, most of them directly supported in COMSOL Multiphysics. A property that is supported by an application mode is automatically incorporated in the proper edit field once you have selected a material. In the cases where a property is not supported by an application mode, you must manually enter a call to the property function. The properties available in the Material Library are:

TABLE 2-1: AVAILABLE MATERIAL PROPERTIES

MATERIAL PROPERTY	SHORT NAME	ARGUMENT	SI UNIT	NUMBER OF MATERIALS WITH THIS PROPERTY	SUPPORTED IN COMSOL MULTIPHYSICS
Linear expansion	dL	Temperature	-	1437	
Instantaneous coefficient of thermal expansion	CTE	Temperature	1/K	1047	
Coefficient of thermal expansion	alpha	Temperature	1/K	1439	√
Thermal conductivity	k	Temperature	W/(m·K)	990	√
Molar heat capacity	HC	Temperature	J/(mol·K)	380	
Heat capacity	C	Temperature	J/(kg·K)	749	√
Dynamic viscosity	eta	Temperature	Pa·s	95	√
Thermal diffusivity	TD	Temperature	m^2/s	284	
Vapor pressure	VP	Temperature	Pa	99	
Young's modulus	E	Temperature	Pa	898	√
Initial bulk modulus	kappa	Temperature	Pa	350	√
Initial shear modulus	mu	Temperature	Pa	374	√
Poisson's ratio	nu	Temperature	-	374	√
Electric resistivity	res	Temperature	ohm·m	382	√
Electric conductivity	sigma	Temperature	S/m	382	√
Surface emissivity	epsilon	Temperature	-	76	√
Normal total emissivity	nemiss	Temperature	-	50	

TABLE 2-1: AVAILABLE MATERIAL PROPERTIES

MATERIAL PROPERTY	SHORT NAME	ARGUMENT	SI UNIT	NUMBER OF MATERIALS WITH THIS PROPERTY	SUPPORTED IN COMSOL MULTIPHYSICS
Tensile strength	Syt	Temperature	Pa	540	
Yield strength level	Sys	Temperature	Pa	480	√
Elongation	elong	Temperature	-	343	
Density	rho	Temperature	kg/m^3	1822	√
Stress rupture	SR	Time	Pa	147	
Creep strength	CS	Time	Pa	43	
Fatigue S-N curve	FSN	Number of cycles	Pa	42	√*
Relative permeability	mur	Norm of H field	-	12	√
Nonlinear magnetic flux density, norm	normfB	Norm of H field	T	12	√
Nonlinear magnetic field, norm	normfH	Norm of B field	A/m	12	√

* Fatigue data is supported through a script interface, see `matlibfatigue` on page 188 in the *Structural Mechanics Module Reference Guide*.

The functions in the Material Library have the following default variables for the arguments:

ARGUMENT	DEFAULT VARIABLE	UNIT
Temperature	`T`	K
Time	`t`	h
Effective plastic strain	`epe`	-
Number of cycles	`n`	-
Norm of H field	`normH_emnc`	A/m
Norm of B field	`normB_emqa`	T

You can change the default variable in the argument of the property functions to match variable names in a model. For example, if you use the variable `T2` for temperature, change the argument of the property function from `T` to `T2`. Note that the argument need not be a modeled variable, it can also be a constant or an expression.

As mentioned earlier, the functions defining the material properties in the Material Library are based on the SI unit system. However, COMSOL Multiphysics' built-in

unit conversion syntax allows you to use these properties for modeling in all base unit systems available in the software. For example, if you use `T` as variable name for temperature, the entry `T[1/K]` in the argument of a property function always gives the numeric temperature value expressed in kelvin as input to the property function, regardless of the current base unit system. If this property function is, say, a density, `rho`, you must also append the corresponding SI unit, kg/m^3, so that the full, dimensionally correct expression reads `rho(T[1/K])[kg/m^3]`.

In cases where property functions are not automatically supported in an application mode (see the rightmost column of Table 2-1), you must manually enter the material property function call. Here you prepend the string `mat`*`i`*`_` to the property's short name from Table 2-1, where *`i`* is the material number in the specific model. The materials are numbered according to the order of selection, which is identical with the order in which they appear in the **Model** node of the **Materials** list in the **Materials/ Coefficients Library** dialog box and the **Library material** list in the **Subdomain Settings** dialog box. For example, typing `mat1_CTE(T[1/K])` in an edit field yields the instantaneous coefficient of thermal expansion for the material that you first added to the model.

Notes on the Material Properties

When using the Material Library, it is important to check the validity of the property function under the conditions that you are interested in investigating.

The following section contains remarks about the definition, error estimate, and conditions for some of the properties included in the Material Library. Note that every property function contains a literature reference where you can find more details about the conditions and validity range for that specific property (see "Reviewing Material Properties" on page 15).

Coefficient of Thermal Expansion This coefficient is defined as $(\Delta L/L)_T/(T - T_{\text{ref}})$. In most cases this property is calculated from the $\Delta L/L$ values. The error is expected to be in the range of 10–15%, but it might be higher near room temperature due to the small value of $T - T_{\text{ref}}$.

Elastic and Initial Shear Modulus The accuracy of this data is estimated to be approximately 5–10%. For solder alloys the literature reports a wide spread of values. Data from several sources (when available) are evaluated, and representative values are given; the error is estimated to be 10–25%. For some polymers the flexural modulus is used as the elastic modulus, and it is typically within 10% of the elastic modulus.

Typically, values measured with a strain gauge are approximately 10% lower than those measured with a dynamic technique. Values measured by a dynamic technique are preferred over those measured by strain gauge techniques.

For cubic materials where the elastic and shear modulus are calculated from the elastic constants (C11, C12, C44), the Material Library uses the average of the Reuss and Voigt equations (see R.F.S. Hearmon, *Advances in Physics*, vol. 5, 1956, p. 232). For isotropic solids (glasses), it uses methods from L.D. Landau and E.M. Lifshitz, *Theory of Elasticity*, Addison-Wesley, New York, 1966.

Poisson's Ratio and Initial Bulk Modulus These properties are calculated from the elastic modulus and the shear modulus using standard relationships, and in this sense they are self-consistent and accurate. The accuracy of this data is estimated to be approximately 10–20%. Because these are derived quantities, though, the error can be significantly higher. The curves for these properties often show improbable shapes that are most likely due to their derived nature and are not believed to be real. If the elastic and shear modulus were determined in a self-consistent manner, the curves would likely be much better behaved. However, all of the data are presented "as is" from the original references and are self-consistent within the Material Library.

Thermal Conductivity This property can be very sensitive to impurities, heat treatment, and mechanical worked state, especially at very low temperatures. This sensitivity is somewhat decreased above room temperature and decreases as the amount of alloying increases. Compare 4340-QT (quenched and tempered) and 4340-NT (annealed).

Thermal Diffusivity For metals this property can be very sensitive to impurities, heat treatment, and mechanical worked state, especially at very low temperatures. This sensitivity is somewhat decreased above room temperature and decreases as the amount of alloying increases. To see an example of this, compare the data for elemental (high purity) Fe and Armco iron (commercial purity).

Electric Resistivity This property is very sensitive to impurities, heat treatment, and mechanical worked state, especially at very low temperatures.

Electric Conductivity This property is very sensitive to impurities, heat treatment, and mechanical worked state, especially at very low temperatures.

Surface Emissivity (ε_T) This property is the measured emissivity over all wavelengths and 2π radians. This is the emissivity used in the Stefan-Boltzmann law.

Normal Total Emissivity ($\varepsilon_{T,n}$) The measured emissivity is over all wavelengths at a direction normal to the surface. This is the most commonly reported value. For polished metal the following assumption is valid: $\varepsilon_T/\varepsilon_{T,n} = 1.15–1.20$. Both emissivities are sensitive to the surface condition (roughness and oxide thickness).

Density (ρ) The density for solids is calculated from the room-temperature density and the linear expansion coefficient and is given by $\rho/(1 + \Delta L/L)^3$. The data for oxides, carbides, and nitrides depend on the material's porosity. For gases the ideal gas law is used.

Tensile Strength, Yield Strength Level, and Elongation Most of the data for these properties are taken from product brochures provided by the material suppliers. Use these data with the understanding that they are only representative of the actual material properties. The variation with temperature is usually not smooth. Many of these materials are precipitation hardening alloys, and the temperature affects the aging processes in different ways at different temperatures. Unless otherwise stated, the data are for "short" times at the indicated temperatures and not for the equilibrium structure. These properties are very sensitive to the details of the processing and heat treatments. Comparison of data from different suppliers indicate that the spread in the published values is approximately 20% for materials with similar processing. The spread in the elongation data can be as high as 50–100%.

Fatigue S-N Curve Fatigue data are given as the maximum stress, σ_{max}, as function of the number of cycles. The stress amplitude, maximum stress, and minimum stress are related through the stress ratio, R.

$$\sigma_a = \frac{(\sigma_{max} - \sigma_{min})}{2} \qquad R = \frac{\sigma_{max}}{\sigma_{min}}$$

The maximum stress, σ_{max}, is given together with the stress ratio for all fatigue data. You can calculate the stress amplitude as

$$\sigma_a = \frac{\sigma_{max}\left(1 - \frac{1}{R}\right)}{2}.$$

A script interface, see `matlibfatigue` on page 188 in the *Structural Mechanics Module Reference Guide* extracts S-N curves on the form σ_a, as function of the number of cycles. That is the definition required for fatigue analysis using the Structural Mechanics Module.

Creep Strength and Stress-Rupture Curves This data is very sensitive to the test atmosphere as well as the microstructure and heat treatment of the material.

Polymers and Polymer-Based Composites Properties of polymers and polymer-based composites are sensitive to moisture and processing conditions, and they can show time-dependence at higher temperatures. The errors/uncertainties can be large compared to those of other materials. Keep these aspects in mind when using the properties of these materials.

General The magnitude of the errors reported by authors for a given property is usually smaller by a factor of 2–3 than the error between different sources for the same data. This is especially true for materials such as ceramics.

3

Material Library Modeling Example

This chapter describes an example model of a MEMS device that uses the Material Library to include the temperature dependencies of the electric and thermal conductivities for the UNS C17500 alloy. A similar model, *Thermal Expansion*, which uses the Material Library to model thermal expansion, is available as part of the MEMS Module and the Structural Mechanics Module.

Joule Heating in a MEMS Device Using the Material Library

Introduction

Joule heating is a common effect at the microscale, where current densities can be very high. This example model estimates the temperatures for a given set of voltages applied across a MEMS device. Such a device could be included in a microgyroscope or any other sensor that measures acceleration or position. The analysis also estimates the influence of temperature on the total current as a function of the voltage.

Model Definition

The model geometry appears in Figure 3-1.

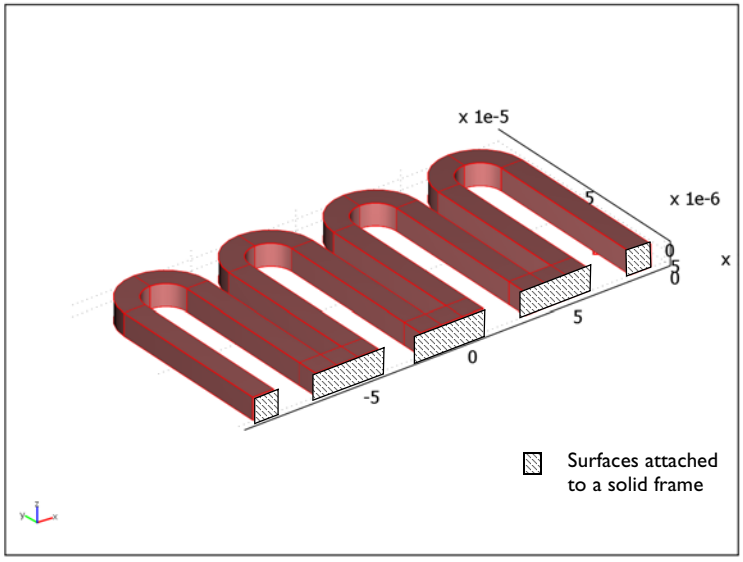


Figure 3-1: Geometry of the MEMS device under study. The coordinate values are given in SI units. The largest dimension of the device is roughly 200 microns.

The model consists of two sets of physics:

- A thermal balance with a heat source in the device, originating from Joule heating (ohmic heating). Air cooling is applied on the boundaries except at the position where the device is attached to a solid frame, where an insulation condition is set.
- A current balance, where all boundaries are electrically insulated except the left and right surfaces attached to the solid frame. Over these surfaces a voltage is applied.

You solve the model using the applied voltage, U, as a parameter ranging between 3 mV and 10 mV in steps of 1 mV.

The device is made of the copper-beryllium alloy UNS C17500.

The thermal balance consists of a balance of flux at steady state. The heat flux is given by conduction only. The heat originates from the ohmic losses and is proportional to the square of the modulus of the electric field and the electric conductivity. The air cooling at the boundaries is expressed using a constant heat transfer coefficient of 10 W/m^2 and an ambient temperature of 298 K (25 °C). The electric-current density is given by Ohm's law, where that density is set to the conductivity times the electric field. A voltage of 3 mV is applied across the left and right surfaces attached to the solid frame.

Both the thermal and electric conductivities are temperature dependent, which means that the electric potential and temperature fields must be solved fully coupled.

The Material Library makes it possible to review the dependencies of the electric and thermal conductivities on temperature for UNS C17500. You can see from the corresponding graphs that the property functions are defined for a wide temperature interval, from 300 K to 1100 K. It is important that you always check the validity of property functions for the conditions in your specific process.

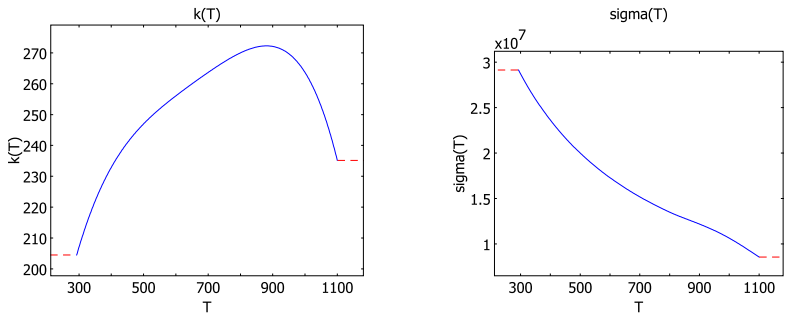


Figure 3-2: Thermal conductivity (left) and electric conductivity (right) for UNS C17500.

Results and Discussion

The following figure shows the temperature distribution in the device for an applied voltage of 3 mV. The heat source increases the temperature from an ambient temperature of 298 K to 378 K, which is well within the temperature range for the property functions. The temperature is almost constant inside the device.

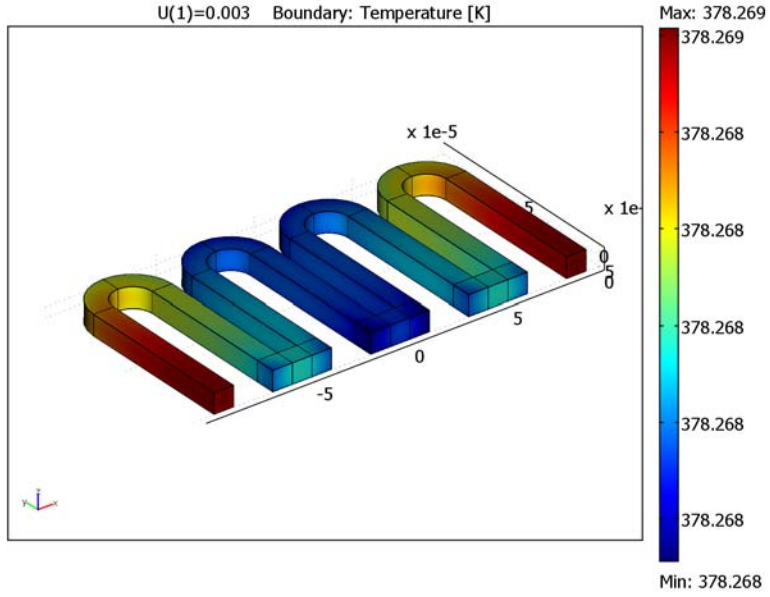


Figure 3-3: Temperature distribution in the device.

Figure 3-4 shows the modulus of the current-density vector. As expected, current density is largest in the device's inner sharp corners. A possible improvement of the model would be to round these corners to their true physical curvature. The inner

surfaces of the U-shaped bends also display a high current density because the current takes a shorter path through the device.

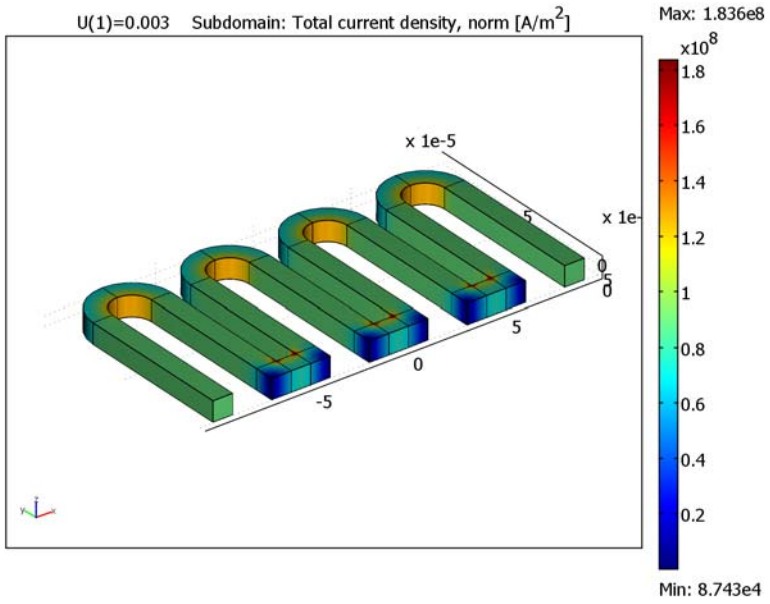


Figure 3-4: The modulus of the current-density vector, [A/m^2].

An interesting issue is the influence of temperature on the linearity of the current density as a function of the total potential difference across the device. The next graphs show total current and temperature as functions of the applied voltage, respectively.

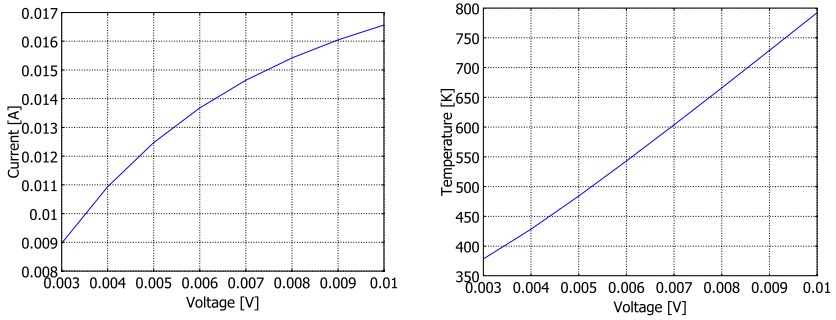


Figure 3-5: Total current through the device (left) and inner temperature (right) as functions of the applied voltage.

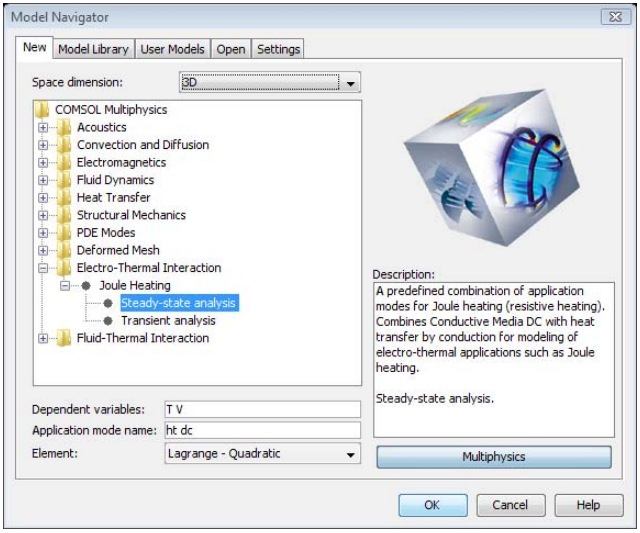
Model Library path:
`COMSOL_Multiphysics/Multiphysics/mems_joule_heating`

Modeling Using the Graphical User Interface

1 Open the **Model Navigator**.

2 Select **3D** from the **Space dimension** list.

3 In the list of application modes select **COMSOL Multiphysics> Electro-Thermal Interactions>Joule Heating>Steady-state analysis**.



4 Click **OK**.

GEOMETRY MODELING

1 From the **Draw** menu select **Work Plane Settings**.

2 Click the **x-y** button in the **Plane** area if it is not already selected. Click **OK**.

3 From the **Options** menu select **Axes/Grid Settings**.

4 Enter `-1.3e-4` in the **x min** edit field, `1.3e-4` in the **x max** edit field, `-0.3e-4` in the **y min** edit field, and `1.3e-4` in the **y max** edit field.

5 Click the **Grid** tab, then clear the **Auto** check box.

6 Enter `1e-5` in both the **x spacing** and **y spacing** edit fields.

7 Click **OK**.

Next draw a projection of the 3D geometry and extrude it to create a 3D object:

1 From the **Draw** menu select **Specify Objects>Rectangle**.

2 In the **Size** area, type `1e-5` in the **Width** edit field and `8e-5` in the **Height** edit field.

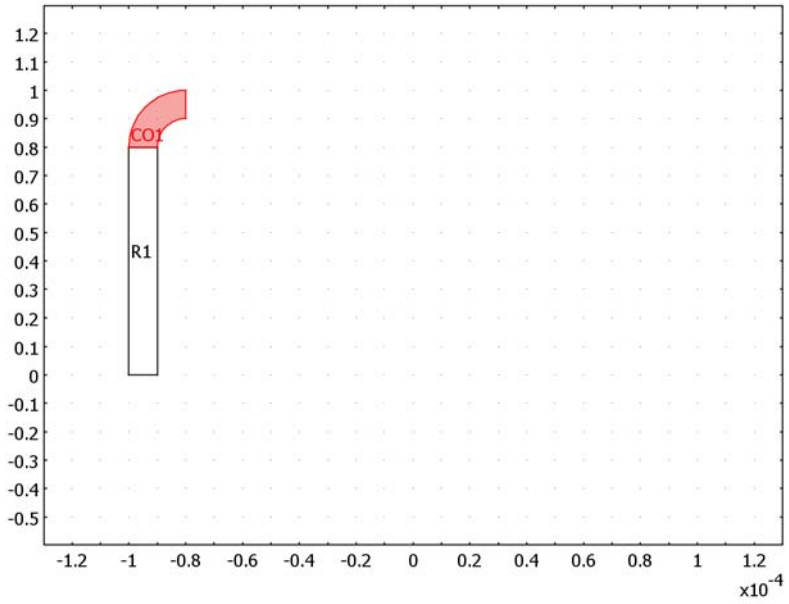
3 In the **Position** area, type `-1e-4` in the **x** edit field. Click **OK**.

4 Click the **2nd Degree Bézier Curve** button on the Draw toolbar to the left in the user interface. Click the coordinates (-9e-5, 8e-5), (-9e-5, 9e-5), and (-8e-5, 9e-5) to create an arc.

5 Click the **Line** button on the Draw toolbar, then click the coordinate (-8e-5, 1e-4).

6 Click the **2nd Degree Bézier Curve** button on the Draw toolbar, then click the coordinates (-1e-4, 1e-4) and (-1e-4, 8e-5).

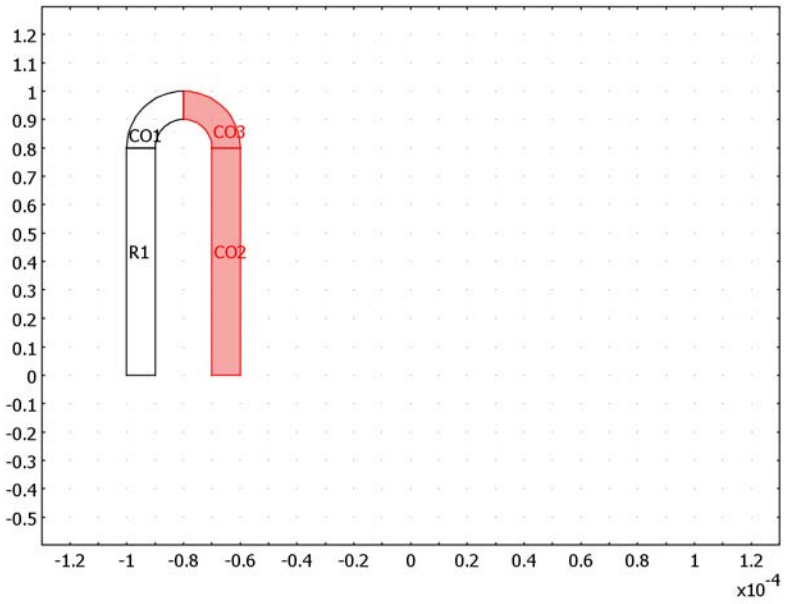
7 Click the right mouse button to form a composite object with the shape of an elbow.



8 Press Ctrl+A to select both objects.

9 Click the **Mirror** button on the Draw toolbar.

10 In the **Mirror** dialog box locate the **Point on line** row. In the cell under the **x** column enter `-8e-5`. Make sure that the **Normal vector** row has the default values **x** = `1` and **y** = `0`. Click **OK**.

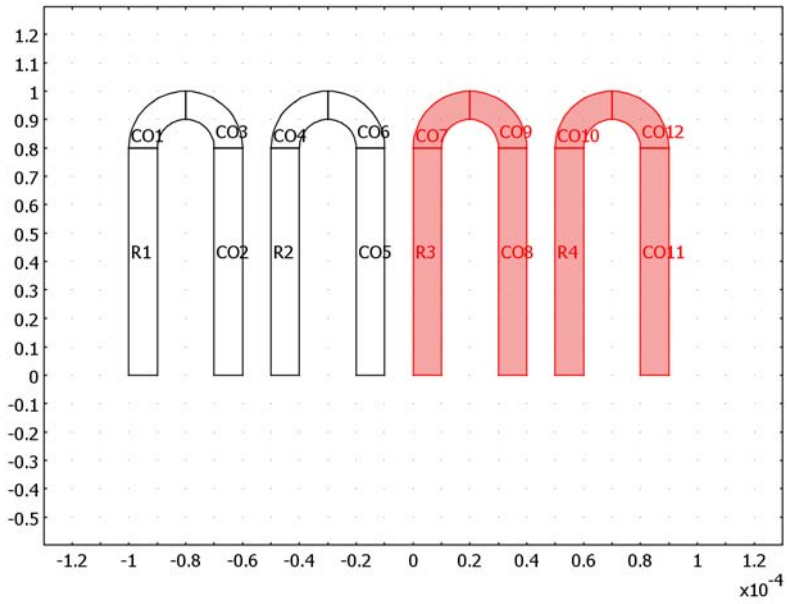


11 Press Ctrl+A to select all the objects and Ctrl+C to copy them.

12 Press Ctrl+V to paste the objects. In the resulting **Paste** dialog box enter `5e-5` in the **x** edit field. Click **OK**.

13 Press Ctrl+A to select all the objects and Ctrl+C to copy them.

14 Press Ctrl+V to paste all objects. In the resulting **Paste** dialog box enter `1e-4` in the **x** edit field. Click **OK**.



15 Click the **Zoom Extents** button on the Main toolbar at the top of the user interface.

16 From the **Draw** menu select **Specify Objects>Rectangle**.

17 In the **Width** edit field enter `3e-5`; in the **Height** edit field enter `1e-5`; and in the **x** edit field enter `-7e-5`. Click **OK**.

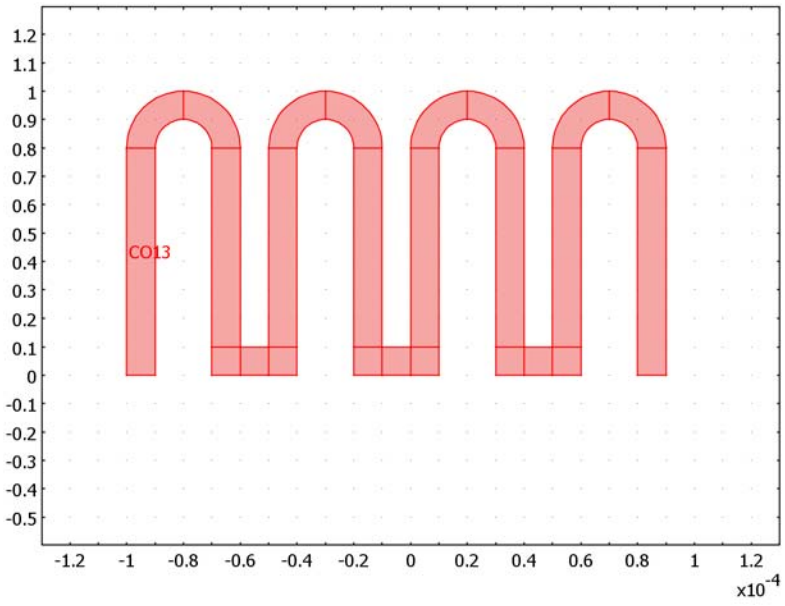
18 Press Ctrl+C followed by Ctrl+V to copy and paste the selected rectangle.

19 In the **Paste** dialog box type `5e-5` in the **x** edit field. Click **OK**.

20 Press Ctrl+C followed by Ctrl+V to copy and paste the selected rectangle.

21 In the **Paste** dialog box type `5e-5` in the **x** edit field. Click **OK**.

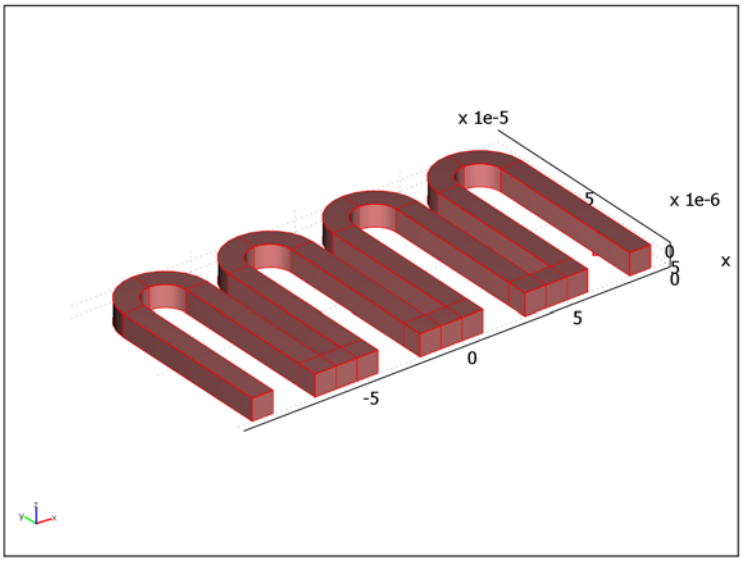
22 Press Ctrl+A and then click the **Union** button on the Draw toolbar to create one composite object.



23 From the **Draw** menu select **Extrude**.

24 Enter `1e-5` in the **Distance** edit field. Click **OK**.

25 Click the **Headlight** button on the Camera toolbar.



PHYSICS SETTINGS

First define a variable for the total electric current through the device.

Boundary Coupling Variables

1 Choose **Options>Integration Coupling Variables>Boundary Variables**.

2 Select Boundary 5.

3 In the first row of the table, type `I` in the **Name** column and `nJ_dc` in the **Expression** column. Leave the default settings for **Integration order** and **Global destination**.

4 Click **OK**.

Proceed by setting the subdomain properties and boundary conditions, starting with the thermal analysis.

Subdomain Settings—Heat Transfer by Conduction

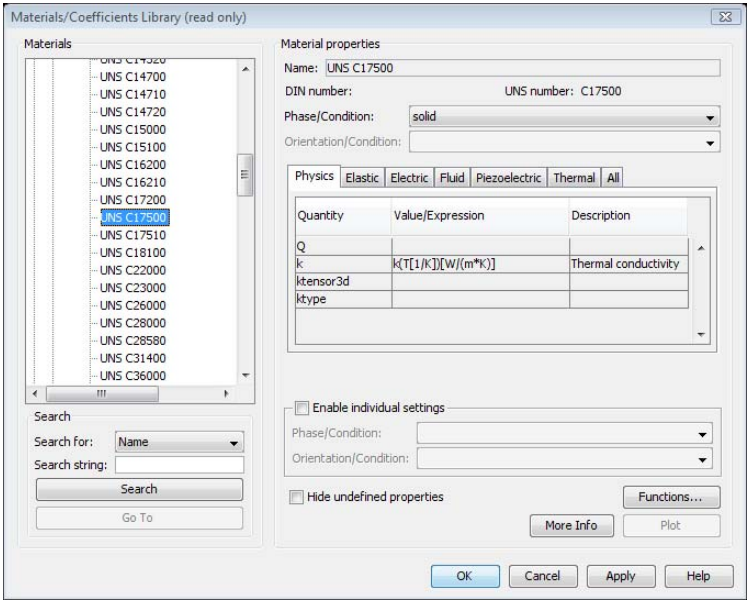
1 From the **Multiphysics** menu select **Heat Transfer by Conduction (ht)**.

2 From the **Physics** menu select **Subdomain Settings**.

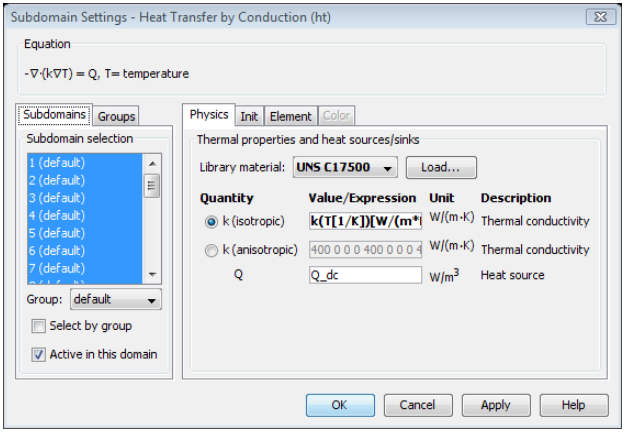
3 Click the **Subdomain selection** list and press Ctrl+A to select all the subdomains.

4 Click the **Load** button.

5 In the **Materials** list select **Material Library>Al & Cu alloys>Copper alloys>UNS C17500**.



6 Click **OK**.



7 Click **OK** to close the **Subdomain Settings** dialog box.

Boundary Conditions—Heat Transfer by Conduction

1 From the **Physics** menu select **Boundary Settings**.

2 Click the **Boundary selection** list.

3 Press Ctrl+A to select all the boundaries.

4 In the **Boundary selection** list, press Ctrl and then click Boundaries 2, 17, 26, 32, 52, 61, 67, 87, 96, 102, and 122 to clear them from the current selection.

Note that you can also do this directly in the user interface by selecting all the boundaries, clicking the right mouse button to keep the selection, and then selecting the boundaries corresponding to the attachment to the base one at the time. When you click on a boundary, it turns green. If this is the boundary you want to clear from the selection list, click the right mouse button. Repeat this procedure until all boundaries just listed are cleared from the selection.

5 From the **Boundary condition** list select **Heat flux**.

6 Enter 10 in the **Heat transfer coefficient** edit field and 298 in the **External temperature** edit field.

7 Click **OK**.

Subdomain Settings—Conductive Media DC

1 From the **Multiphysics** menu select the **Conductive Media DC (dc)** application mode.

2 From the **Physics** menu select **Subdomain Settings**.

3 Select all the subdomains in the **Subdomain selection** list, if they are not already selected.

4 Click the σ **(isotropic)** button.

5 In the **Library material** list select **UNS C17500**.

6 Click **OK**.

Boundary Settings—Conductive Media DC

1 From the **Physics** menu select the **Boundary Settings**.

2 Click the **Boundary selection** list, then press Ctrl+A to select all the boundaries.

3 From the **Boundary condition** list select **Electric insulation**.

4 Select Boundary 2, then select **Ground** from the **Boundary condition** list.

5 Select Boundary 122, then select **Electric potential** from the **Boundary condition** list.

6 In the V_0 edit field type U.

7 Click **OK**.

MESH GENERATION

1 Click the **Interactive Meshing** button on the Mesh toolbar.

2 Select Boundary 2, which is the left-most boundary attached to the solid frame.

3 Click the **Decrease Mesh Size** button on the Mesh toolbar to decrease the mesh size from normal to fine.

4 Click the **Decrease Mesh Size** button on the Mesh toolbar a second and a third time to decrease the mesh size to extra fine.

5 Click the **Mesh Selected (Mapped)** button on the Mesh toolbar.

6 Click the **Subdomain Mode** button on the Main toolbar.

7 Select Subdomains 1–5, which are the five first domains from left to right. Note that you can do this by clicking the mouse until you get the desired subdomain highlighted, then right-click to save that selection. Continue to the next subdomain, highlight it by clicking on it, and right-click to save that selection. Repeat this process until you have selected all five subdomains. Alternatively, you can open the **Subdomain Settings** dialog box and do the selection in the **Subdomain selection** list before clicking **Cancel** to close the dialog box.

8 Click the **Mesh Selected (Swept)** button on the Mesh toolbar.

There is a good reason for not sweeping the mesh throughout all subdomains: the meshing of the cubic sections, which unite the U-shaped sections of the geometry, requires that you change the sweep direction in order to create only hexagonal mesh elements. If you instead mesh all U-shaped sections first, COMSOL Multiphysics detects the sweep dimension automatically by the fact that two opposite faces of the cubes are meshed. You can therefore first create a swept mesh for all U-shaped sections and then mesh the cubes to create a hexagonal mesh for the entire geometry.

9 Click the **Boundary Mode** button on the Main toolbar.

10 Select Boundaries 32, 67, and 102. The easiest way to locate these boundaries is by doing the selection in the **Boundary selection** list in the **Boundary Settings** dialog box. Alternatively, you can use the technique outlined earlier—that is, click on the desired boundary until it gets highlighted, then right-click to save the selection, and so on for multiple selections.

11 Click the **Mesh Selected (Mapped)** button on the Mesh toolbar.

12 Click the **Subdomain Mode** button on the Main toolbar.

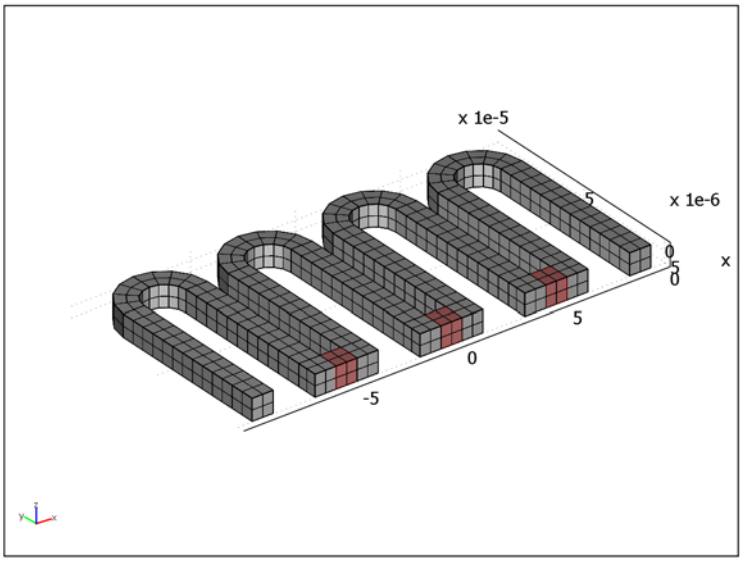
13 Press Ctrl+D to clear the current selection.

14 Select Subdomains 7–12, 14–19, and 21–25 by using the one of the techniques outlined in Step 7.

15 Click the **Mesh Selected (Swept)** button.

16 Select Subdomains 6, 13, and 20.

17 Click the **Mesh Selected (Swept)** button.



COMPUTING THE SOLUTION

1. Click the **Solver Parameters** button on the Main toolbar to open the **Solver Parameters** dialog box.
2. From the **Solver** list select **Parametric**.
3. In the **Parameter** area, type `U` in the **Parameter name** edit field and type `3e-3:1e-3:10e-3` in the **Parameter values** edit field. When solving the model this gives solutions for applied voltages of 3 mV, 4 mV, …, 10 mV.
4. From the **Linear system solver** list select **Direct (UMFPACK)**.
5. Click **OK** to close the **Solver Parameters** dialog box.
6. Click the **Solve** button on the Main toolbar. Note that the solution is fully coupled.

POSTPROCESSING AND VISUALIZATION

To reproduce the plot in Figure 3-3, displaying the surface temperature distribution for an applied voltage of 3 mV, perform the following steps:

1. Click the **Plot Parameters** button on the Main toolbar.
2. On the **General** page, clear the **Slice** check box and select the **Boundary** check box.

3 In the **Solution to use** area, select **0.003** from the **Parameter value** list.

4 Click the **Boundary** tab.

5 Enter `T` in the **Expression** edit field.

6 Click **OK** to generate the plot.

Finally, generate the plots in Figure 3-5 of the total current and the temperature as functions of the applied voltage by following these steps:

1 From the **Postprocessing** menu select **Cross-Section Plot Parameters**.

2 Click the **Point** tab. In the **Expression** edit field type `I`.

3 Click the **General** tab. Click the **Title/Axis** button.

4 Click the option button next to the **Title** edit field. Leave the edit field empty to obtain a plot without a title.

5 Click the option button next to the **First axis label** edit field, then enter the label `Voltage [V]`.

6 Click the option button next to the **Second axis label** edit field, then enter the label `Current [A]`.

7 Click **OK** to close the **Title/Axis Settings** dialog box, then click **Apply** to generate the left plot in Figure 3-5.

8 Click the **Point** tab. In the **Expression** edit field type `T`.

9 In the **Coordinates** area, enter the **x**, **y**, and **z** values, `-5e-6`, `5e-6`, and `5e-6`, respectively.

These settings correspond to a point in the center of the central cubic subdomain (number 13). Because the temperature distribution is essentially uniform, the choice of point inside the device is arbitrary.

10 Return to the **General** page. From the **Plot in** list select **New figure**.

11 Click the **Title/Axis** button.

12 Click the **Auto** option button for the **Second axis label**, then click **OK**.

13 Click **OK** to close the **Cross-Section Plot Parameters** dialog box and generate the right plot in Figure 3-5.

4

Functions

The Material Library describes material properties with functions, usually functions of temperature, and for this purpose it uses piecewise analytic functions. For user-defined property functions you can define three types of functions—inline, piecewise analytic, or interpolation.

This chapter details the Functions feature that describes the material properties in the Material Library and the functions that you can use to define custom properties.

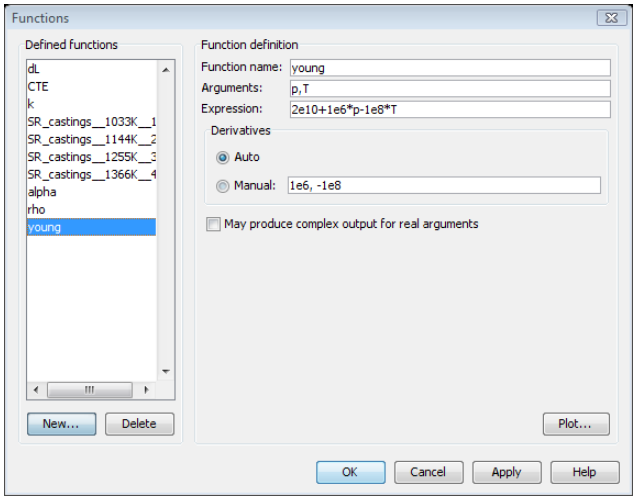
Using Inline Functions

Just as you can define variables in COMSOL Multiphysics, you can define inline functions. They extend variables with the ability to bind parameters during function calls. In other words, you do not need to know the actual names of the variables in an expression when you write the function. You define inline functions in the **Functions** dialog box.

Assume that you want to define Young's modulus for a material as a function of pressure and temperature. You can name the function `young(p,T)` and use the expression `2e10+1e6*p-1e8*T` to define the function. Follow these steps:

1. From the **Options** menu open the **Materials/Coefficients Library** dialog box.
2. Click the **+** sign in the **Material Library** node in the **Materials** list to expand the **Material Library** node.
3. Click the **+** sign in the **Cast Irons & Mold materials** node.
4. Click the **+** sign in the **Cast Irons** node.
5. Select material **A297 HI (UNS J94003)** in the **Cast Irons** node. Note that this material entry does not contain the Young's modulus.
6. Click the **Copy** button.
7. Click the **Model** node in the **Materials** tree, then click **Paste** to add this material to those available inside the model.
8. Click the **Functions** button.
9. Click the **New** button.
10. In the **New Function** dialog box that appears, select **Analytic** and type `young` in the **Function name** edit field. Click **OK** to return to the **Functions** dialog box.
11. In the **Arguments** edit field type `p,T`.
12. In the **Expression** edit field type `2e10+1e6*p-1e8*T`.

I3 Click the **Manual** button in the **Derivatives** area, then type `1e6,-1e8` in the associated edit field.



I4 Click **OK**.

I5 The function `young` can now be used to define the Young's modulus in your material.

I6 Enter `young(p[1/Pa],T[1/K])[Pa]` in the **Value/Expression** column in the Young's modulus row.

I7 Click **OK** to close the **Materials/Coefficients Library** dialog box.

COMSOL Multiphysics must know the derivative of a function if you are using a variable that depends on the solution in a function argument. This is the reason in the previous exercise for clicking the **Manual** button and entering the derivatives in the associated edit field. Note that you can use of the `diff` operator to compute derivatives of a function (see "Using Special Operators" on page 155 in the *COMSOL Multiphysics User's Guide* for more information). If you click the **Auto** button in the **Derivatives** area, COMSOL Multiphysics uses the `diff` operator on the expression to get the derivatives. Select the **May produce complex output for real arguments** check box if the defined function works similarly to `sqrt`, that is, if it sometimes returns complex values for a real-valued input.

Using Functions Based on Interpolated Data

To define functions based on interpolated data, use the **Functions** dialog box, which you open through the **Functions** button in the **Materials/Coefficients Library** dialog box. To define a new interpolation function, click the **New** button to open the **New Function** dialog box. Specify a name for the function, then click the **Interpolation** button. Next choose a method for entering data and, if applicable, a data source, then click **OK**.

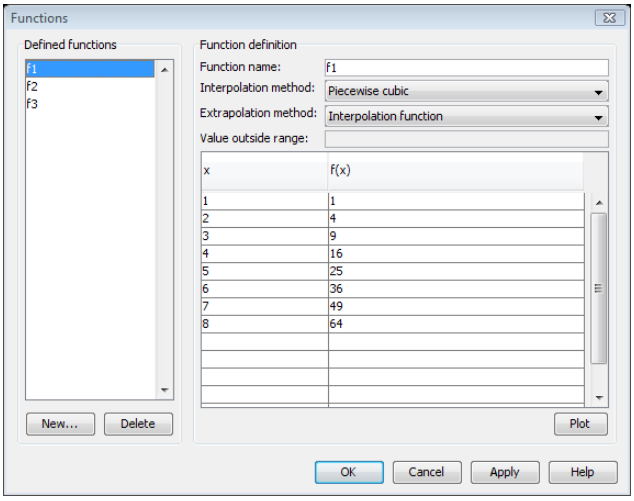


Figure 4-1: The Functions dialog box, used here to edit an interpolation function.

For functions of one variable, you can choose between the following interpolation methods:

- Nearest neighbor
- Linear
- Piecewise cubic
- Cubic spline

For functions of more than one variable, COMSOL Multiphysics supports only the nearest-neighbor and linear interpolation methods.

Piecewise-cubic interpolation is a method using a piecewise-cubic Hermite polynomial with continuous first derivatives. It preserves the shape of the data and respects monotonicity. The cubic-spline method also performs interpolation with a piecewise cubic polynomial. Here even second derivatives are continuous; however, the method does not necessarily respect monotonicity.

You must also specify how COMSOL Multiphysics treats arguments that fall outside the grid. There are three extrapolation methods to choose from:

- Constant
- Interpolation function
- Specific number

Constant means that the extrapolation method uses the value from the closest point inside the grid, while Interpolation Function evaluates the polynomial from the closest grid point at the actual point where a value is requested. If selecting Specific Number, you can assign a single value, usually zero or NaN, to all points outside the grid.

For functions of one variable you can enter the data directly into a lookup table. In this case you can get a preview of the function by clicking the **Plot** button.

For functions of one to three variables, you can either retrieve data from a text file, COMSOL Script, or MATLAB. The file format is the same as that for a file produced when exporting in the format **Grid, data** on a regular grid using the selection **Export>Postprocessing Data** from the **File** menu:

```
% Grid
x grid points separated by spaces
y grid points separated by spaces (optional)
z grid points separated by spaces (optional)
% Data
Data values separated by spaces
```

Each row contains values for different x grid points for fixed values of y and z. The rows first increase the y grid value and then the z grid value. The grid points can also represent another independent variable that the data values depend on. For example, the "grid points" can be temperature values and the data values can represent the thermal conductivity at these temperatures (see the example in "Interpolation of Measured Data and Nonlinear Materials" on page 219 in the *COMSOL Multiphysics User's Guide*). It is important to use a comment line starting with `%` to separate the grid points or other interpolation points and the data values that are associated with these coordinates or interpolation points.

To retrieve data from COMSOL Script or MATLAB, create a structure on the command line with the fields `x`, `y` (optional), `z` (optional), and `data`. Then `x`, `y`, and `z` are vectors specifying the grid, and `data` is a multidimensional array of the same format as produced by the function call `[xx,yy,zz] = meshgrid(x,y,z);`. For example, to define the function $f(x,y,z) = xy\sin(z)$ on a unit-cube grid and prepare it for export to COMSOL Multiphysics, type the following on the COMSOL Script or MATLAB command line:

```
x = linspace(0,1,11); y = linspace(0,1,11); z = linspace(0,1,11);
[xx,yy,zz] = meshgrid(x,y,z);
data = xx.*yy.*sin(zz);
f.x = x; f.y = y; f.z = z; f.data = data;
```

When COMSOL Multiphysics evaluates the function, the software performs a structured interpolation from the data values on the grid to the coordinates where the function is evaluated. See "A Rock Fracture Flow Model" on page 250 in the *COMSOL Multiphysics Model Library* for an example using data interpolation.

COMSOL Multiphysics stores the data it retrieves from COMSOL Script or MATLAB in the function when it is created, and the connection to the original structure is lost. When the data is stored in a text file, the function stores only the name of the text file and reads data from the file during the analysis.

Using Piecewise Analytic Functions

To define your own piecewise analytic functions, use the **Functions** dialog box, which you open through the **Functions** button in the **Materials/Coefficients Library** dialog box.

To define a new piecewise analytic function, click the **New** button to open the **New Function** dialog box. Specify a name for the function in the **Function name** edit field, then click the **Piecewise analytic** option button and finally click **OK**.

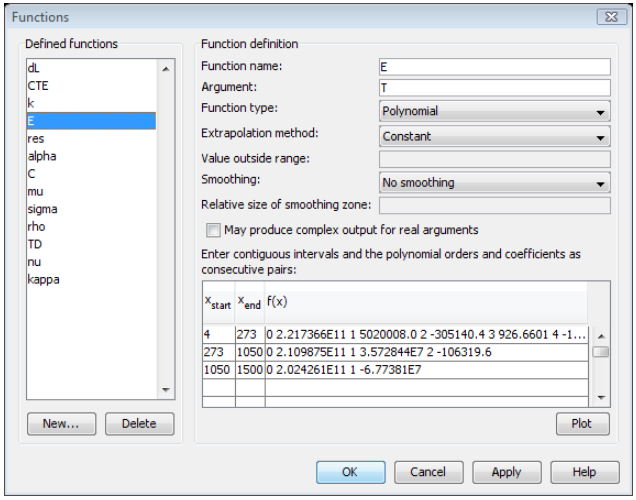


Figure 4-2: The Functions dialog box, used here to edit a piecewise analytic function defining the Young's modulus for the material 1010 (G10100) in the Material Library.

You can choose between three different function types in the **Function type** list:

- **Polynomial**
- **Exponential polynomial**
- **General**

POLYNOMIAL

Use the Polynomial function type to define functions using different polynomials on the intervals, that is

$$f(x) = \sum_i a_{ij} x^i \qquad x_{j\text{start}} < x \le x_{j\text{end}}$$

where i can be any integer.

EXPONENTIAL POLYNOMIAL

Use the Exponential polynomial function type to define functions using different exponential functions with a polynomial exponent on the intervals, that is

$$f(x) = e^{\sum_i a_{ij} x^i} \qquad x_{j\text{start}} < x \le x_{j\text{end}}$$

where i can be any nonnegative integer.

GENERAL

Use the General function type to create functions that use an analytic expression on the different intervals. For the **General** type you must also specify a name in the **Argument** edit field.

It is also necessary to specify how COMSOL Multiphysics treats arguments that fall outside the intervals. There are four extrapolation methods to choose from in the **Extrapolation method** list:

- **No extrapolation**

  The function is not defined outside the interval. Trying to evaluate the function generates an error and evaluates to NaN.

- **Constant** (default)

  The extrapolation method uses the value from the start point of the first interval and the end point of the last interval on the corresponding sides.

- **Nearest function**

  The function at the first or last interval (depending of the side) is used to evaluate at the actual point where a value is requested.

- **Specific number**

  If selecting the Specific Number method you can assign a single value (usually zero or NaN) to all points outside the intervals. Enter the single value in the **Value outside range** edit field.

Functions defined in the different intervals can create a discontinuous function, which can cause problems for the solvers. One way to avoid this is to smooth the function at the interval borders. You choose among four levels in the **Smoothing** list:

- **No smoothing** (default)

- **Continuous function**
- **Continuous first derivative**
- **Continuous second derivative**

You specify the size of the smoothing zone in the **Relative size of smoothing zone** edit field. "Relative size" here means in relation to the size of the intervals on both sides of the border.

Select the **May produce complex output for real arguments** check box if the defined function works similarly to `sqrt`; that is, it sometimes returns complex values for a real-valued input.

You enter the start and end points together with the definition of the function on the interval directly into a table. The table has three columns:

- x_{start}
- x_{end}
- $f(x)$

Specify the interval limits in the x_{start} and x_{end} columns.

Note: The intervals must be contiguous and in ascending order.

Specify the function definition in the $f(x)$ column. You define the function differently depending of the **Function type**. The Polynomial and Exponential polynomial function types are defined using consecutive pairs specifying the polynomial order and the corresponding coefficient. For example, to specify the function

$$f(x) = 1.23 + 1.2 \cdot 10^3 x^3 - 6.58 x^5$$

enter `0 1.23 3 1.2e3 5 -6.58` in the $f(x)$ column. You specify a General function by simply entering the expression using the argument you have specified in the **Argument** edit field. Enter the above function as `1.23+1.2e3*x^3-6.58*x^5` if you specify x as the argument.

You get a preview of a function by clicking the **Plot** button.

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