

INTRODUCTION TO Optimization Module



5.2a

Introduction to the Optimization Module

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Introduction

This introduction is intended to give you a jump-start in your modeling work. It contains examples of the typical use of the Optimization Module and two tutorial examples that introduce the workflow. The first tutorial solves a curve fitting problem and the second example contains a topology optimization of a structural beam.

You can use the Optimization Module in combination with essentially any of the other products in the COMSOL Multiphysics product suite. The module is a general interface for computing optimal solutions to engineering problems to, for example, improve a design so that it minimizes energy consumption or maximizes the output. Any model inputs such as geometric dimensions and part shapes, material properties, and material distribution can be treated as design variables, and any model output can be an objective function.

Problems that may benefit from the systematic exploratory processes provided by the Optimization Module can be divided broadly into two classes:

• Design problems with a single objective.

Here, the problem is to find the values of control variables or design variables that yield the best performance of a model, quantified by means of an objective function. Problems of this kind arise, for example, in structural optimization, antenna design, and process optimization. In many cases, improving the objective function in a robust way is more important than finding the absolute optimum.

• Inverse problems, and in particular parameter estimation in PDEs.

Here the problem is to reliably determine the values of a set of parameters that provide simulated data that best matches measured data. Such problems arise in applications such as geophysical imaging, nondestructive testing, biomedical imaging, and weather data assimilations. *Curve fitting* also belongs to this category.

Problems of the above types can often be formulated more generally as optimization problems. The Optimization interface, Optimization study step, and Parameter Estimation study step in COMSOL Multiphysics are useful for solving design problems as well as inverse problems and parameter estimation.

Work Flow and Examples

The work flow in the Optimization Module is quite straightforward and can be described by the following steps:

- For classical optimization, not involving any Multiphysics model, add a Stationary study and an Optimization study step to an empty model. Define parameters and help variables under Global Definitions, then set up an objective function, control variables, bounds and constraints in the Optimization study step. Constraints and objectives are written as explicit functions of the control variables.
- For Multiphysics optimization, first create the *forward model* containing the geometry and the physics. Define parameters under Global Definitions, or by adding control variables to an Optimization interface. Make sure the forward model solves properly for some reasonable values of the control variables before proceeding with defining the objective function and constraints, and then finally solving the optimization problem.

Note that if your optimization problem only requires global scalar control variables, objective functions and constraint expressions, you can set everything up directly in the Optimization study step. The Optimization interface is only needed if control variables are spatially dependent fields, if constraints must be applied at each mesh node individually, or if the objective function is of a least-squares type more complex than transient curve fitting.

Examples using the Optimization Module exist in the application library for the Optimization Module, as well as in the Application Libraries for several other modules. Search for *optimization* in the Application Libraries window search field to find models that use the Optimization Module in the products that your license includes. These describe the Optimization interface and its different features through tutorial and benchmark examples for various types of optimization. The set includes models of topology optimization, shape optimization, flow minimization, maximization of the reaction rate, and inverse modeling.

An Overview of Optimization Terminology

Assuming that you have solved a COMSOL model of a physical design, it is common to ascribe to it some figure of merit, a cost function, or — using a more general term — an *objective function*. This objective function can quantify almost anything about the performance of the system.

It is natural to question how this objective function changes when you vary some parameters or *control variables*. These variables or parameters can control any part of the design: dimensions, loads, boundary conditions, material properties, material distribution, and so forth. The control variables often have a set of *bounds* and *design constraints* associated with them: dimensions must be within some limits, geometric features must not come to close to each other, only certain materials are possible, and so on.

When optimizing a system modeled as a Multiphysics model, there may also be *performance constraints* present, which depend on the model solution. For example, when minimizing the weight of a part, it is often important to keep the maximum stress or temperature below a predefined safety limit.

In general, an *optimization problem* is when you want to improve the *objective function* by varying the *control variables* within some set of *constraints*. Optimization problems can be further categorized as *topology*, *size*, *shape*, and *parameter* optimization.

Optimization Algorithms

The Optimization Module contains the framework and functionality needed to perform *gradient-based* and *gradient-free* optimization on an existing COMSOL model.

There are three optimization algorithms for gradient-based optimization available in the module. The first algorithm is based on the SNOPT code developed by Philip E. Gill of the University of California San Diego, and Walter Murray and Michael A. Saunders of Stanford University. When using SNOPT, the objective function can have any form and any constraints can be applied. The algorithm uses a gradient-based optimization technique to find optimal designs, and when the underlying PDE is stationary, frequency- or time-dependent, analytic sensitivities of the objective function with respect to the control variables can be used.

The second algorithm is the MMA solver, which is based on the globally convergent method of moving asymptotes by Krister Svanberg of KTH (Royal Institute of Technology, Stockholm). The MMA solver can handle objective functions and constraints of the same very general form as SNOPT. It is well suited to handle problems with a large number of control variables, such as topology optimization.

The third algorithm is a Levenberg-Marquardt solver. When this solver is used, the objective function must be of least-squares type. Also, constraints are not supported. Since the Levenberg-Marquardt method is derived to solve problems of least-squares type, it typically converges faster than SNOPT and MMA for such problems.

In addition, the Optimization Module provides a number of gradient-free (derivative-free) optimization algorithms. Currently Nelder-Mead, BOBYQA, COBYLA and a coordinate search are supported. These methods can optimize a model with respect to design parameters (model parameters) including those that control the geometry sequence that defines the model geometry. There is also a Monte Carlo method, useful for exploring the design space.

All optimization solvers are accessible from the same Optimization study step, which contains the ordinary solver sequence over which the optimization method iterates. The gradient-free methods can contain any other study sequence, including Study Reference links which make it possible to evaluate different objective function contributions and constraints in different studies. The gradient-based methods are limited to optimizing over a single study step for types supporting the computation of analytic sensitivities: currently Stationary, Time Dependent and Frequency Domain studies.

Optimization Module Applications

The Optimization Module provides versatile tools for optimization, curve fitting, parameter estimation, and inverse modeling. Optimization can involve solving a basic linear or quadratic programming problem, but you can also seamlessly incorporate optimization and parameter estimation as additions to, for example, models of structural mechanics, fluid flow, or chemical reactions. The optimizations can be an optimal shape or topology, or a maximization or minimization of some quantity, just to name a couple of examples.

The plot in Figure 1 shows the hydraulic conductivity obtained by inverse modeling using 24 observations in a model where the aim is to characterize an aquifer. The model is in the Subsurface Flow Module application library and combines the Optimization interface with a Darcy's Law interface for the fluid flow in the aquifer. The inverse problem in this model is to estimate the

hydraulic-conductivity field in the aquifer using experimental data in the form of hydraulic-head measurements from four dipole-pump tests.

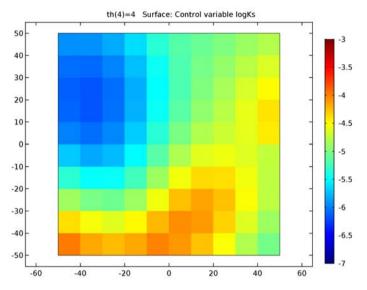


Figure 1: Hydraulic conductivity obtained by inverse modeling in the Aquifer Characterization model.

Another application of the Optimization Module is to find the optimal distribution of porous material in a microchannel, where the objective is to minimize the horizontal velocity at the center of the channel. The plot in Figure 2

shows the *x*-component of the velocity field for the optimal solution and the distribution of the filling material in the open channel:

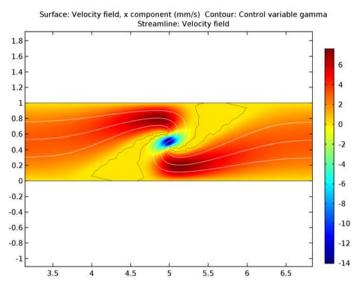


Figure 2: The horizontal velocity (surface plot) and velocity field (streamlines) after optimization. In addition, the contour $\gamma = 0.5$ indicates the border between open channel and filling material.

This model is in the COMSOL Multiphysics application library. It combines a Laminar Flow interface for the single-phase flow in the channel and an Optimization interface, where the objective is a scaled *x*-direction velocity that the optimization solver minimizes. The design variable gamma (γ) can be interpreted as the local porosity, ranging between 0 (filled) and 1 (open channel), so the contour $\gamma = 0.5$ indicates the border between the open channel and the filling.

About Parameter Estimation

You can use the Optimization Module to perform parameter estimation: to determine input values so that the output matches some experimental data — that is, to solve an *inverse problem*. The first tutorial (Tutorial Example — Curve Fitting) describes how to use the Optimization Module for parameter estimation. When solving an inverse problem, there is some set of experimental data that can be compared to the output of the model. Parameter estimation is used to adjust model inputs or properties such that the results agree with the experimental data. Typical objectives include estimating material properties or loads.

For several reasons, inverse problems are inherently the most difficult problems to solve. They are often ill-posed in the sense that they have multiple locally optimal

solutions where the optimization algorithm may get stuck, or entire subspaces of equal merit may exist where the algorithm wanders around forever. In addition, the particular local optimum that is found depends strongly on the initial guess and on small perturbations in the experimental data. For these reasons, it is best to approach inverse problems with a good understanding of the underlying physics and mathematics of the problem. In particular, some problem-dependent regularization strategy is usually needed to make the optimization process robust. Consider a COMSOL Multiphysics model of a physical system, such as a sample of a rubber-like material in simple uniaxial tension. One way to model rubber-like materials is using a Mooney-Rivlin model, which requires empirically determined material constants to describe the structural deformation. Assuming that there are experimental results relating load and deformation, as shown in Figure 3, it is possible to use parameter estimation to determine the material model constants that best fit this data. The curve shown in Figure 3 is computed based upon the results of a parameter estimation; it is a least-squares fit of a COMSOL model with Mooney-Rivlin material parameters to the experimental data.

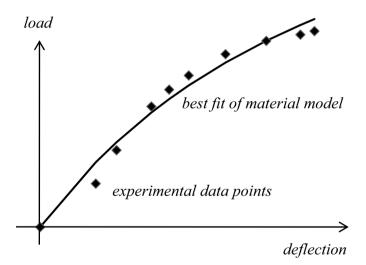


Figure 3: Experimental data and a best fit curve of the Mooney-Rivlin material model based upon a finite element model of a test sample.

About Topology Optimization

The second tutorial model in this guide (Tutorial Example — Topology Optimization) shows how to solve a model using topology optimization.

Consider a COMSOL model of a physical system, such as the bracket shown in Figure 4. The part is constrained at the top and loaded on the side. The part must

support a known load while staying within acceptable limits on the deflection. However, an experienced structural engineer can quickly recognize that the part is overdesigned. It is possible to remove material from the part, which would reduce the total mass (the cost) of the part, while still staying within the limits on the deflection (the constraints). A closely related problem which is often easier to solve can be stated as: Minimize the compliance (the deflection) of the structure under the condition that the total mass must be reduced by at least some predefined factor.

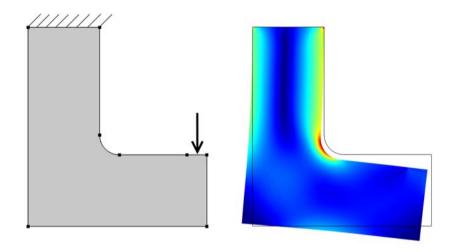


Figure 4: A simple bracket design, and the solved finite element model showing stresses and deflections. This design has room for improvement.

One way to address this is to use *topology optimization*. Topology optimization treats the material distribution as the design variable. Design variables of this type are treated in the same way as the solution variables; they are interpolated using shape functions on the finite element mesh. Therefore, there is one design variable per mesh node or per mesh element, associated with a position in the geometry. We call this a *control variable field*.

The Optimization Module computes the *derivative*, or the *sensitivity*, of the objective function with respect to these discrete design variables. For topology optimization, the *adjoint method* is by far the most efficient. The optimization solver uses the sensitivity information to manipulate the design variables, within the limit of any user-defined constraints, in the direction of improved objective function values.

This is an iterative procedure, as illustrated in Figure 5. Starting with the initial design, the solver adjusts the control variables representing a fictitious material density in each element. This is repeated as long as some improvement in the objective function is possible and the constraints are not violated.

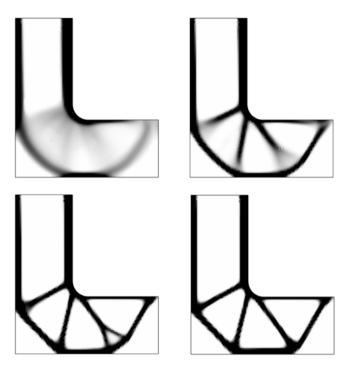


Figure 5: Topology optimization of the bracket, the material distribution, as defined by the finite element mesh, is modified to minimize the weight while satisfying a constraint on peak displacement. The design evolution is shown after 8, 16, 32 and 100 iterations.

A structural engineer will recognize that the resulting design is essentially a truss structure. This result also highlights an issue with topology optimization: The optimal design is often not a candidate for manufacture, it is only an approximation of a better design, as found via the current finite element mesh. With a modicum of engineering knowledge, it is still possible to use the results of a topology optimization as a design guide to build the next design iteration.

Although topology optimization is quick to set up, it has a couple of drawbacks. First, the resulting design does have some dependency on the mesh used. There are techniques known as *regularization* that you can use to avoid this, but they do make the setup more complex. The topology model example in this guide includes regularization. Second, it is difficult to incorporate geometric constraints

(constraints on bend radius or feature thickness, for example) into the optimization algorithm. Without incorporating such constraints, topology optimization can often come up with designs that are impractical. Therefore, topology optimization should be used early in the design process as a guide for the overall structure of the system. It becomes more difficult to use efficiently when the design is already quite rigid and only minor modifications to the design are possible. In such situations, *size optimization* and *shape optimization* become more useful.

The Optimization Module is a general purpose add-on to COMSOL Multiphysics and its other modules. It consists of a physics interface, special study steps, solvers, and an application library.

The Optimization Interface

The Optimization Module adds the Optimization interface () to the list of available physics interfaces. The interface can be found under the Mathematics>Optimization and Sensitivity branch when you are adding physics to your model.

The Optimization interface includes a wide range of advanced features for defining an optimization problem separately, or in connection to a physics model:

- Global objectives, including least-squares objectives
- Global constraints
- Global control variables
- Integral objectives on all geometry levels: domains, boundaries, edges, and points
- Integral constraints on all geometry levels
- Pointwise constraints on all geometry levels
- · Control variable fields on all geometry levels
- Probe objectives in domains (an objective defined by a point evaluation of an expression)

The Optimization Study Step

The Optimization study step (1) acts as the central control panel for any optimization problem. It can be added to any study, where it will appear as the first step. The remaining steps in the study define the simulation which is being optimized. Note that the Optimization study step replaces and cannot be used together with some other study steps, notably Parametric Sweep and its variants.

In the Optimization study step, you can set up objective function contributions, select control variables and set constraints. Objectives, constraints and control variables defined in an Optimization interface are displayed in the study step, where they can be disabled or enabled. Note that most optimization tasks can be specified using the Optimization study step alone, needing no Optimization Interface.

The Optimization study step also contains an optimization solver choice, including the most important solver settings, as well as extensive settings for controlling graphics and table output during the solution process.

The Parameter Estimation Study Step

The Parameter Estimation study step $(\dot{\dot{}}\dot{}\dot{}\dot{}\dot{}})$ is a specialized version of the Optimization study step, intended to simplify some typical parameter estimation tasks. In particular, it contains a user interface for specifying a least-squares objective function based on time-dependent measurements entered or imported into an interpolation function.

The Optimization Solvers

The Optimization Module contains the following optimization solvers:

SNOPT: A robust, gradient-based, general-purpose, sequential quadratic programming algorithm for nonlinear constrained problems.

MMA: A general-purpose, interior point method based on successive convex approximations constructed from objective and constrain gradient information, particularly suited to topology optimization.

Levenberg-Marquardt: A special-purpose solver for least-squares fitting, using the special problem structure to estimate second-order derivatives from first order gradient data. Constraints are ignored.

Nelder-Mead: A robust derivative-free, heuristic, simplex search algorithm, including a penalty method for constraint handling.

BOBYQA: An algorithm sampling the objective function to construct and maintain a quadratic approximation of the objective inside a moving trust region. General constraints can be handled in an augmented Lagrangian wrapper, solving a sequence of unconstrained problems.

COBYLA: An algorithm sampling both objective function and constraint values to create and maintain a linear approximation inside a moving trust region. General constraints are accepted but may be violated at intermediate solution steps.

Coordinate search: A method which searches for the optimum by successive sampling along the control variable axes, typically changing one control variable at a time.

Monte Carlo: A basic stochastic sampling algorithm useful for exploring the design space, extracting statistical information.

This tutorial model demonstrates how to use the Optimization Module to estimate unknown function parameters based on measured data. The two-parameter Mooney-Rivlin solid material model is used as an example, but the procedure is generally applicable when you need to fit a parametrized analytic function to measured data.

The two-parameter incompressible Mooney-Rivlin material model describes the local behavior of rubber-like materials. The model assumes that the local strain energy density in an incompressible solid is a simple function of local strain invariants.

In a standard tensile test, a rotationally symmetric test specimen is pulled in such a way that it extends in one direction and contracts symmetrically in the other two. For this case of uniaxial extension, the relationship between an applied force, F, and the resulting extension, ΔL , of a true Mooney-Rivlin material is

$$\frac{F}{A_0} = 2 \Big(C_{10} + C_{01} \frac{L_0}{L_0 + \Delta L} \Big) \Big(\frac{L_0 + \Delta L}{L_0} - \Big(\frac{L_0}{L_0 + \Delta L} \Big)^2 \Big)$$

where A_0 is the original cross-sectional area of the test specimen and L_0 is its reference length. The constants C_{10} and C_{01} are material parameters that must be determined by fitting the above equation to the experimental data from the tensile test.

In practice, tensile test data is delivered in a form which is independent of the geometry of the test specimen used. There are multiple possible formats. The one used here contains corresponding measured values of engineering stress, P_i , representing force per unit reference area

$$P = \frac{F}{A_0}$$

and stretch, λ_i , representing relative elongation

$$\lambda = \frac{L_0 + \Delta L}{L_0}$$

The expected relationship between these variables for a Mooney-Rivlin material is

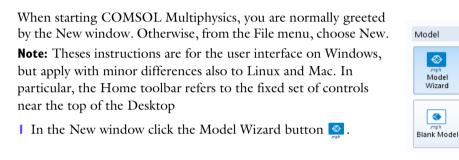
$$P(\lambda) = 2\left(C_{10} + \frac{C_{01}}{\lambda}\right) \left(\lambda - \frac{1}{\lambda^2}\right)$$

Given *N* pairs of measurements (λ_i, P_i) , i = 1..N, the values of C_{10} and C_{01} that best fit the measured data are considered to be those which minimize the total squared error

$$e = \sum_{i=1}^{N} (P(\lambda_i) - P_i)^2$$

The curve fitting problem is therefore identical to an optimization problem.

Creating a New Model



Model Wizard

This pure optimization example does not refer to any geometry. Any model must, however, contain at least one component. Zero-dimensional components are useful for this type of optimization problem, as well as, for physics modeled using only ordinary differential equations (ODEs). The Stationary study is necessary as a placeholder signaling the problem type, even if there are no equations to solve in this case.

- I In the Model Wizard window, click the 0D button · .
- 2 In the Select Physics tree under Mathematics>Optimization and Sensitivity, click Optimization (opt)
- 3 Click Add.
- 4 Click the Study button 🚭.
- 5 In the tree under Preset Studies, click Stationary 🗁.
- 6 Click Done 🗹.

	Search
 ▲ Δu Mathematics ▷ 4/ct, ODE and DAE Interfaces ④ Optimization and Sensitivity ④ Optimization (opt) ↓ Sensitivity (sens) 	
	Add
dded physics interfaces: & Optimization (opt)	Add
	Add

Global Definitions

When your control variables are independent of geometry, it is easiest to set them up initially as global parameters. Also add the stretch parameter lambda that has been varied in the measured data as a global parameter.

Parameters

Note that you can click the double-arrow button in the upper left corner of parameter and variable tables to expand them, making editing easier.

- I On the Home toolbar click Parameters P_i .
- 2 In the Settings window locate the Parameters section.

3 In the table, enter the following settings:

Setting	S		~
– Parameter	rs		
Param	eters		
* Name	Expression	Value	Description
lambda	1	1	Stretch
C10	1[MPa]	1E6 Pa	Mooney-Rivlin parameter
C01	1[MPa]	1E6 Pa	Mooney-Rivlin parameter

Variables 1

- I On the Home toolbar click Variables a= and choose Global Variables a= .
- 2 In the Settings window for Variables locate the Variables section.
- **3** In the table, enter the following settings:

Name Expression Unit Description P 2*(C10+C01/lambda)*(lambda-1/lambda^2) Pa Engineering stress	Settings Variables	5			÷ 1
" Name Expression Unit Description					
P 2*(C10+C01/lambda)*(lambda-1/lambda^2) Pa Engineering stress	10		Unit	Description	
	P	2*(C10+C01/lambda)*(lambda-1/lambda^2)	Pa	Engineering stress	

Optimization

You can import tensile test data from file in the form of comma-separated values or, as demonstrated here, enter the data manually into a local table.

Global Least-Squares Objective 1

I On the Optimization toolbar, click Global Least-Squares Objective (i).



- 2 In the Settings window for Global Least-Squares Objective, locate the Experimental Data section.
- **3** From the Data source list, choose Local table.
- 4 Click Add Column.
- **5** In the table, enter the following settings:

I	2
I	0
1.075	1.052E6
1.103	1.3633E6
1.15	1.844E6
1.174	2.101E6
1.2004	2.330E6
1.25	2.745E6
1.305	3.129E6
1.351	3.441E6
1.37	3.543E6

- 6 From the Parameter type list, choose Parameter.
- 7 In the Parameter name text field, type lambda.
- 8 From the Parameter column list, choose 1.
- **9** In the table, enter the following settings:

** Data column	Unit	Model expression	Weight
2	Pa	P	1

Study |

The Optimization study step controls several aspects of the optimization problem. Here, you choose solver, set fundamental solver parameters, review the optimization problem contributions from the Optimization interfaces, and optionally add objective function contributions, control variables and constraints.

Optimization

The Levenberg-Marquardt solver exploits — and requires — the special structure of least-squares problems, which it can solve very efficiently. Other solvers can solve least-squares problems, but are generally slower.

▼ Exp	erimental Data	
Data so	urce:	
Local	table	-
** 1	2	

I On the Study toolbar, click Optimization 🙋.



2 In the Settings window for Optimization locate the Optimization Solver section. From the Method list, choose Levenberg-Marquardt.

In this case, the objective function is set up in the Optimization interface. Note how it shows up as Active in the Objective functions from physics interface column in the Objective function section. You can click in the Active column to disable any such contribution from an Optimization interface.

Under Control Variables and Parameters, you can add parameters from the Global Parameters node. This transforms them into global control variables for which you can specify an initial guess, as well as, lower and upper bounds. For parameter estimation problems such as this, bounds should in general not be specified. If the problem is well-posed, it should have a unique solution anyway.

- **3** Locate the Control Variables and Parameters section and click Add + twice.
- **4** In the table, enter the following settings:

** Parameter name II	nitial value	Scale	Lower bound	Upper bound
C10 (Mooney-Rivlin parameter) 🔹 1	[MPa]	1[MPa]		
C01 (Mooney-Rivlin parameter) 🔹 1	MPa]	1[MPa]		
(

Results

Add a plot of the least-squares fitted stress-strain curve together with the measured data.

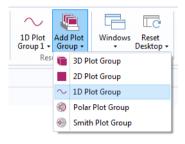
I D Plot Group I

On the Home toolbar, click Add Plot Group $\overline{[m]}$ and choose 1D Plot Group \sim .

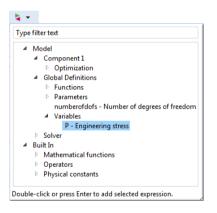
Global I

I On the 1D plot group toolbar, click Global 🕞.





- 2 In the Settings window for Global, locate the y-axis data section.
- 3 Click Replace Expression ↓ → in the upper-right corner of the y-axis data section. From the menu, choose Model>Global Definitions>Variables> P Engineering stress.



GLOBAL 2

- On the 1D Plot Group 1 toolbar, click Global.
- 2 In the Settings window for Global, locate the y-axis data section.
- 3 Click Replace Expression ↓ in the upper-right corner of the y-axis data section. From the menu, choose Model>Component 1>Optimization> comp1.opt.glsobj1.col1 Least squares experimental value.

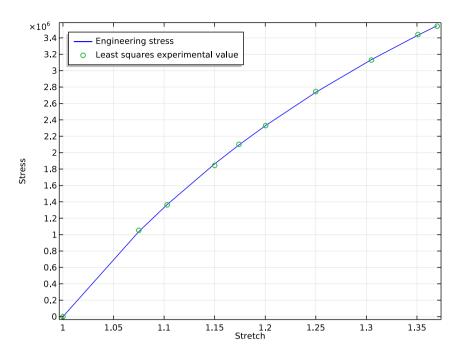
- 4 Click to expand the Coloring and style section.
- **5** Find the Line style subsection. From the Line list, choose None.
- 6 Find the Line markers subsection. From the Marker list, choose Circle.
- 7 From the Positioning list, choose In data points.
- 8 On the 1D plot group toolbar, click Plot 💿 .

Finish the plot by adjusting the title, axis labels, and legend positioning.

- 9 In the Model Builder click 1D Plot Group 1 \sim .
- **10** In the Settings window for 1D Plot Group 1 click to expand the Title section. From the Title type list, choose None.
- II Locate the Plot Settings section.
 - Select the x-axis label check box.
 - In the x-axis label text field, type Stretch.
 - Select the y-axis label check box.
 - In the y-axis label text field, type Stress.
- ¹²Click to expand the Legend section. From the Position list, choose Upper left.

 Coloring 	and Style
— Line style —	
Line:	None 🔻
Color:	Cycle 🔹
Width:	1
<u> </u>	1 1 1 1 1 1 1
— Line marke	rs
Marker:	Circle 🔹
Positioning:	In data points 🔹 👻

▼ Title
Title type: None 🔻
 Plot Settings
x-axis label: 📝 Stretch
y-axis label: 🖉 Stress
Axis
> Grid
▼ Legend
Show legends
Position: Upper left •



Derived Values

Use the predefined Objective value node to evaluate the estimated values of material parameters C01 and C10.

- I In the Model Builder expand the Results>Derived Values node 405, then click Results>Derived Values>Objective Value (15).
- **2** In the Settings window for Global Evaluation locate the Data section. From the Parameter selection (lambda) list, choose Last.
- 3 Click Replace Expression ↓ → in the upper-right corner of the Expression section. From the menu, choose Model>Solver>Control parameters>C10 Mooney-Rivlin parameter.
- 4 Click the Evaluate button =.

Repeat steps 3 and 4 for the other Mooney-Rivlin parameter C01.

Global Evaluation = Evaluate -			
Label: Objective value			
▼ Data			
Data set: Parameter selection (lambda):	Study 1/Solution 1		•
- Expression		+ •	۰.
Expression:			
C10			
Unit:			
Pa			•
Description:			

Tutorial Example — Topology Optimization

Topology optimization in a structural mechanics context can answer the question: Given that you know the loads on the structure, which distribution of the available material maximizes stiffness? Or, conversely, how much material is necessary to obtain a predefined stiffness, and how should it be distributed? Such investigations typically occur during the concept design stages.

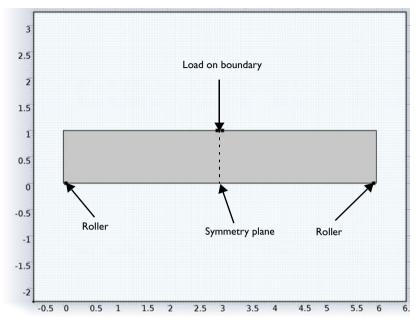
The conflicting goals of stiffness maximization and mass minimization lead to a continuum of possible optimal solutions, depending on how you balance the goals against each other. This topology optimization example demonstrates how to use a penalization method (SIMP) to obtain an optimal distribution of a fixed amount of material such that stiffness is maximized. Changing the amount of material available leads to a different solution that is also Pareto optimal, representing a different balance between the conflicting objectives.

The geometry and load pattern are similar to the Messerschmitt-Bölkow-Blohm beam (MBB) commonly used as a validation test for topology optimization.

Model Definition

The model studies optimal material distribution in the beam, which consists of a linear elastic material, structural steel. The dimensions of the beam region -6 meters by 1 meter by 0.5 meters — means an original total weight of 23,550 kg.

The beam is symmetric about the plane x = 3. Both ends rest on rollers while an edge load acts on the top middle part.



The objective functional for the optimization, which defines the criterion for optimality, is the total *strain energy*. Note that the strain energy exactly balances the work done by the applied load, so minimizing the strain energy minimizes the displacement induced at the points where load is applied, effectively minimizing the compliance of the structure — maximizing its stiffness. The other, conflicting, objective is minimization of total mass, which is implemented as an upper bound on the mass of the optimized structure.

Another condition that is more difficult to enforce is the requirement that the optimized topology is truly binary — any given point is either solid or void, nothing in between — but still without excessively fine details or "checkerboard" patterns. The SIMP penalization method accomplishes the first part. In the SIMP model, the stress tensor is considered to be a function of the true Young's modulus E_0 and the artificial density, ρ_{design} , which acts as control variable in the optimization problem:

$$E(\mathbf{x}) = \rho_{\text{design}}(\mathbf{x})^p E_0$$
$$\mathbf{x} \in \Omega,$$

Since the stiffness must, for numerical reasons, not vanish completely anywhere in the model, the density parameter is constrained such that $10^{-9} \le \rho^p \le 1$. The

exponent $p \ge 1$ is a penalty factor that makes intermediate densities provide less stiffness compared to what they cost in weight.

When there is an overall limit on the fraction $\gamma = 0.5$ of the domain area, *A*, occupied by solid material

$$0 \leq \int_{\Omega} \rho_{\text{design}}(\mathbf{x}) d\Omega \leq \gamma A$$

the SIMP penalization forces ρ_{design} toward either of its bounds. Increasing *p* therefore leads to a sharper solution.

At the same time, the solution must not contain too much fine detail, since that would compromise the reliability of the final design. Also, it is desirable to make the solution as independent of the mesh resolution as possible. To accomplish this, some kind of regularization is needed. There are many possibilities. One of the easiest to implement is based on a combination of successive mesh refinements and a penalty applied to the gradient of the design variable.

The integral of the squared norm of the gradient of the design variable ρ_{design} measures, in some sense, the total variation of the design variable. For a sharp topology solution represented by linear shape functions, the magnitude of the gradient is inversely proportional to the mesh element size. The zone of intermediate densities is at the same time one element thick, and its area is proportional to the mesh element size. A reasonably mesh- and problem-independent dimensionless penalty term is therefore of the form

$$\frac{h_0 h_{max}}{A} \int_{\Omega} \left| \nabla \rho_{\text{design}}(\mathbf{x}) \right|^2 d\Omega$$

where h_0 is an initial mesh size, governing the size of details in the solution and h_{max} is the current mesh size at a given level in the process.

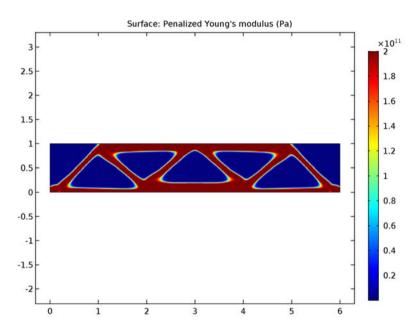
This penalty term is, for the worst possible solution, on the order of **1**. In order to balance it against the real strain energy objective, it is also necessary to normalize the strain energy. This can be accomplished quite easily by simply solving the structural problem for an initial configuration consisting of homogeneous density $\rho_{design} = \gamma$ and then divide the strain energy functional by the total strain energy, W_{s0} , found for that configuration.

In addition, the objective and the penalty term must be balanced against each other, for example as a linear combination controlled by a parameter, q, to create a final composite objective function:

$$f = \frac{(1-q)}{W_{s0}} \int_{\Omega} W_s(\mathbf{x}) d\Omega + q \frac{h_0 h_{max}}{A} \int_{\Omega} \left| \nabla \rho_{\text{design}}(\mathbf{x}) \right|^2 d\Omega$$

Results

The following plot shows the stiffness distribution for the optimized solution. The resulting design is an approximation of a truss structure, which is expected for this beam size. Note that the optimal design for a longer or shorter beam may be quite different, and also that there may exist stiffer solutions using the same amount of material. Such solutions typically consist of thinner members that have been eliminated here by the regularization and refinement procedure..



Notes About the COMSOL Implementation

A Solid Mechanics interface represents the structural properties of the beam, while an Optimization interface allows adding the control variable, objective, and constraints for the optimization problem. The internal strain energy is a predefined variable, solid.Ws, readily available to use as the objective function for the optimization problem.

Only the left half of the beam geometry must be modeled, because of the assumed symmetry, which is implemented as a Roller condition on the symmetry plane. Plots for postprocessing and inspection of the solution while solving are set up using a Mirror data set, to show the complete solution. The geometry is parametrized, making it easy to experiment with different beam sizes.

The optimization solver is selected and controlled from an Optimization study step. For topology optimization, either the MMA or the SNOPT solver can be used. They have different merits and weaknesses. MMA tends to be braver in the beginning, proceeding quickly towards an approximate optimum. SNOPT is more cautious, but converges more efficiently close to the final solution due to its second-order approximation of the objective.

This example demonstrates a strategy based on using MMA with a limited number of iterations on successively finer meshes. It quickly and reliably produces trustworthy topologies showing good improvement of the objective function value. These solutions are not necessarily globally optimal, which may, however, be of less importance in practice.

Creating a New Model

When starting COMSOL Multiphysics, you are normally greeted by the New window. Otherwise, from the File menu, choose New. **Note:** Theses instructions are for the user interface on Windows but apply with minor differences also to Linux and Mac. In particular, the Home toolbar refers to the fixed set of controls near the top of the Desktop



In the New window click the Model Wizard button 🙎.

Model Wizard

- In the Model Wizard window, click 2D 🤏.
- 2 In the Select Physics tree under Structural Mechanics, click Solid Mechanics (solid) ⇒.
- 3 Click Add.
- 4 In the Select physics tree under Mathematics>Optimization and Sensitivity, click Optimization (opt) 💣.
- 5 Click Add.
- 6 Click the Study button 🚭.
- 7 In the tree under Preset Studies for Selected Physics Interfaces, click Stationary <u>></u>.

8 Click Done 🗹.

4	Preset Studies for Selected Physics Interfaces Interfaces Interfaces Interfaces Stationary Mar Time Dependent	
ddad	study:	
	Stationary	
	physics interfaces:	
	 Solid Mechanics (solid) Optimization (opt) 	
	Physics	

Global Definitions

Set up named parameters for any quantity that you might perceivably want to change later on. The global Parameters node then gives you a direct overview of the values that are used in the model, making it easier to reproduce and modify.

Parameters

I On the Home toolbar click Parameters P_i .

2 In the Settings window for Parameters locate the Parameters section and enter the following settings:

* Name	Expression	Value	Description
9	3	3	Half beam width
b	1	1	Beam hight
h0	0.05	0.05	Initial mesh size
nmax	0.05	0.05	Current mesh size
p	5	5	SIMP penalization factor
9	0.25	0.25	Regularization factor
gamma	0.5	0.5	Maximum area fraction
domainArea	a*b	3	Area of design domain
Ws0	1	1	Reference objective value
	1		

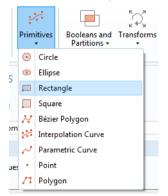
Note: The reference objective value is initially set equal to 1 and must be updated before optimization is started.

Geometry I

The actual beam geometry consists of a rectangle of width 2a and height b; however, because of the mirror symmetry, you only need to draw the left half. Also insert two points to delimit boundary segments where the central load and the roller condition in the lower left corner can be applied. Applying the boundary conditions on small boundaries of fixed size avoids the mesh dependency caused by point conditions.

Rectangle I (rI)

I On the Geometry toolbar, click Primitives and choose Rectangle 📃 .



- 2 In the Settings window for Rectangle locate the Size section.
 - In the Width text field, type a.
 - In the Height text field, type b.
- 3 Click the Build Selected button 🖷 .

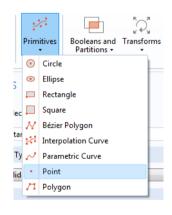
Point I (ptl)

- 4 On the Geometry toolbar, click Primitives and choose Point
- 5 In the Settings window for Point locate the Point section. In the x text field, type 0.1.

Point 2 (pt2)

- I On the Geometry toolbar, click Primitives and choose Point .
- **2** In the Settings window for Point locate the Point section.
 - In the x text field, type a-0.1.
 - In the y text field, type b.
- 3 Click the Build Selected button 🖷 .

▼ Size		
Width:	a	m
Height:	b	m



•	Point	
x:	a-0.1	m
y:	b	m

Add Material

Add structural steel as the domain material in the beam. Note that Young's modulus and Poisson's ratio are defined in their own property group subnode under the material.

- I On the Home toolbar click Add Material 🏭.
- In the Add Material window tree under Built-In, click Structural steel. Click + Add to Component.



Definitions

Set up the penalized Young's modulus. Material property values can be accessed using the material identifier and the property group identifier as namespace. Since the control variable rho_design is not yet defined, the expression will be temporarily displayed in red.

Variables 1

- I On the Home toolbar click Variables a= and choose Local Variables a= .
- 2 In the Settings window for Variables locate the Variables section.
- **3** In the table, enter the following settings:

** Name	Expression	Unit	Description
E_SIMP	mat1.Enu.E*rho_design^p	Pa	Penalized Young's modulus

Solid Mechanics (solid)

- In the Model Builder under Component 1, click Solid Mechanics 🚍 .
- 2 In the Settings window for Solid Mechanics locate the 2D Approximation section. From the 2D approximation list, choose Plane stress.

•	2D Approximation		
2D a	approximation:		
Plane stress 🔹			

Linear Elastic Material I

Set Young's modulus to the modified, penalized, expression.

- I In the Model Builder under Solid Mechanics (solid), click Linear Elastic Material 1.
- 2 In the Settings window for Linear Elastic Material locate the Linear Elastic Material section.
- **3** From the *E* list, choose User defined. In the associated text field, type E_SIMP.

 ✓ Solid Mechanics (solid) Linear Elastic Material 1 ⇒ Free 1 ➡ Initial Values 1
 Linear Elastic Material
Nearly incompressible material
Solid model:
Isotropic 🔹
Specify:
Young's modulus and Poisson's ratio
$C = C(E, \nu)$
Young's modulus:
E User defined 🔹
E_SIMP Pa
Poisson's ratio:
ν From material •
Density:
ho From material $ullet$

Roller 1

Use a Roller condition to represent the mirror symmetry boundary. If you have access to the Structural Mechanics Module, you can use a Symmetry condition instead.

I On the Physics toolbar click Boundaries — and choose Roller.



2 Select Boundary 6 only.

Note: There are many ways to select geometric entities. When you know the geometric entity to add, such as in this exercise, you can click the Paste Selection button \square and enter the boundary number in the Selection field. For more information about selecting geometric entities in the Graphics window, see the *COMSOL Multiphysics Reference Manual*.

Roller 2

Add another roller condition for the lower left corner of the beam.

I On the Physics toolbar click Boundaries — and choose Roller.

2 Select Boundary 2 only.

Boundary Load I

Since this is a linear problem, the magnitude of the applied force does not affect the optimal topology.

- I On the Physics toolbar click Boundaries and choose Boundary Load.
- 2 Select Boundary 5 only.
- **3** In the Settings window for Boundary Load locate the Force section.
 - From the Load type list, choose Total force.

Specify the \mathbf{F}_{tot} vector as -100[kN] in t	he
y direction.	

Optimization (opt)

Use the Optimization interface to set up the control variable field, objective contributions and constraints.

Control Variable Field I

Use linear elements to represent the artificial density rho_design. This is important since higher-order elements produce over- and under-shoots near sharp edges, which cannot be prevented just by bounding the control variable degrees of freedom. Set the initial value of the control variable field equal to the maximum allowed area fraction, which means that the initial value will certainly be a feasible solution.

- In the Model Builder under Component 1, click Optimization 💣.
- 2 On the Physics toolbar click Domains 🔵 and choose Control Variable Field.

Optimization Add Physics	Domains	Boundaries	Points Pairs	Global	Attributes	Ν
Physics	Least-	Squares Objective	🛑 Integral Obje	ective	Probe Objective	
Model Builder	Integr	al Inequality Constraint	🛑 Pointwise In	equality Co	nstraint 🛑 Control Variable Field	

3 Select Domain 1 only.

▼ F	orce		
Load	type:		
Total force 🔹			
Total	force:		
Ftot	0	x	N
Ftot	-100[kN]	У	N.

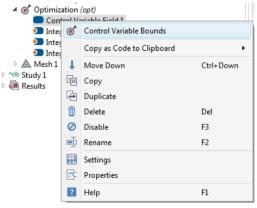
- 4 In the Settings window for Control Variable Field locate the Control Variable section.
 - In the Control variable name text field, type rho_design.
 - In the Initial value text field, type gamma.
- 5 Locate the Discretization section. From the Element order list, choose Linear.

 Control Variable 				
Control variable name:				
rho_design				
Initial value:				
gamma				
Control Variable Scaling				
 Discretization 				
Shape function type:				
Lagrange 🔹				
Element order:				
Element order:				
Element order: Linear				
Linear				
Linear Frame:				

Control Variable Bounds 1

Limit the range of the control variable rho_design such that the difference in penalized stiffness between solid and void areas is nine orders of magnitude. This makes the void areas weak enough not to stiffen the design appreciably, but at the same time stiff enough to avoid severe ill conditioning for the solvers.

I Under Optimization (opt), right-click Control Variable Field 1 and choose Control Variable Bounds ♂.



- 2 In the Settings window for Control Variable Bounds locate the Bounds section.
 - In the Lower bound text field, type 1e-9^(1/p).
 - In the Upper bound text field, type 1.

•	Bounds			
7	Lower bound			
1e-9^(1/p)				
✓ Upper bound				
1				

Integral Objective 1

Set up the compliance objective as an integral of the strain energy. Note the normalization factor Ws0, which is initially set equal to 1, as well as, how the regularization weight q enters the expression.

- I On the Physics toolbar click Domains 🔵 and choose Integral Objective.
- **2** Select Domain 1 only.
- **3** In the Settings window for Integral Objective locate the Objective section.
- 4 In the Objective expression text field, type (1-q)*solid.Ws/Ws0.

Obje	ctive expression:			
(1-q)*solid.Ws/Ws0			

Integral Objective 2

Add the regularization penalty term as a second integral objective contribution on the domain level. Note that the term is normalized by the mesh scale and domain area.

- 1 On the Physics toolbar click Domains 🔵 and choose Integral Objective.
- **2** Select Domain 1 only.
- 3 In the Settings window for Integral Objective locate the Objective section.
- 4 In the Objective expression text field, type q*h0*hmax*(d(rho design,x)^2+d(rho design,y)^2)/domainArea.

•	Objective
0	bjective expression:
c	*h0*hmax*(d(rho_design,x)^2+d(rho_design,y)^2)/domainArea

Integral Inequality Constraint I

Constrain the total amount of material available by limiting the domain integral of the control variable rho_design.

- On the Physics toolbar click Domains 🔵 and choose Integral Inequality Constraint.
- **2** Select Domain 1 only.

- 3 In the Settings window for Integral Inequality Constraint locate the Constraint section. In the Constraint expression text field, type rho_design.
- 4 Locate the Bounds section. In the Upper bound text field, type gamma*domainArea.

 Constraint 					
Constraint expression:					
rho_design					
Quadrature Settings					
 Bounds 					
Lower bound					
0					
🔽 Upper bound					
gamma*domainArea					

Mesh I

For topology optimization, it is typically necessary to take manual control over the mesh size, since it does at least to some extent affect the result.

I On the Mesh toolbar click Free Triangular 🔕 .



Size

Set the maximum element size to the previously defined constant hmax. The mesh size you specify is an upper limit. Small features in the geometry may lead to smaller elements being created in some places.

In the Model Builder under Mesh 1, click Size 🔬.

2 In the Settings window for Size locate the Element Size section. Click the Custom button.

Element Size			
Calibrate for:			
General physics 🔹			
Predefined Normal	-		
O Custom			
 Element Size Parameters 			
Maximum element size:			
hmax	m		
Minimum element size:			
9E-4	m		
Maximum element growth rate:			
1.3			
Curvature factor:			
0.3			
Resolution of narrow regions:			
1			

- **3** Locate the Element Size Parameters section. In the Maximum element size text field, type hmax.
- 4 Click the Build All button 🟢 .

Study I

First compute only a stationary solution on which you can evaluate a reference value for the objective, as well as, set up suitable plots.

On the Home toolbar click Compute = .



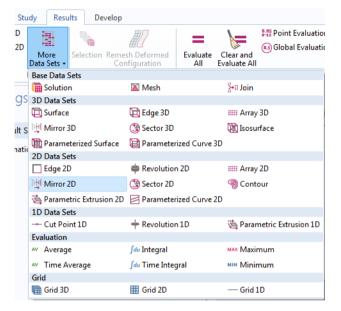
Results

Use a Mirror data set to plot the whole beam rather than just the left half. Also, customize one of the plots for plotting the topology as it evolves when solving using an optimization solver.

Data Sets

For the Mirror data set, specify two points on the symmetry plane.

I On the Results toolbar click More Data Sets 📗 and choose Mirror 2D 🕌.



- 2 In the Settings window for Mirror 2D locate the Axis Data section.
 - In row Point 1, set X to a.
 - In row Point 2, set X to a.
 - In row Point 2, set Y to b.

Stress (solid)

Modify the predefined von Mises stress plot to use the Mirror data set.

In the Model Builder under Results, click Stress (solid) ■.

▼ Data				
Data set: Study 1/Solution 1				
▼ Axis	Data			
Axis entry	method: Two point	s	•	
	X:	Y:		
Point 1:	a	0	m	
Point 2:	a	b	m	

- 2 In the Settings window for 2D Plot Group locate the Data section. From the Data set list, choose Mirror 2D 1.
- **3** On the 2D plot group toolbar click Plot on .

2D Plot Group	
Label: Stress (solid)	
▼ Data	
Data set: Mirror 2D 1	•
▷ Title	

2D Plot Group 2

Modify the predefined control variable plot, originally showing rho_design, to use the Mirror data set. This plot is later used during solution.

- In the Model Builder under Results, click 2D Plot Group 2
- 2 In the Settings window for 2D Plot Group locate the Data section. From the Data set list, choose Mirror 2D 1.
- **3** Click 2D Plot Group 2 **and press F2**.
- 4 Go to the Rename 2D Plot Group dialog box and type Topology in the New name text field. Click OK.

Topology

Plotting the penalized Young's modulus gives a sharper and fairer picture of the topology, as seen by the Solid Mechanics interface.

- In the Model Builder expand the Results>Topology node, then click Surface 1
- 2 In the Settings window for Surface locate the Expression section. In the Expression text field, type E_SIMP.

 Expression 	+ • 🛓 •
Expression:	
E_SIMP	
Unit:	
Pa	•
Description:	
Penalized Young's modulus	
- Parameters	

3 On the 2D plot group toolbar click Plot $\overline{\mathbf{o}}$.

Derived Values

Evaluate a predefined Global Evaluation node to get a reference value for the strain energy objective.

- I In the Model Builder expand the Results>Derived Values node 405, then click Objective Value 43.
- **2** On the Global Evaluation toolbar click Evaluate **=**.

The result, which should be near 64.7, is displayed in the Table window.

Global Definitions

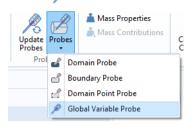
Read the value from the results table and update the value of the parameter Ws0. This will make the initial value of the integral strain energy objective equal to 1 when optimization is started, making it easier to tune the regularization.

Parameters

- In the Model Builder under Global Definitions, click Parameters P_i .
- 2 In the Settings window locate the Parameters section.
- 3 Change the Expression column for parameter Ws0 to 64.7.

gamma	0.5	0.5	Maximum area fraction
domainArea	a*b	3	Area of design domain
Ws0	64.7	64.7	Reference objective value

Definitions

Set up probes for the objective functions and constraint, which will make it easier to follow the optimization progress. Scale the objectives such that the values displayed become independent of the regularization factor. This makes the results obtained using different amounts of regularization comparable to each other. 

- 2 In the Settings window for Global Variable Probe locate the Expression section. In the Expression text field, type opt.iobj1/(1-q).
- **3** Select the Description check box.
- 4 In the associated text field, type Normalized strain energy.

 Expression 	+• 🛓•
Expression:	
opt.iobj1/(1-q)	
Table and plot unit:	
J/m	-
Description:	
Normalized strain energy	

5 Repeat steps 1-4 to add probes for the expressions opt.iobj2/q with description Gradient penalty and opt.iconstr1/(gamma*domainArea) with description Mass utilization.

Study I

Add the Optimization study step; select a solver and limit the number of iterations. Also switch on plotting while solving.

Optimization

I On the Study toolbar, click Optimization 🙋.



2 In the Settings window for Optimization locate the Optimization Solver section.

 Optimization Solver
Method:
MMA
Optimality tolerance:
1E-6
Study step:
Stationary
Maximum number of objective evaluations:
100

- From the Method list, choose MMA.
- In the Maximum number of objective evaluations text field, type 100.
- **3** Locate the Output While Solving section.
 - Select the Plot check box.
 - From the Plot group list, choose Topology.
- 4 On the Home toolbar click Compute =.

 Output While Solving 	
Plot Plot	Topology •
Probes:	All

Global Definitions

Now reduce the maximum mesh element size to half of its original value. This will increase the time required for each iteration, but only a few iterations are needed to produce a sharp solution on the refined mesh.

Parameters

- I In the Model Builder under Global Definitions, click Parameters P_i .
- 2 In the Settings window locate the Parameters section.
- 3 Change the Expression column for parameter hmax to 0.025.

* Name	Expression	Value	Description
a	3	3	Half beam width
b	1	1	Beam hight
h0	0.05	0.05	Initial mesh size
hmax	0.025	0.05	Current mesh size
р	5	5	SIMP penalization factor
q	0.25	0.25	Regularization factor

Return to Study 1, reduce the maximum number of iterations and restart the solver using the current topology as the initial guess.

Optimization

- In the Model Builder under Study 1, click Optimization 🙋.
- **2** In the Settings window for Optimization locate the Optimization Solver section.
- 3 In the Maximum number of objective evaluations text field, type 50.

 Optimization Solver
Method:
MMA 🔹
Optimality tolerance:
1E-6
Study step:
Stationary •
Maximum number of objective evaluations:
50

Step 1: Stationary

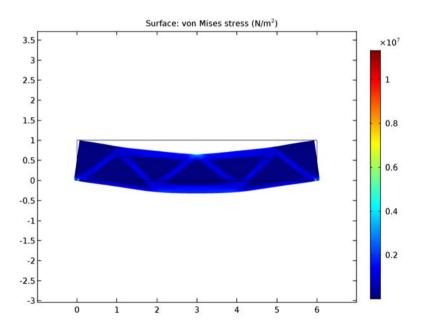
Change the Stationary step to use the current solution as the initial value for all variables. This automatically triggers a mapping from the old coarse mesh to the new, finer mesh.

- In the Model Builder under Study 1, click Step 1: Stationary 🚬.
- **2** In the Settings window for Stationary click to expand the Values of dependent variables section.

- **3** Find the Initial values of variables solved for subsection.
 - From the Settings list, choose User controlled.
 - From the Method list, choose Solution.
 - From the Study list, choose Study 1..

 Values of Dependent Variables 	
- Initial values of variables solved for	
Settings:	User controlled 🗸
Method:	Solution -
Study:	Study 1 🔹
Selection:	Automatic 👻
Values of variables not solved for	
Settings:	Physics controlled 🔹
- Store fields in output	
Settings:	All

4 On the Home toolbar click Compute = .



The default plots show the stress distribution in the optimized structure, clearly indicating that the load paths follow the optimized topology. Switch to the other plot group to display a sharper picture of the final design.