



# Granta EduPack White Paper

## Materials Selection

Harriet Parnell<sup>1</sup>, Kaitlin Tyler<sup>1</sup>, and Mike Ashby<sup>2</sup>

<sup>1</sup>Ansys Academic Development Team

<sup>2</sup>Department of Engineering, University of Cambridge

## Abstract

The aim of this white paper is to guide the learner through the fundamental steps of the materials selection methodology and basic understanding of performance indices. Details on how to implement performance indices in Ansys Granta EduPack and related resources are also included. More information about the methodology and advanced applications can be found in subject textbooks [1].

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## 1. Materials Selection Methodology

The materials selection methodology is a process used during the design of a product. This means it uses the requirements of a design as guiding inputs. It doesn't matter if the design is original (i.e., new concept) or evolutionary (i.e., redesign), materials selection is relevant to both, and is explored at all stages.

A designer aims to find the best match between the attribute profiles of materials and processes, which must also be compatible, and those required by the design. The materials selection methodology is shown in Figure 1 and highlights four key steps: 1) **Translation**, 2) **Screening**, 3) **Ranking**, and 4) **Documentation**.

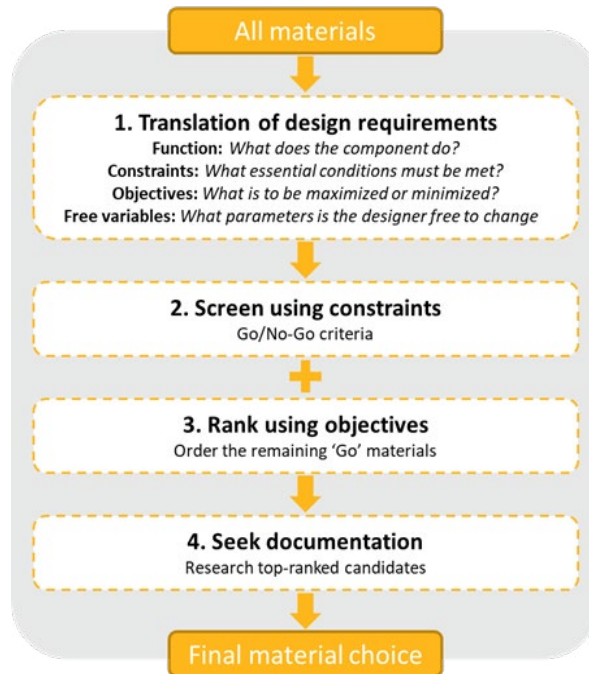


Figure 1: The materials selection methodology showing four main steps: translation, screening, ranking, and documentation.

### 1.1 Translation

The first step of the methodology is to **translate** design requirements into a set of conditions for selecting a material. As shown in Figure 1, there are four key phases, exploring the component's: *function* and identifying the *constraints*, *objectives*, and *free variables* imposed by the design.

#### **Phase 1: function- what does the component do?**

Engineering components have one or more functions e.g. they might have to support a load, contain a pressure, or transmit heat. For mechanical engineering design, the key elements are the geometry and the mode of load situation, which can generally be condensed into a combination of axial tension or compression, bending, and torsion. Almost always, one mode dominates.

#### **Phase 2: constraints- what essential conditions must be met?**

Depending on the component there will be a set of non-negotiable conditions that must be met by the material for it to perform appropriately. For example, it may need to support external loads without failing, be electrically conductive, withstand a corrosive environment or operate safely over a defined temperature range.

### **Phase 3: objectives- what is to be maximized or minimized?**

Objectives relate to the function of the component and allow the designer to optimize an aspect of its performance. Most commonly, the objective is to minimize the component's weight or cost, but it could be to maximize the energy stored per unit volume (a spring) or maximize heat transfer per unit area (a heat exchanger).

### **Phase 4: free variables- what parameter is the designer free to change?**

These are the parameters that can be adjusted to optimize the objective. Aspects of the geometry are free variables. A beam might have a fixed length but a shape and area of cross-section that can be varied to minimize weight. Initially, the choice of material is itself a free variable, allowing a choice that meets the constraints while minimizing cost, for example.

It is worth spending time on the **translation** step since the best materials can only be identified through this selection methodology if all the final design requirements are correctly included. As shall be seen in sections 1.2. and 1.3 respectively, the constraints identified in translation become set property limits, and the objectives go on to define performance indices for which extreme values are sought.

## **1.2 Screening**

The second step of the materials selection methodology is **screening**. Constraints act as gates. If a material meets the demands of the constraints, it passes through to the next selection step. If not, it is screened out.

Some constraints translate directly into simple limits on material properties. If the component must operate at 250 °C, then all materials with a maximum service temperature less than this are eliminated. If it must be electrically insulating, then all material with an electrical resistivity less than about  $10^{10} \mu\Omega\cdot\text{cm}$  are rejected.

Constraints on stiffness, strength and many other component characteristics are used in a different way. This is because stiffness (to take an example) can be achieved in more than one way: by choosing a material with a high modulus, certainly; but also, by simply increasing the cross-section; or, in the case of bending-stiffness or stiffness in torsion, by giving the section an efficient shape (a box, or I-section, or a tube). Achieving a specified stiffness (the constraint) involves a trade-off between these, and to resolve it we need to invoke an objective. The outcome of doing so is a performance index, see section 2.

Although it is possible to screen material by hand (*i.e.* using a database of attribute values), Ansys Granta EduPack allows quick and visual progression through the selection process, using property charts.

The selection tools available in Granta EduPack allow simple constraints to be applied, screening out all the materials that fail to meet them. Materials that fall outside the acceptable limit appear gray, as seen Figure 2 which shows the tool in action. Frame (a) plots the range of a material attribute, unscreened. In frame (c) all materials with values of the attribute below the horizontal line have been screened out, appearing now only in gray. Frames (b) and (d) show the same things when two attributes are plotted. All those outside the box in frame (d) are screened out.

## What is a property chart?

A property chart is a diagram with one (or a combination of) material attribute plotted on each axis. Figure 2 illustrates this concept for a single axis bar chart (Figure 2a) and a double axes bubble chart (Figure 2b). The scales are logarithmic and span a range so wide that all materials are included.

When data for a given material class such as metals is plotted on a bubble chart, it is found that they occupy a field which can be visualized as a 'balloon'. Ceramics also form a field, and so do polymers, elastomers, composites, and so on. The fields may overlap but are nonetheless distinct. Property charts, therefore, allow general comparison between material families.

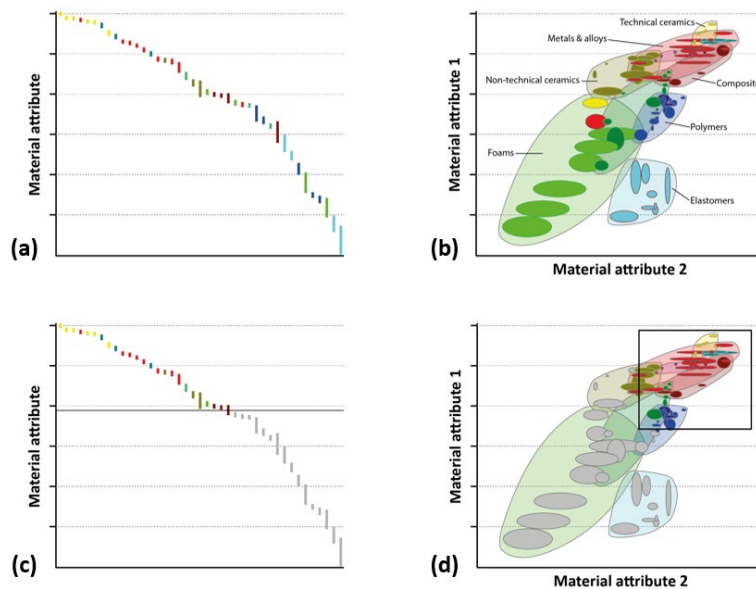


Figure 2: Schematic of property charts taken from Granta EduPack showing a) a bar chart; b) a bubble chart; c) a bar chart with a selection line; and d) a bubble chart with a selection box.

## 1.3 Ranking

Once screening has removed unsuitable materials, the next step is *ranking*. Here, surviving candidates are ordered by their ability to meet a criterion of excellence, such as minimizing weight or cost. The criterion uses the objectives identified during translation to derive a *performance index*.

In simple cases, performance is limited by a single property, but more often, a combination of properties is involved. For example, when designing for a light stiff panel in bending, materials with the greatest values of the specific stiffness ( $E^{1/3}/\rho$ ) perform best. This ranking can be visualized on a property chart in the way illustrated by Figure 3a. The performance index relevant for a panel in bending is denoted by  $M_p$  and is shown as a line with a gradient of 3 on a log-log chart. Two more performance index examples are also shown in Figure 3a: that for a light stiff beam loaded in bending ( $M_b = E^{1/2}/\rho$ ) and that for a light stiff tie loaded in tension ( $M_t = E/\rho$ ).

The Granta EduPack allows an index line to be added to a property chart and provides the option to 'minimize' or 'maximize' its value. For a light stiff panel, materials with a higher Young's modulus and lower density would perform best. Figure 3b demonstrates that by moving this index line to the top left

corner, the performance index  $E^{1/3}/\rho$  increases in value (0.2 to 5). By choosing to maximize the index, any materials that fall to the lower right-hand side of the line no longer pass this ranking step; those that remain on the upper left-hand side continue to be shortlisted.

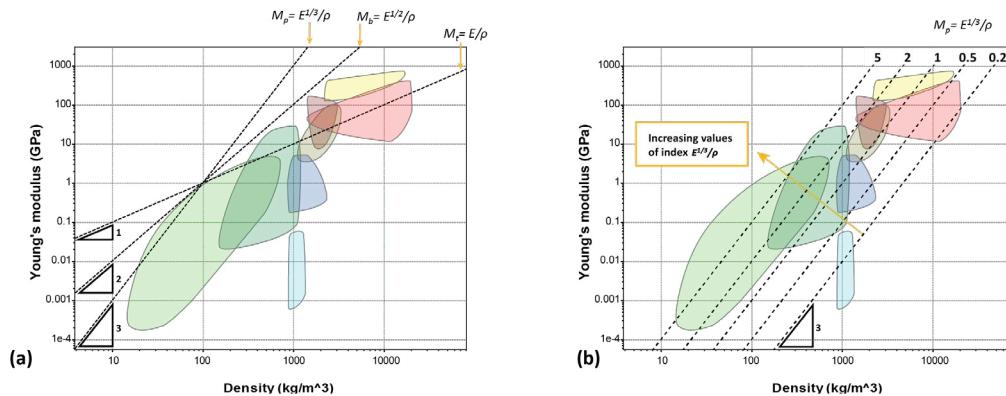


Figure 3: Schematic  $E - \rho$  property charts showing a) selection lines for three performance indices for stiff, lightweight design and b) a grid of lines for the performance index  $M_p = E^{1/3}/\rho$ .

## 1.4 Documentation

The final step in the materials selection methodology is to research the shortlisted candidates. Although a material may have successfully passed the screening stage, and demonstrated the best performance during ranking, there may be hidden considerations that would prevent it from being a viable option. Consider case histories of failures, manufacturing limitations, and even global issues that might affect its availability. This step requires designers to think more holistically, and appropriately involves real-life decision-making skills.

## 2. Performance Indices

Performance indices are a key tool in materials selection. These properties or combinations of properties define the slope of selection lines used in the ranking step. The relevant index depends on the functional design of the part, as described in Section 1.3. How are they derived? This question is the focus of this section.

### 2.1 Origin of Performance Indices: the Performance Equation

The performance index for material selection depends on the function of the component of which it will be made. Performance can be expressed as a general equation which combines three aspects of the design: the functional requirements (the need to carry loads, transmit heat, store elastic or thermal energy, etc.), the geometry, and the properties of the material of which it is made, including its cost.

$$p = f \left[ \left( \begin{array}{c} \text{specified Functional} \\ \text{requirements, } F \end{array} \right), \left( \begin{array}{c} \text{Geometric} \\ \text{parameters, } G \end{array} \right), \left( \begin{array}{c} \text{Material} \\ \text{properties, } M \end{array} \right) \right] \quad (1)$$

where  $p$  describes the aspect of performance of the component that is to be optimized- its mass, or volume, or cost, or life for example- and  $f( )$  means 'a function of'. Optimum design means the selection of material and geometry which maximize (or minimize)  $p$ . The optimization is subject to constraints, some of them imposed by the material properties.

Frequently, the three groups of parameters in equation (1) are ‘separable’, which allows for the rearrangement of the equation shown below

$$p = f_1(F) \cdot f_2(G) \cdot f_3(M) \quad (2)$$

where  $f_1$ ,  $f_2$ , and  $f_3$  are functions. The function  $f_3(M)$  is the performance index. The separable nature of equation (2) means that the optimum material found using this index is valid for all geometries  $G$  and all values of the functional requirements  $F$ . The performance for all Functions and Geometries is maximized by maximizing  $f_3(M)$ , greatly simplifying the selection of a short-list of materials in the early stages of a design. Of course, to truly complete the product design, all aspects of the performance equation must be considered.

### What is a material index?

In other documents that discuss the materials selection methodology, the term *material index* may be used. This refers to  $f_3(M)$ , and is the same as the performance index in this document. This is simply a nomenclature difference.

## 2.2 Performance Index Derivation

Echoing the flow described in Section 1, the combination of function, objectives, constraints, and free variables (if applicable) leads to the material performance index. Figure 4 walks through the general thought process behind deriving the performance indices.

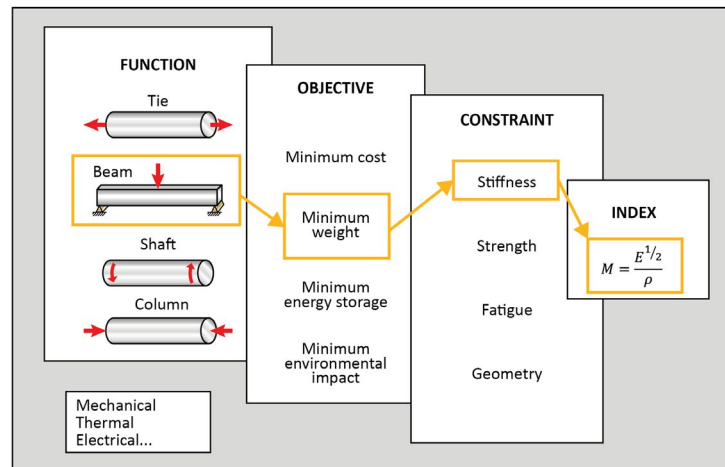


Figure 4: General performance index derivation workflow

The derivation starts by identifying the function of the design—this describes the loading situation, or how the forces are applied and the geometry. This could be mechanical, electrical, thermal, or more. Figure 4 shows a beam in bending.

The next derivation step is identifying relevant equations for the objectives. These equations will often include variables related to the function and geometry of the design, which will be dealt with later in the derivation.

Third, determine if any equations related to the objectives also include constraints. As mentioned previously, not all performance indices have coupled constraints and objectives. But many do. If there is no equation relevant to the constraints, that is okay.

At this point in the derivation, there could be multiple equations at play. This is where the free variable, if any, comes in. By identifying the free variable in the established equations, one equation can be solved for the free variable and inserted into the other.

#### What if there is no free variable?

If the geometric or functional constraints of a design are already known, there may be no free variable from the translation step. In this case, the material performance index would simply be a single material property, rather than a coupled set of properties.

Our equation can now be rearranged to take the form of Equation 2 in Section 2.1. Simply separate out the terms related to material properties and the material performance index has been successfully derived. These derivations are general and apply to all relevant functions and geometries. A reference booklet of pre-derived indices can be found linked in Section 3. Here you will find more pre-derived indices for stiffness-limited design, strength-limited design, thermos-mechanical design, and electro-mechanical design- just to name a few.

To aid understanding of how specific performance indices can be defined, two example derivations can be found below.

#### 2.2.1 Example 1: Cheap thermal-storage materials

Thermal storage heaters are designed to heat up at night (utilizing lower cost electricity) and release heat during the day. The material of the core, in which the heat is stored, must have low cost but high thermal capacity. The goal, then, is a performance index characterizing materials that can store the most thermal energy per unit cost.

The table lists the translation.

<b>Function</b>	Heat-storing medium
<b>Objective</b>	Maximize thermal energy stored per unit material cost
<b>Constraints</b>	Adequate working temperature $100^{\circ}\text{C} < T_{\text{max}} < 150^{\circ}\text{C}$

The thermal energy  $E$  stored in a mass  $m$  of solid when heated through a temperature interval  $\Delta T$  is

$$E = mC_p\Delta T \quad (3)$$

where  $C_p$  is the heat capacity of the solid. The material cost is

$$C = mC_m$$

where  $C_m$  is the cost per kg of the solid. The energy stored per unit cost is therefore

$$\frac{E}{C} = \left( \frac{C_p}{C_m} \right) \Delta T \quad (4)$$



The quantity  $\Delta T$  is prescribed — it is a functional requirement, in this case 100 to 150°C. The remaining term on the right (in brackets) is the *performance index*. The energy per unit cost is maximized by maximizing

$$M = \frac{C_p}{C_m} \quad (5)$$

### 2.2.2 Example 2: A light, stiff beam with fixed section-shape

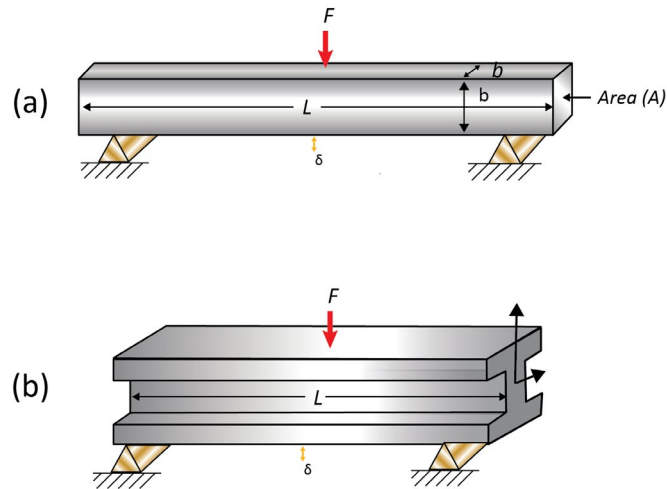


Figure 5 (a) square cross section beam and (b) I-beam

Figure 5(a) shows a simple beam, loaded in bending. The beam has a length  $L$  and a square, solid cross-section with second moment of area  $I$ . The goal is to minimize the mass of the beam while still giving it a prescribed stiffness.

The translation can be found in the table below.

<b>Function</b>	Beam in bending
<b>Objective</b>	Minimize the mass
<b>Constraints</b>	(a) Length $L$ specified (b) Support bending load $F$ without deflecting too much

The mass  $m$  of the beam is

$$m = AL\rho \quad (6)$$

where  $A$  is the area of the cross-section and  $\rho$  is the density of the material. The mass can be made as small as we please by reducing the section area  $A$ ; but if it is reduced too much the beam will not be stiff enough. The prescribed stiffness thus imposes a constraint on  $A$  which can be calculated as follows.

The deflection of a simply-supported beam with a central load  $F$  is

$$\delta = \frac{FL^3}{C_1EI}$$

with  $C_1 = 48$ . Other supports or distributions of load change  $C_1$ , but nothing else. The stiffness  $S$  for a square section beam of side  $b$  (as shown in Figure 5a) is

$$S = \frac{F}{\delta} = \frac{C_1 EI}{L^3} \quad (7)$$

The stiffness  $S$  and length  $L$  are constraints prescribed by the design. The area  $A$  is the ‘free’ variable. We wish to choose  $A$  such as to minimize the weight, while meeting the constraint on stiffness.

$$I = \frac{b^4}{12} = \frac{A^2}{12} \quad (8)$$

Substituting in  $I$  from equation (8) into equation (7) and eliminating  $A$  between this and (6) gives an equation for the mass

$$m = \left( \frac{12S}{C_1} \right)^{1/2} (L)^{5/2} \left( \frac{\rho}{E^{1/2}} \right) \quad (9)$$

The first bracket contains the functional requirement  $F$ , the second contains the geometry  $G$ , both of which are specified by the design, and the third bracket contains the material properties  $M_b$ . It can be seen that equation (9) is separable in accordance with equation (2). The weight of the beam can be minimized (and performance maximized) by seeking the material with the largest value of the performance index. This selection is independent of the stiffness  $S$ , the length  $L$ , and of the loading details contained in  $C_1$ .

$$\boxed{M_b = \frac{E^{1/2}}{\rho}} \quad (10)$$

The same material choice is optimal for all square section beams loaded in bending, or indeed for all beams of the *same* shape (round, square or I-section, as in Figure 5(b)).

## 2.3 Using Performance Indices in Granta EduPack

### Performance Indices as Selection Lines

Figure 3 shows that selection lines can be used to identify the materials that optimize the objectives during Ranking. The slope of this line can be identified from the performance index when the chart used log axis. To identify the slope of the line, we start with a performance index. For example, we will use equation 10.

First step is to rearrange the equation so no fractions are found, as shown below.

$$E = \rho^2 M_b^2 \quad (11)$$

Then, take the log of both sides of eq. 11

$$\log E = 2 \log \rho + 2 \log M_b \quad (12)$$

Because the chart has log axis, equation 12 plots as a straight selection line with a slope 2 as shown in Figure 6a. As  $M_b$  increases, the line moves upwards and to the left.

## Performance Indices as Chart Axis using the Granta EduPack

An alternative, when using performance indices for ranking, is to set the performance index as the chart axis (Figure 6(b)). The materials with the greatest values of the performance index are those highest on the chart.

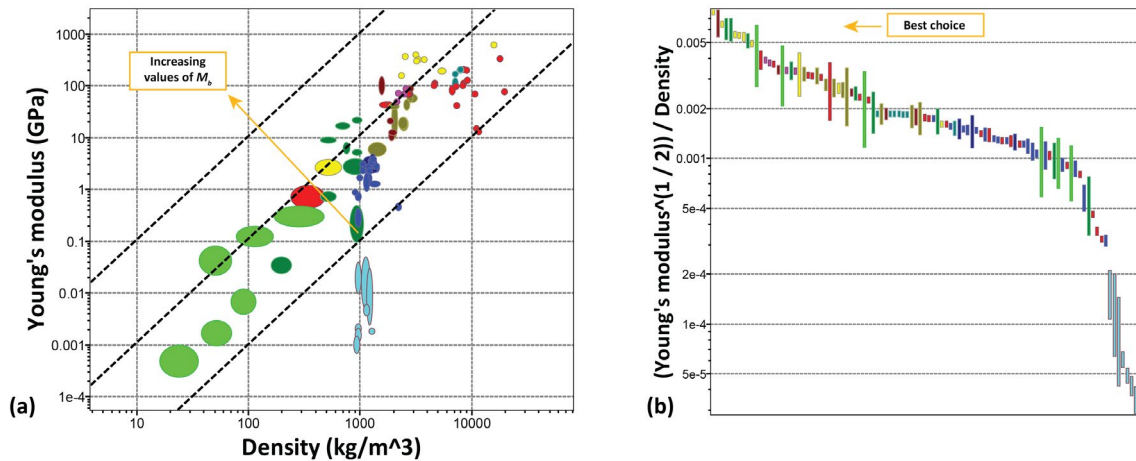


Figure 6 (a) Chart with performance index selection lines of slope 2 and (b) chart with performance index as the y-axis

## Performance Index Finder in Granta EduPack

In the advanced subject databases of Granta EduPack, there is a “Performance Index Finder” option within the Chart Stage box (see Figure 7).

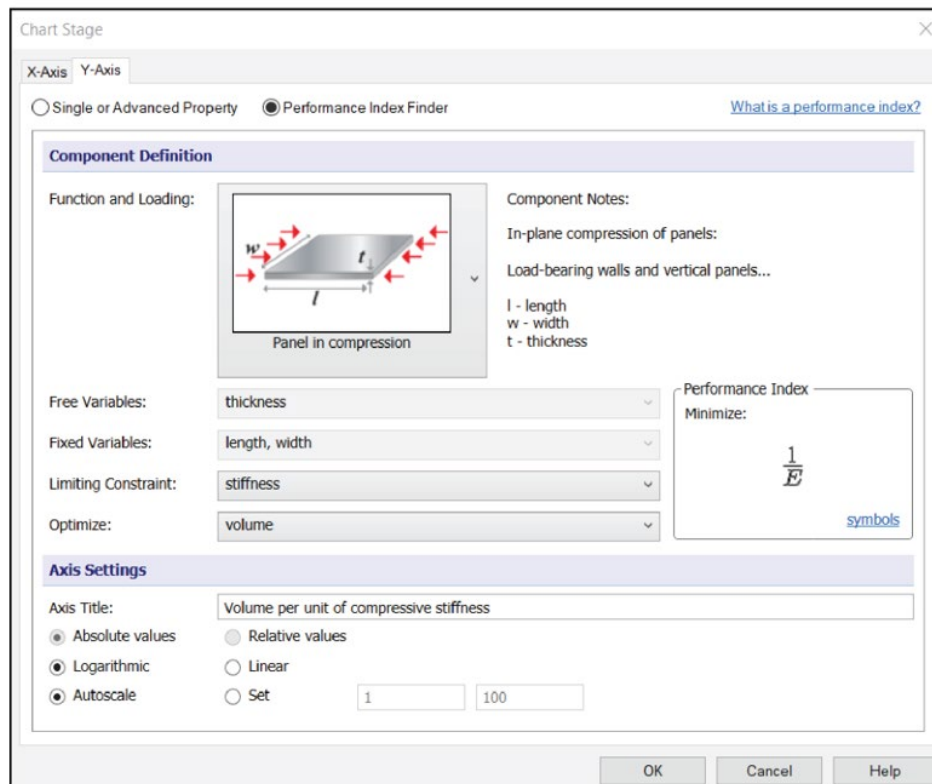


Figure 7: Screenshot of the Performance Index Finder tool within Granta EduPack, demonstrating how selecting various translation step information allows for the selection of a performance index

This tool allows entry of the function, the constraints, the objectives, and free variables, as identified during the translation step. The relevant performance index is automatically calculated and a chart like Figure 6(b), with the performance index on the axis, is generated.

### 3. References and Relevant Links

#### 3.1 References

The key reference for the materials selection methodology is that listed below.

[1] Ashby, M. F. (2017). Materials Selection in Mechanical Design (Fifth Edition). Elsevier Ltd. ISBN 978-0-08-100599-6

#### 3.2 Relevant Links

Here are some links to additional resources that can aid in learning and using the materials selection methodology and performance indices.

#### **Ansys Innovation Courses**

[Basic Systematic Materials Selection](#)

#### **Video Tutorials**

- [Creating Charts using Ansys Granta EduPack](#)
- [How to use the Limit Stage in Ansys Granta EduPack](#)
- [Performing a Basic Materials Selection in Ansys Granta EduPack](#)

#### **Ansys Education Resources**

- [Performance Indices Booklet](#)
- [Selection Case Study: Mechanical Applications](#)
- [Selection Case Study: Thermo-Mechanical Applications](#)
- [Selection Case Study: Electro-Mechanical Application](#)

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