

# Overview of the latest developments in Multiscale.Sim, a virtual material testing tool to accelerate materials design

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Multiscale.Sim from CYBERNET SYSTEMS is a versatile, easy-to-use Ansys add-on tool for multiscale analysis. Using an analytical approach based on the homogenization method, it can perform virtual material tests and identify anisotropic material constants from macroscopic material responses in different deformation modes. A particularly unique feature is the support for many types of non-linear and non-structural problems. As a stand-alone tool, it is very powerful for facilitating material design, offers maximum advantage when used in combination with a variety of Ansys solutions. This article introduces the latest developments with analysis examples, focusing on the integration with Ansys products.

## Overview of Multiscale.Sim

The first version of Multiscale.Sim™ [1] was released in 2007. Initially, many customers had problems preparing material properties, despite the high anisotropy of the material. This is particularly noticeable with fibre-reinforced plastic (FRP) and other fibre-based composites. Adding additional fillers results in a very large number of possible material combinations, so an approach based on testing of actual materials is not suitable for material design. We proposed to solve these problems with virtual material testing.

Fig. 1 summarises the main differences between real and virtual material testing procedures to illustrate the advantages of analysis-based material testing. Testing of actual materials is very costly from preparation to execution of test specimens and processing of test results. Special jigs may be required to obtain the anisotropic properties. If the material property to be evaluated is creep or fatigue resistance, the time requirement is often in the range of days or months. Above all, the same running costs are incurred for every material studied. This is very incompatible with composites which have a myriad of combinations. Virtual material testing techniques can be used to significantly address these problems.

With this approach, all steps are carried out virtually with the whole process being enabled by our solution. It consists of several steps and all the Ansys products or additional Ansys tools work together seamlessly in an integrated GUI environment, which is one of the unique features of our solution. The functions of each work step are summarized in Fig. 2. We provide virtual material testing technology based on the homogenization method. In this method, firstly, an analytical model (hereafter referred to as a micromodel) is created to represent the microstructural heterogeneity of the specimen. This model is created as a rectangle with periodic symmetry in all directions. Micromodels are the most important information characterizing the accuracy of virtual material tests and should be prepared with care. On the other hand, since so many case studies are required for material design, it is also important for them to be easy to create. Due to the complexity of

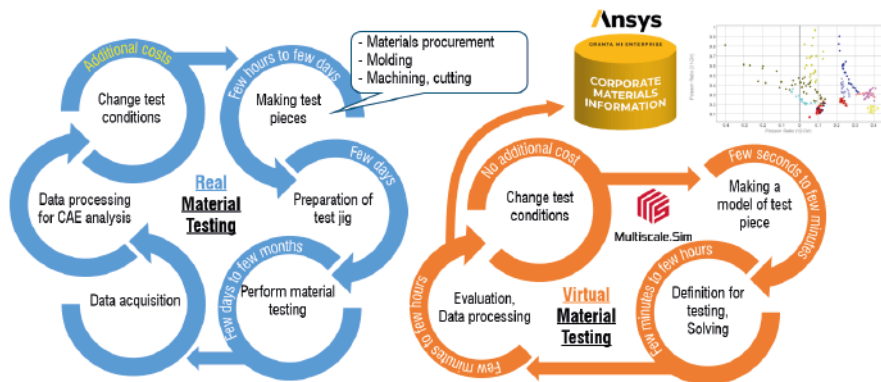


Fig. 1. Comparison of virtual and numerical material testing with a focus on cost.

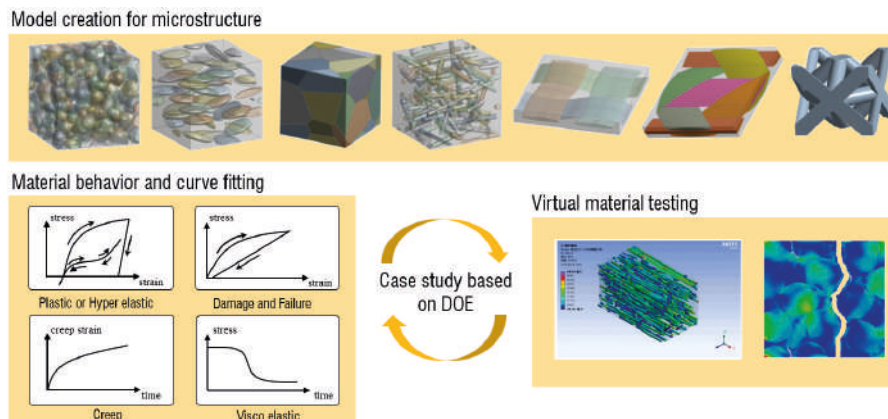


Fig. 2. Overview of Multiscale.Sim.

the material microstructure, manual modelling is not feasible. This can be solved using the template function we provide. For randomness, statistical information can be used. For short fibre dispersion materials, the fibre orientation ratio; for filler dispersion materials, the probability distribution of the existing dimensions or the degree of cohesion, etc. It is also not practical to model this information manually in a standard CAD system; script-based approaches are more effective. The virtual material test is achieved by defining strict boundary conditions that reflect the ideal deformation modes of the actual material tests. This feature is extremely versatile and can easily reproduce any deformation mode, not just general uniaxial testing, making it a very important feature for understanding the behaviour of anisotropic materials. Needless to say, observing the behaviour of a material over a long period of time in a simulated environment is not a problem.

The output is a macroscopic material response and corresponds to various results obtained by averaging the volume of the results within the microstructure using a microscopic model. In addition to the elastic response, it is possible to evaluate the behaviour of various non-linear materials such as elastoplasticity, fracture damage, viscoelasticity and creep. When performing large structural analyses that reflect the behaviour of macroscopic materials, it is also necessary to prepare macroscopic material constants to describe the material behaviour. We provide macroscopic material constitutive laws for this purpose as well as curve-fitting functions to identify the constants. The combination of these functions allows multiscale analysis for sequential coupling of micro and macro models.

### Multiscale.Sim development trends

This section describes the latest developments in Multiscale.Sim. All features are designed to make virtual material testing technology more convenient and accurate.

### SpaceClaim migration of the micro modelling function

Due to the wide variety of microstructures in composites, expanding modelling capabilities has always been a top priority. Therefore, we

listen to our customers' needs and actively incorporate them into our development plans. So far, this functionality has mainly been implemented in Ansys DesignModeler™, but we are actively migrating it to SpaceClaim®. This is also an effort to keep pace with Ansys' development strategy. This allows users of Ansys Mechanical™ Enterprise to create models without additional licenses. Our goal is to migrate all the modelling functionality currently implemented in DesignModeler to SpaceClaim by the end of this year.

### Granta MI interface for managing and using the material database

The response obtained from the virtual material test is converted into material constants by curve fitting and recorded in the engineering data, which is a standard function of Ansys Workbench™. However, aggregating the material data locally is not sufficient to achieve maximum benefit. The high-end materials database system Ansys Granta™ solves all these problems. Multiscale.Sim has developed an interface that works with Granta MI™. It allows bi-directional data association between Multiscale.Sim and Granta MI. Granta MI allows users to record not only the material constants used in the analysis, but also various other information about the material. This means that both input and output information can be managed for homogenization analysis, which not only improves data traceability,

but also enables the use of AI in materials informatics [2].

Let's take a look at a simple example of how to use it. The material to be analysed is a lattice structure created by 3D printing consisting of columns of various cross-sectional shapes and angles. By changing the thickness and angle of the columns, not only the density but also the material properties such as modulus of elasticity, change significantly. This feature can be used to create the optimal material behaviour for the product. The lattice structure is controlled by several shape parameters such as topology, column thickness (assuming a circular cross-section), and the aspect ratio. The raw material used to construct the lattice is fixed to titanium.

Fig. 3 shows a visualization of an aggregated dataset in Granta MI. The modulus of elasticity and Poisson's ratio are placed on the axes, respectively. The microstructure of four typical conditions is also shown in the same figure. With Granta MI users can not only see the general trend of the data, but also refine their search to find the optimal lattice structure for their product.

Composites also facilitate the creation of materials with unsampled area properties. Finally, we use AI to try to predict a lattice structure that matches the desired material

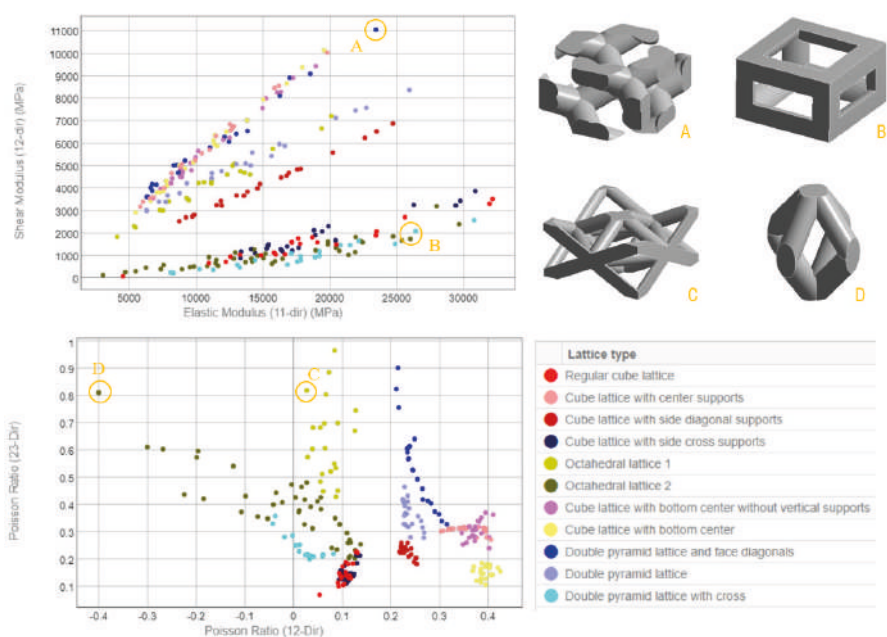
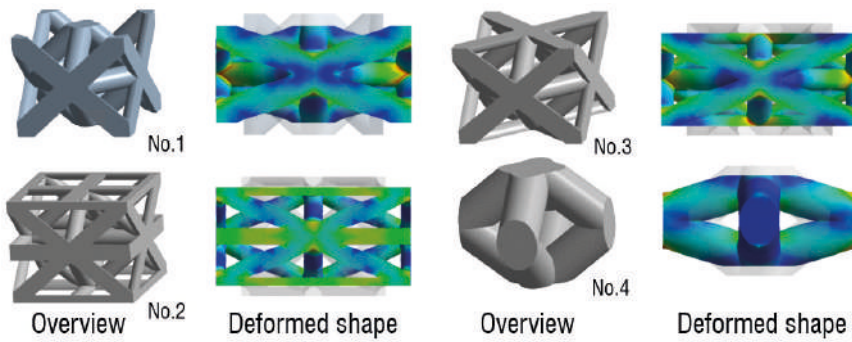


Fig. 3. An example of the materials database displayed by Granta MI



Elastic constants obtained by virtual material testing

Properties	Direction	Candidate ID No.			
		1	2	3	4
Young Modulus [GPa]	X	10.001	9.9885	9.9890	9.9704
	Y and Z	7.1713	3.9354	4.7810	8.0266
Poisson's Ratio [-]	XY	0.0079	0.0071	0.2516	-0.1280
	YZ and XZ	0.4982	0.5035	0.4999	0.5019
Shear Modulus [GPa]	XY	4.0840	0.4391	5.4378	0.6039
	YZ and XZ	5.8174	2.6447	4.5385	5.3495

Fig. 4. Example of inverse lattice structure identification by AI trained on a materials database.

behaviour (which does not exist in the materials database). This problem can be solved by response surface optimization analysis. Suppose we need a lattice structure with a longitudinal modulus of 10 [GPa] in the x-direction and a Poisson's ratio of 0.50 [-] in the yz-direction. Fig. 4 shows four candidates for the lattice structure predicted by AI. Virtual material tests were performed on these lattice structures to validate the results, which are also summarized in Fig. 4. It can be seen that the modulus and Poisson's ratio given as target values are reproduced with very high accuracy for all lattice structures. Of course, the properties of other components vary from lattice structure to lattice structure.

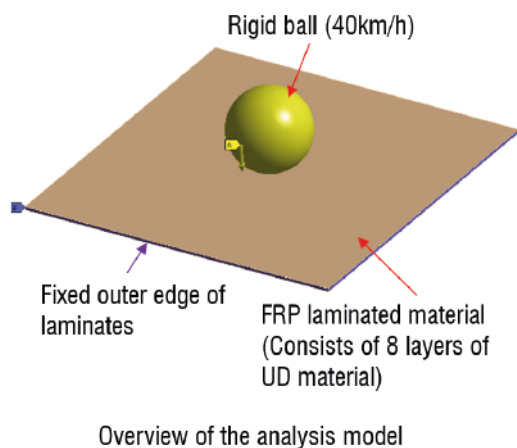
### LS-DYNA interface supporting strong non-linearity such as impact fracture problems

In composites, which are a mixture of materials with very different stiffnesses, high stresses are concentrated at the material interface, which is the starting point for failure. Such problems are highly non-linear and implicit analysis approaches have limited applicability. We are also developing an explicit virtual material testing technique which can be carried out by coupling with LS-DYNA®. This allows multi-scale analysis, mainly for composite fracture problems. A simple analysis example is shown in Fig. 5. A rigid ball is dropped onto a composite material made of unidirectional

reinforcing fibres (referred to as UD material). Three different lamination patterns were prepared. Each of them has a very different tendency to anisotropy and therefore shows very different fracture behaviour on impact. This analysis is possible by accurately observing the anisotropic fracture behaviour of the UD material through virtual material testing. Fig. 6 shows the actual results of this analysis. The material behaviour can be observed, considering various failure modes such as de-bonding at the material interface and transverse cracking and propagation. The obtained anisotropic fracture strength can be used to perform the fracture analysis of any macrostructure made of the UD material.

### Resin flow analysis tools to incorporate moulding history

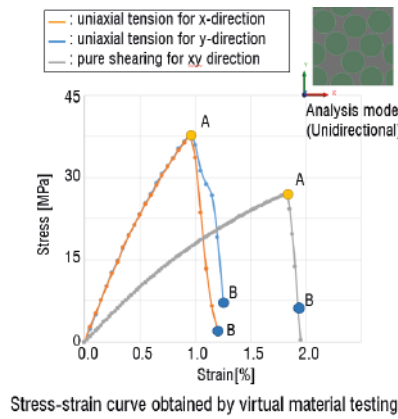
It is important to consider the moulding history when analysing material behaviour as injection moulded products contain discontinuous fibres and their orientation is not uniform throughout the product. Multiscale.Sim can map the distribution of fibre orientations based on the moulding history and the corresponding material constants. The microstructure of injection-moulded parts varies from region to region. Of course, it is not possible to carry out virtual material tests of every region. Therefore, independent of the moulding analysis, the equivalent material constants for the microstructure of a typical fibre orientation pattern are evaluated. By converting these results into response surfaces as material constants equivalent to directional pairs, it is possible to interpolate material constants other than the sampling points. It is then possible to



Fracture behavior for different lamination patterns (equivalent stress distribution)

Timing	Lamination Pattern		
	[0/0/0/0] <sub>sym.</sub>	[0/90/0/90] <sub>sym.</sub>	[0/90/45/-45] <sub>sym.</sub>
Immediately after impact			
After impact			

Fig. 5. Fracture analysis of a laminated unidirectional reinforcement



Equivalent stress distribution inside a microstructure

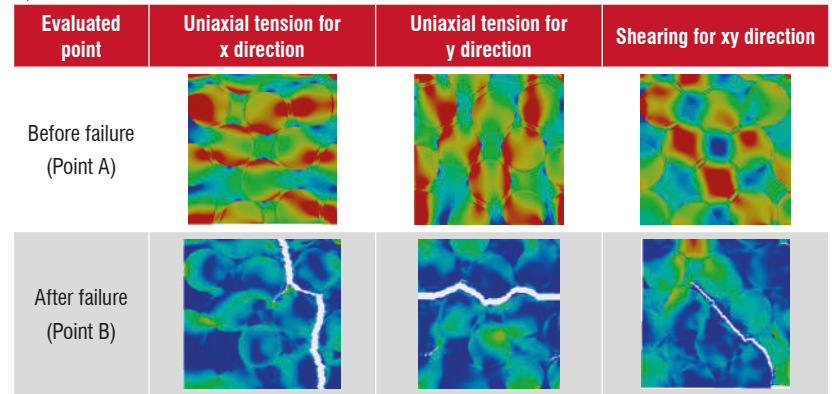


Fig. 6. Example of observed fracture behaviour of unidirectionally reinforced material using virtual material testing

use this response surface to map the material constants onto the fibre distribution obtained from the resin flow analysis. The advantage of using this method is that it can be used to map any constitutive law. This includes not only problems related to elasticity, but also any material non-linearities.

### Link to Rocky for the creation of microstructures based on physical phenomena

For some composites such as porous materials and powders, it is not always possible to achieve sufficient analytical accuracy without preparing microstructures based on physical phenomena. To overcome this problem, you can use a modelling approach in combination with particle simulation software Rocky. The forming process of the material is analysed in Rocky and the results are used as a micromodel in Multiscale.Sim.

To outline the function, we will use a powder made of spherical particles as an example. Fig. 7 shows the results of a powder material with a particle size distribution that has been used to fill a container by free falling and tapping. Smaller particles fall through the spaces created between the large particles.

As a result, the microstructure of the filling material shows features of segregation. Towards the bottom surface, the proportion of smaller particles increases. An interface currently under development can be used to extract the microstructure of a particular region from the results of this analysis. Since the material behaviour of powders cannot be represented by elasto-plastic material models such as those used for metallic materials, it is necessary to use the Drucker Prager model which is specialized for powder materials. We are also developing a curve-fitting function for this purpose. An example of a real analysis of powdered materials was introduced in a previous issue of this magazine [3]. For segregated materials, as in the case of injection moulding described in the previous section, the material properties are not uniform. This can also be overcome with a mapping technique based on the response surface.

### Conclusion

This paper provided an overview of the functionality of Multiscale.Sim, an Ansys add-in tool for performing multiscale analysis, as well as the latest development trends. We are constantly developing this product to help you in your material design process. While

focusing on the integration of Multiscale.Sim and Ansys products, we are also actively working with our customers to develop specific functional requirements..

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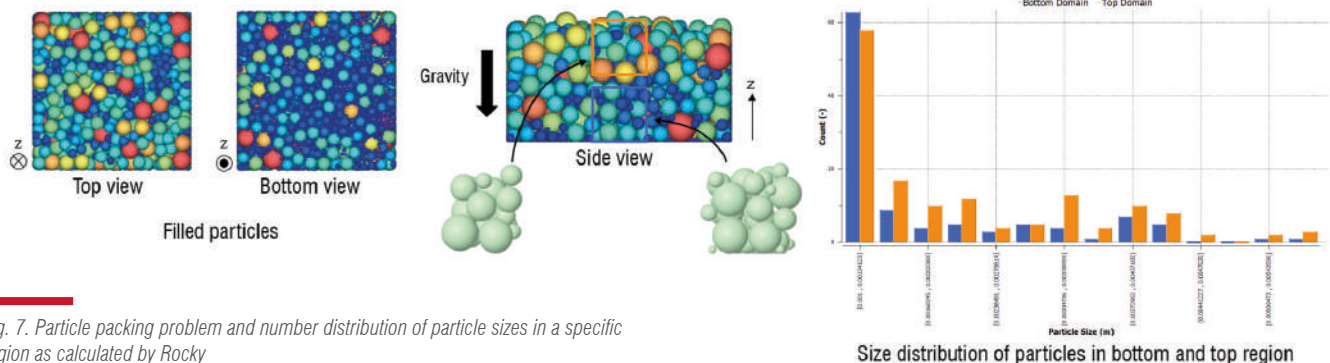


Fig. 7. Particle packing problem and number distribution of particle sizes in a specific region as calculated by Rocky