# MUL2-UC

**Micromechanics code: beam modeling
of periodically heterogeneous
composites**

June 9th, 2017

A.G. de Miguel[1]

[1] Politecnico di Torino, 24 Corso Duca degli Abruzzi, 10129 Turin (TO), Italy

Mail to: alberto.garcia@polito.it

# Table of contents

# 1. Introduction

The micromechanics code MUL2-UC is developed to work as an efficient and high-fidelity tool for the computation of the effective stiffness matrix and the recovering of the local fields of periodically heterogeneous composite structures. The main novelty is that higher-order beam theories are employed to model the microstructure of composite structures, differing from conventional micromechanics numerical tools which usually make use of 2D/3D finite models to solve the problem. The code implements the Mechanics of Structure Genome (MSG) [1] to decouple the multiscale problem into global and local analysis, and uses the Carrera Unified Formulation (CUF) [2] to generate lower-cost refined beam models to solve the constitutive problem posed by MSG.

# 2. Functionalities and general description

MUL2-UC makes use of standard 1D elements to discretize the various constituents along the longitudinal direction of the microstructure and a higher-order non-local theory of structure, denominated to as Hierarchical Legendre Expansions (HLE) [3], to expand the unknowns of the problem over the remaining two directions. An advanced mapping technique is also implemented in the tool to model the exact geometry of the different constituents (fibers, matrix, particles, plies, etc…) over the cross-section of the beam. If different phases are located along the beam axis, these can be captured by the 1D finite element discretization. It is important to note that, following this modeling approach, the geometrical description of the microstructure is fixed at the beginning of the analysis, and the accuracy of the solutions is controlled by the polynomial order of the expansions, $p$, which is introduced by the user during the analysis.

A visual scheme of the MUL2-UC operation is illustrated in Figure 1. The user defines the inputs of the problem, including the section geometry, the beam discretization, the properties of the constituents, the boundary constraints and the polynomial order of the beam theory. Then, the code generates the arrays of the problem, solves the linear system and computes the fluctuation variables. The complete 3D stiffness matrix is automatically generated with only a single run of the code. If the local fields are required, the user must only input the values of the global strains, and the code computes the local strain and stress fields over the microstructure using the same fluctuation unknowns previously obtained. This process can be repeated indefinitely without launching the tool again, enabling the user to save precious time in the multiscale analysis. If the user wants to increase the accuracy of the solutions, this can be done by simply relaunching the tool again introducing a higher polynomial order, $p$, with no need of remeshing.
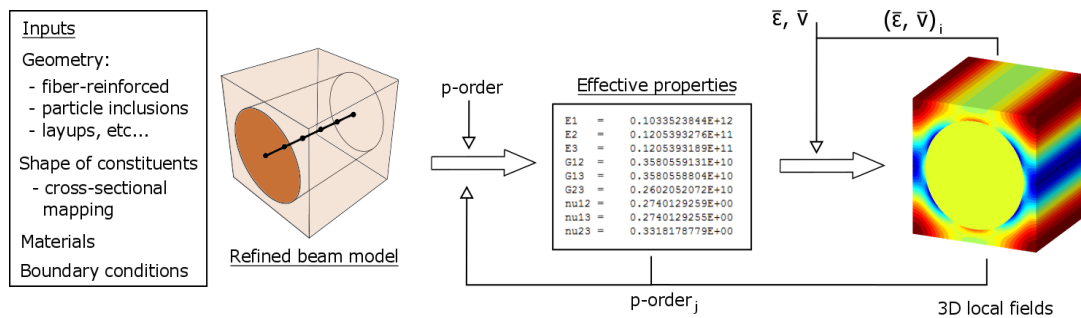
Figure 1. Micromechanics analysis using MUL2-UC.

MUL2-UC couples the already established capabilities of MSG for the accurate micromechanics analysis with the efficiency of refined beam models for representative volumes in which the heterogeneities are predominant in one or two directions, such as fiber reinforced or particle reinforce composites. In these cases, but not limited to, refined beam models are very convenient in terms of computational efforts, and can provide the same level of accuracy as commonly used 2D or 3D models. In addition, the exact geometry of the constituents can be represented regardless of the size of the discretization, for instance, the fiber section can be modeled by only a single HLE expansion domain.

The code is entirely written in Fortran 77/90. The present version of the software is available in https://cdmhub.org/resources/downloads as a downloadable folder for Windows operating systems. It contains an executable file 'MUL2-UC_v1.1.exe' and several text files including inputs and outputs. For the purposes of the present competition, several pre-arranged models of typical microstructures are available for any user to easily try and test the code, including common fiber-reinforced UCs and particle inclusions with variable geometries. The outputs of the micromechanical analysis are presented in .dat files and can be found in the folder 'Matrices'. A Gmsh file is also generated so as to allow the post-processing of the local fields in a more user-friendly environment. Gmsh is free finite element mesh generator released under the GNU General Public License and can be downloaded at http://gmsh.info/ .

This document contains some important information for users to understand, setup, launch and use the code. Section 3 describes the different modules defined inside MUL2-UC to generate HLE beam models for microstructures. Section 4 includes useful information on how to run the code and a description of the common microstructures that are available in the present version of the tool. Finally, Section 5 shows a tutorial example with a step-by-step explanation of the code features.

# 3. Model setting

To generate HLE beam models for the micromechanics analysis, MUL2-UC splits the modeling procedure into several modules. These correspond to the different sets of inputs that the user must define to launch the code, counting:

1.  <u>Materials</u>: number of materials, properties and orientation (if needed). Isotropic, monoclinic and orthotropic materials can be introduced through the engineering constants.
2.  <u>Beam mesh</u>: number and type of beam elements along the beam axis. The user can select 2-node (*beam2*), 3-node (*beam3*) or 4-node (*beam4*) line elements. For the case of unidirectional microstructures, e.g. fiber reinforced, a single *beam2* element is enough to obtain the effective properties and the local fields with no lack of accuracy.
3.  <u>Cross-sectional expansion</u>: refinement theory of structure, including sub-domain distribution of the section surface, polynomial order of the expansions and mapping parameters for curved constituents (e.g. for fibers). The materials are assigned in a component-wise sense, that is accounting for the exact geometry and properties of the different constituents.
4.  <u>Boundary conditions</u>: definition of the periodic boundary conditions. These are automatically introduced by the code along the beam axis and the user only needs to take care of the periodicity over the cross-section.

# 4. Running the code

The user can initialize the tool by launching the executable file 'MUL2-UC_v1.1.exe' located in the downloadable folder 'MUL2-UC_ASC'. Several common microstructures are available and ready for the user to straightforwardly use the code. The code also allows to do free modeling for generic microstructures by modifying the input files located in the folder 'Input_Files_FreeModel'. Up to date, the code has been developed for academic purposes and the free modeling option requires the user to be familiar with the format of the inputs. For this reason, the present document focuses on the common microstructures deployed in the proposed version of MUL2-UC, which are sufficient to demonstrate the capabilities of HLE higher-order beam models for the efficient micromechanics analysis. If the reader is interested in the free modeling option, more information and support can be provided by Eng. A.G. de Miguel to [alberto.garcia@polito.it](mailto:alberto.garcia@polito.it) or through the cdmHUB channels.

## 4.1. Pre-arranged microstructures

For the rapid and straightforward testing of the code, four common examples of microstructures are included: fiber reinforced square pack, hexagonal pack, cubic particle inclusion and cylindric particle inclusion. In all cases the user has the freedom to introduce the materials properties of the constituents, the geometry of the UC, the fiber volume fraction, and the polynomial order of the beam theory. A brief description of these models is provided in the following.

### 4.1.1. Square pack

The model corresponds to the typical square pack illustrated in Figure 2. The dimensions of the UC are 1x1x1 and the volume fiber is introduced by the user during

the analysis. Due to the unidirectional arrangement of the constituents, only one section is enough to represent the microstructure. The curvature of the fiber section is directly mapped into the cross-section of the model, enabling to use only one domain for the fiber, being a total of 5 the number of sub-domains employed for the cross-section expansion. The fiber volume fraction is introduced by the user as desired.
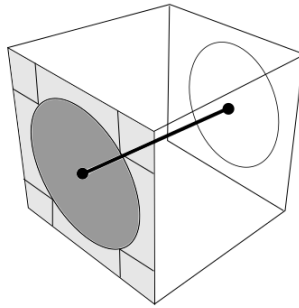
Figure 2. Model of the square pack generated by the MUL2-UC.

### 4.1.2. Hexagonal pack

The hexagonal pack (shown in Figure 3) is also a well-known example of microstructure used by engineers for multiscale analyses. The dimensions of the UC are 1x1x1.73 and, as for the square pack, only a single section is required to model the problem. The total number of section sub-domains is 15, including one for each fiber. The fiber volume fraction is defined by the user.
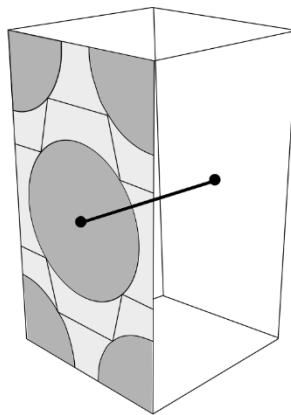
Figure 3. Model of the hexagonal pack generated MUL2-UC.

### 4.1.3. Parallelepiped inclusion

This common microstructure consists in a cubic UC with an embedded parallelepiped inclusion. The particle is located in the center. The user defines the geometrical dimensions of the inclusion as, i.e length, width and height. The beam model generated by MUL2-UC for the given inputs is equivalent to the one in Figure 4. One can note that the sections of the beam placed at the center in correspondence to the particle account for the fiber material.
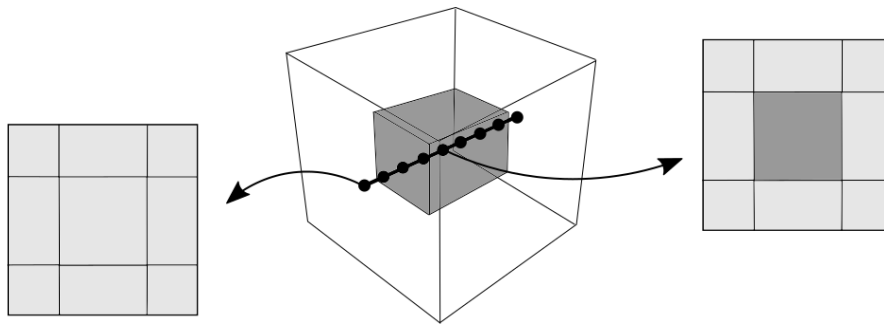
Figure 4. Model of the parallelepiped inclusion generated by MUL2-UC.

### 4.1.4. Cylindric inclusion

The cylindric inclusion, shown in Figure 5, is very similar to the previous one, with the difference that the inclusion is now curved. The user can input the length of the particle and the radius of its section.
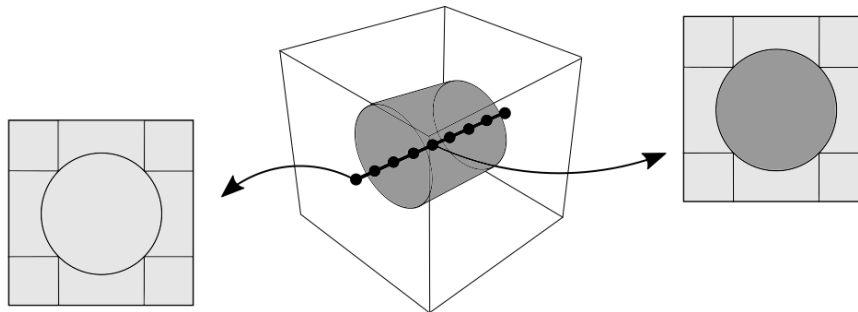


Figure 5. Model of the cylindric inclusion generated by MUL2-UC.

# 5. Tutorial example

This section shows how to perform the homogenization and dehomogenization of a UC through an example case using the common microstructures available in the tool. The hexagonal pack is selected for this example.

When the code is launched, a command window opens in the screen similar to the one shown in Figure 6.

Figure 6. Initializing MUL2-UC.

To select the hexagonal pack, the user must type 2, as indicated in the Figure 2. By doing this, the code reads the predefined parameters of the model and then asks for the material inputs. Starting for the fiber properties, the user must input 1 if an isotropic material is considered, or 2 if orthotropic. Once this is done, the engineering constants of the material can be introduced, see Figure 7. The procedure to input the matrix properties is the same. For the present example, a G40-800 carbon fiber and 8552 epoxy matrix are used. Their properties are:

- G40-800: orthotropic ($E_1 = 290$ GPa, $E_2 = 19$ GPa, $E_3 = 19$ GPa, $\upsilon_{12} = 0.2$, $\upsilon_{13} = 0.2$, $\upsilon_{23} = 0.36$, $G_{12} = 27$ GPa, $G_{13} = 27$ GPa, $G_{23} = 7$ GPa)
- Epoxy: isotropic ($E = 4.08$, $\upsilon = 0.38$)



Figure 7. Introducing the material properties.
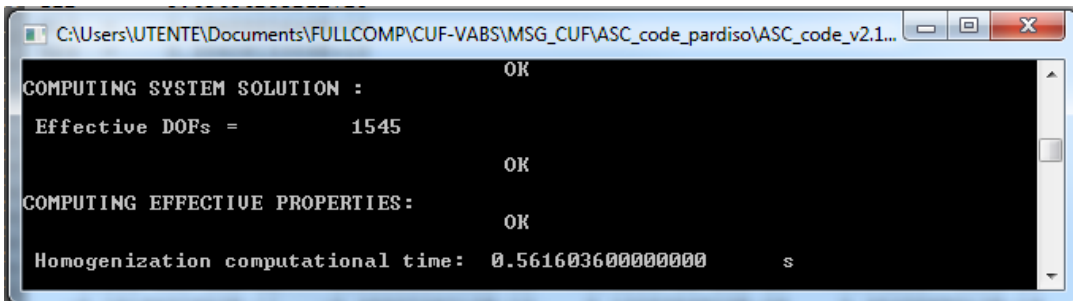
Once the material properties have been defined, the code requires the fiber volume fraction of the hexagonal UC. For example, a value of 0.6 can be introduced. The code automatically generates the expansion domains of the curved fibers and those correspondent to the matrix (see Figure 2). The next step is to introduce the polynomial order of the HLE beam model. This parameter determines the refinement of the model and controls the accuracy of the solutions, mainly for the computation of the local fields at the end of the analysis. Polynomial orders between 2 and 8 can be selected. An 8$^{th}$ order is introduced for the present analysis.



Figure 8. Geometry and polynomial order of the HLE.

At this point, all the necessary inputs for the micromechanical study have been introduced and the code proceeds to run the homogenization analysis and computes the effective properties of the material. During this process, the command window shows some relevant information of the analysis, such as the effective number of degrees of freedom of the beam model and the computational time for the homogenization process.



Figure 9. Effective degrees of freedom and computational time of the homogenization.

A file with the constitutive information automatically opens containing the stiffness and compliance matrices of the equivalent homogeneous material, as well as the engineering constants (see Figure 10).

Figure 10. File generated by MUL2-UC with the constitutive information.

If this file does not open automatically, the user can find it inside the folder 'Matrices' under the name 'Effective_stiffness.dat'.

The next step of the study is to obtain the local fields for the given global solution. In order to continue with the analysis, the user must first close the file of the constitutive information. By entering 1, the user can now introduce the global strains to compute the local strains and stress fields within the microstructure. The usual coordinate system is employed, i.e. X is the fiber direction (beam axis) and Y and Z the remaining two over the cross-section. For this tutorial example, a unitary longitudinal strain is introduced, leaving the remaining components as zero.



Figure 11. Inputs of the global strains for the dehomogenization.

Once this is done, the code generates the outputs of the dehomogenization. If the user has already installed Gmsh in his/her workstation, a .msh file will automatically open containing all the local solutions.
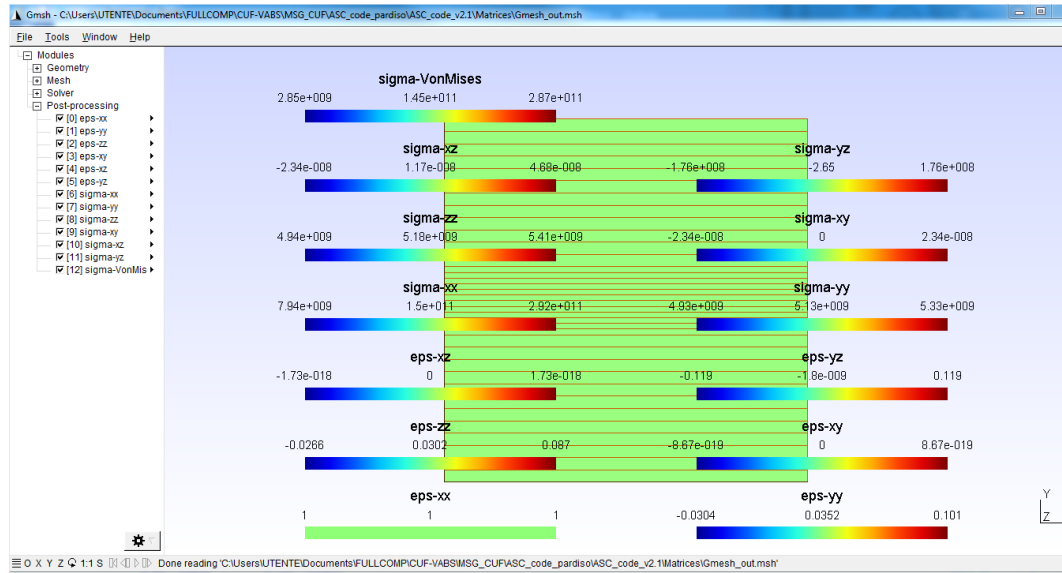


Figure 12. Post-processing of the local solutions in Gmsh.

This file can also be found in the folder 'Matrices' under the name 'Gmesh_out.msh', together with another text files that contain the numerical values of all the local solutions for the different sections of the beam nodes (ris2D_SEC001_001 and ris2D_SEC002_001 in the present example). Figures 13 and 14 show the results of von-Mises and transverse stresses, respectively.
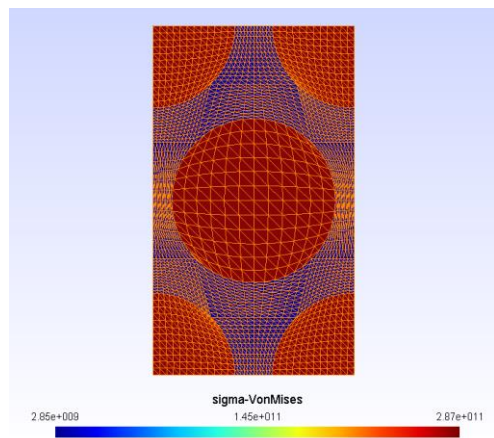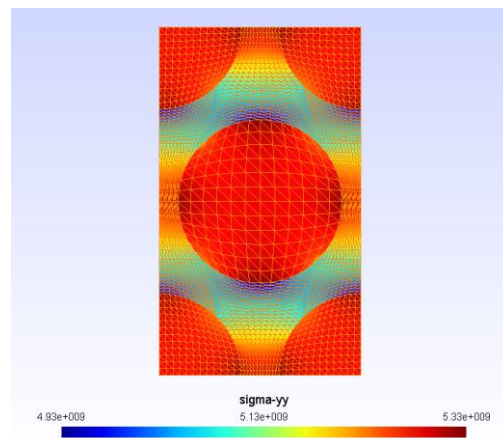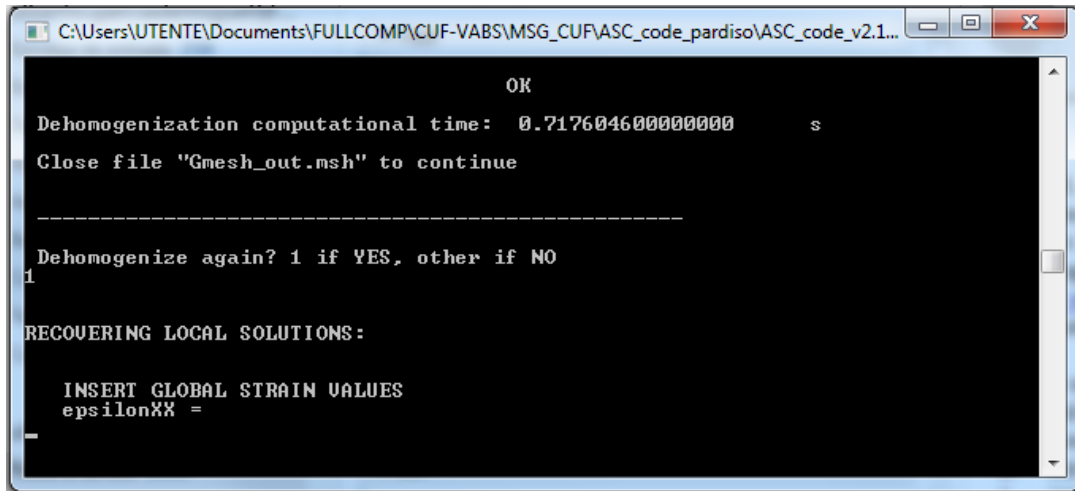


Figure 13. Von Mises stress



Figure 14. Transverse stress

It is important to note that in order to capture the curvature of the fibers' sections and to represent accurately the high-gradients of the local fields, high polynomial orders are required in the analysis. To demonstrate the capabilities of the HLE high

order beams, the fibers are modeled by only a single expansion in all the common examples. For more information about the formulation and results of the code, interested readers are referred to the companion conference paper [4].

Coming back to the command window, the user can see the computational time used for the dehomogenization process. The code asks whether the user wants to dehomogenize again, or just finish the analysis. If new local solutions are wanted, the user must enter 1 and the code returns to the previous step in which one can introduce again the global strains.



Figure 15. Iterative dehomogenization for multiple global inputs.

This action can be indefinitely done with no need of solving the homogenization problem, allowing the most efficient evaluation of the strains and stresses of the multiscale problem.

# 6. Acknowledgements

# 7. References

[1] W. Yu. "A Unified Theory for Constitutive Modeling of Composites", *Journal of Mechanics of Materials and Structures*, vol. 11, no. 4, 2016, pp. 379-411.

[2] E. Carrera. "Theories and finite elements for multilayered, anisotropic, composite plates and shells". *Archives of Computational Methods in Engineering*, vol. 9, no. 2, 2002, pp. 87–140.

[3] E. Carrera, A.G. de Miguel and A. Pagani. "Hierarchical theories of structures based on Legendre polynomial expansions with finite element applications", *Int'l Journal of Mechanical Sciences*, vol. 120, 2017, pp. 286-300.

[4] A.G. de Miguel, A. Pagani, E. Carrera and W. Yu. "Micromechanics modeling of unit cells using CUF beam models and the Mechanics of Structure Genome", to be presented at the ASC 32nd Annual Technical Conference, October 23-25, 2017.