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MIDAS-VT-Pre: Software to generate 2D finite element model of particle/fiber embedded composites with cohesive zones

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ABSTRACT

Studying the behavior of particle/fiber embedded composites has been a common and challenging problem in mechanics of materials area. Analysis of these materials can be effectively conducted by computational simulations such as finite element (FE) analyses. Creating a model that represents the actual microstructure of the composite is crucial to obtain a trustable result, but is often labor-intensive. Microstructure Inelastic Damage Analysis Software (MIDAS) Virtual Tester Preprocessor (MIDAS-VT-Pre) was developed to facilitate construction of two-dimensional microstructure FE models of particle/fiber embedded composites. MIDAS-VT-Pre is able to insert automatically cohesive zone interface elements in the mesh structure in order to simulate crack initiation and propagation. This program is tailored to generate the FE model of standard mechanical test configurations that are frequently used in laboratory settings. The output of this program includes mesh structure and boundary conditions. This information can be used to run FE simulation (i.e. virtual testing) using common FE software such as ABAQUS.

Code metadata

Current code version	v1.0.0
Permanent link to code/repository used for this code version	https://github.com/ElsevierSoftwareX/SOFTX_2018_270
Legal Code License	GNU General Public License v3.0
Code versioning system used	git
Software code languages, tools, and services used	MATLAB
Compilation requirements, operating environments & dependencies	Microsoft Windows
If available Link to developer documentation/manual	https://github.com/K1-ZR/midas-vt-pre/blob/master/documents/MIDAS-VT-User'sGuide.pdf
Support email for questions	keyvan.zare@gmail.com

Software metadata

Current software version	v1.0.0
Permanent link to executables of this version	https://github.com/K1-ZR/midas-vt-pre/releases/tag/v0.1.2
Legal Software License	GNU General Public License v3.0
Computing platforms/Operating Systems	Microsoft Windows
Installation requirements & dependencies	MATLAB Runtime 9.5
If available, link to user manual–if formally published include a reference to the publication in the reference list	https://github.com/K1-ZR/midas-vt-pre/blob/master/documents/MIDAS-VT-User'sGuide.pdf
Support email for questions	keyvan.zare@gmail.com

1. Motivation and significance

A large portion of the mechanics of material science usually deals with the study of the behavior of heterogeneous materials.

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The overall properties of a heterogeneous material are governed by its microstructure and the properties of its components [1,2]. Accurate analysis of heterogeneous materials' behavior requires to take into account these factors accordingly. Creating a FE model that fully represents the features of the actual microstructure including random spatial distribution and irregular shapes of particles is sometimes difficult and time-consuming. A review of composite modeling approaches in the literature shows that simplified particle geometries such as circles and ellipses are often used to approximate the actual microstructure of composites [3–6]. This approach may be reasonable for some cases, but it fails to capture the accurate behavior of the composites when the particles have irregular shapes and random distribution. In more recent studies, microstructure images have been widely used to create accurate microstructural FE model of heterogeneous materials [7–17]. Fortunately, there are various imaging technologies such as optical imaging, optical microscopy, scanning electron microscope (SEM), and atomic force microscopy (AFM) that allow capturing the microstructure of materials at different length scales. MIDAS-VT-Pre is designed to assist with generating the two-dimensional FE mesh of particle/fiber embedded composites directly from given microstructure images without losing significant morphological details.

In addition, a considerable amount of studies in mechanics of material science area has investigated the simulation of cracking in materials. Among many approaches to simulate cracking, cohesive zone model (CZM) is one of the most popular methods that can simulate material debonding effectively [14,18–20]. This method assumes that there is a fictitious fracture process zone ahead of the crack tip that follows a softening behavior. The fracture process zone is simulated using cohesive interface elements. Interface elements connect two nodes shared between two adjacent continuum elements. The softening behavior of the cohesive zone is simulated by the traction–separation relation of the interface elements. The cohesive zone interface element is a core component in simulation of potential debonding using CZM. While there are many applications that generate continuum FE mesh of a given geometry, to the knowledge of the authors, there is quite limited software available to generate FE mesh with cohesive zone interface elements. Hence, MIDAS-VT-Pre is equipped with a feature to embed cohesive zone interface elements within the FE mesh structure for simulating potential crack propagation.

The primary objective of MIDAS-VT-Pre is to generate the FE model of frequently used mechanical tests for particle/fiber embedded composites. These FE model simulations can be used along with the laboratory tests to better select component materials and thus better design the composite. It can also be potentially useful as a replacement of repetitive laboratory tests.

2. Software description

MIDAS-VT-Pre is a user-friendly software that is developed to generate 2D FE model of any particle/fiber embedded composite from given microstructure of the composite. The current version is applicable to two-phase particulate composites that are composed of distinct particles and continuous matrix phase. In order to have a straightforward process, MIDAS-VT-Pre is tailored to generate FE models for specific test settings. The schematic view of the available tests are shown in Fig. 1. The only information that MIDAS-VT-Pre requires to generate FE models is the sample's geometry: dimensions and microstructure.

MIDAS-VT-Pre uses the specimen's dimensions and a microstructure image, either physically scanned or artificially–virtually fabricated, of the specimen as inputs. It identifies the microstructure of the composite using an image processing module. Then the software meshes the microstructure geometry and classifies individual phases for proper material properties. The initial FE mesh contains only three-node bulk elements without cohesive zone interface elements. If the cohesive zone elements are desired to be embedded, users can define areas to locate cohesive zone elements so that cracking (initiation and propagation) can be effectively simulated.

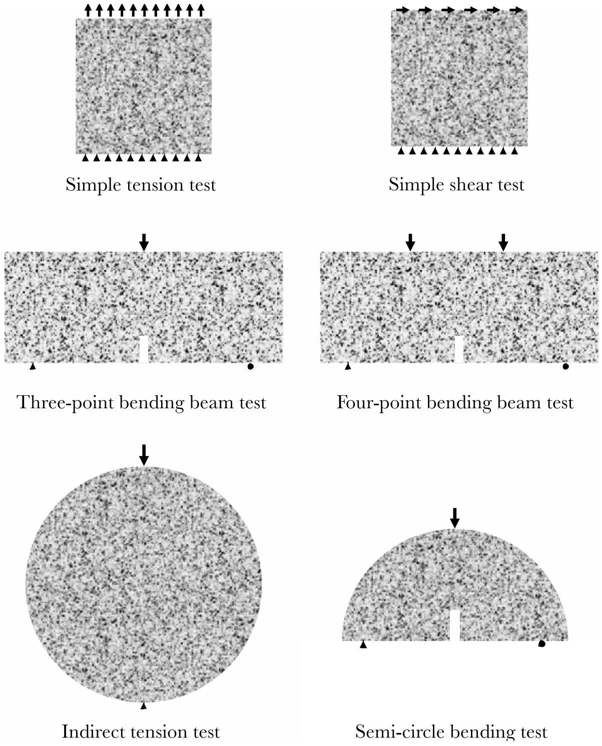


Fig. 1. Test configurations.

The output of MIDAS-VT-Pre is FE mesh data and boundary conditions for certain laboratory test pursued by users. The mesh data contains nodal coordinates and elemental connectivity for both three-node bulk elements and four-node cohesive zone interface elements. The output can be used in any common FE software (e.g. ABAQUS) and MIDAS-VT which is a separate software developed by the authors to run FE models and conduct post-processing of simulations [21]. MIDAS-VT-Pre is also able to create homogeneous (one-phase) FE models of the aforementioned laboratory tests with or without embedding cohesive zone elements within a user-defined area when such simulation is deemed.

2.1. Software architecture

The overall flow of MIDAS-VT-Pre is illustrated in Fig. 2. MIDAS-VT-Pre offers two options to generate the FE model. The first option (Case I) is useful when the user generates a FE model from the sample's geometry, i.e. shape and microstructure image. In this case, MIDAS-VT-Pre distinguishes different phases from the microstructure image and meshes the resulting geometry accordingly. The initial FE mesh includes only three-node bulk elements. Once meshing is completed, interface elements are embedded within the CZ area which is defined by user to simulate cracking. The second option (Case II) is used when the user is only interested in inserting cohesive zone elements within a regular FE structure which was created in advance by a separate meshing program.

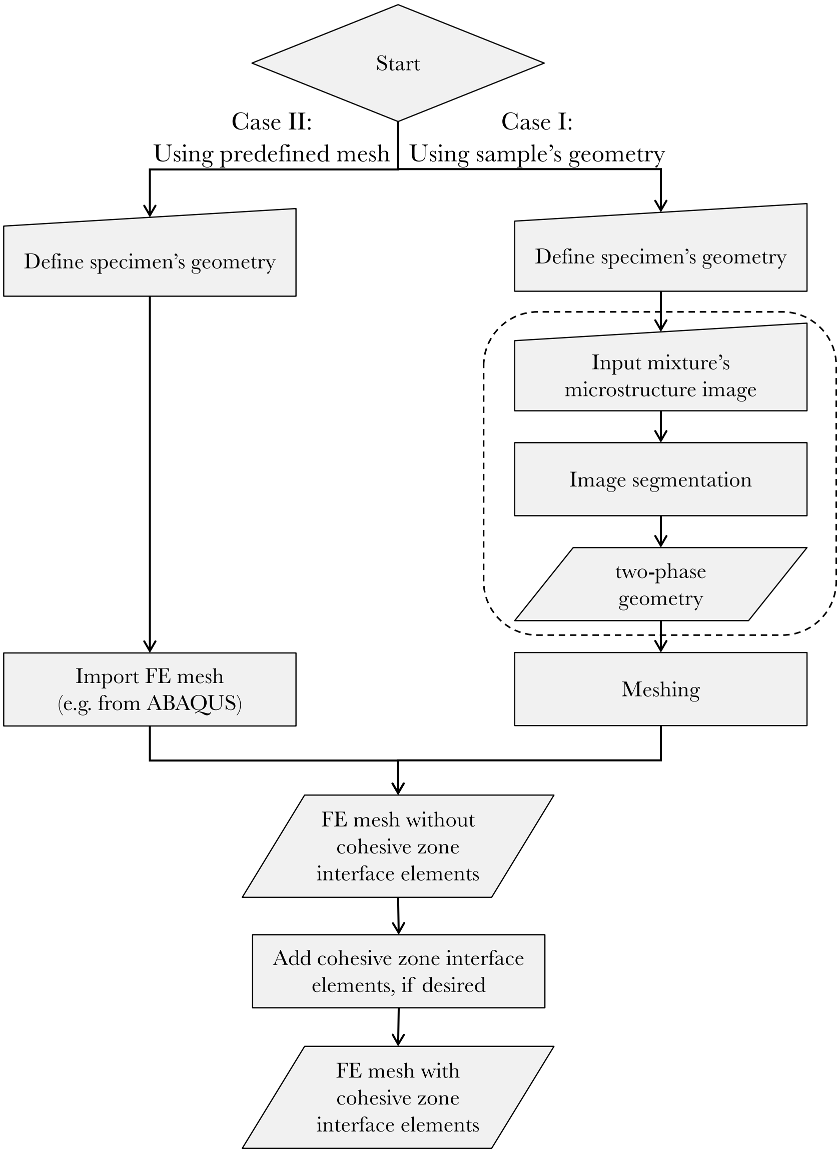


Fig. 2. MIDAS-VT-Pre flowchart.

3. Software features

MIDAS-VT-Pre automatically generates the 2D FE model for a sample, either homogeneous or heterogeneous with particles/fibers, to simulate the mechanical behavior of the sample subjected to several different testing conditions (as illustrated in Fig. 1). It, first, treats the complex microstructure of the composite using an image processing feature, then meshes the sample with or without cohesive zone interface elements. These two steps are explained in detail as follows.

3.1. Image processing

MIDAS-VT-Pre is equipped with an image processing module which recognizes the microstructure geometry of the sample. This module uses color segmentation tools available in Image Processing Toolbox of MATLAB [22]. Color segmentation method requires each phase to be represented in different color intensity. The current version of MIDAS-VT-Pre is able to handle two-phase media which includes distinct heterogeneities within a continuous matrix phase. The steps of obtaining an accurate 2D microstructure of the particle/fiber embedded composite is illustrated in Fig. 3. The program distinguishes heterogeneities from the background matrix based on the difference in their color intensities and converts the original image to a binary one. In the image processing module, it is assumed that the particles are lighter than the background, as shown in Fig. 3(a). Fig. 3(b) shows the resulting binary image where the white objects represent particles, while the surrounding matrix phase is presented as the black background. In the next step, the particles' boundary pixels are transformed into a vectorial format to describe the geometry of each particle in form of a polygon (Fig. 3(c)). The resulting geometry consists of polygons with a copious number of vertices which may induce an undesired extremely fine mesh. Therefore, the program removes unnecessary vertices of each polygon in order to define each particle with a much smaller number of vertices while salient geometric features are retained (Fig. 3(d)). The image analysis module defines the microstructure in terms of a coordinate system defined by pixels of the image. So, before meshing the geometry, the preliminary microstructure needs to be scaled from pixel coordinates to the actual size of the sample.

3.2. Cohesive zone interface element insertion

MIDAS-VT-Pre meshing module comes with an automated interface element insertion feature. As mentioned earlier, cohesive zone elements are four-node interface elements that allow simulation of crack initiation and propagation within FE framework. They are zero thickness elements that link pair nodes of neighboring bulk elements that share the same location. The insertion process of cohesive interface elements is exemplified in Fig. 4. The example assumes that the two bulk elements at the right side are in the non-cracking region, while the two left side elements are in the cracking region. In this method, the interface elements are added within the cracking region (between element 1 and 2) and along the boundary of the cracking region (between element 2 and 3). Algorithm 1 describes the pseudocode for insertion of interface elements. In order to be able to add interface elements into the existing mesh structure, the nodes within the cracking region first are duplicated in such a way that the elements do not share any nodes. Thus, unlike the regular FE mesh, multiple nodes may have the same coordinates (Fig. 4(b)). Once the new nodes are generated, the element connectivity matrix is updated accordingly. The cohesive interface elements are then defined between adjacent bulk elements using the nodes of the overlapped edges as shown in Fig. 4(c) and Algorithm 1 lines 10 to 20. Since node duplication changes the node numbering order, the Reverse Cuthill–McKee algorithm is used to optimize the nodal numbering in order to minimize the size of stiffness matrix [23].

Algorithm 1 Embedding interface elements between bulk elements. This algorithm is implemented into *AddCohEl* function.

```
    Duplicate nodes and update element connectivity
 1: for $i = 1 : number\ of\ bulk\ elements$ do
 2:     if $element\ i \in cracking\ zone$ then
 3:         for $j = 1 : 3$ do                          ▷ Loop over element's nodes
 4:             $NewNode(c, 1{:}3) = OldNode(OldConn(i, j), 1{:}3)$
 5:             $NewConn(i, j) = c$                     ▷ Update the element connectivity matrix
 6:             $c = c + 1$
 7:         end for
 8:     end if
 9: end for

    Define interface elements
10: for $i = 1 : number\ of\ bulk\ elements$ do
11:     if $element\ i \in cracking\ zone$ then
12:         for $j = 1 : 3$ do                          ▷ Loop over element's edges
13:             $k \leftarrow neighboring\ element\ number$
14:             $m \leftarrow the\ first\ node\ of\ the\ overlapped\ edge$
15:             $n \leftarrow the\ second\ node\ of\ the\ overlapped\ edge$
16:             $CohConn(c, 1 : 4) = [NewConn(i, m : n)\ NewConn(k, m : n)]$
17:             $c = c + 1$
18:         end for
19:     end if
20: end for
```

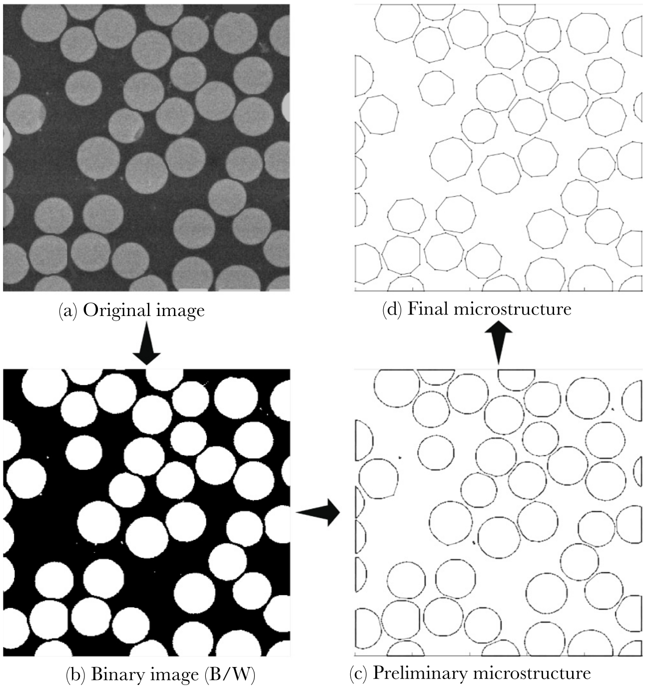
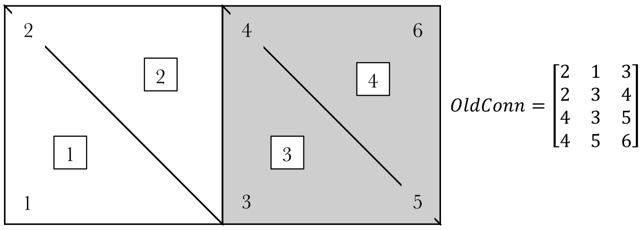

(a) Original image
(d) Final microstructure
(b) Binary image (B/W)
(c) Preliminary microstructure

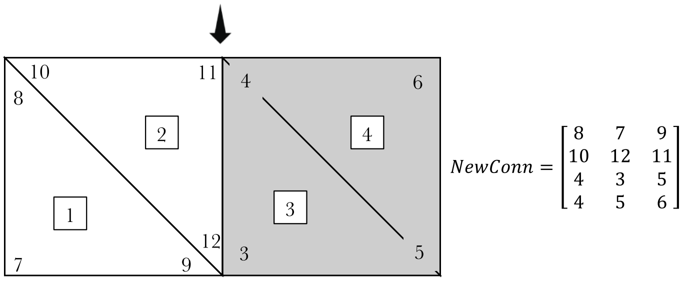
Fig. 3. Steps of generating 2D microstructure of a heterogeneous composite.

4. Illustrative example

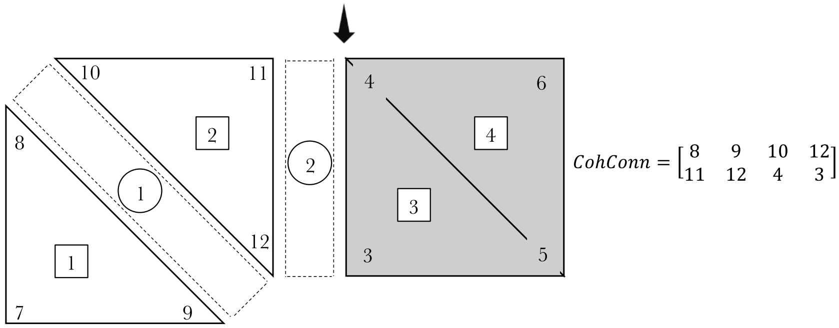
An illustrative example is given in this section to demonstrate how MIDAS-VT-Pre can be used to generate a FE model of a testing configuration. As shown in Fig. 5, the FE model of a Semicircular Bending (SCB) test is generated from a specimen image. To create the FE model, MIDAS-VT-Pre requires that the user inputs specimen's dimensions including the notch size and a user-defined cracking area for embedding cohesive zone interface elements. For instance, as Fig. 5(b) shows, the rectangular zone above the notch was defined as a potential cracking zone. This method can avoid adding unnecessary cohesive zone interface elements which can reduce computational costs. If the model requires prediction/representation of potential cracking of the entire area, it can certainly be pursued. After defining the specimen dimensions, the user can bring the specimen's microstructure image for microstructural FE simulation. Then, MIDAS-VT-Pre identifies the particles' perimeters and specimen geometry to create the final geometry. When the accuracy of the geometry is confirmed, the user can start meshing. The software also allows the user to adjust the global element size using *max mesh size* parameter. The cohesive zone interface elements can then be added at this step if it is desired. Once meshing is completed, MIDAS-VT-Pre identifies boundary conditions automatically. Mesh information and boundary conditions are then exported to a text file that can be used in standard FE software such as ABAQUS. The model is completed by adding appropriate material properties of individual phases. The result of the SCB simulation is exemplified in Fig. 5(c). The readers may refer to MIDAS-VT-Pre User's Manual [24] which provides details of each step.



(a) Original mesh



(b) Duplicating nodes



(c) Embedding cohesive interface elements

Fig. 4. Embedding cohesive zone elements between bulk elements.

5. Impact

MIDAS-VT-Pre helps FE virtual testing of heterogeneous materials that are subjected to fracture damage due to crack initiation and propagation. Comparing simulation results with experimental results can help design heterogeneous materials in a much more efficient manner by reducing costs and time to conduct repetitive laboratory tests [14]. Also, the ease of creating an FE model for various microstructures is greatly helpful when studying the effect of microstructure on the overall behavior of composites [25]. This practice is also useful in determining representative volume elements (RVE) of composite structures when conducting micromechanical and/or multiscale methods. The effective properties of the composites can be easily obtained virtually by conducting RVE analysis under various loading scenarios [15]. MIDAS-VT-Pre can vastly help those as a supporting tool.

6. Conclusions

MIDAS-VT-Pre was developed to easily and accurately create FE models of testing specimens, in particle/fiber embedded composites where cracking can occur within matrix phase and along two-phase boundaries. The software in a form of user-friendly interface is equipped with an image processing module to detect the microstructural features and an FE meshing module to embed optimized cohesive interface elements for user-defined potential cracking area. The MIDAS-VT-Pre output is fully compatible with common FE software such as ABAQUS and MIDAS-VT, which is a separate software that the authors developed, for a more target-oriented simulation of materials that present nonlinear viscoelastic fracture [21]. The source code and the standalone version of MIDAS-VT-Pre is accessible online [24]. The authors welcome other researchers' comments, suggestions, and contributions to make the program more useful.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Acknowledgment

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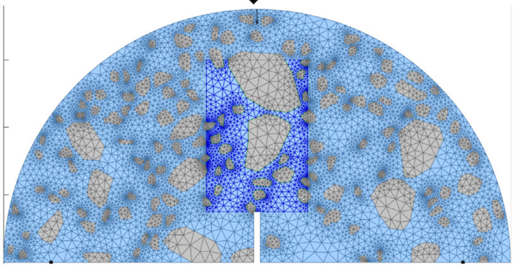
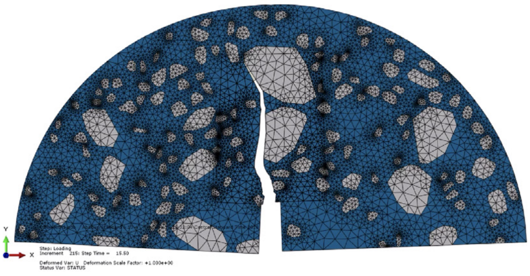
(a) Original Image



(b) Mesh with cohesive zone elements



(c) FE simulation with ABAQUS

Fig. 5. Generating semicircular bending model using MIDAS-VT-Pre.

Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.softx.2019.100292.

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